



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 07:11 pm BST

PDB ID : 2XOK
Title : Refined structure of yeast F1c10 ATPase complex to 3 Å resolution
Authors : Stock, D.; W Leslie, A.G.; Walker, J.E.
Deposited on : 2010-08-18
Resolution : 3.01 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

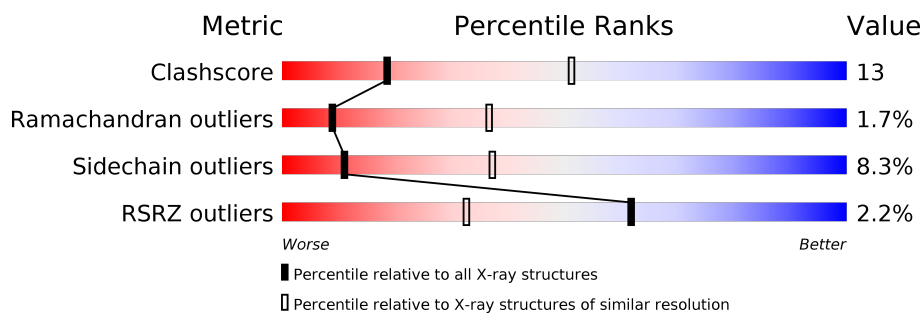
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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	545	<div> <div></div> <div> <div></div> <div>61%</div> <div>26%</div> <div>• 11%</div> </div> </div>
1	B	545	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>30%</div> <div>• 11%</div> </div> </div>
1	C	545	<div> <div></div> <div> <div></div> <div>62%</div> <div>26%</div> <div>• 11%</div> </div> </div>
2	D	511	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>24%</div> <div>• 8%</div> </div> </div>
2	E	511	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>29%</div> <div>• 8%</div> </div> </div>
2	F	511	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>29%</div> <div>• 8%</div> </div> </div>
3	G	311	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>26%</div> <div>• 14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	H	160	
5	I	61	
6	K	76	
6	L	76	
6	M	76	
6	N	76	
6	O	76	
6	P	76	
6	Q	76	
6	R	76	
6	S	76	
6	T	76	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 30113 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, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	1
			3665	2314	649	699	3			
1	B	484	Total	C	N	O	S	0	0	1
			3670	2317	650	700	3			
1	C	485	Total	C	N	O	S	0	0	1
			3674	2319	651	701	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	471	Total	C	N	O	S	0	0	1
			3550	2250	605	689	6			
2	E	469	Total	C	N	O	S	0	0	1
			3537	2243	603	685	6			
2	F	470	Total	C	N	O	S	0	0	1
			3544	2247	604	687	6			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	266	Total	C	N	O	S	0	0	1
			2031	1277	356	388	10			

- Molecule 4 is a protein called ATP SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	119	Total	C	N	O	S	0	0	0
			751	470	133	146	2			

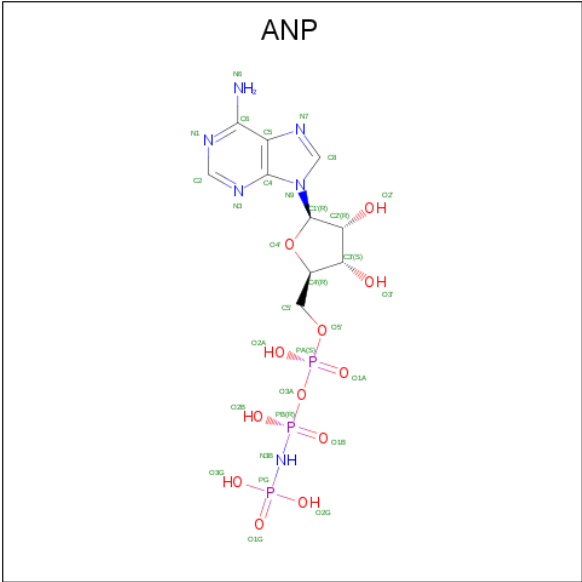
- Molecule 5 is a protein called ATP SYNTHASE CATALYTIC SECTOR F1 EPSILON SUBUNIT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	49	Total	C	N	O	0	0	1
			325	201	57	67			

- Molecule 6 is a protein called ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	73	Total	C	N	O	S	0	0	1
			517	347	80	87	3			
6	L	72	Total	C	N	O	S	0	0	1
			507	337	80	87	3			
6	M	73	Total	C	N	O	S	0	0	1
			515	342	81	88	4			
6	N	73	Total	C	N	O	S	0	0	1
			515	342	81	88	4			
6	O	74	Total	C	N	O	S	0	0	1
			523	348	82	89	4			
6	P	75	Total	C	N	O	S	0	0	1
			534	357	83	90	4			
6	Q	75	Total	C	N	O	S	0	0	1
			534	357	83	90	4			
6	R	74	Total	C	N	O	S	0	0	1
			523	348	82	89	4			
6	S	74	Total	C	N	O	S	0	0	1
			523	348	82	89	4			
6	T	73	Total	C	N	O	S	0	0	1
			515	343	81	88	3			

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

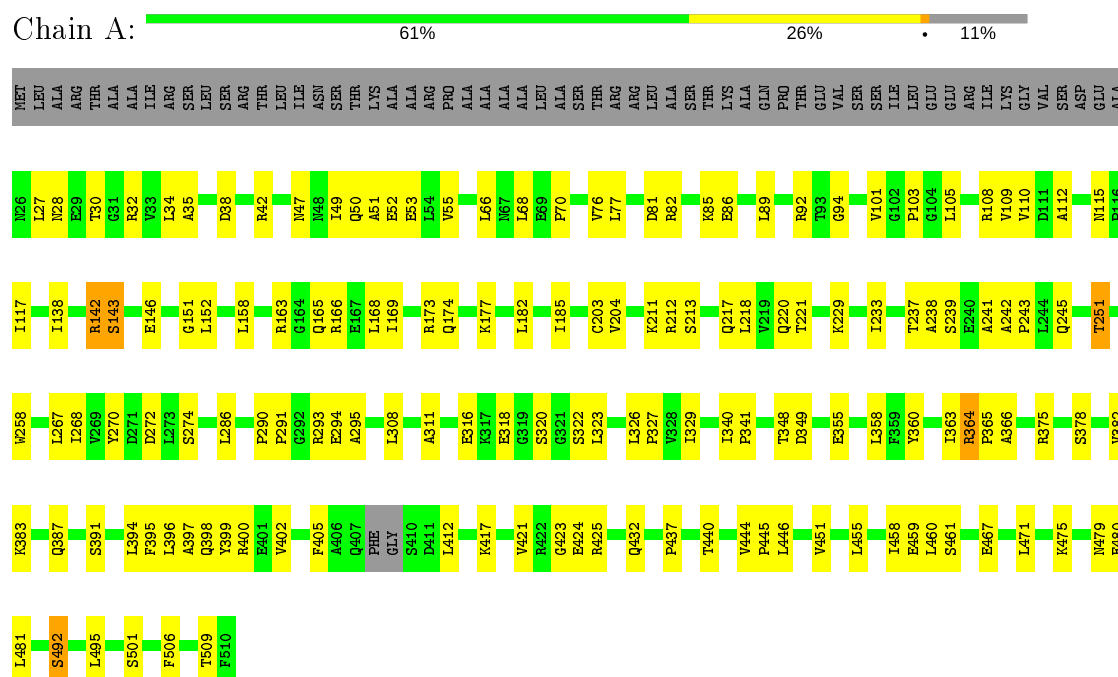
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

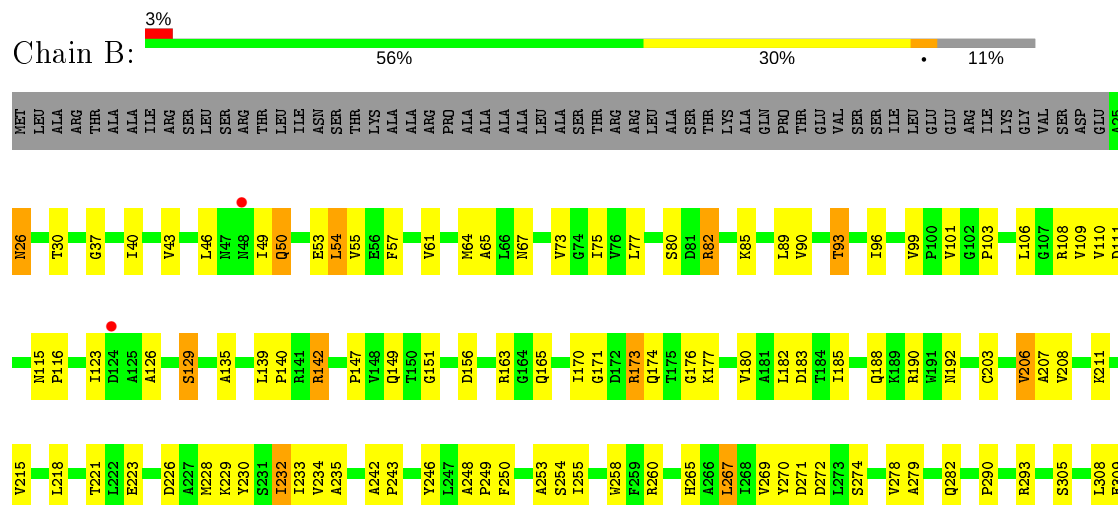
3 Residue-property plots

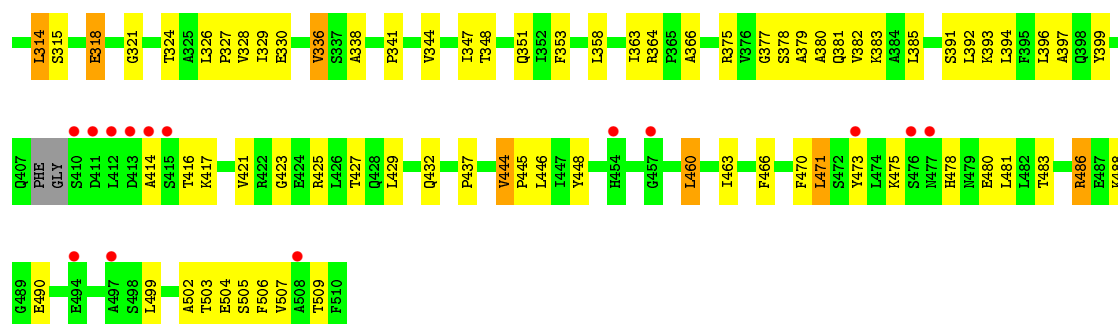
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

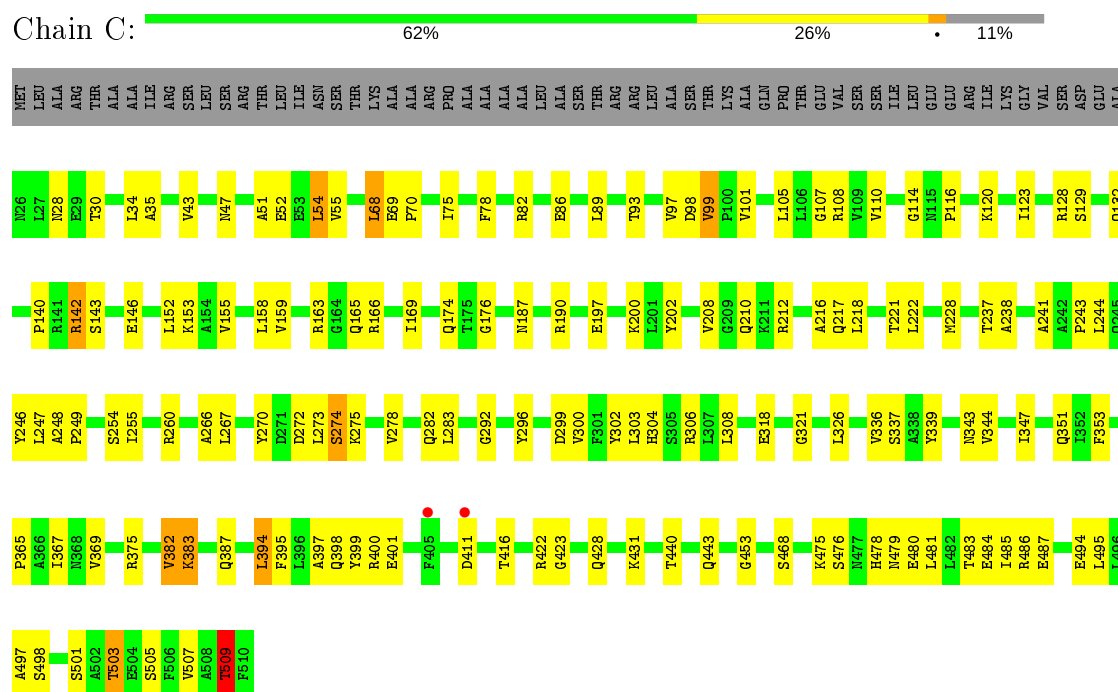


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

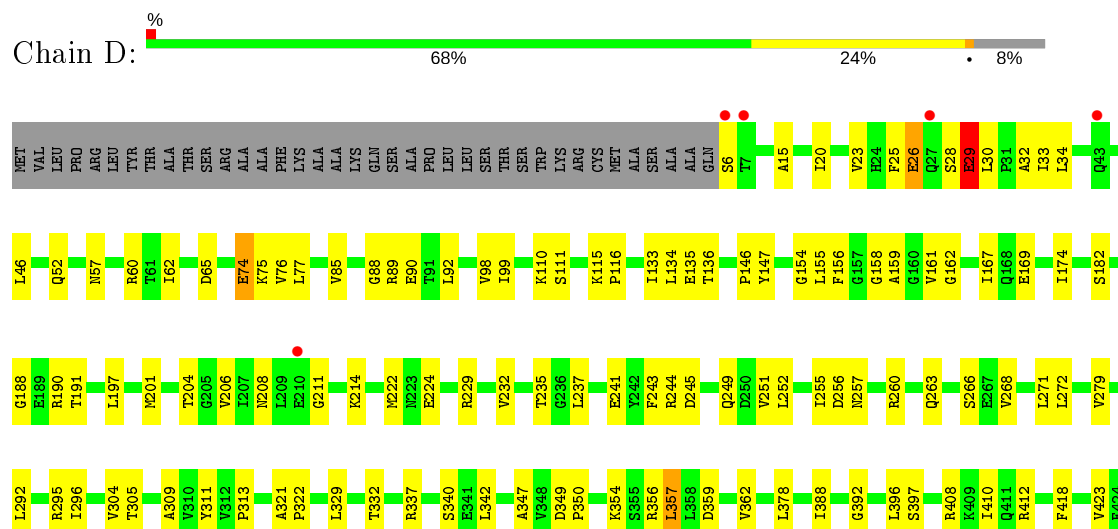


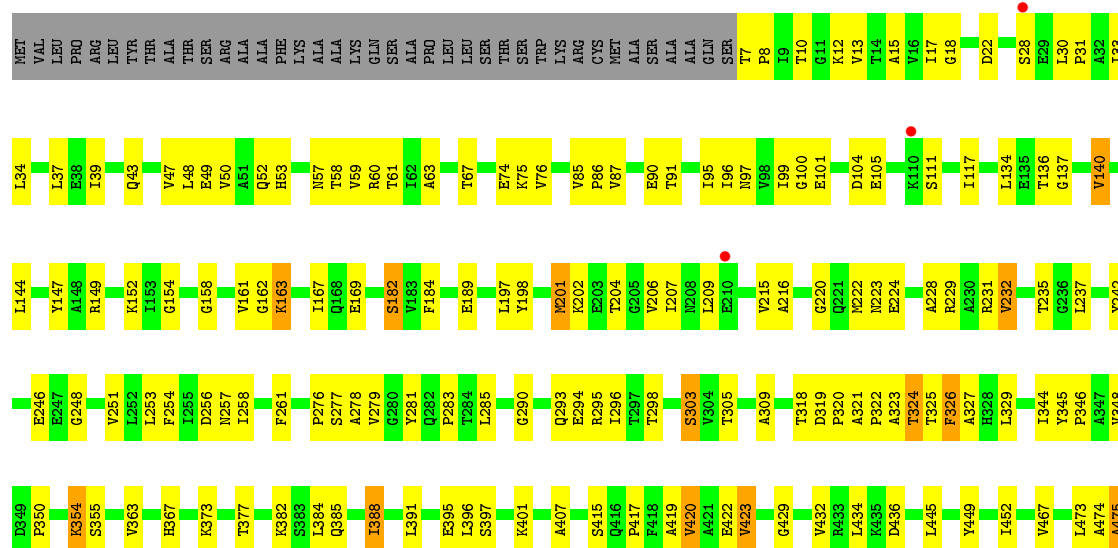


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



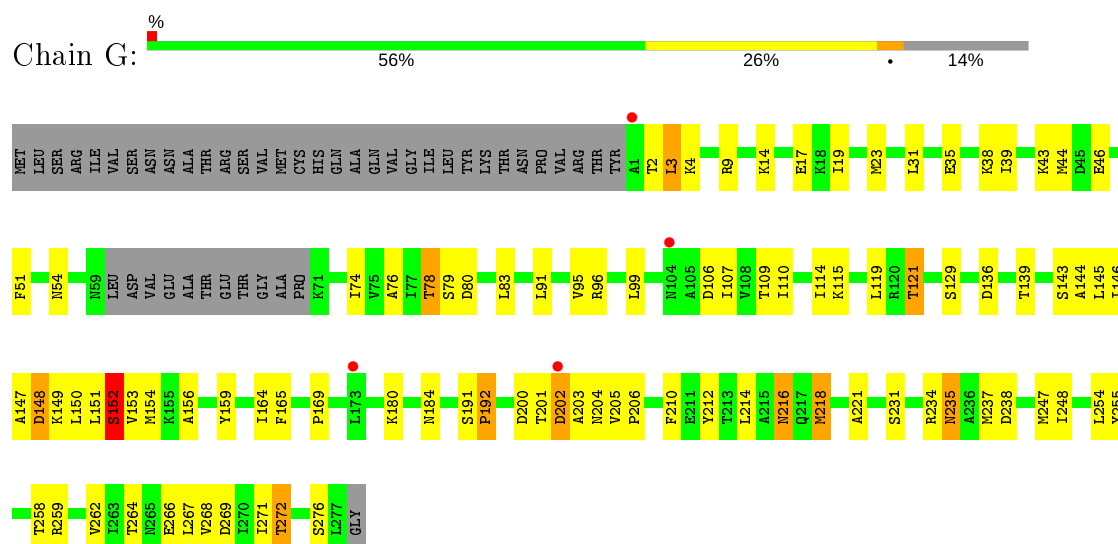
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



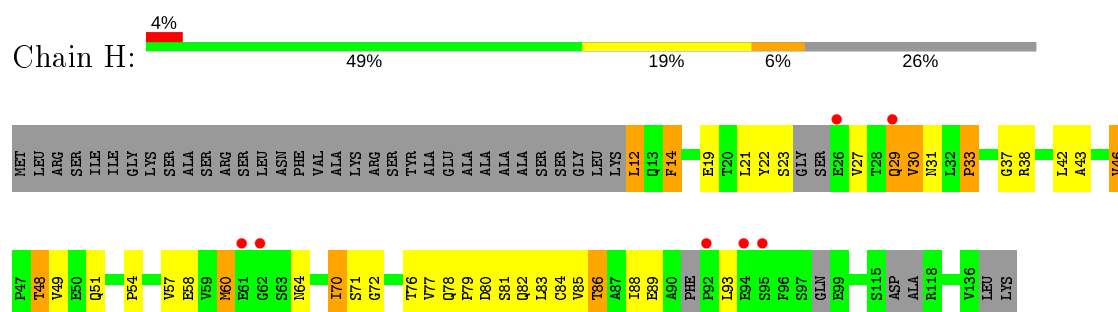




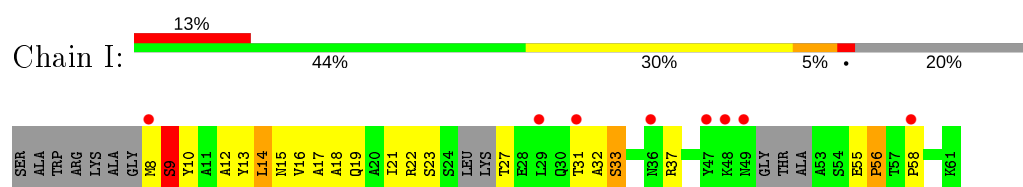
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



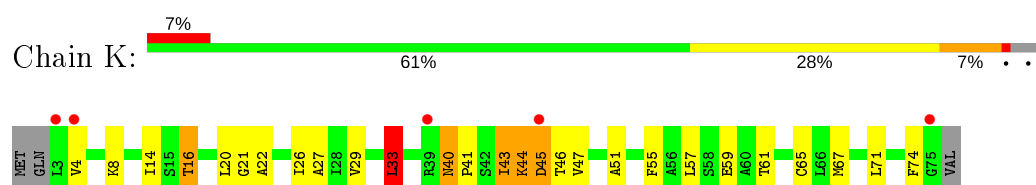
• Molecule 4: ATP SYNTHASE



• Molecule 5: ATP SYNTHASE CATALYTIC SECTOR F1 EPSILON SUBUNIT

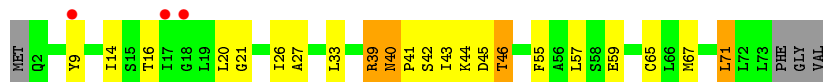


• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

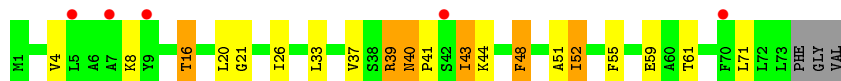


• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL

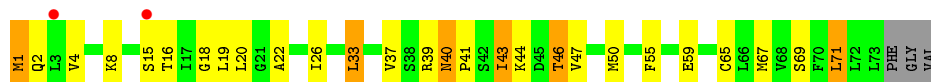




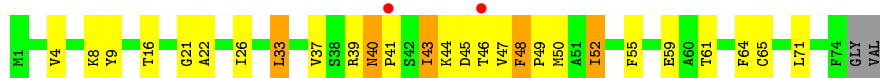
- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



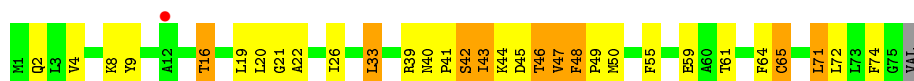
- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



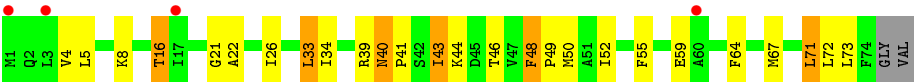
- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



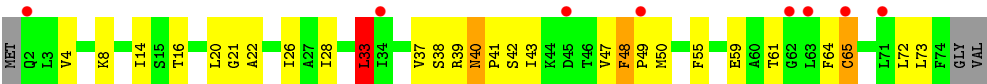
- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



- Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



• Molecule 6: ATP SYNTHASE SUBUNIT 9, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.35Å 173.71Å 137.89Å 90.00° 91.77° 90.00°	Depositor
Resolution (Å)	20.00 – 3.01 20.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	74.8 (20.00-3.01) 74.8 (20.00-3.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.253 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	88.3	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 79.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.004 for h,-k,-l 0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30113	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0/3719	0.66	0/5034
1	B	0.46	0/3724	0.63	0/5041
1	C	0.57	0/3729	0.72	2/5049 (0.0%)
2	D	0.55	0/3606	0.67	0/4891
2	E	0.44	0/3593	0.59	1/4872 (0.0%)
2	F	0.52	0/3600	0.69	0/4883
3	G	0.45	0/2056	0.58	0/2768
4	H	0.46	0/759	0.59	0/1040
5	I	0.53	0/327	0.82	2/447 (0.4%)
6	K	0.48	1/525 (0.2%)	0.61	1/712 (0.1%)
6	L	0.46	0/514	0.57	0/697
6	M	0.47	0/522	0.60	0/707
6	N	0.47	0/522	0.61	0/707
6	O	0.47	0/530	0.59	0/718
6	P	0.46	1/542 (0.2%)	0.56	0/734
6	Q	0.48	1/542 (0.2%)	0.60	0/734
6	R	0.46	0/530	0.59	0/718
6	S	0.46	0/530	0.63	1/718 (0.1%)
6	T	0.47	0/522	0.58	1/708 (0.1%)
All	All	0.50	3/30392 (0.0%)	0.64	8/41178 (0.0%)

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
5	I	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	74	PHE	C-N	-5.30	1.23	1.33
6	K	74	PHE	C-N	-5.25	1.23	1.33
6	Q	74	PHE	C-N	-5.16	1.23	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	56	PRO	N-CA-CB	6.34	110.90	103.30
5	I	58	PRO	N-CA-CB	5.81	110.27	103.30
6	K	33	LEU	CA-CB-CG	5.54	128.03	115.30
6	S	33	LEU	CA-CB-CG	5.38	127.67	115.30
2	E	285	LEU	CA-CB-CG	5.29	127.45	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	I	9	SER	Peptide

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	3665	0	3747	90	0
1	B	3670	0	3752	120	0
1	C	3674	0	3753	90	0
2	D	3550	0	3620	75	0
2	E	3537	0	3610	88	0
2	F	3544	0	3615	108	0
3	G	2031	0	2081	50	0
4	H	751	0	598	31	0
5	I	325	0	249	19	0
6	K	517	0	559	26	0
6	L	507	0	547	18	0
6	M	515	0	559	18	0
6	N	515	0	559	22	0
6	O	523	0	570	19	0
6	P	534	0	579	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	534	0	579	25	0
6	R	523	0	570	24	0
6	S	523	0	570	20	0
6	T	515	0	558	26	0
7	A	31	0	13	1	0
7	B	31	0	13	1	0
7	C	31	0	13	2	0
7	D	31	0	13	3	0
7	F	31	0	13	7	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
All	All	30113	0	30740	805	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 13.

The worst 5 of 805 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)
6:P:40:ASN:HB3	6:P:41:PRO:HA	1.35	1.09
6:M:40:ASN:HB3	6:M:41:PRO:HA	1.40	1.04
2:F:7:THR:HB	2:F:8:PRO:HD2	1.41	1.02
6:S:40:ASN:HB3	6:S:41:PRO:HA	1.44	0.98
3:G:23:MET:HB3	3:G:237:MET:HG3	1.48	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	479/545 (88%)	427 (89%)	50 (10%)	2 (0%)	34	71
1	B	480/545 (88%)	434 (90%)	44 (9%)	2 (0%)	34	71
1	C	483/545 (89%)	443 (92%)	36 (8%)	4 (1%)	19	55
2	D	469/511 (92%)	430 (92%)	37 (8%)	2 (0%)	34	71
2	E	467/511 (91%)	424 (91%)	37 (8%)	6 (1%)	12	43
2	F	468/511 (92%)	417 (89%)	42 (9%)	9 (2%)	8	34
3	G	262/311 (84%)	231 (88%)	24 (9%)	7 (3%)	5	25
4	H	109/160 (68%)	89 (82%)	15 (14%)	5 (5%)	2	13
5	I	43/61 (70%)	27 (63%)	10 (23%)	6 (14%)	0	1
6	K	71/76 (93%)	66 (93%)	2 (3%)	3 (4%)	3	15
6	L	70/76 (92%)	67 (96%)	0	3 (4%)	2	14
6	M	71/76 (93%)	67 (94%)	3 (4%)	1 (1%)	11	41
6	N	71/76 (93%)	61 (86%)	7 (10%)	3 (4%)	3	15
6	O	72/76 (95%)	65 (90%)	5 (7%)	2 (3%)	5	24
6	P	73/76 (96%)	68 (93%)	2 (3%)	3 (4%)	3	15
6	Q	73/76 (96%)	64 (88%)	3 (4%)	6 (8%)	1	3
6	R	72/76 (95%)	65 (90%)	5 (7%)	2 (3%)	5	24
6	S	72/76 (95%)	66 (92%)	4 (6%)	2 (3%)	5	24
6	T	71/76 (93%)	65 (92%)	5 (7%)	1 (1%)	11	41
All	All	3976/4460 (89%)	3576 (90%)	331 (8%)	69 (2%)	9	37

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	29	GLU
2	F	28	SER
3	G	152	SER
3	G	202	ASP
3	G	204	ASN

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	A	388/437 (89%)	369 (95%)	19 (5%)	25	60
1	B	388/437 (89%)	351 (90%)	37 (10%)	8	31
1	C	388/437 (89%)	360 (93%)	28 (7%)	14	44
2	D	380/411 (92%)	360 (95%)	20 (5%)	22	57
2	E	378/411 (92%)	357 (94%)	21 (6%)	21	54
2	F	379/411 (92%)	359 (95%)	20 (5%)	22	57
3	G	218/266 (82%)	191 (88%)	27 (12%)	4	19
4	H	54/131 (41%)	40 (74%)	14 (26%)	0	2
5	I	23/48 (48%)	20 (87%)	3 (13%)	4	18
6	K	53/56 (95%)	48 (91%)	5 (9%)	8	31
6	L	52/56 (93%)	47 (90%)	5 (10%)	8	30
6	M	53/56 (95%)	45 (85%)	8 (15%)	3	13
6	N	53/56 (95%)	47 (89%)	6 (11%)	6	23
6	O	54/56 (96%)	46 (85%)	8 (15%)	3	13
6	P	55/56 (98%)	50 (91%)	5 (9%)	9	33
6	Q	55/56 (98%)	46 (84%)	9 (16%)	2	11
6	R	54/56 (96%)	43 (80%)	11 (20%)	1	5
6	S	54/56 (96%)	47 (87%)	7 (13%)	4	18
6	T	53/56 (95%)	45 (85%)	8 (15%)	3	13
All	All	3132/3549 (88%)	2871 (92%)	261 (8%)	11	37

5 of 261 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	380	THR
3	G	3	LEU
6	R	48	PHE
2	E	433	ARG
2	F	251	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	50	GLN

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Mol	Chain	Res	Type
2	D	195	ASN
6	M	2	GLN
1	C	210	GLN
1	C	407	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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	ANP	C	600	8	29,33,33	2.70	8 (27%)	31,52,52	1.88	10 (32%)
7	ANP	B	600	8	29,33,33	2.93	6 (20%)	31,52,52	1.78	8 (25%)
7	ANP	D	600	8	29,33,33	3.08	9 (31%)	31,52,52	2.04	9 (29%)
7	ANP	F	600	8	29,33,33	2.96	7 (24%)	31,52,52	2.17	10 (32%)
7	ANP	A	600	8	29,33,33	2.76	7 (24%)	31,52,52	1.80	9 (29%)

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	ANP	C	600	8	-	2/14/38/38	0/3/3/3
7	ANP	B	600	8	-	3/14/38/38	0/3/3/3
7	ANP	D	600	8	-	2/14/38/38	0/3/3/3
7	ANP	F	600	8	-	1/14/38/38	0/3/3/3
7	ANP	A	600	8	-	2/14/38/38	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	600	ANP	PG-O1G	9.60	1.61	1.46
7	A	600	ANP	PG-O1G	8.77	1.60	1.46
7	F	600	ANP	PG-O1G	8.66	1.59	1.46
7	B	600	ANP	PG-O1G	8.65	1.59	1.46
7	D	600	ANP	PB-O1B	8.18	1.59	1.46

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	600	ANP	O1B-PB-N3B	-5.45	103.75	111.77
7	B	600	ANP	PA-O3A-PB	-4.69	116.12	132.62
7	D	600	ANP	PA-O3A-PB	-4.61	116.38	132.62
7	A	600	ANP	PA-O3A-PB	-4.19	117.87	132.62
7	D	600	ANP	C4-C5-N7	-4.18	105.04	109.40

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	600	ANP	PG-N3B-PB-O1B
7	A	600	ANP	PB-N3B-PG-O1G
7	A	600	ANP	PG-N3B-PB-O1B
7	C	600	ANP	PB-N3B-PG-O1G
7	C	600	ANP	PG-N3B-PB-O1B

There are no ring outliers.

5 monomers are involved in 14 short contacts:

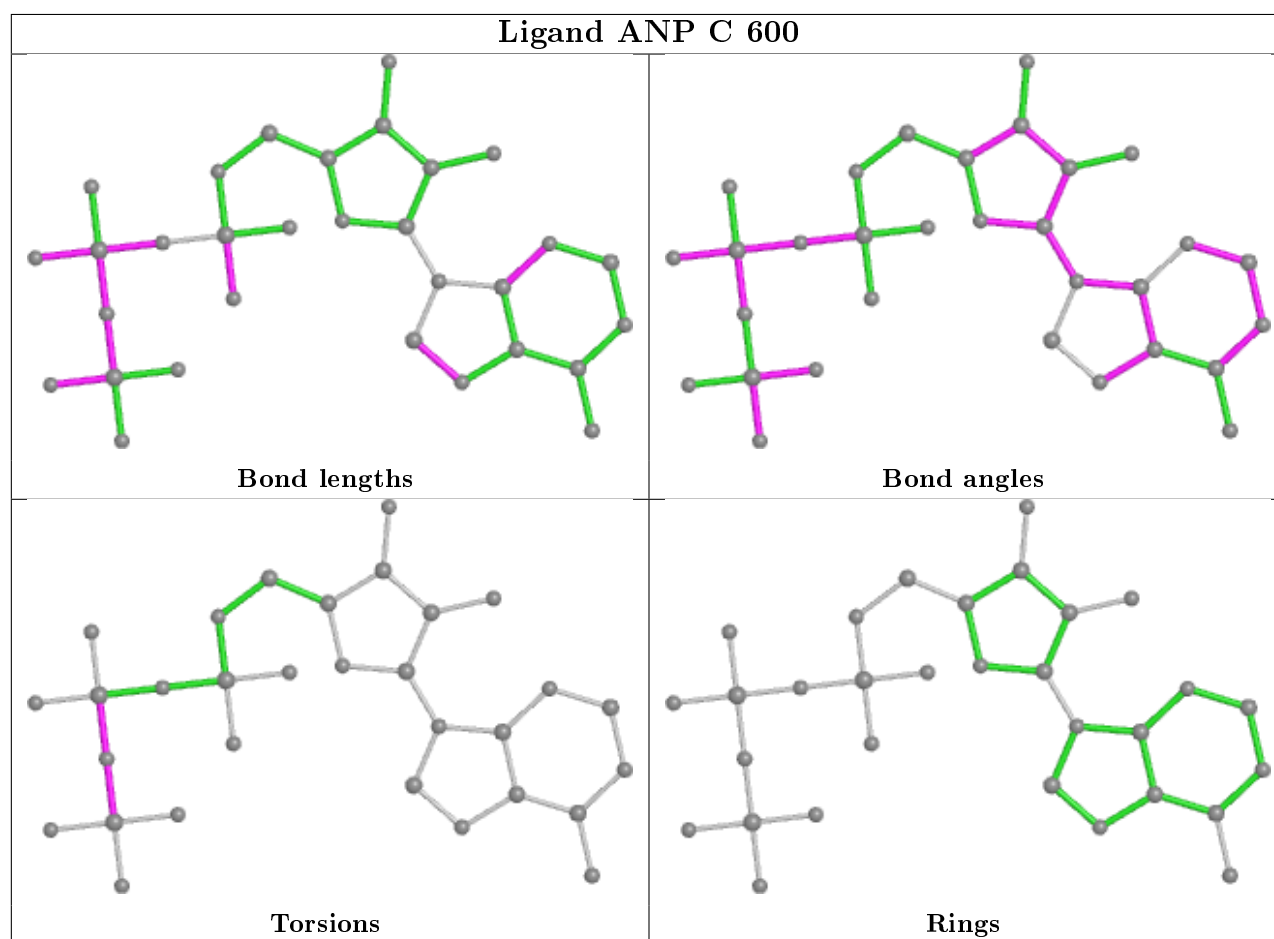
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	600	ANP	2	0

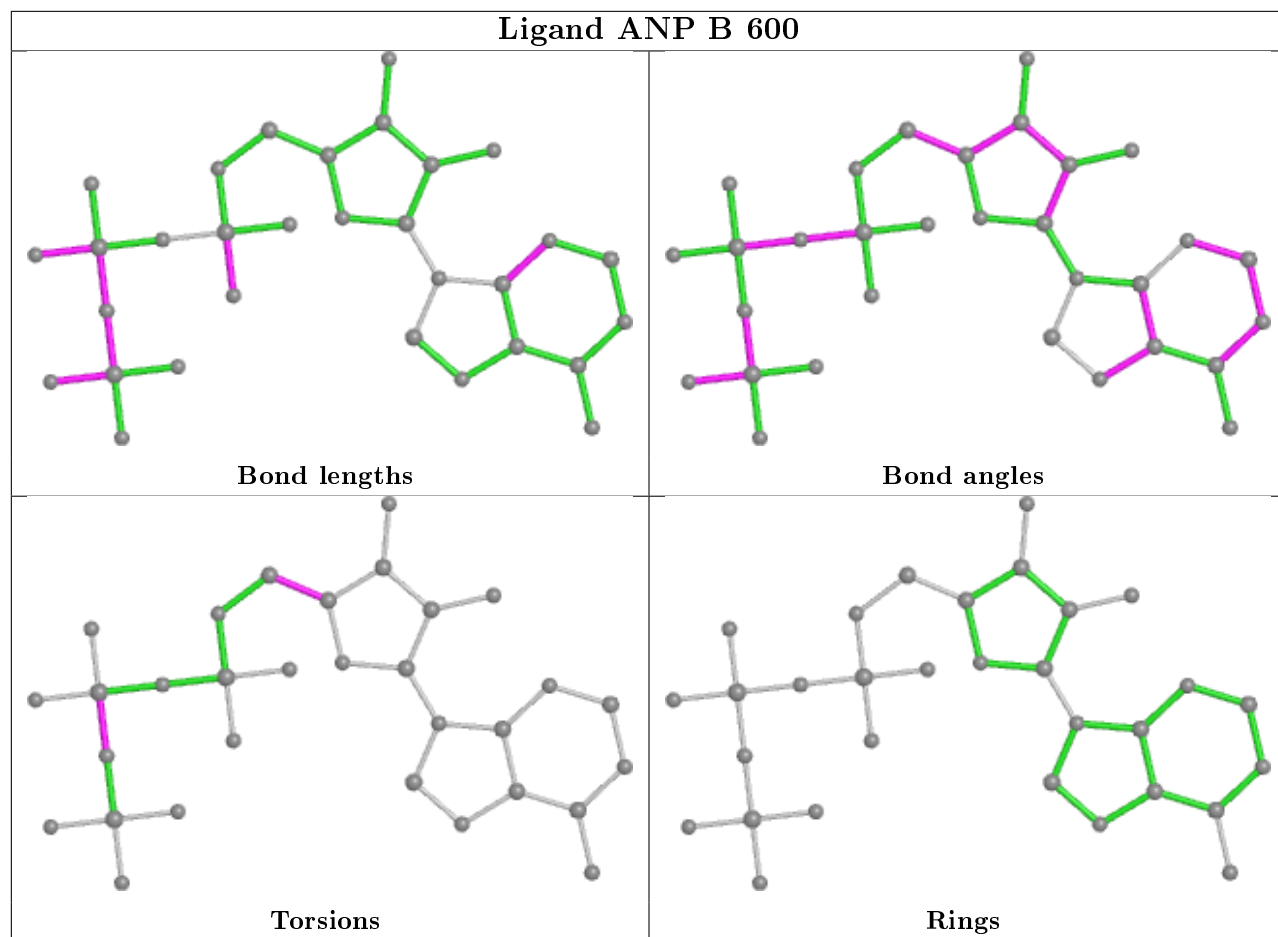
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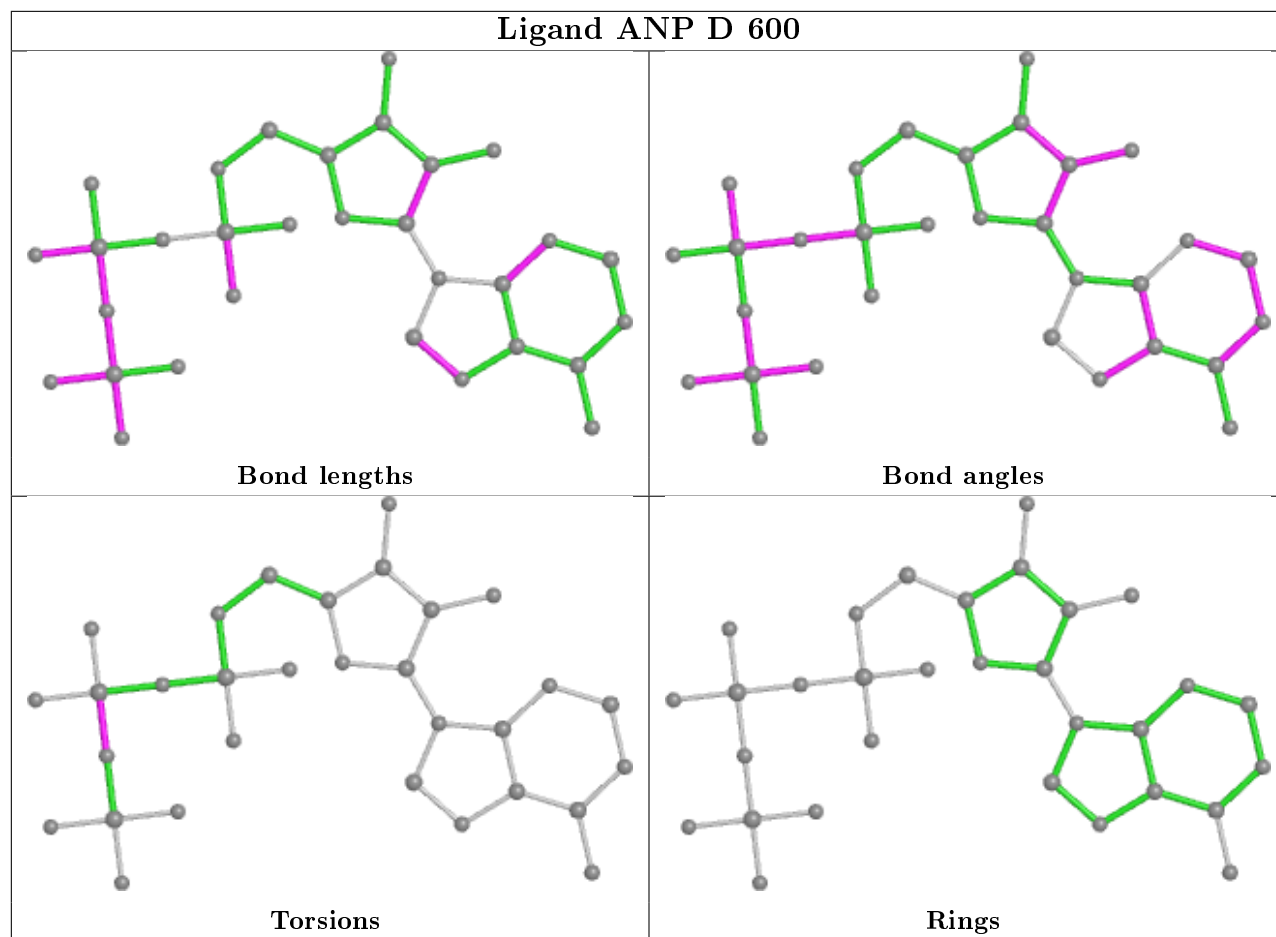
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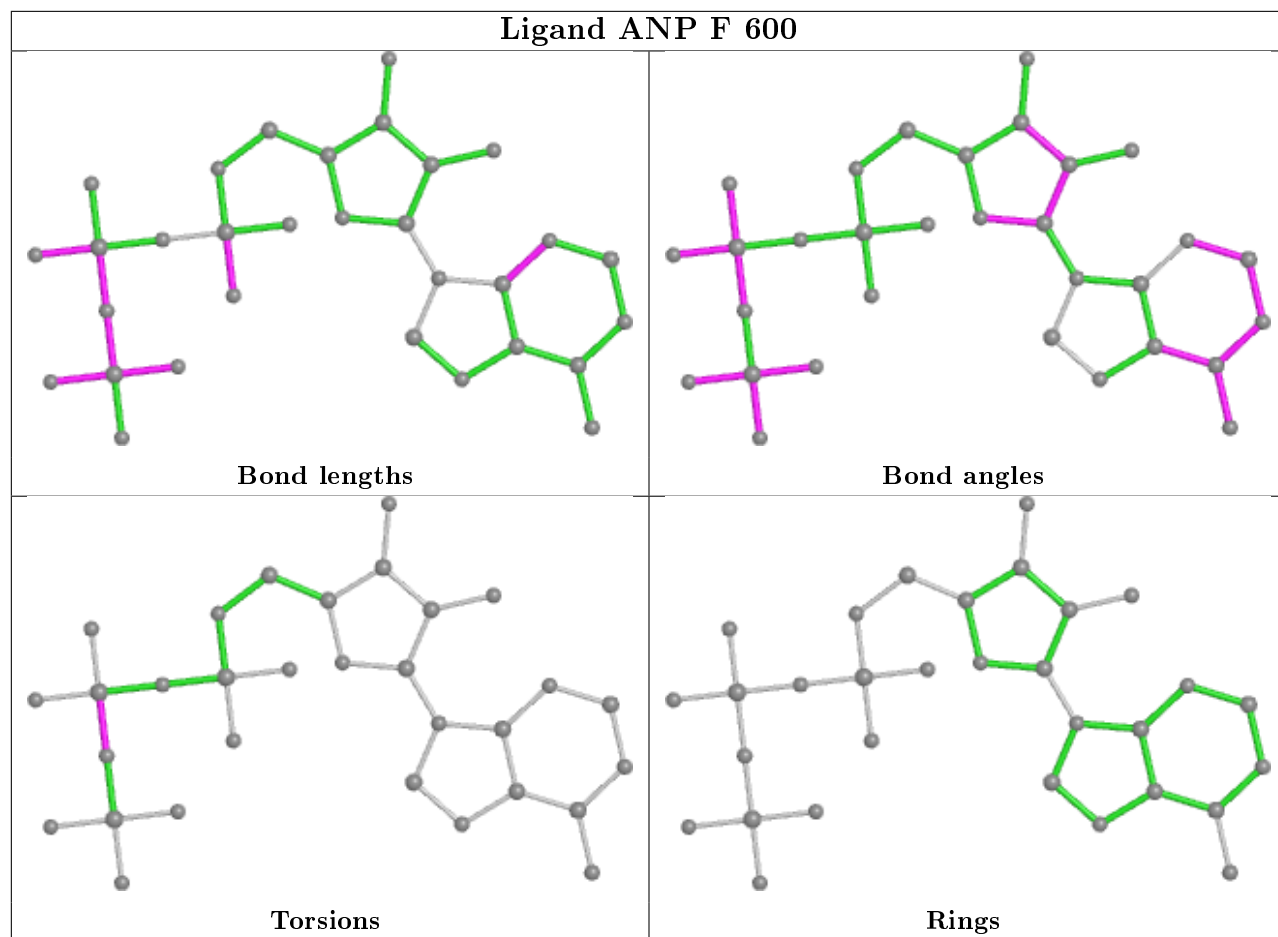
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	600	ANP	1	0
7	D	600	ANP	3	0
7	F	600	ANP	7	0
7	A	600	ANP	1	0

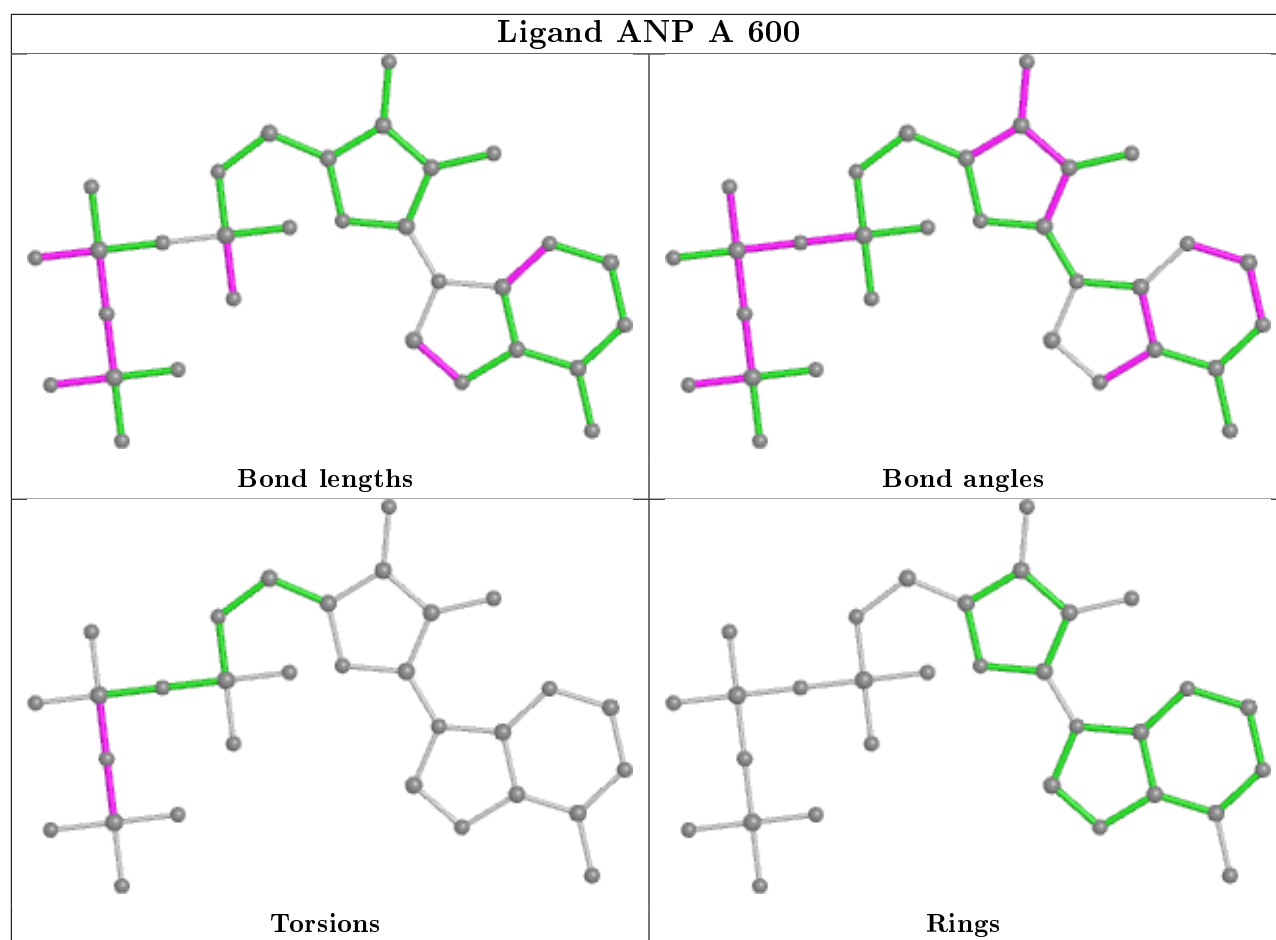
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	483/545 (88%)	-0.59	0 100 100	61, 89, 128, 145	0
1	B	484/545 (88%)	-0.20	16 (3%) 46 20	66, 116, 205, 226	0
1	C	485/545 (88%)	-0.59	2 (0%) 92 78	56, 81, 125, 176	0
2	D	471/511 (92%)	-0.55	5 (1%) 80 55	64, 85, 123, 160	0
2	E	469/511 (91%)	-0.27	13 (2%) 53 24	71, 114, 176, 213	0
2	F	470/511 (91%)	-0.55	3 (0%) 89 72	51, 93, 137, 165	0
3	G	266/311 (85%)	-0.30	4 (1%) 73 46	64, 122, 155, 172	0
4	H	119/160 (74%)	0.09	7 (5%) 22 7	102, 146, 195, 216	0
5	I	49/61 (80%)	0.51	8 (16%) 1 0	134, 162, 208, 228	0
6	K	73/76 (96%)	0.38	5 (6%) 17 5	151, 188, 222, 243	0
6	L	72/76 (94%)	0.36	3 (4%) 36 14	149, 188, 213, 217	0
6	M	73/76 (96%)	0.35	5 (6%) 17 5	144, 180, 200, 210	0
6	N	73/76 (96%)	0.16	2 (2%) 54 26	131, 166, 183, 195	0
6	O	74/76 (97%)	0.03	2 (2%) 54 26	123, 154, 171, 184	0
6	P	75/76 (98%)	-0.02	0 100 100	118, 150, 164, 175	0
6	Q	75/76 (98%)	0.05	1 (1%) 77 51	117, 152, 169, 189	0
6	R	74/76 (97%)	0.05	2 (2%) 54 26	125, 164, 183, 196	0
6	S	74/76 (97%)	0.35	4 (5%) 25 9	138, 175, 204, 221	0
6	T	73/76 (96%)	0.52	8 (10%) 5 2	147, 187, 218, 225	0
All	All	4032/4460 (90%)	-0.29	90 (2%) 62 32	51, 109, 193, 243	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	29	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
6	L	9	TYR	4.9
6	T	2	GLN	4.6
2	E	27	GLN	4.1
1	B	454	HIS	4.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

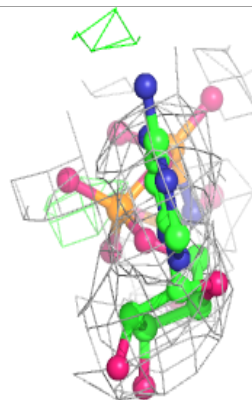
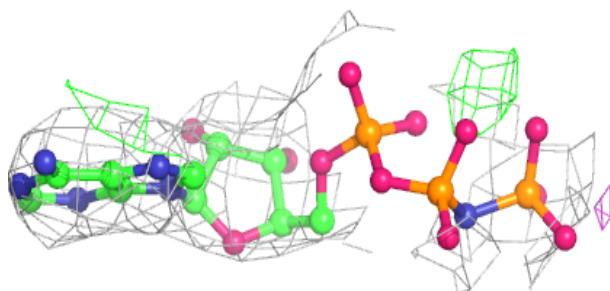
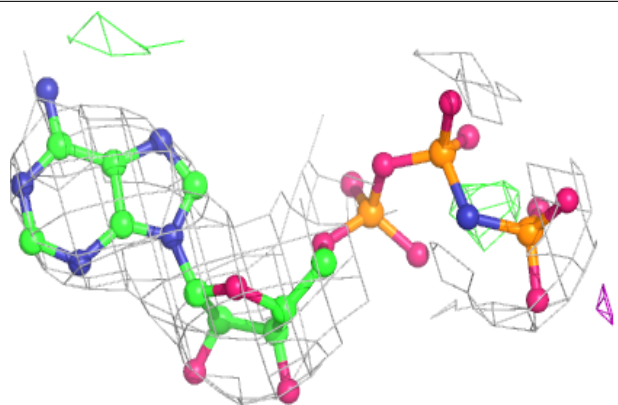
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MG	A	700	1/1	0.94	0.27	66,66,66,66	0
7	ANP	B	600	31/31	0.94	0.16	110,134,145,146	0
7	ANP	D	600	31/31	0.95	0.17	66,73,116,122	0
8	MG	D	700	1/1	0.95	0.27	71,71,71,71	0
7	ANP	C	600	31/31	0.97	0.12	51,69,77,83	0
7	ANP	F	600	31/31	0.97	0.16	39,72,95,95	0
7	ANP	A	600	31/31	0.97	0.12	60,71,80,88	0
8	MG	C	700	1/1	0.98	0.22	80,80,80,80	0
8	MG	B	700	1/1	0.98	0.22	86,86,86,86	0
8	MG	F	700	1/1	0.99	0.22	52,52,52,52	0

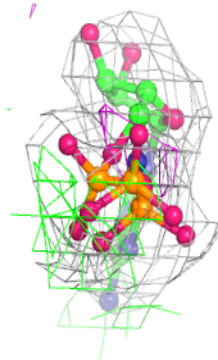
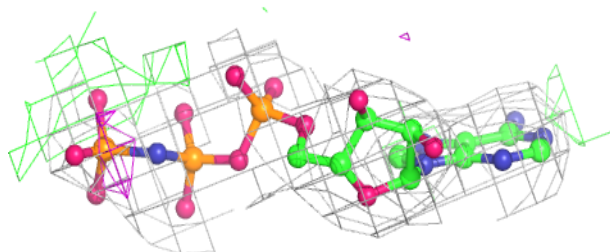
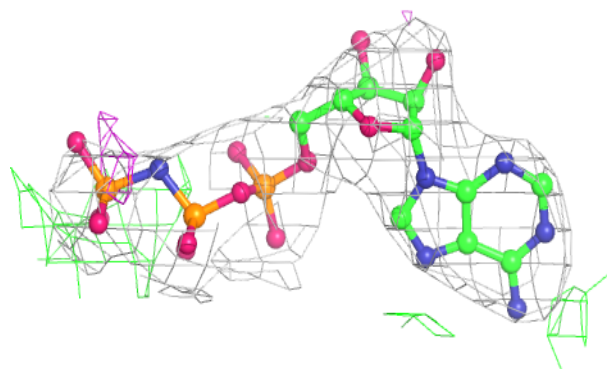
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

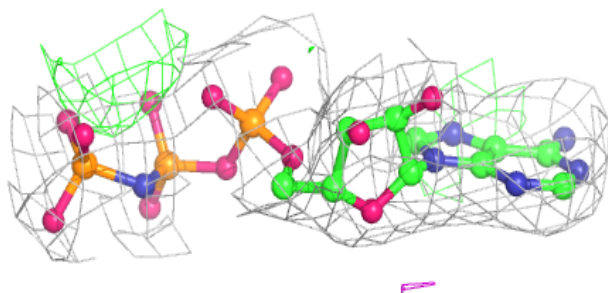
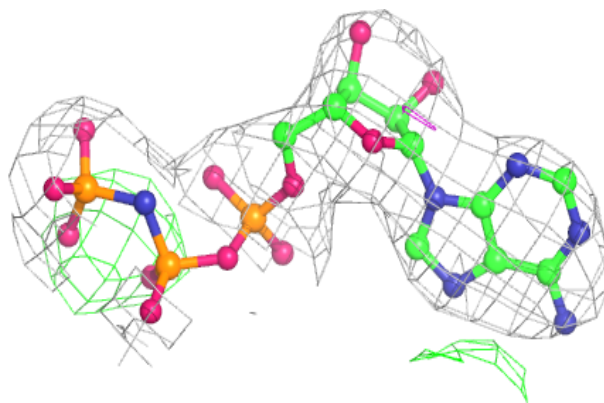
**Electron density around ANP D 600:**

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

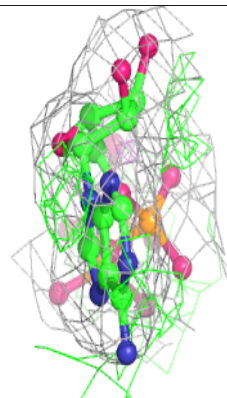
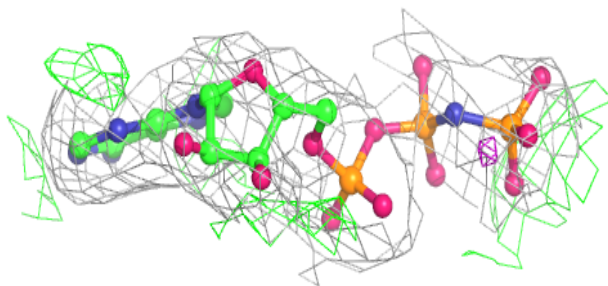
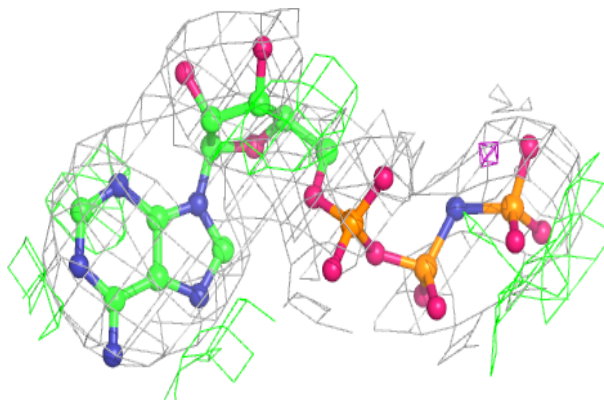


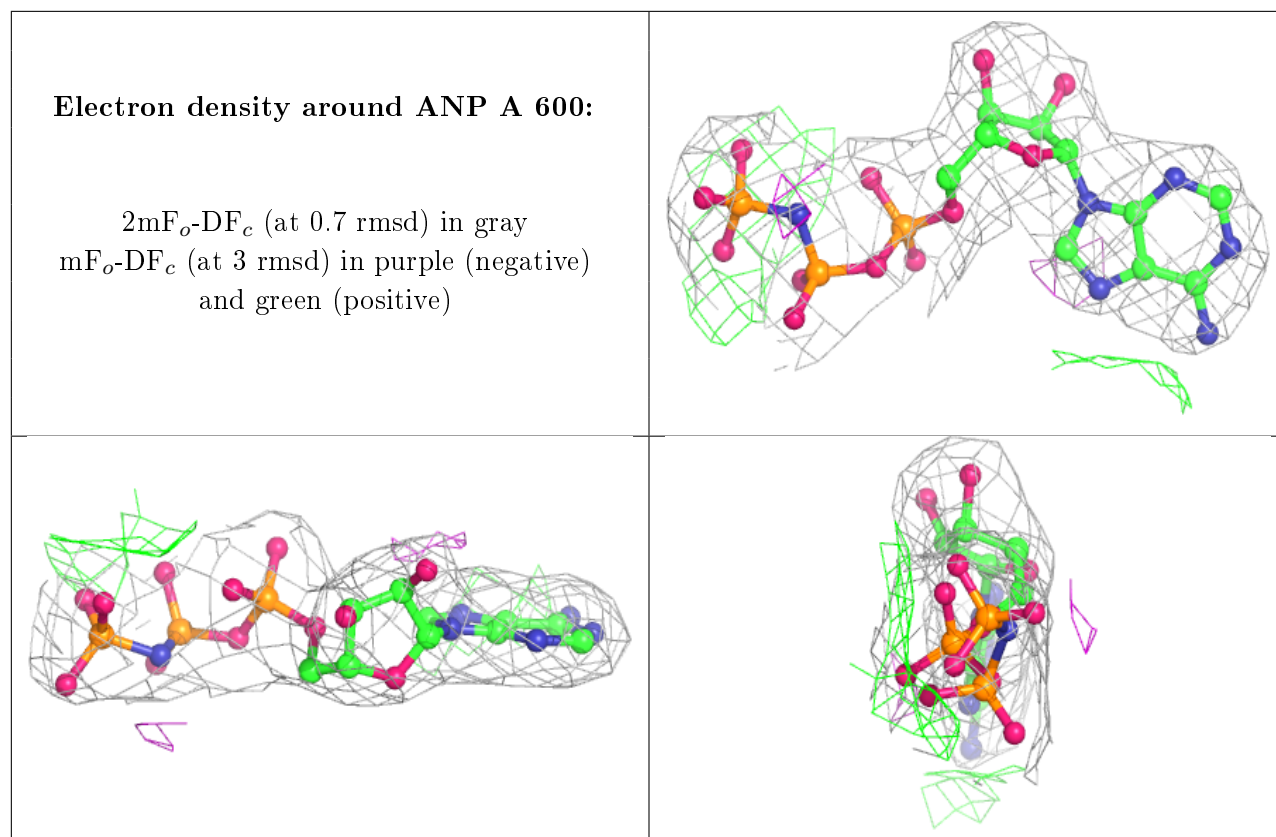
Electron density around ANP C 600:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.