wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 04:59 PM EST

PDB ID	:	1COW
Title	:	BOVINE MITOCHONDRIAL F1-ATPASE COMPLEXED WITH AUROVERTIN B
Authors	:	van Raaij, M.J.; Abrahams, J.P.; Leslie, A.G.W.; Walker, J.E.
Deposited on	:	1996-05-08
Resolution	:	3.10 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:

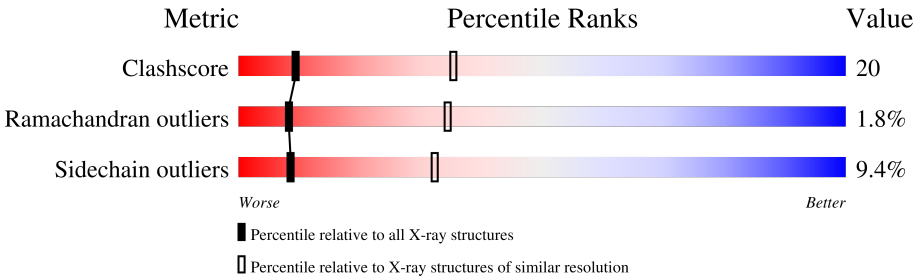
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.10 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	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	510	49% 35% 10% • 5%
1	B	510	47% 38% 10% • 5%
1	C	510	53% 37% 5% • •
2	D	482	52% 38% 6% • •
2	E	482	43% 40% 11% • •
2	F	482	55% 34% 7% • •
3	G	272	25% 15% 5% • 55%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 23462 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	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	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			

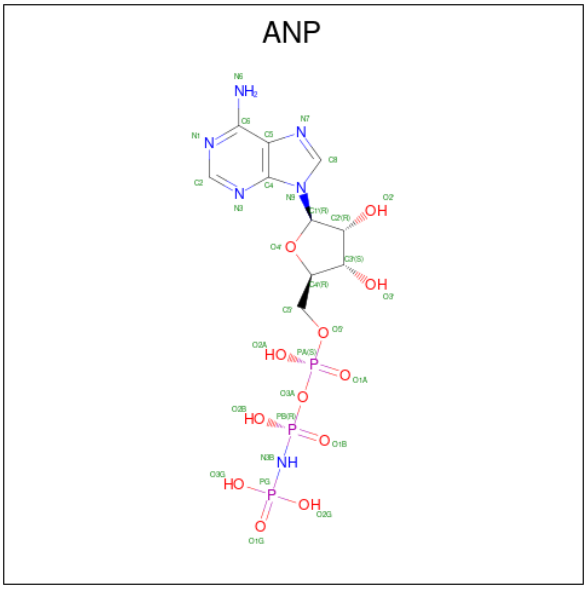
- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

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

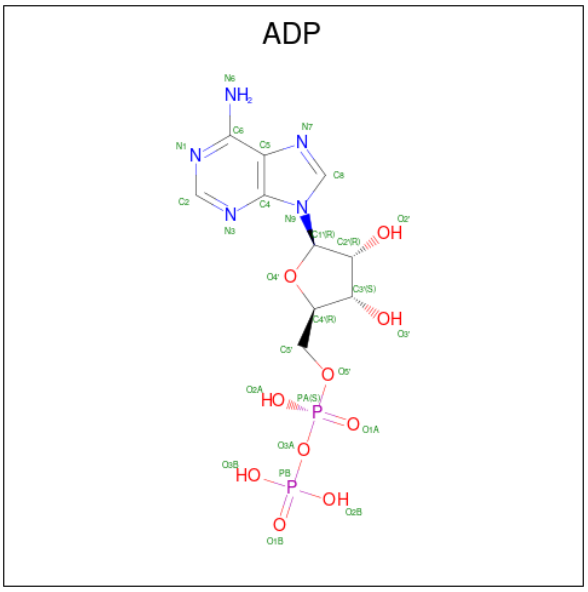
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



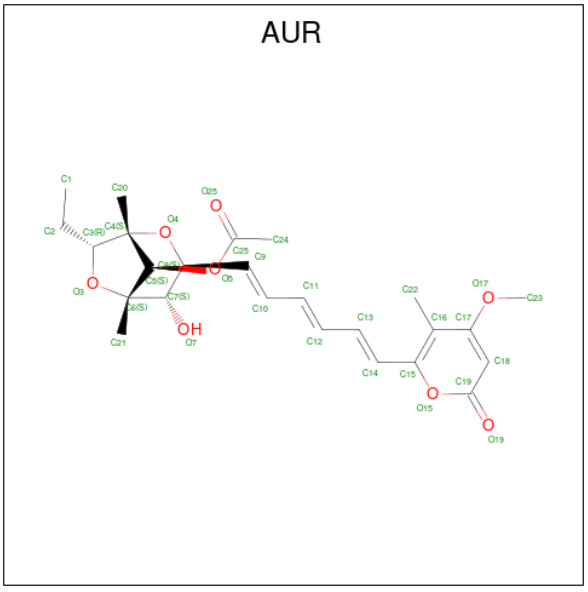
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 31 10 6 12 3	0	0
5	B	1	Total C N O P 31 10 6 12 3	0	0
5	C	1	Total C N O P 31 10 6 12 3	0	0
5	F	1	Total C N O P 31 10 6 12 3	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 7 is AUROVERTIN B (three-letter code: AUR) (formula: $C_{25}H_{32}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	C	O	0	0
			33	25	8		
7	F	1	Total	C	O	0	0
			33	25	8		

- Molecule 8 is water.

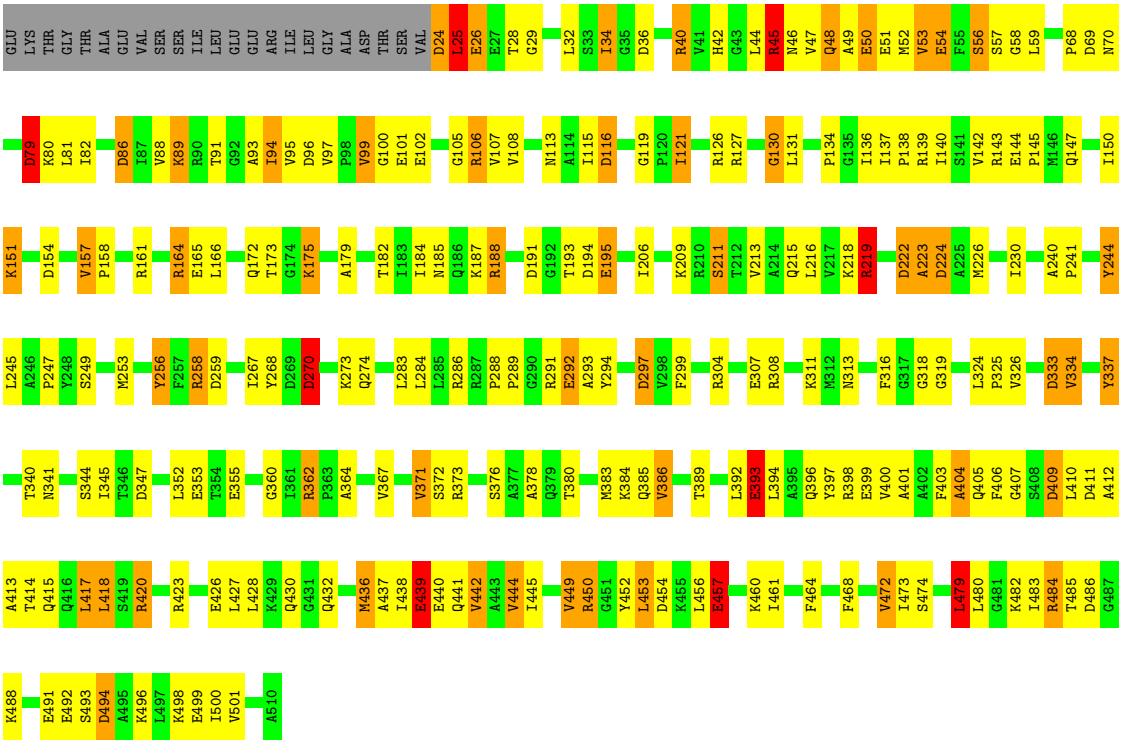
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	80	Total O 80 80	0	0
8	B	84	Total O 84 84	0	0
8	C	98	Total O 98 98	0	0
8	D	94	Total O 94 94	0	0
8	E	47	Total O 47 47	0	0
8	F	92	Total O 92 92	0	0
8	G	23	Total O 23 23	0	0

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. 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. 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.

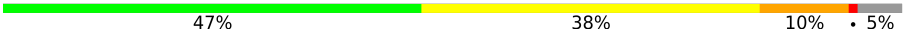
• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

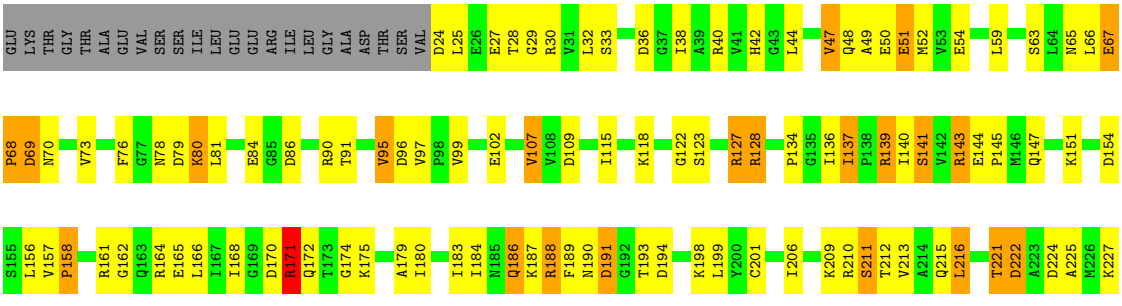
Chain A:

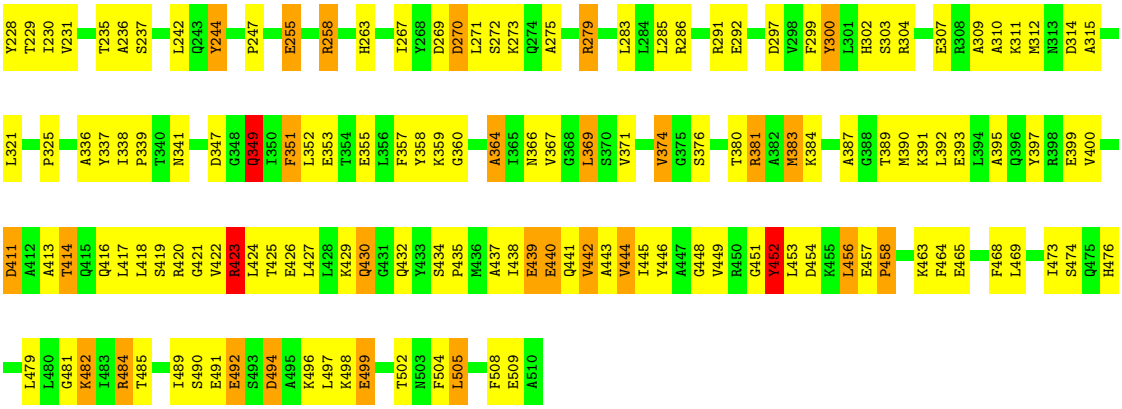


• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

Chain B:

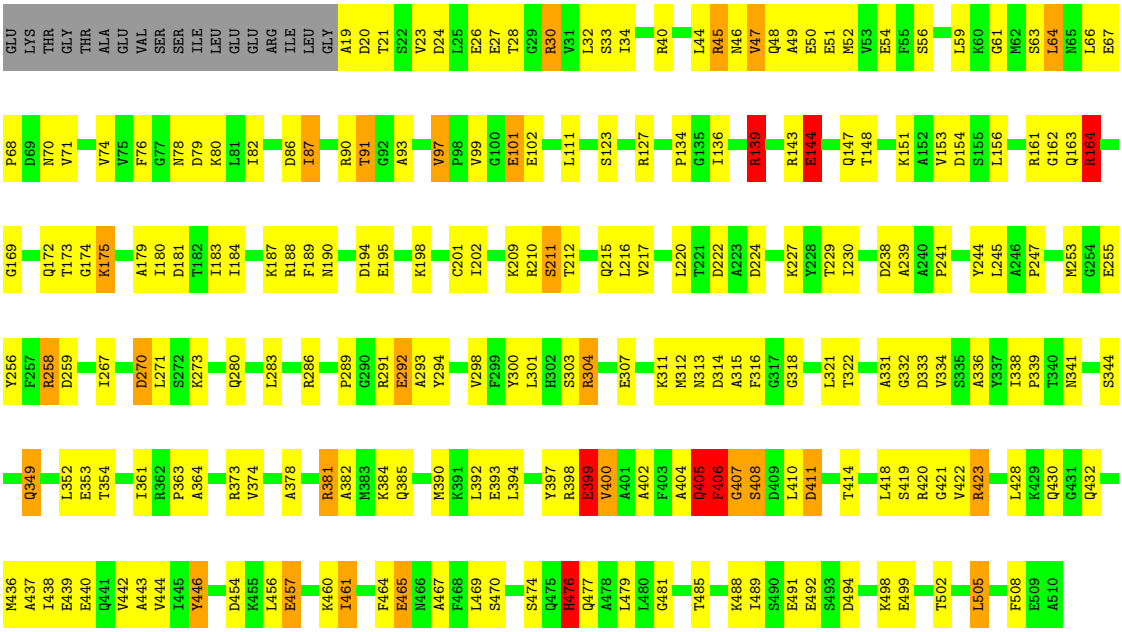






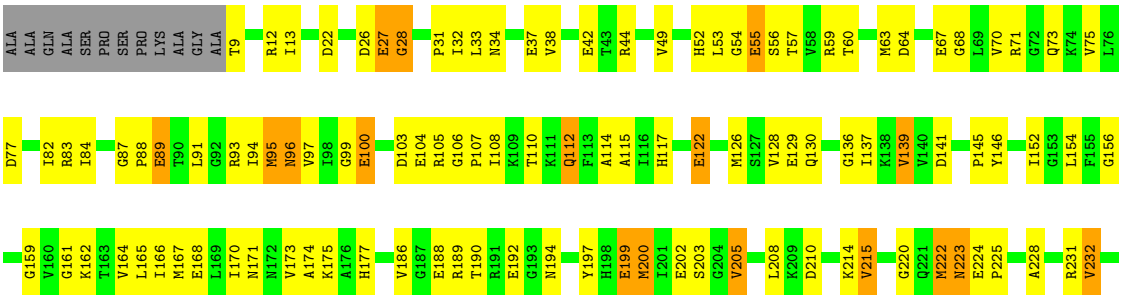
• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

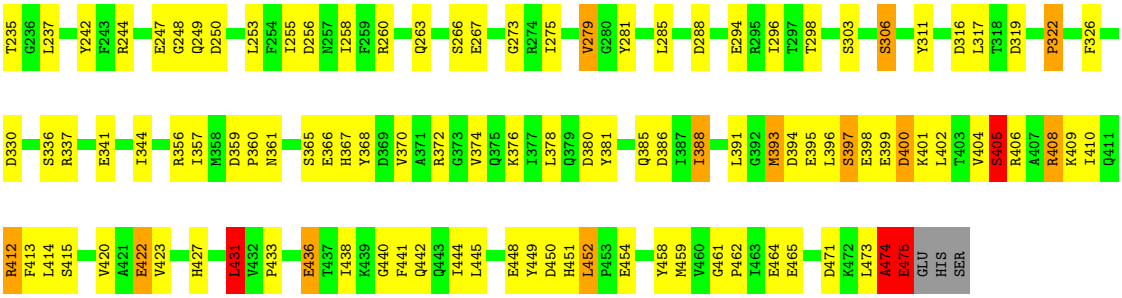
Chain C:



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

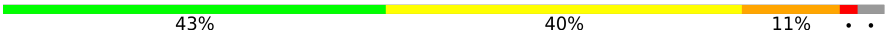
Chain D:

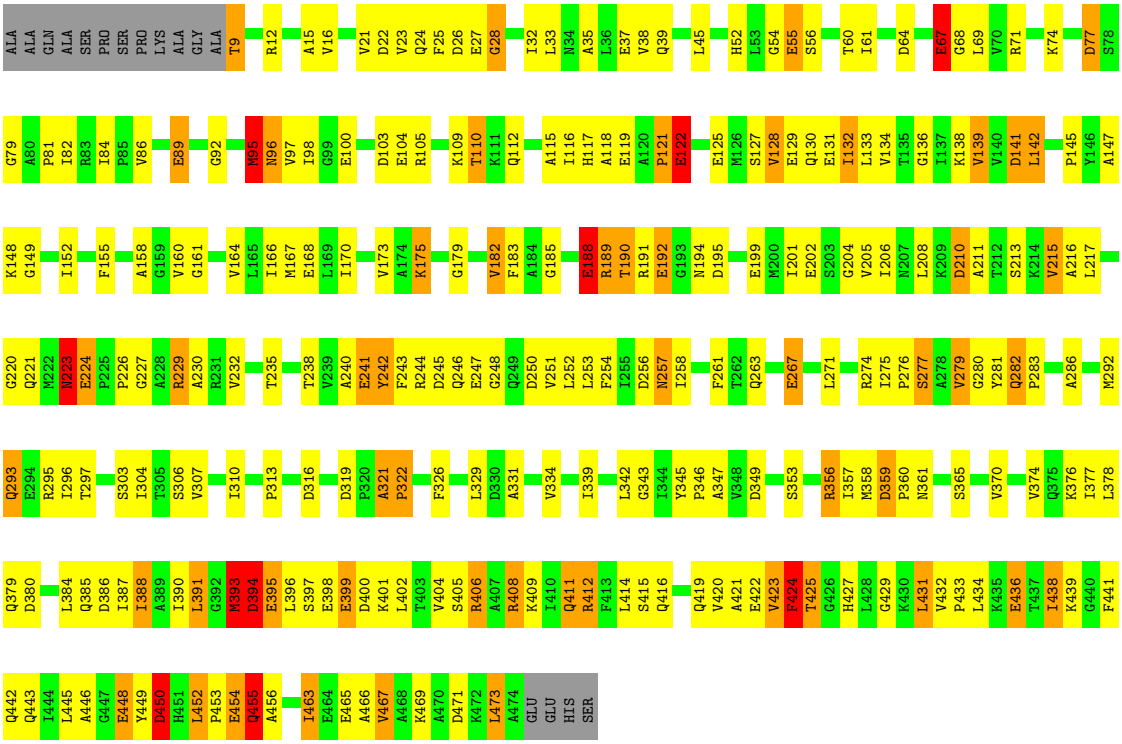




• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

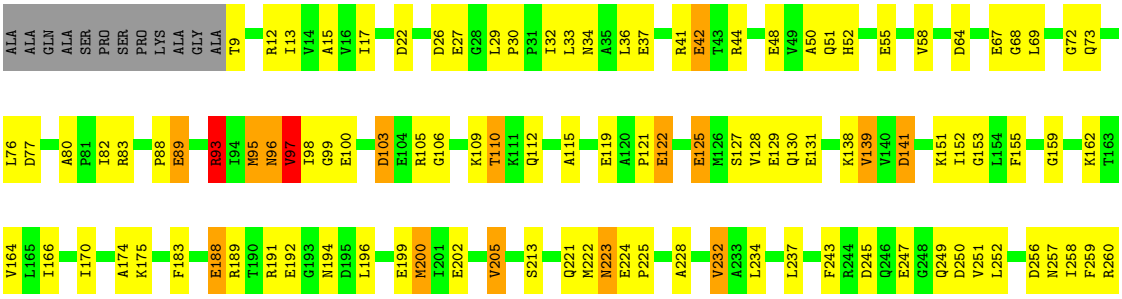
Chain E:

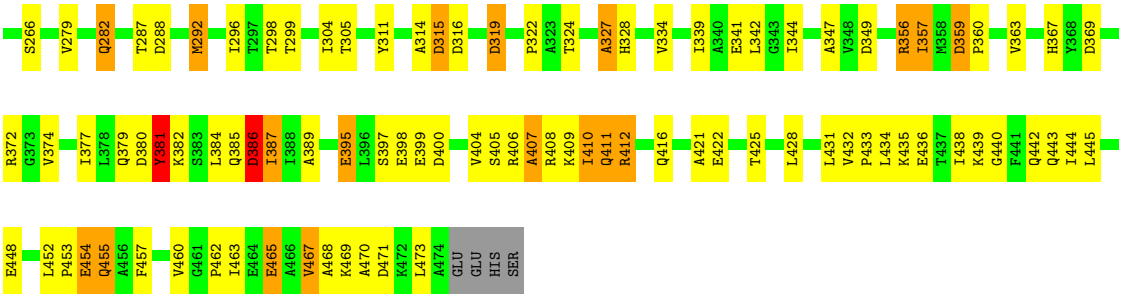




• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

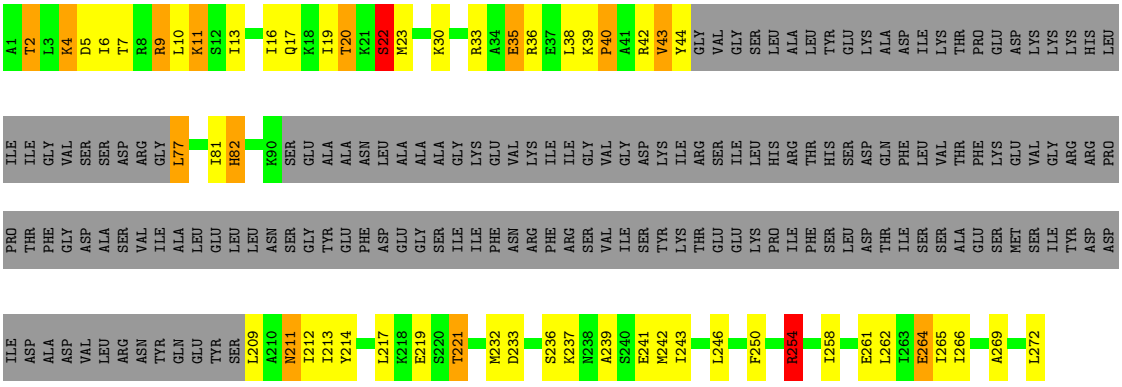
Chain F:





• Molecule 3: BOVINE MITOCHONDRIAL F1-ATPASE

Chain G: 25% 15% 5% 55%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	283.40Å 107.60Å 140.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.10) 99.4 (20.00-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.44 (at 3.09Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , 0.280 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 91.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	23462	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage'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.*

[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.

5 Model quality

5.1 Standard geometry

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

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	0.99	17/3766 (0.5%)	1.38	45/5080 (0.9%)
1	B	1.00	16/3766 (0.4%)	1.40	41/5080 (0.8%)
1	C	1.00	19/3799 (0.5%)	1.38	39/5126 (0.8%)
2	D	1.01	24/3596 (0.7%)	1.40	41/4879 (0.8%)
2	E	1.02	25/3587 (0.7%)	1.36	47/4867 (1.0%)
2	F	1.07	26/3587 (0.7%)	1.39	55/4867 (1.1%)
3	G	0.99	7/949 (0.7%)	1.42	18/1266 (1.4%)
All	All	1.01	134/23050 (0.6%)	1.39	286/31165 (0.9%)

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
1	A	0	1
1	B	0	2
1	C	0	2
2	D	0	1
2	E	0	2
3	G	1	3
All	All	1	11

The worst 5 of 134 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	GLU	CD-OE1	8.28	1.34	1.25
2	F	42	GLU	CD-OE2	8.05	1.34	1.25
2	F	224	GLU	CD-OE2	7.94	1.34	1.25
2	D	436	GLU	CD-OE2	7.43	1.33	1.25
1	A	491	GLU	CD-OE1	7.19	1.33	1.25

The worst 5 of 286 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	408	ARG	NE-CZ-NH2	-16.74	111.93	120.30
2	D	408	ARG	NE-CZ-NH1	15.40	128.00	120.30
1	A	143	ARG	NE-CZ-NH2	-13.38	113.61	120.30
2	D	408	ARG	CD-NE-CZ	11.78	140.09	123.60
3	G	9	ARG	NE-CZ-NH1	11.37	125.99	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	209	LEU	CA

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	PHE	Mainchain
1	B	369	LEU	Mainchain
1	B	432	GLN	Mainchain
1	C	363	PRO	Mainchain
1	C	405	GLN	Mainchain

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	3815	162	0
1	B	3715	0	3814	168	0
1	C	3748	0	3845	137	0
2	D	3539	0	3593	140	0
2	E	3530	0	3587	184	0
2	F	3530	0	3587	137	0
3	G	945	0	1019	39	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	31	0	13	1	0
5	B	31	0	13	8	0
5	C	31	0	13	4	0
5	F	31	0	12	2	0
6	D	27	0	12	3	0
7	E	33	0	32	14	0
7	F	33	0	32	6	0
8	A	80	0	0	6	0
8	B	84	0	0	12	0
8	C	98	0	0	11	0
8	D	94	0	0	11	0
8	E	47	0	0	9	0
8	F	92	0	0	11	0
8	G	23	0	0	2	0
All	All	23462	0	23387	914	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 20.

The worst 5 of 914 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:215:GLN:HG3	2:F:356:ARG:HH22	1.07	1.15
1:C:127:ARG:HH12	1:C:255:GLU:HB2	0.97	1.07
1:C:30:ARG:HE	1:C:87:ILE:HD11	1.24	1.01
2:F:223:ASN:HD22	2:F:223:ASN:H	1.06	1.00
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.80	0.96

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%)	430 (89%)	44 (9%)	11 (2%)	6 28
1	B	485/510 (95%)	430 (89%)	45 (9%)	10 (2%)	7 30
1	C	490/510 (96%)	438 (89%)	46 (9%)	6 (1%)	13 44
2	D	465/482 (96%)	415 (89%)	45 (10%)	5 (1%)	14 46
2	E	464/482 (96%)	401 (86%)	46 (10%)	17 (4%)	3 19
2	F	464/482 (96%)	422 (91%)	40 (9%)	2 (0%)	34 69
3	G	116/272 (43%)	98 (84%)	16 (14%)	2 (2%)	9 36
All	All	2969/3248 (91%)	2634 (89%)	282 (10%)	53 (2%)	8 34

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	57	SER
1	A	405	GLN
1	B	25	LEU
1	B	364	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%)	341 (87%)	52 (13%)	4 17
1	B	393/412 (95%)	351 (89%)	42 (11%)	6 26
1	C	397/412 (96%)	365 (92%)	32 (8%)	11 39
2	D	377/386 (98%)	348 (92%)	29 (8%)	13 41
2	E	376/386 (97%)	339 (90%)	37 (10%)	8 29
2	F	376/386 (97%)	349 (93%)	27 (7%)	14 44
3	G	102/230 (44%)	94 (92%)	8 (8%)	12 40
All	All	2414/2624 (92%)	2187 (91%)	227 (9%)	8 32

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	334	VAL
3	G	77	LEU
2	D	337	ARG
3	G	4	LYS
2	F	127	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	223	ASN
2	F	282	GLN
2	D	194	ASN
1	C	260	ASN
2	F	443	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	$\#\|Z\|>2$
6	ADP	D	600	4	24,29,29	1.18	1 (4%)	29,45,45	1.32	4 (13%)
7	AUR	E	479	-	29,35,35	1.94	6 (20%)	28,52,52	1.90	7 (25%)
5	ANP	B	600	4	29,33,33	1.40	7 (24%)	31,52,52	2.22	7 (22%)
5	ANP	A	600	4	29,33,33	1.65	7 (24%)	31,52,52	2.39	10 (32%)
5	ANP	C	600	4	29,33,33	1.69	8 (27%)	31,52,52	2.12	6 (19%)
5	ANP	F	600	4	29,33,33	1.53	7 (24%)	31,52,52	2.73	8 (25%)
7	AUR	F	602	-	29,35,35	1.64	5 (17%)	28,52,52	2.45	9 (32%)

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
6	ADP	D	600	4	-	1/12/32/32	0/3/3/3
7	AUR	E	479	-	-	2/16/55/55	0/4/3/3
5	ANP	B	600	4	-	2/14/38/38	0/3/3/3
5	ANP	A	600	4	-	3/14/38/38	0/3/3/3
5	ANP	C	600	4	-	8/14/38/38	0/3/3/3
5	ANP	F	600	4	-	5/14/38/38	0/3/3/3
7	AUR	F	602	-	-	1/16/55/55	0/4/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	479	AUR	C7-C8	-5.64	1.47	1.53
5	C	600	ANP	PB-O3A	5.06	1.65	1.59
5	A	600	ANP	PB-O3A	4.45	1.64	1.59
7	F	602	AUR	C7-C8	-4.31	1.48	1.53
7	E	479	AUR	O5-C5	-4.17	1.36	1.44

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	600	ANP	O1G-PG-N3B	-9.57	97.68	111.77
7	F	602	AUR	O17-C17-C16	-7.29	109.39	115.01
5	F	600	ANP	O2G-PG-O3G	6.96	126.17	107.64
5	A	600	ANP	O2B-PB-O1B	6.53	123.61	109.92
5	B	600	ANP	O2G-PG-O3G	6.14	124.00	107.64

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	600	ANP	PB-N3B-PG-O1G
5	A	600	ANP	PG-N3B-PB-O1B
5	A	600	ANP	PG-N3B-PB-O3A
5	B	600	ANP	PB-N3B-PG-O1G
5	B	600	ANP	PG-N3B-PB-O1B

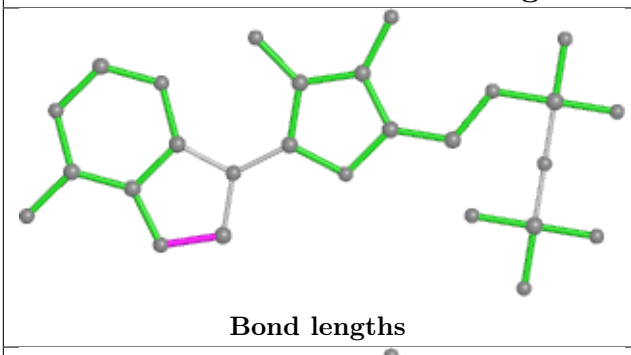
There are no ring outliers.

7 monomers are involved in 38 short contacts:

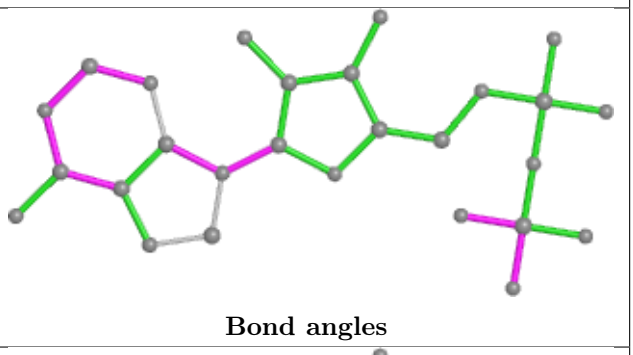
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	600	ADP	3	0
7	E	479	AUR	14	0
5	B	600	ANP	8	0
5	A	600	ANP	1	0
5	C	600	ANP	4	0
5	F	600	ANP	2	0
7	F	602	AUR	6	0

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 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.

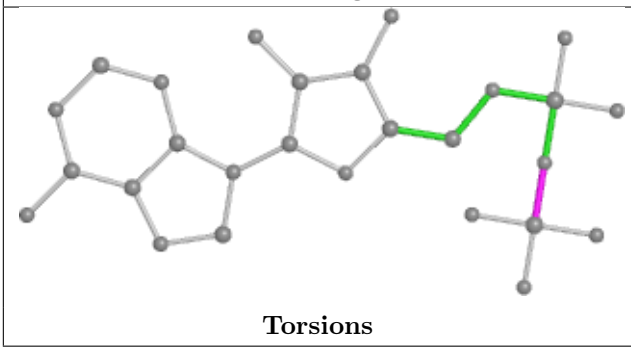
Ligand ADP D 600



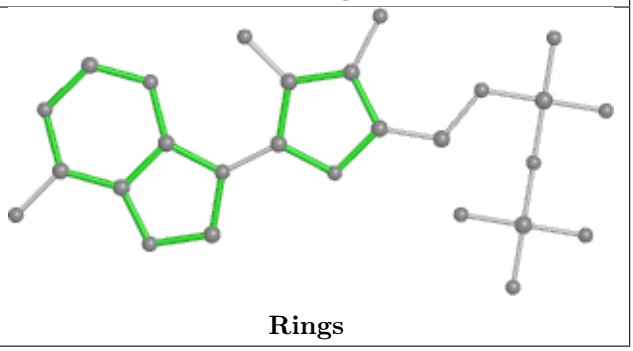
Bond lengths



Bond angles

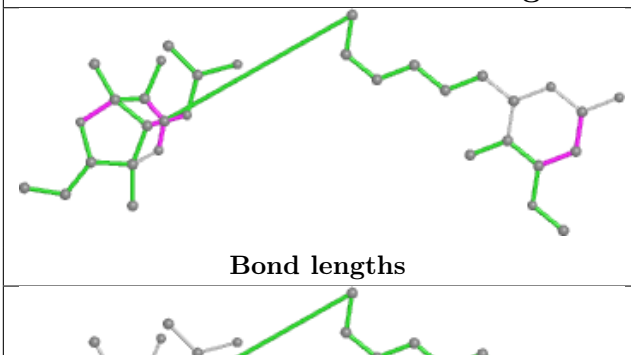


Torsions

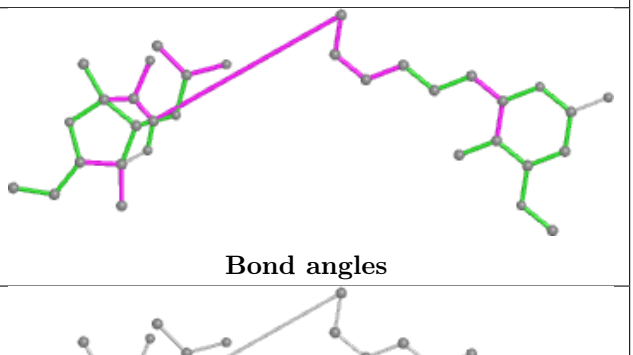


Rings

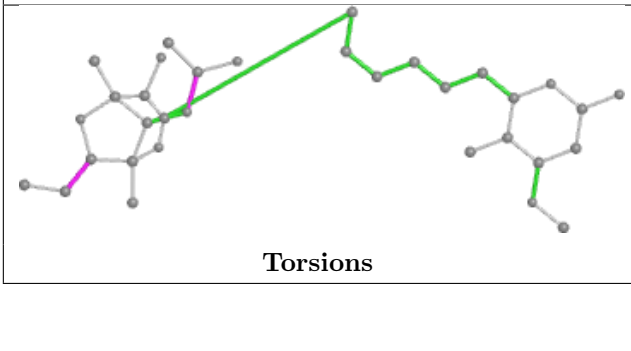
Ligand AUR E 479



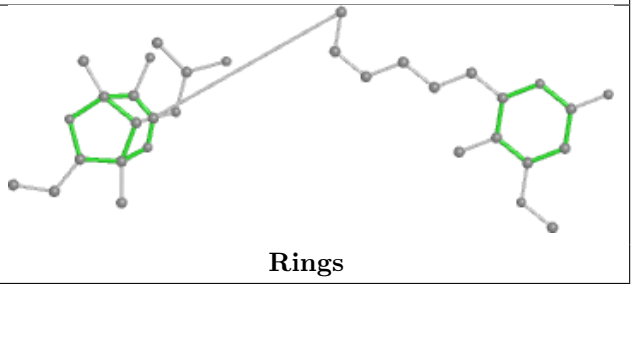
Bond lengths



Bond angles

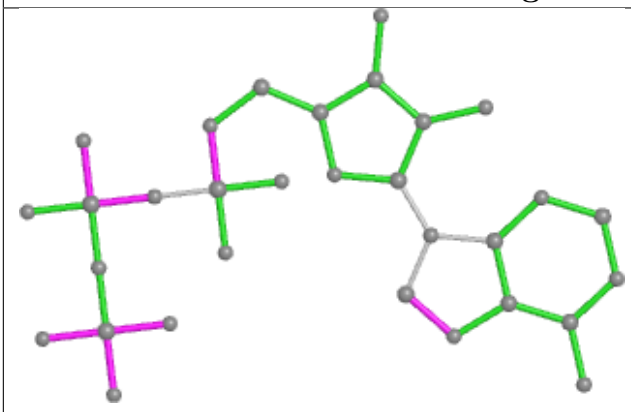


Torsions

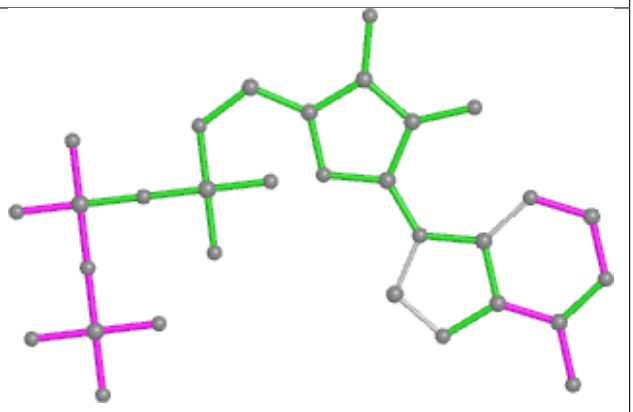


Rings

Ligand ANP B 600



Bond lengths



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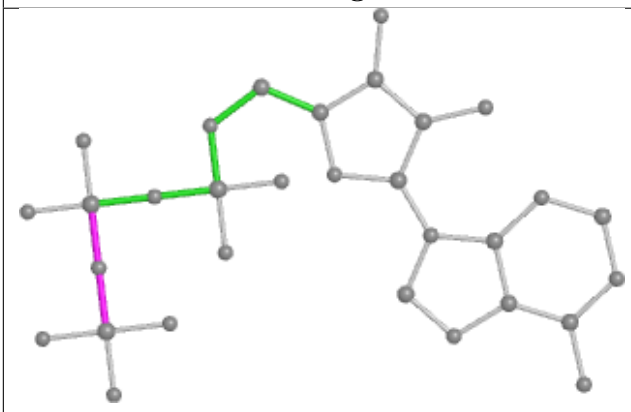
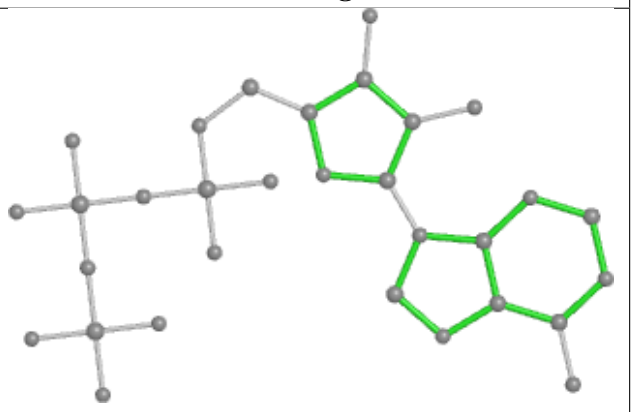
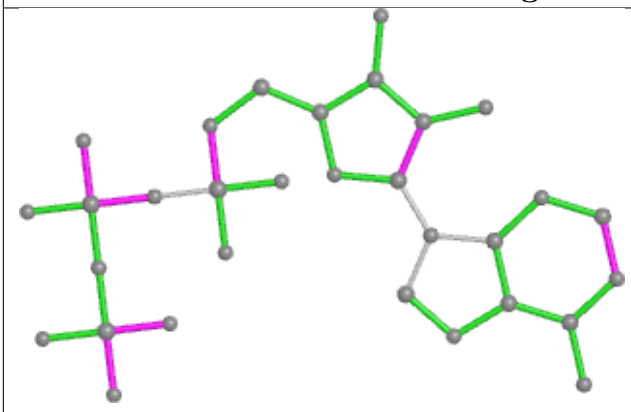


Torsions

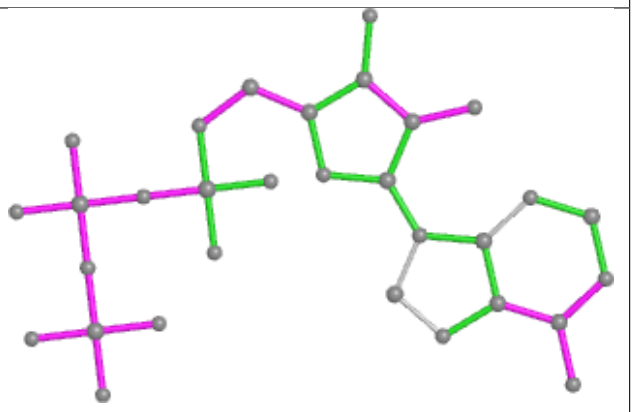


Rings

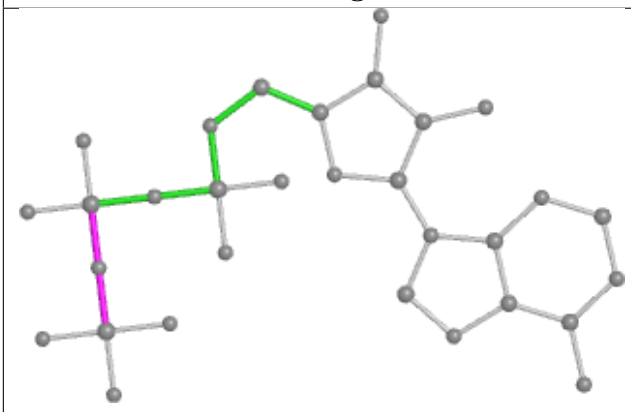
Ligand ANP A 600



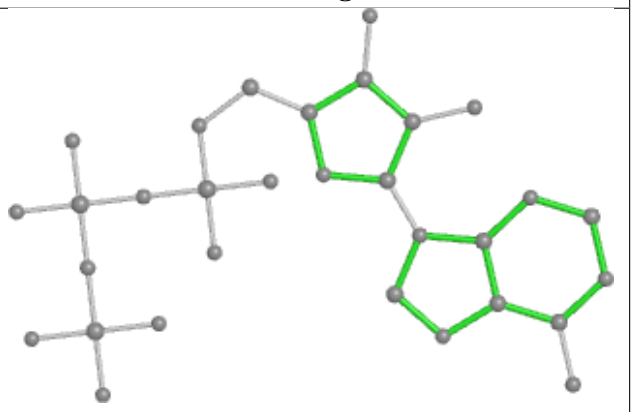
Bond lengths



Bond angles

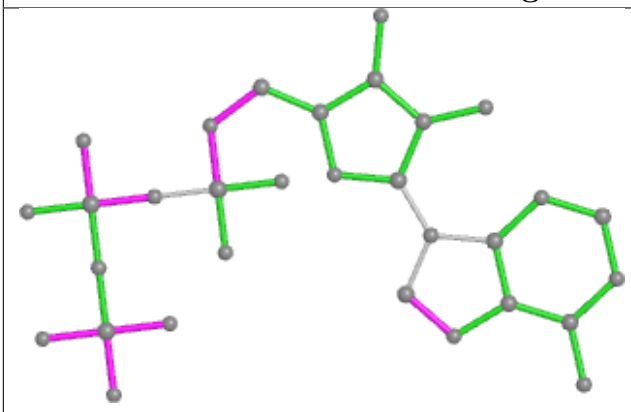


Torsions

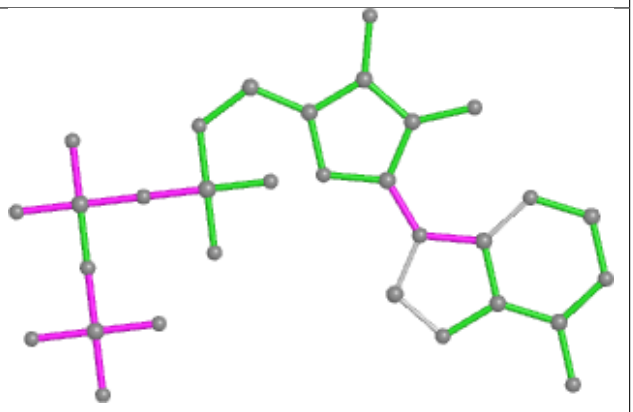


Rings

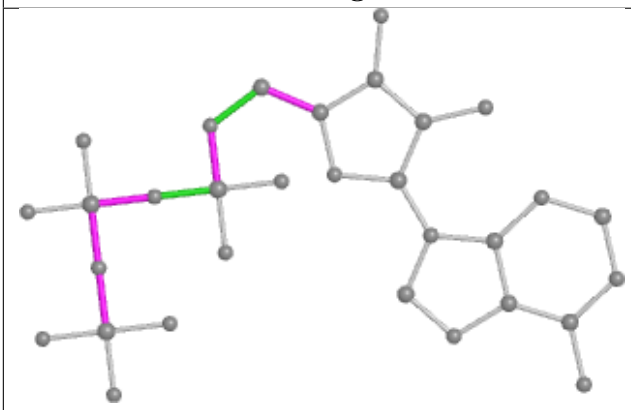
Ligand ANP C 600



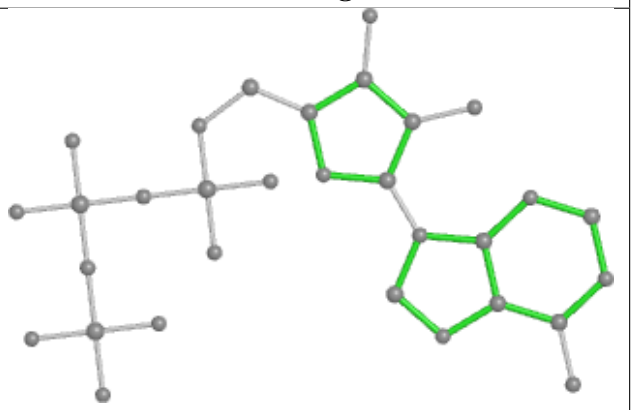
Bond lengths



Bond angles

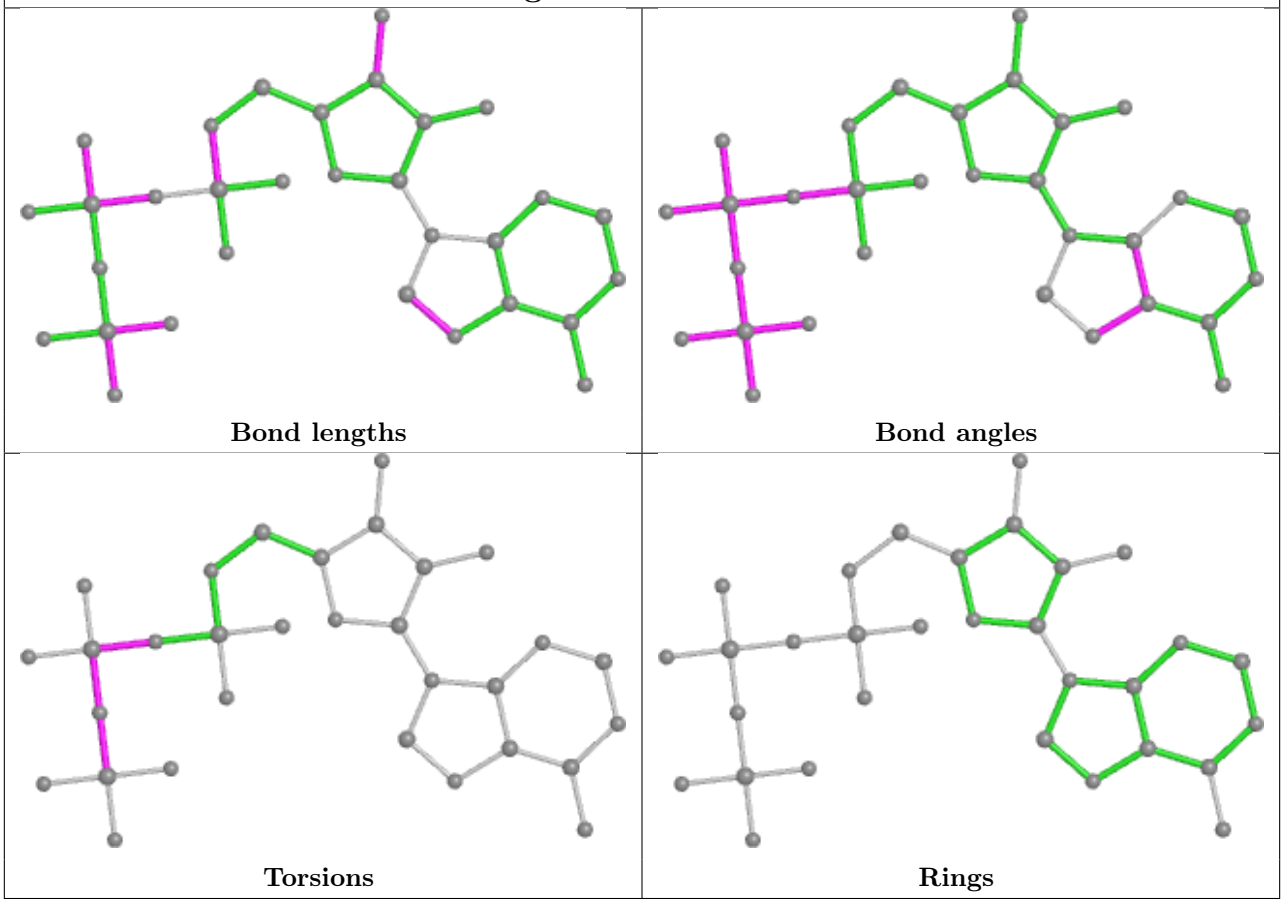


Torsions

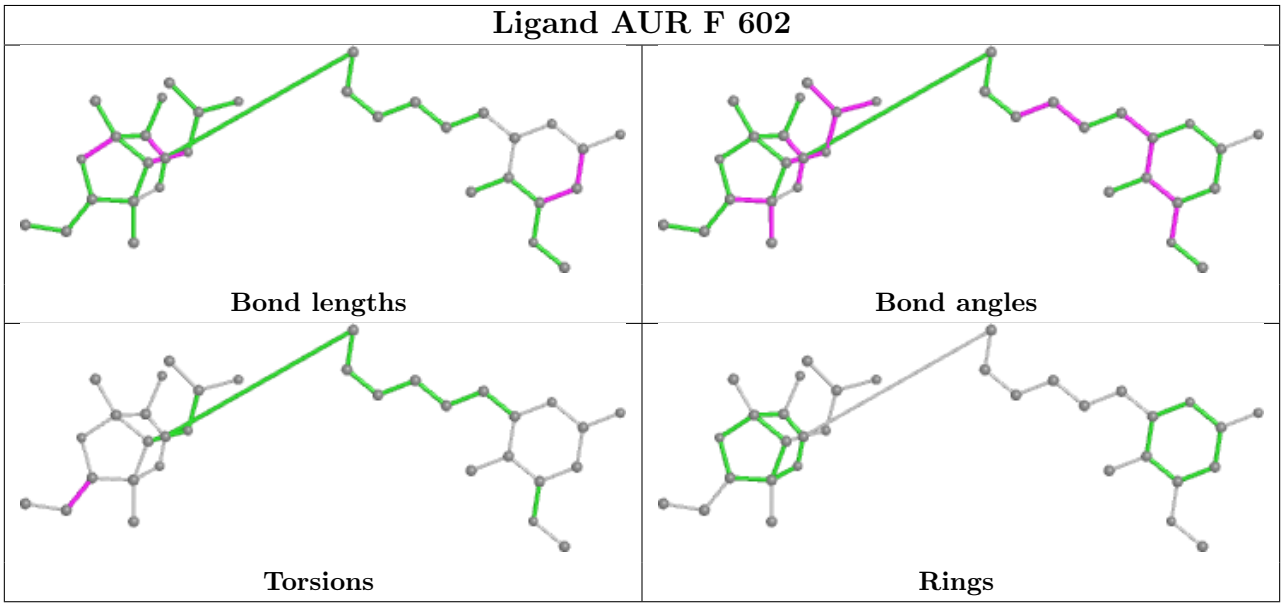


Rings

Ligand ANP F 600



Ligand AUR F 602



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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

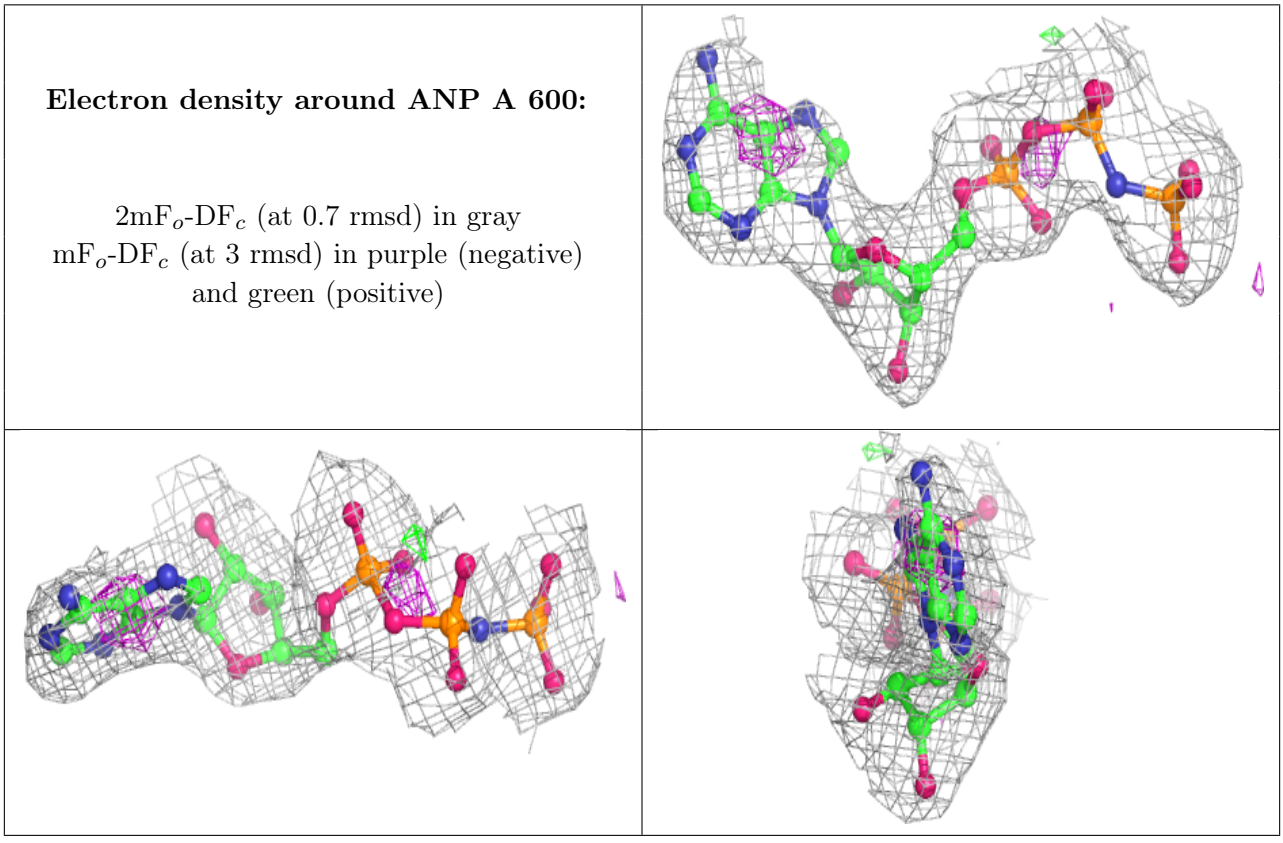
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

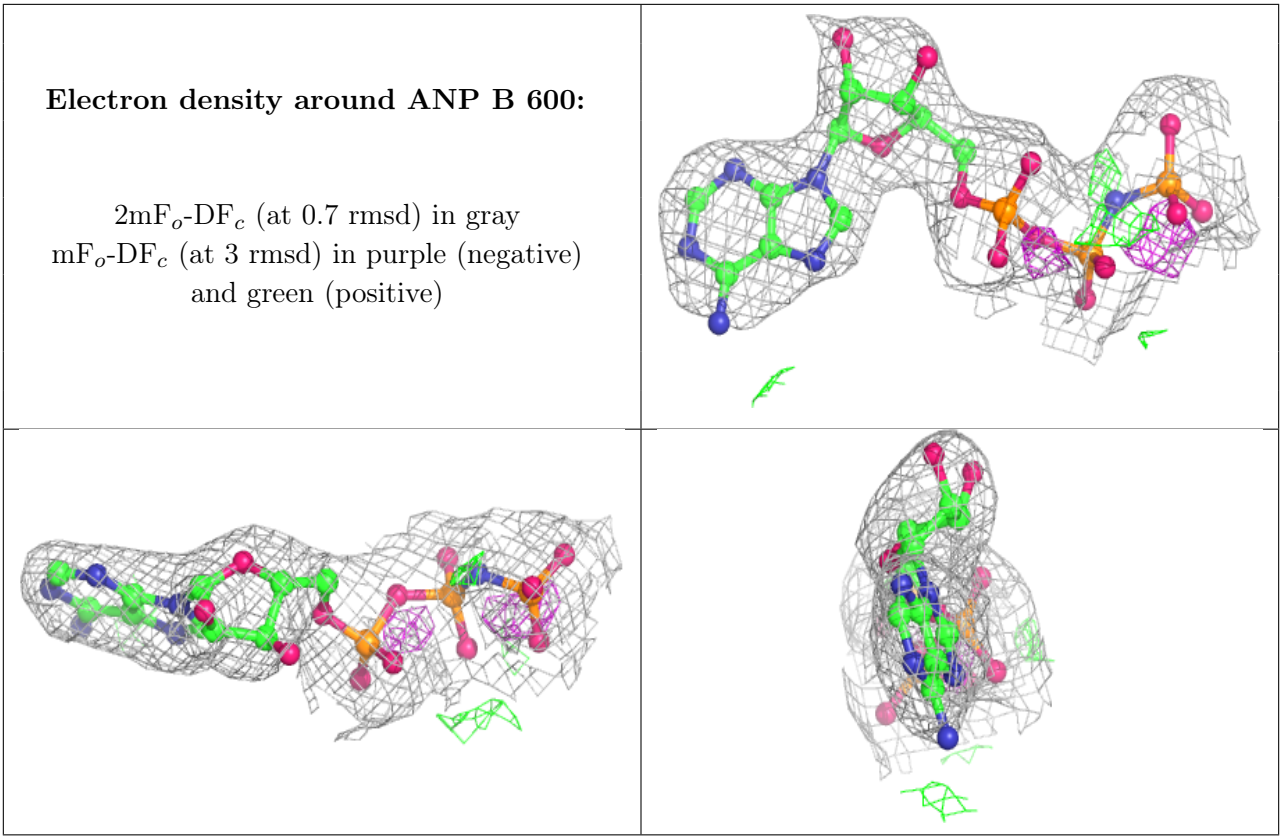
Electron density around ANP A 600:

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



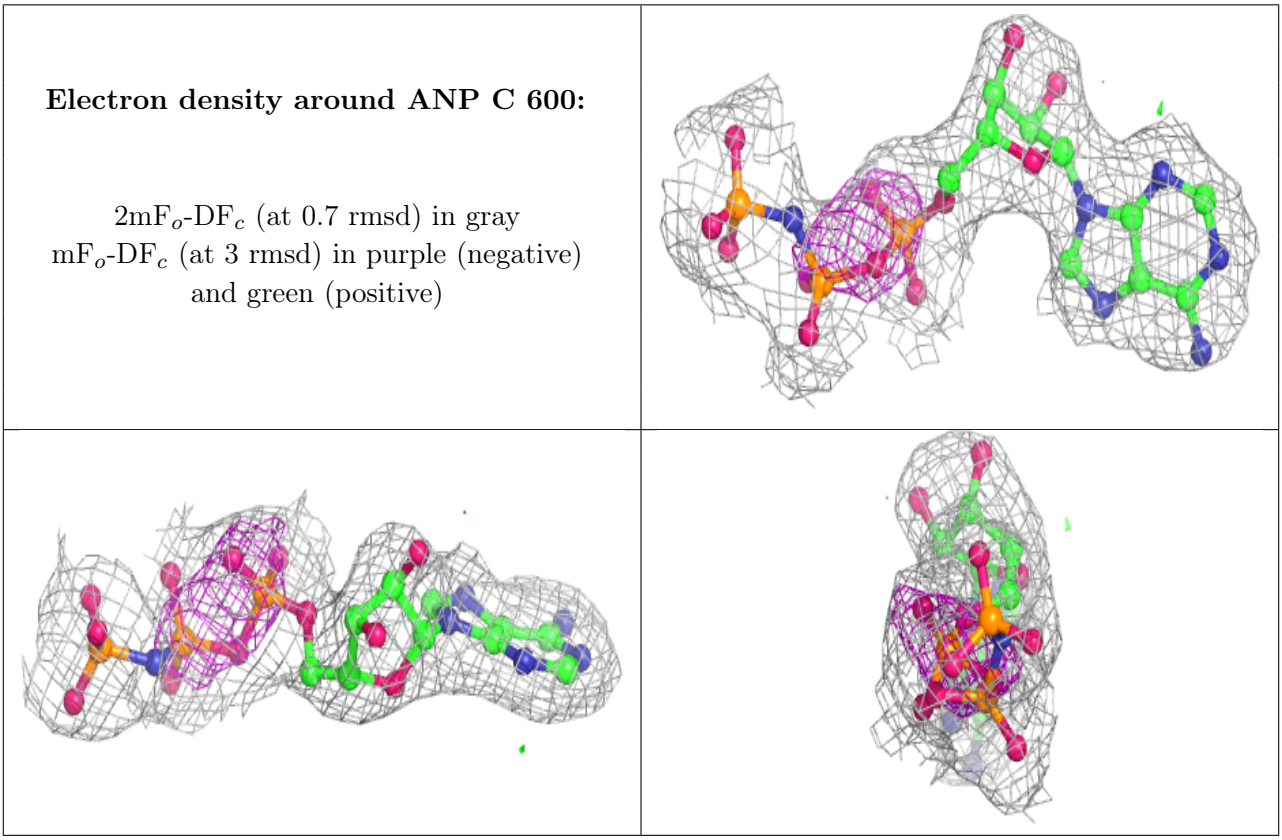
Electron density around ANP B 600:

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



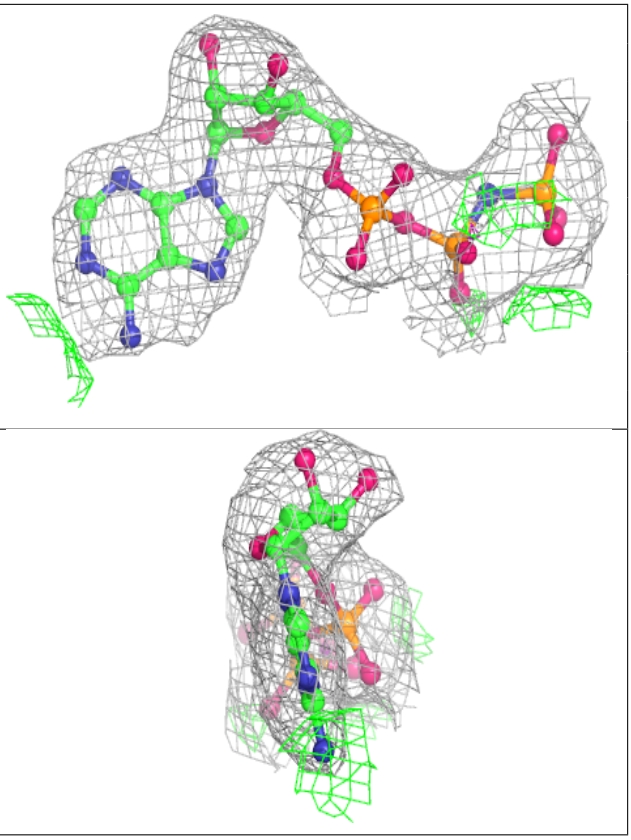
Electron density around ANP C 600:

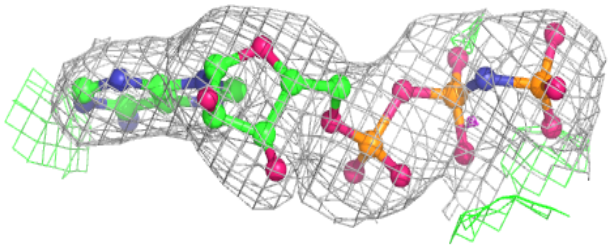
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



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 ADP D 600:

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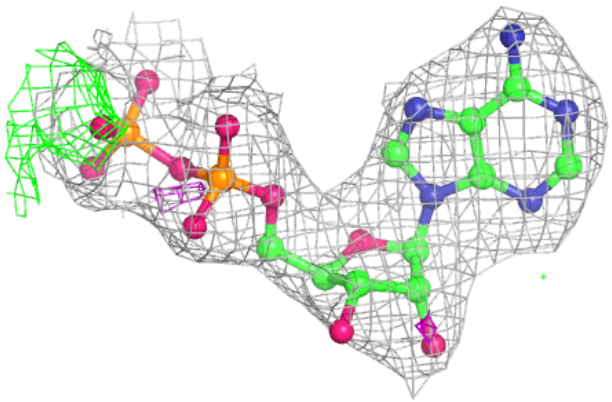
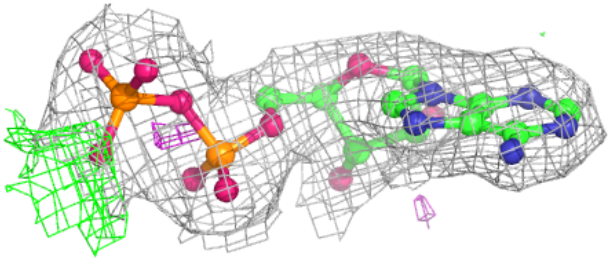
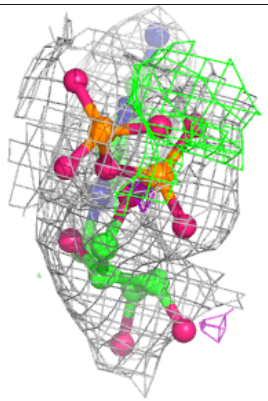
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

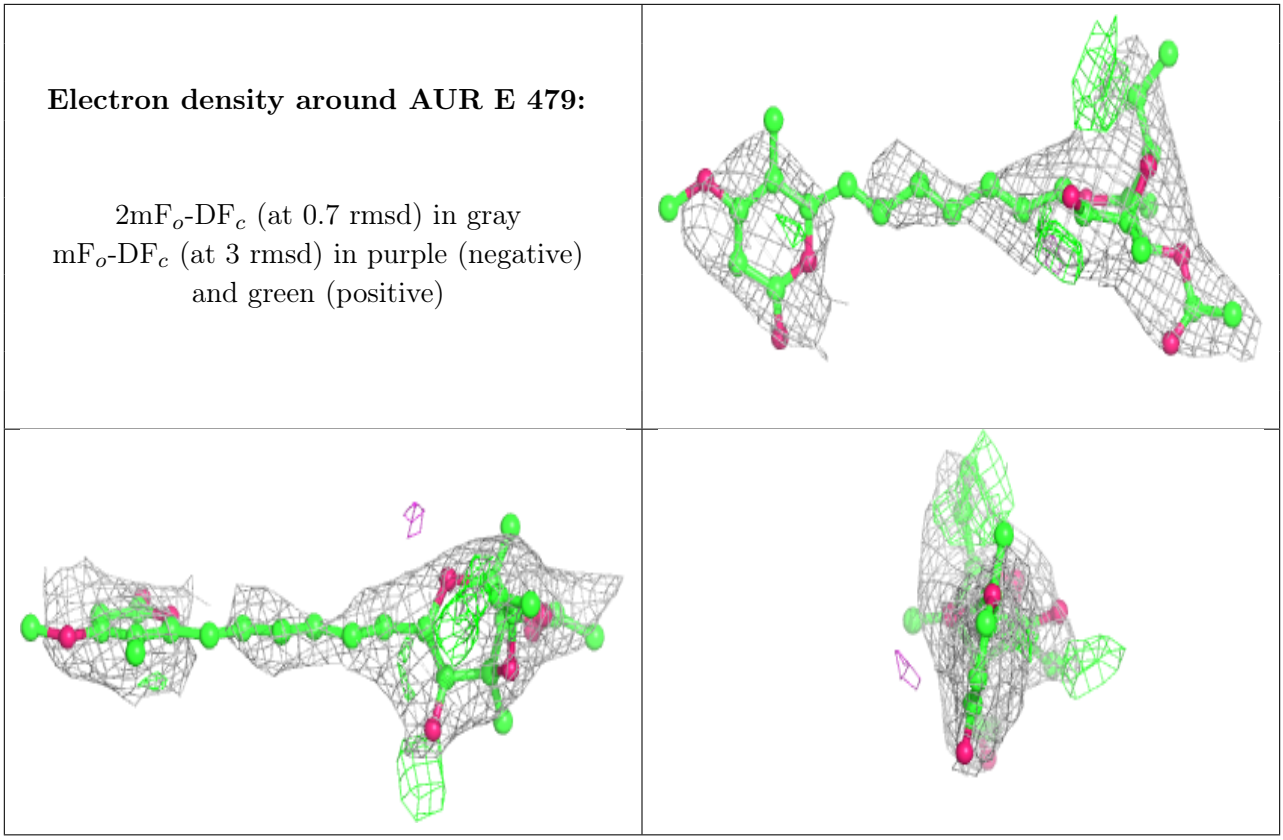






Electron density around AUR E 479:

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



Electron density around AUR F 602:

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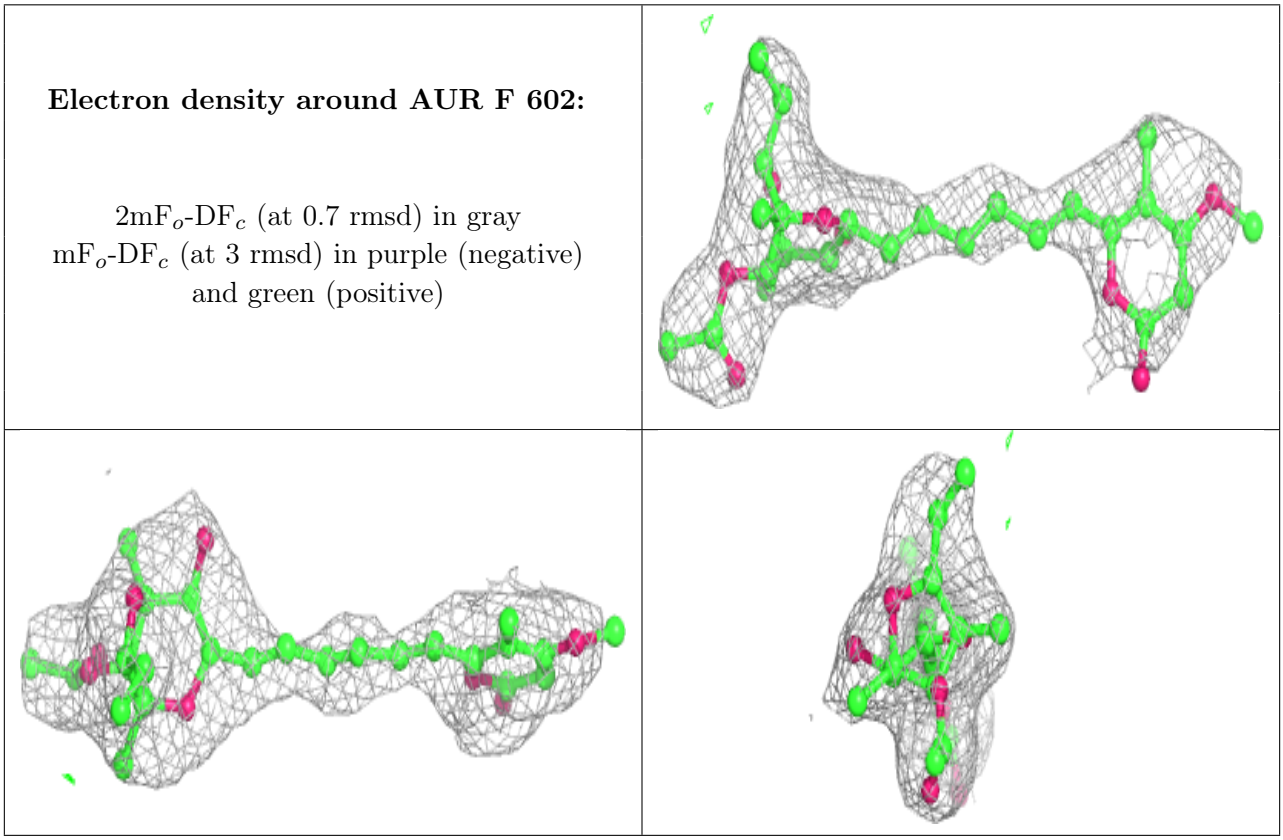
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.