



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:43 AM UTC

PDB ID : 2WSS / pdb_00002wss
Title : The structure of the membrane extrinsic region of bovine ATP synthase
Authors : Rees, D.M.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2009-09-09
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

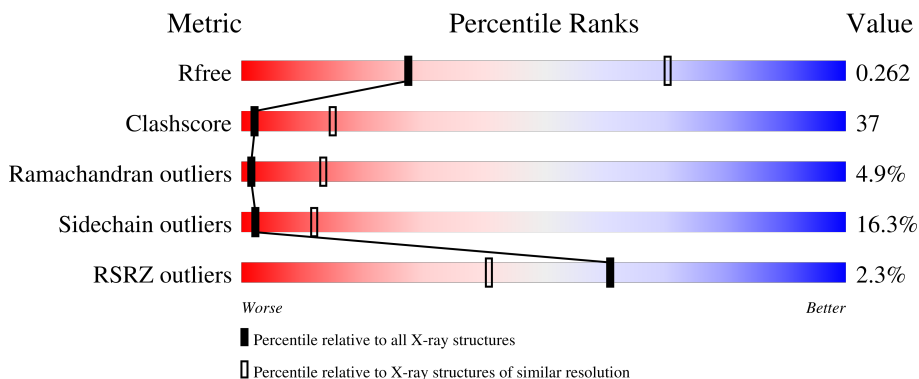
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
1	J	510	
1	K	510	

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Mol	Chain	Length	Quality of chain
1	L	510	
2	D	482	
2	E	482	
2	F	482	
2	M	482	
2	N	482	
2	O	482	
3	G	272	
3	P	272	
4	H	146	
4	Q	146	
5	I	50	
5	R	50	
6	S	190	
6	W	190	
7	T	116	
7	X	116	
8	U	118	
9	V	76	
9	Z	76	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ANP	B	600	X	-	-	-
10	ANP	F	600	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 54949 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
			Total	C	N	O	S			
1	A	510	Total 3882	C 2442	N 684	O 744	S 12	0	0	0
1	B	480	Total 3663	C 2308	N 648	O 695	S 12	0	0	0
1	C	484	Total 3684	C 2323	N 653	O 696	S 12	0	0	0
1	J	487	Total 3715	C 2341	N 656	O 706	S 12	0	0	0
1	K	480	Total 3663	C 2308	N 648	O 695	S 12	0	0	0
1	L	481	Total 3670	C 2315	N 650	O 693	S 12	0	0	0

There are 6 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
J	481	GLY	SER	conflict	UNP P19483
K	481	GLY	SER	conflict	UNP P19483
L	481	GLY	SER	conflict	UNP P19483

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	467	Total 3539	C 2243	N 601	O 684	S 11	0	0	0
2	E	466	Total 3530	C 2238	N 600	O 681	S 11	0	0	0
2	F	466	Total 3534	C 2242	N 600	O 681	S 11	0	1	0

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	260	Total	C	N	O	S	0	0	0
			2027	1273	351	395	8			
3	P	260	Total	C	N	O	S	0	0	0
			2027	1273	351	395	8			

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

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

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	S	167	Total	C	N	O	S	Se	0	0	0
			1292	820	223	242	1	6			
6	W	146	Total	C	N	O	S	Se	0	0	0
			1120	712	191	212	1	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	129	THR	ALA	conflict	UNP P13621
W	129	THR	ALA	conflict	UNP P13621

- Molecule 7 is a protein called ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	T	86	Total	C	N	O	S	Se	0	0	0
			733	459	139	130	1	4			
7	X	41	Total	C	N	O	S	Se	0	0	0
			336	211	62	59	1	3			

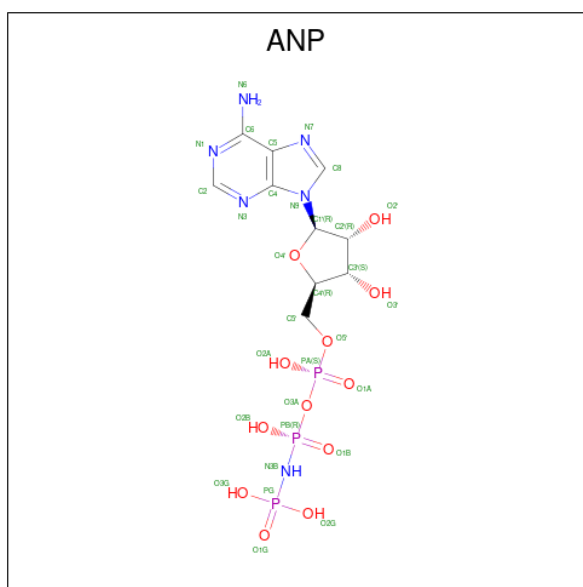
- Molecule 8 is a protein called ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	U	28	Total	C	N	O	0	0	0
			234	149	38	47			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	V	66	Total	C	N	O	Se	0	0	0
			551	352	92	105	2			
9	Z	17	Total	C	N	O		0	0	0
			160	101	33	26				

- Molecule 10 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

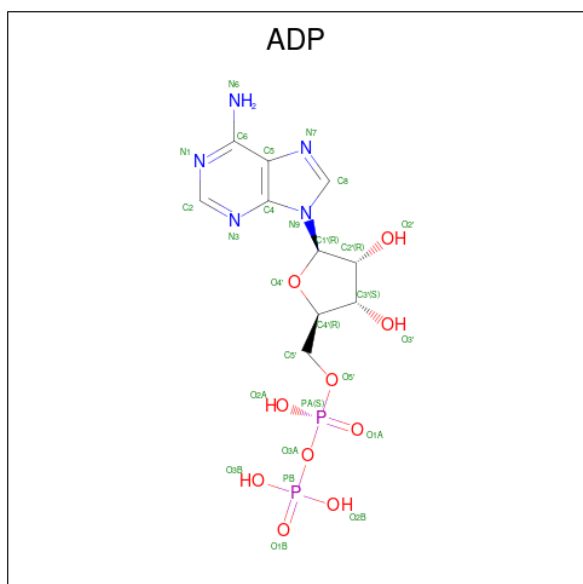
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Mg	0	0
			1	1		
11	B	1	Total	Mg	0	0
			1	1		
11	C	1	Total	Mg	0	0
			1	1		
11	D	1	Total	Mg	0	0
			1	1		

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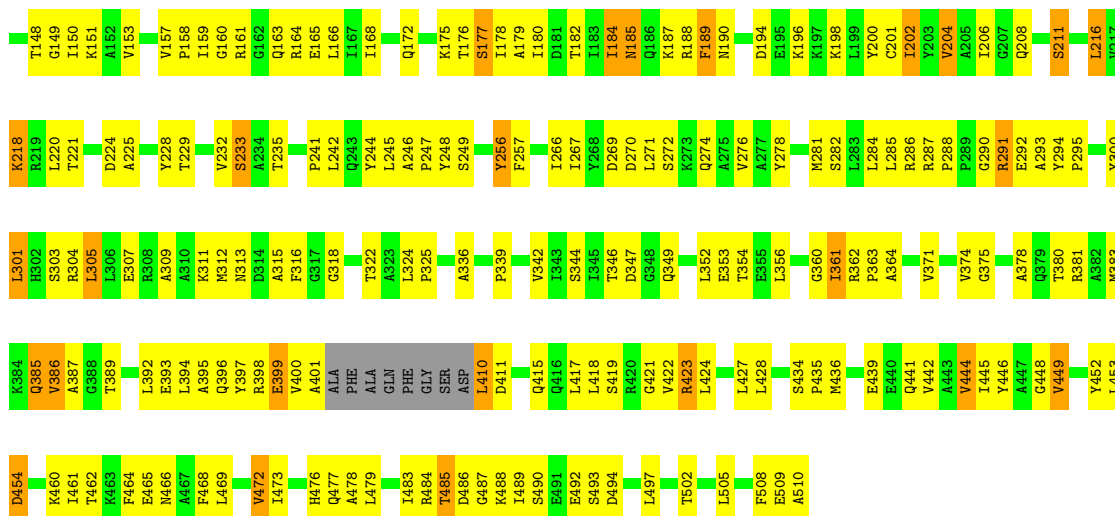
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	F	1	Total Mg 1 1	0	0
11	J	1	Total Mg 1 1	0	0
11	K	1	Total Mg 1 1	0	0
11	L	1	Total Mg 1 1	0	0
11	M	1	Total Mg 1 1	0	0
11	O	1	Total Mg 1 1	0	0

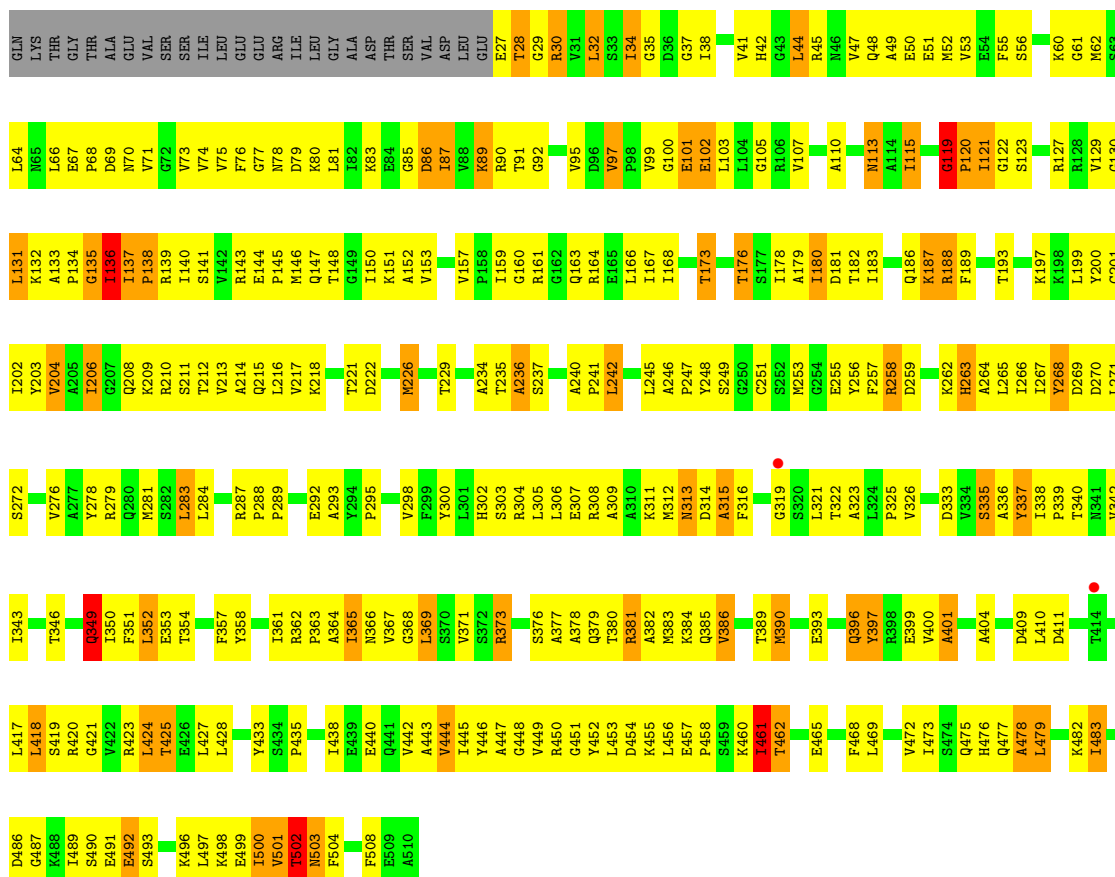
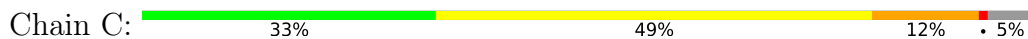
- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



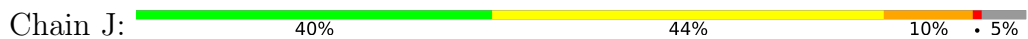
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	D	1	Total C N O P 27 10 5 10 2	0	0
12	M	1	Total C N O P 27 10 5 10 2	0	0

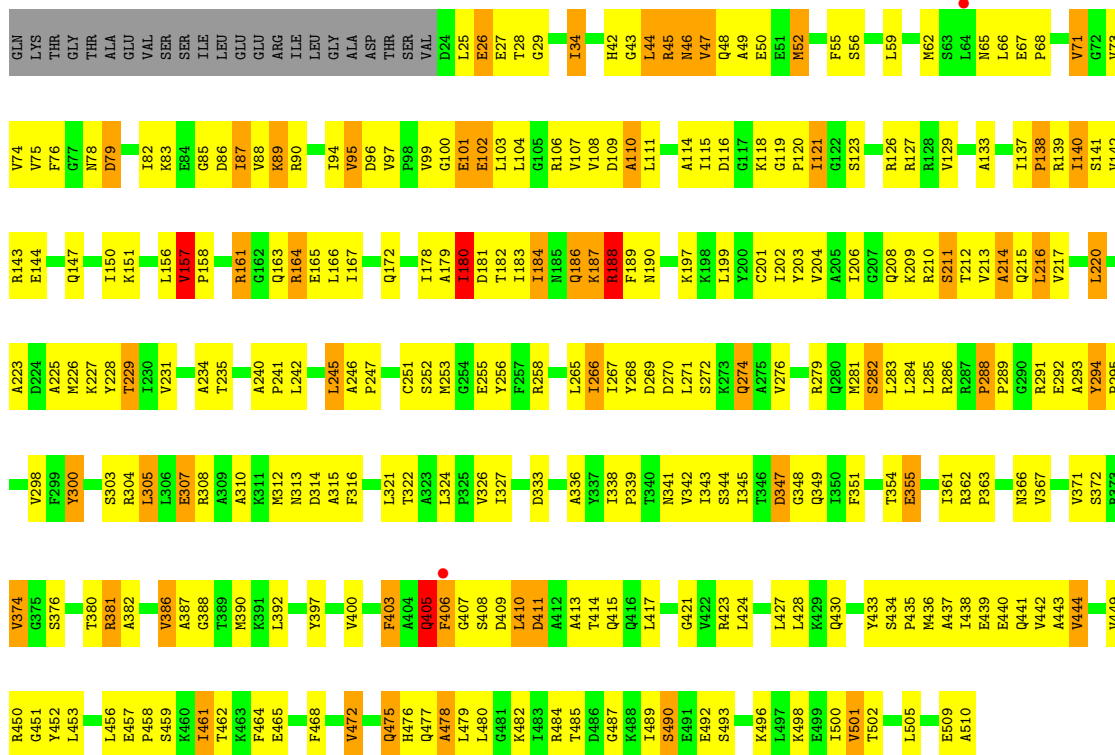


● Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

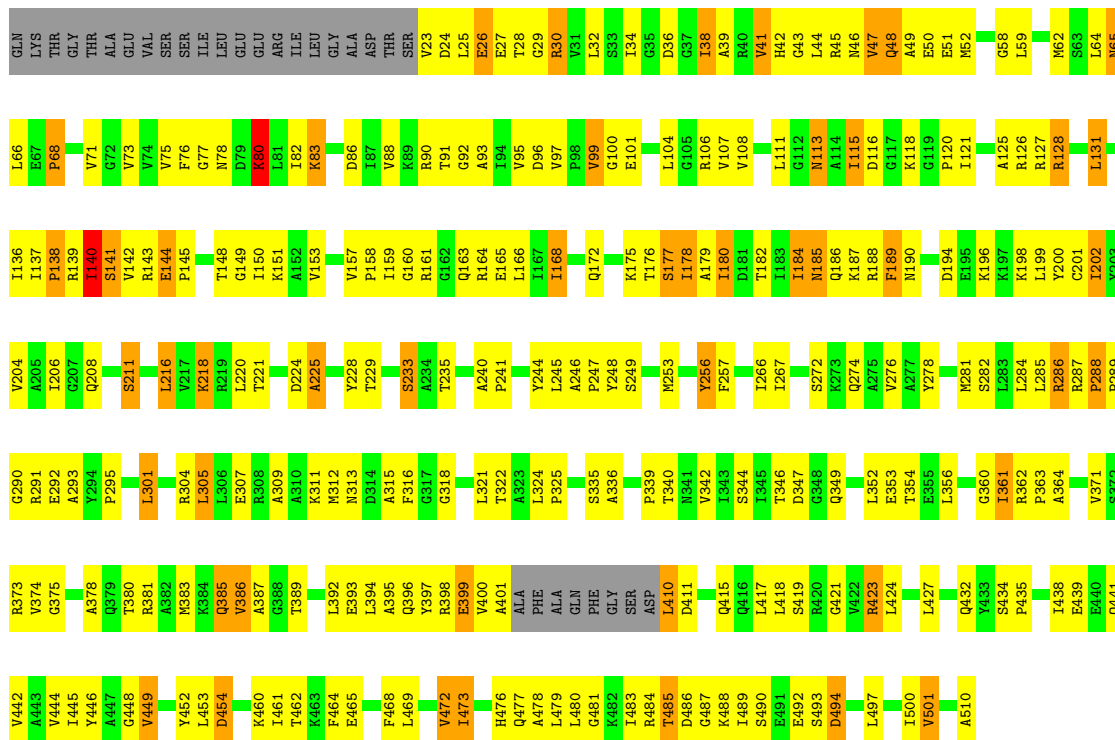


● Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

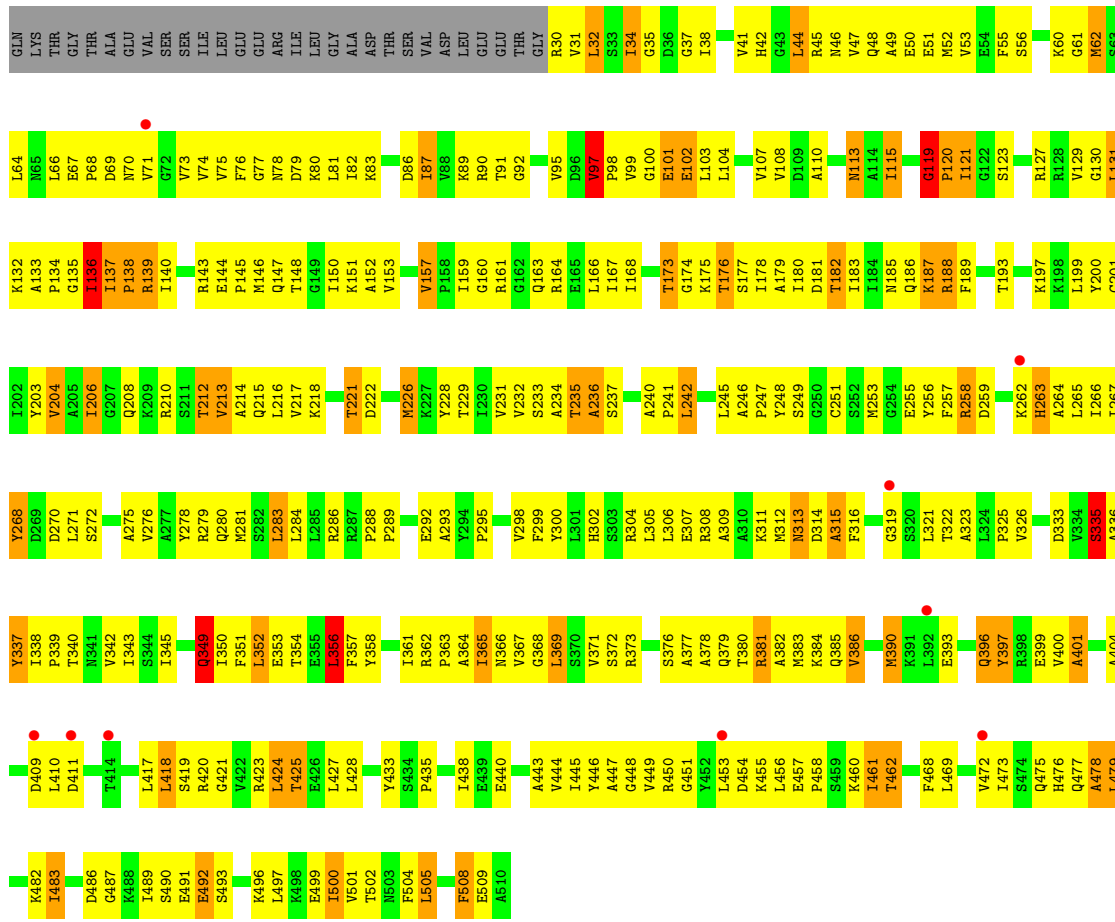




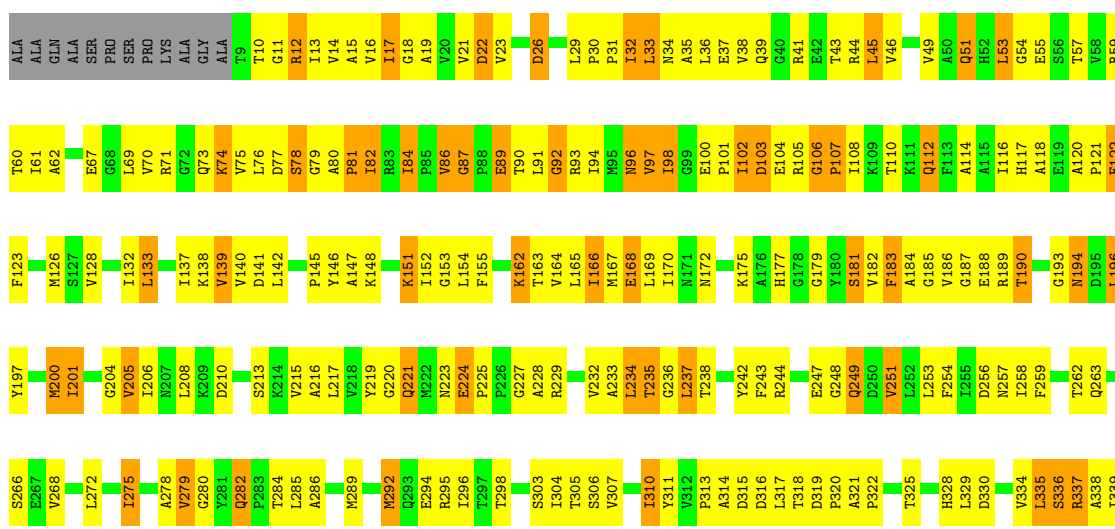
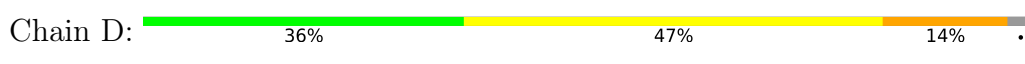
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

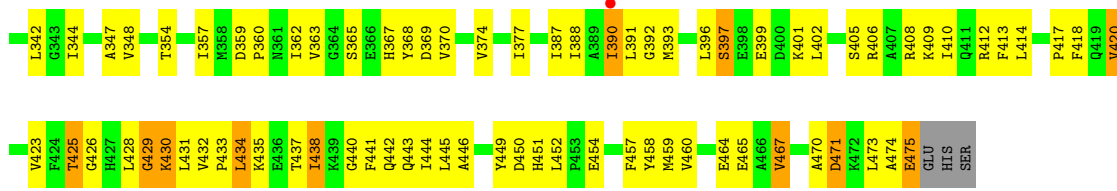


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



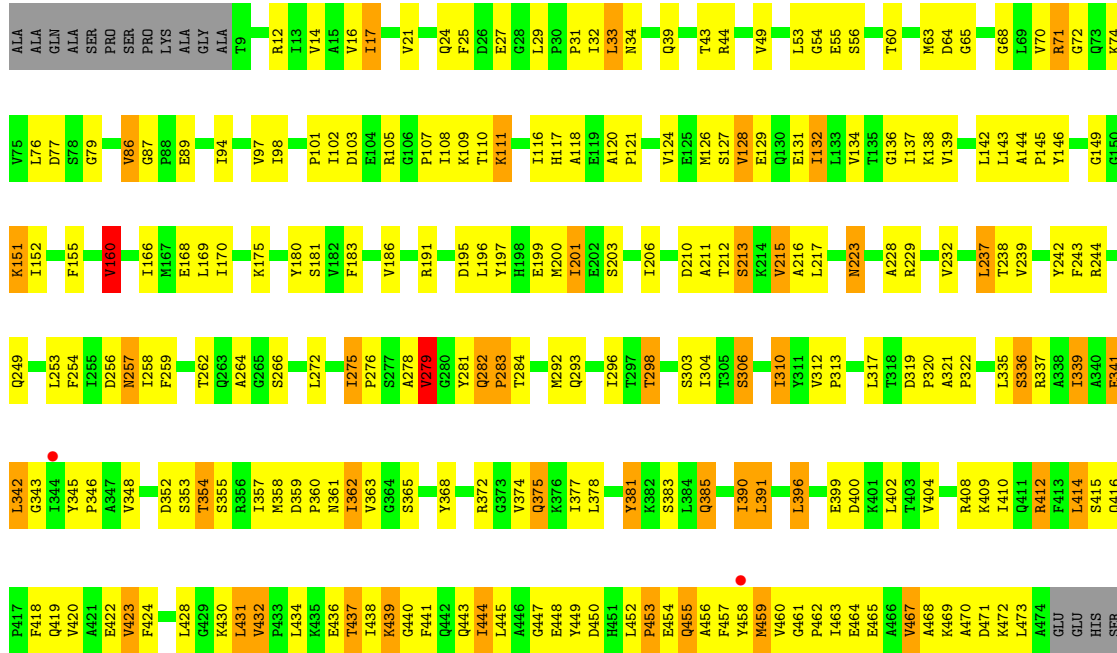
● Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL





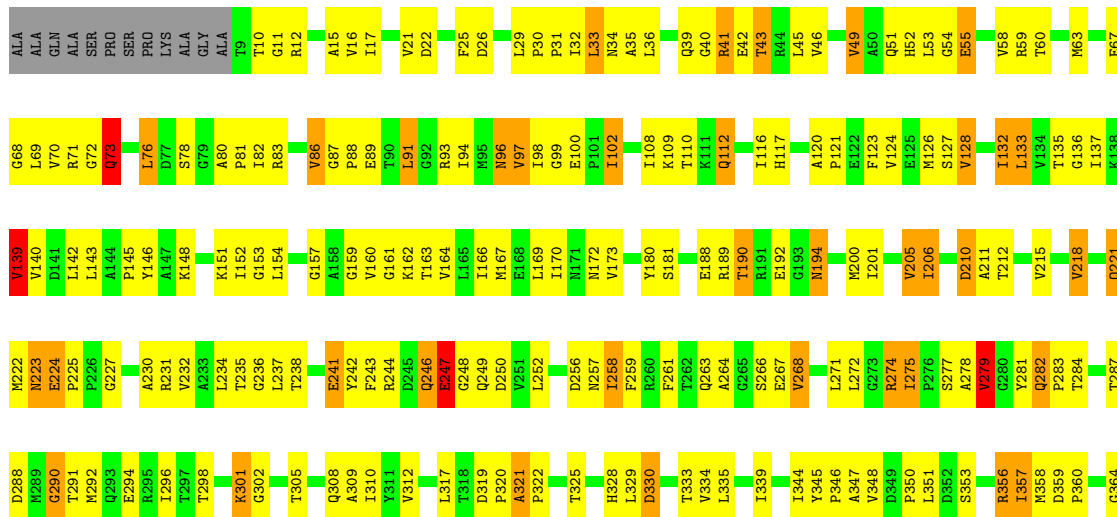
● Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

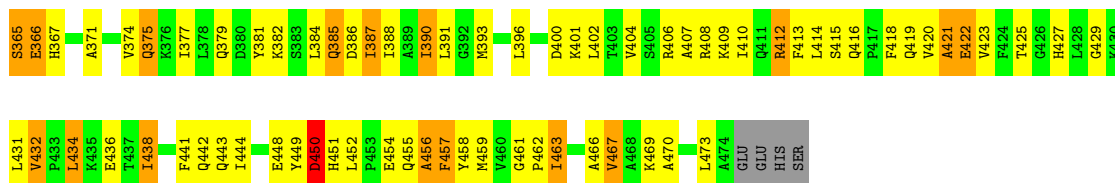
Chain E: 48% 39% 9%



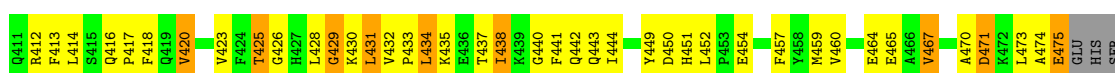
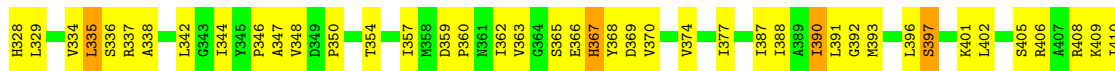
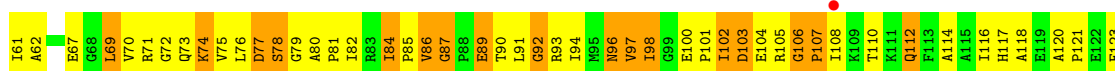
● Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain F: 39% 45% 11%



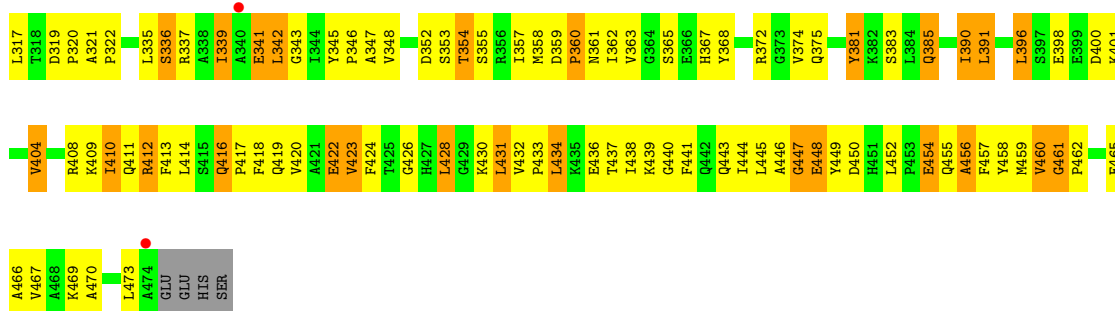


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

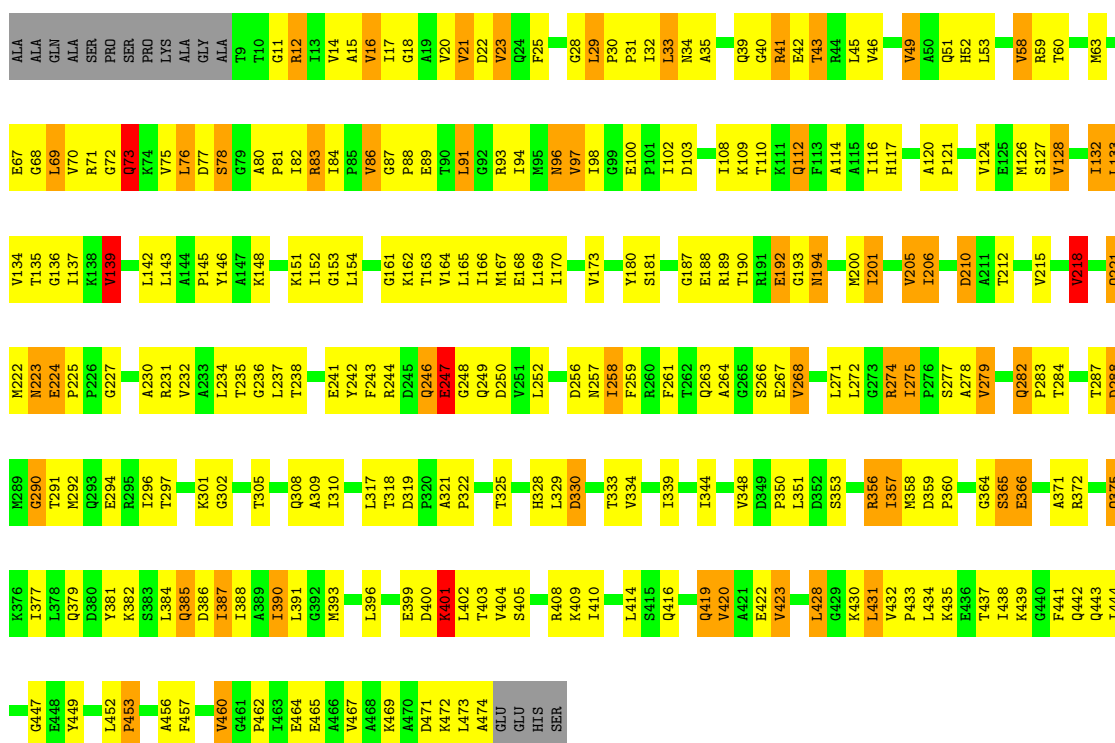


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

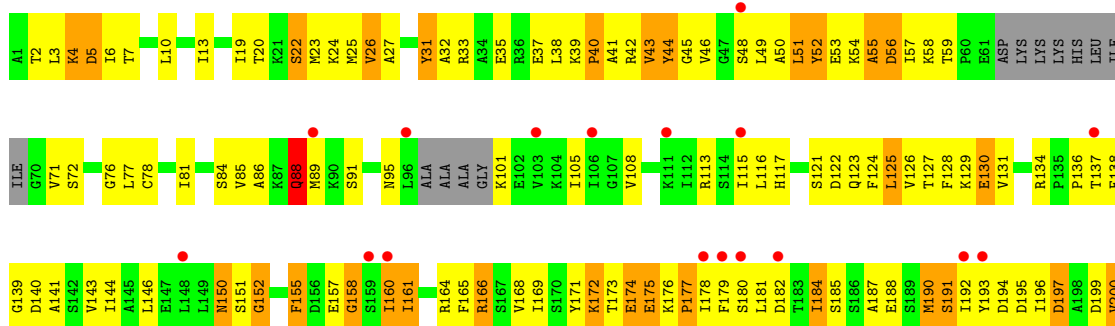


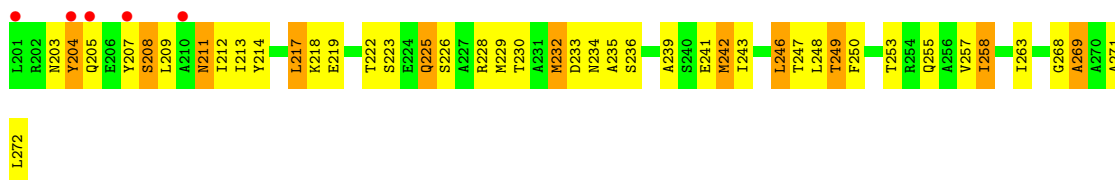


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

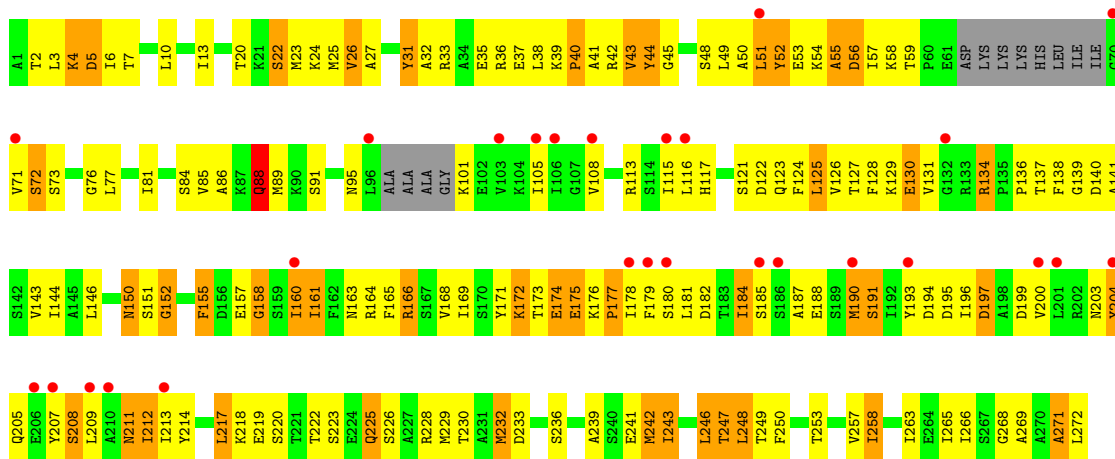


• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

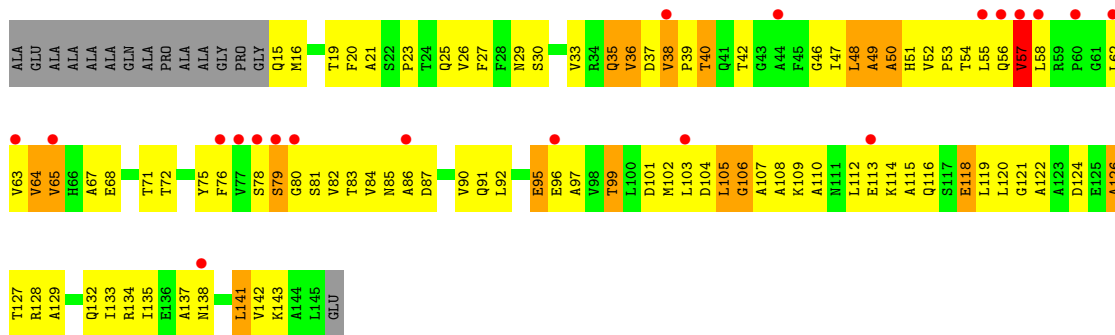




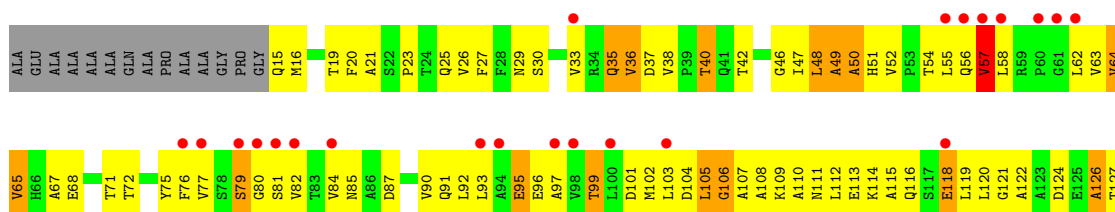
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

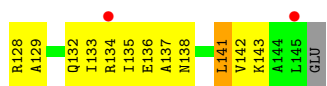


• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

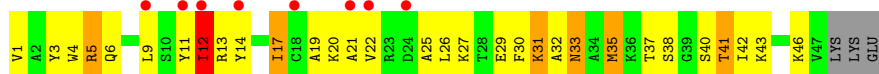


• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL

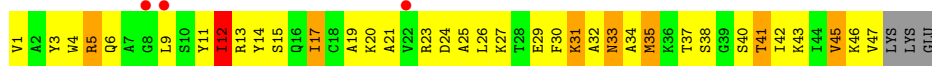




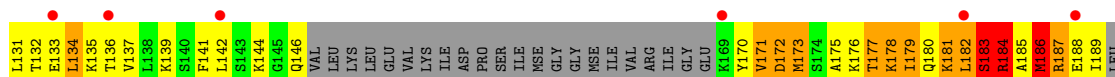
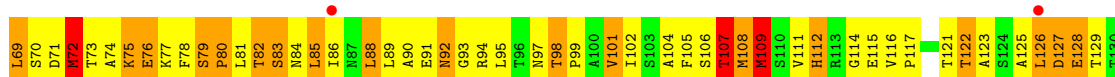
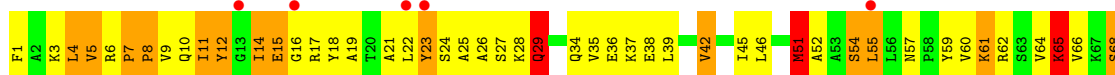
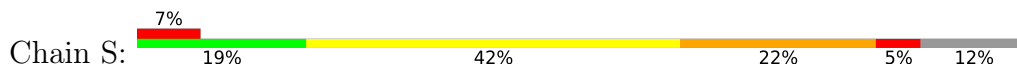
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



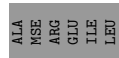
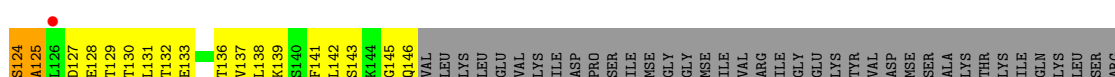
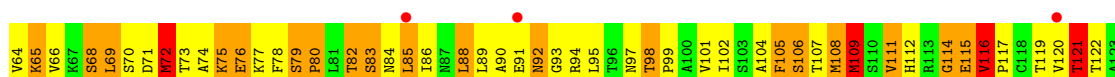
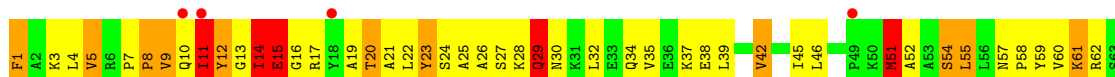
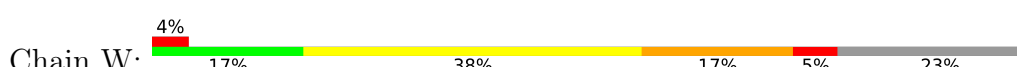
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



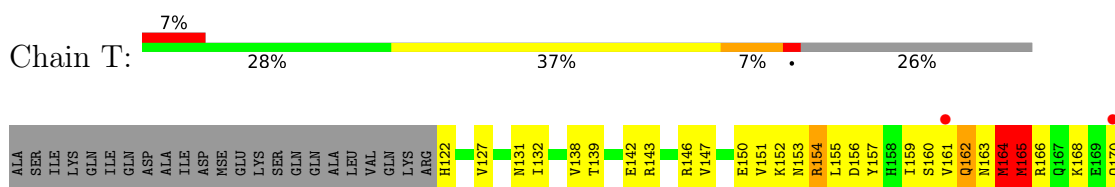
• Molecule 6: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL



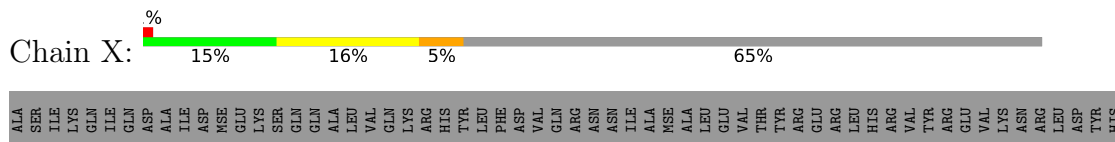
• Molecule 6: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL



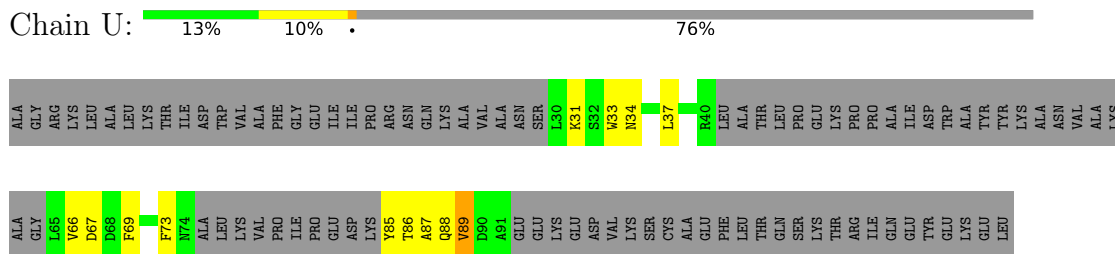
• Molecule 7: ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL



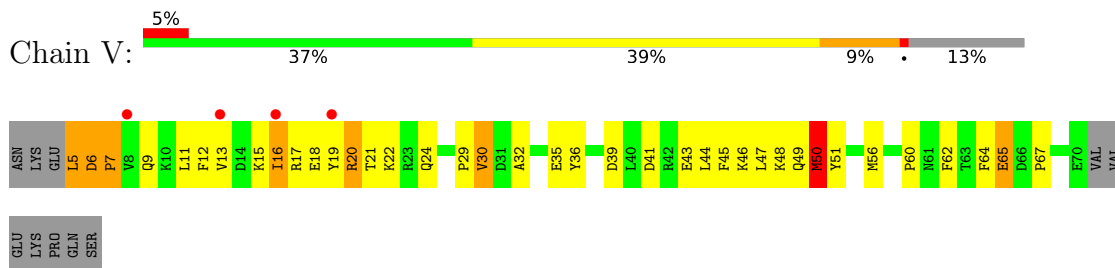
- Molecule 7: ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL



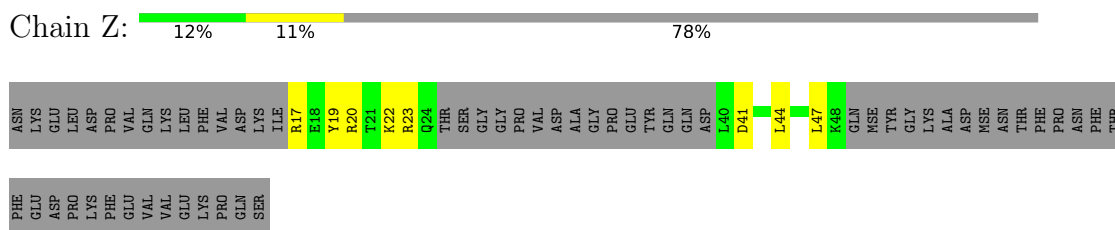
- Molecule 8: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL



- Molecule 9: ATP SYNTHASE-COUPPLING FACTOR 6, MITOCHONDRIAL



- Molecule 9: ATP SYNTHASE-COUPPLING FACTOR 6, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	158.24Å 231.25Å 286.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.77 – 3.20 41.77 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.1 (41.77-3.20) 93.0 (41.77-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, R_{free}	0.217 , 0.271 0.208 , 0.262	Depositor DCC
R_{free} test set	8036 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtrriage
Anisotropy	0.069	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 74.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	54949	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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, ADP, 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	0.97	1/3933 (0.0%)	1.14	22/5306 (0.4%)
1	B	0.69	0/3711	1.06	7/5005 (0.1%)
1	C	0.58	0/3735	1.01	18/5038 (0.4%)
1	J	0.70	0/3766	1.11	16/5080 (0.3%)
1	K	0.71	0/3711	1.08	9/5005 (0.2%)
1	L	0.57	0/3721	1.00	17/5019 (0.3%)
2	D	0.63	0/3596	1.04	18/4879 (0.4%)
2	E	0.71	0/3587	1.06	16/4867 (0.3%)
2	F	0.64	0/3594	1.06	19/4877 (0.4%)
2	M	0.60	0/3596	1.04	23/4879 (0.5%)
2	N	0.67	0/3587	1.09	20/4867 (0.4%)
2	O	0.63	0/3587	1.08	24/4867 (0.5%)
3	G	0.59	0/2050	0.94	6/2752 (0.2%)
3	P	0.62	0/2050	0.92	9/2752 (0.3%)
4	H	0.41	0/982	0.79	0/1337
4	Q	0.39	0/982	0.80	0/1337
5	I	0.38	0/374	0.77	1/501 (0.2%)
5	R	0.36	0/374	0.73	1/501 (0.2%)
6	S	0.57	0/1301	1.09	15/1740 (0.9%)
6	W	0.55	0/1131	1.07	7/1521 (0.5%)
7	T	0.45	0/739	0.91	5/982 (0.5%)
7	X	0.51	0/334	0.91	4/437 (0.9%)
8	U	0.40	0/236	0.94	2/315 (0.6%)
9	V	0.49	0/562	0.92	4/751 (0.5%)
9	Z	0.36	0/160	0.66	0/207
All	All	0.66	1/55399 (0.0%)	1.04	263/74822 (0.4%)

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	J	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ASP	C-N	37.35	1.94	1.33

The worst 5 of 263 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	191	ASP	CA-C-N	-17.55	100.28	122.75
1	A	191	ASP	C-N-CA	-17.55	100.28	122.75
2	N	365	SER	N-CA-C	-10.83	100.18	113.50
2	E	365	SER	N-CA-C	-10.61	100.45	113.50
1	C	29	GLY	N-CA-C	8.42	122.90	111.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	ASP	Peptide
1	J	269	ASP	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	3882	0	3986	280	0
1	B	3663	0	3774	217	0
1	C	3684	0	3785	319	0
1	J	3715	0	3814	270	0
1	K	3663	0	3774	237	0
1	L	3670	0	3778	341	0
2	D	3539	0	3592	273	0
2	E	3530	0	3587	211	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3534	0	3595	261	0
2	M	3539	0	3592	302	0
2	N	3530	0	3587	227	0
2	O	3530	0	3586	268	0
3	G	2027	0	2082	182	0
3	P	2027	0	2082	180	0
4	H	970	0	972	103	0
4	Q	970	0	972	98	0
5	I	369	0	395	36	0
5	R	369	0	395	41	0
6	S	1292	0	1382	182	0
6	W	1120	0	1191	157	0
7	T	733	0	751	88	0
7	X	336	0	362	23	0
8	U	234	0	222	15	0
9	V	551	0	534	62	0
9	Z	160	0	171	12	0
10	A	31	0	13	2	0
10	B	31	0	12	1	0
10	C	31	0	13	0	0
10	F	31	0	13	9	0
10	J	31	0	13	2	0
10	K	31	0	13	4	0
10	L	31	0	13	2	0
10	O	31	0	13	5	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
11	F	1	0	0	0	0
11	J	1	0	0	0	0
11	K	1	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
11	O	1	0	0	0	0
12	D	27	0	12	3	0
12	M	27	0	12	4	0
All	All	54949	0	56088	4115	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 37.

The worst 5 of 4115 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:A:191:ASP:C	1:A:192:GLY:N	1.93	1.25
1:C:212:THR:HG23	2:F:356:ARG:HH21	1.07	1.15
1:L:179:ALA:HB1	1:L:267:ILE:HD13	1.23	1.15
1:L:212:THR:HG23	2:O:356:ARG:HH21	1.10	1.14
1:A:16:ILE:HD13	6:S:22:LEU:HD21	1.29	1.14

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	508/510 (100%)	423 (83%)	61 (12%)	24 (5%)	2	14
1	B	476/510 (93%)	410 (86%)	60 (13%)	6 (1%)	9	40
1	C	482/510 (94%)	365 (76%)	88 (18%)	29 (6%)	1	10
1	J	485/510 (95%)	404 (83%)	61 (13%)	20 (4%)	2	17
1	K	476/510 (93%)	414 (87%)	54 (11%)	8 (2%)	7	35
1	L	479/510 (94%)	354 (74%)	100 (21%)	25 (5%)	1	12
2	D	465/482 (96%)	360 (77%)	84 (18%)	21 (4%)	2	15
2	E	464/482 (96%)	392 (84%)	61 (13%)	11 (2%)	4	28
2	F	465/482 (96%)	368 (79%)	78 (17%)	19 (4%)	2	17
2	M	465/482 (96%)	356 (77%)	79 (17%)	30 (6%)	1	8
2	N	464/482 (96%)	392 (84%)	60 (13%)	12 (3%)	4	26
2	O	464/482 (96%)	375 (81%)	70 (15%)	19 (4%)	2	17
3	G	254/272 (93%)	172 (68%)	65 (26%)	17 (7%)	1	7
3	P	254/272 (93%)	175 (69%)	62 (24%)	17 (7%)	1	7
4	H	129/146 (88%)	95 (74%)	22 (17%)	12 (9%)	0	3
4	Q	129/146 (88%)	95 (74%)	22 (17%)	12 (9%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	45/50 (90%)	28 (62%)	13 (29%)	4 (9%)	0	3
5	R	45/50 (90%)	28 (62%)	13 (29%)	4 (9%)	0	3
6	S	163/190 (86%)	97 (60%)	44 (27%)	22 (14%)	0	1
6	W	144/190 (76%)	81 (56%)	37 (26%)	26 (18%)	0	0
7	T	84/116 (72%)	68 (81%)	12 (14%)	4 (5%)	2	14
7	X	37/116 (32%)	25 (68%)	10 (27%)	2 (5%)	1	12
8	U	22/118 (19%)	20 (91%)	2 (9%)	0	100	100
9	V	64/76 (84%)	43 (67%)	19 (30%)	2 (3%)	3	22
9	Z	13/76 (17%)	5 (38%)	8 (62%)	0	100	100
All	All	7076/7770 (91%)	5545 (78%)	1185 (17%)	346 (5%)	1	13

5 of 346 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	22	SER
1	A	24	ASP
1	A	361	ILE
1	A	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	412/412 (100%)	345 (84%)	67 (16%)	2	12
1	B	389/412 (94%)	322 (83%)	67 (17%)	2	10
1	C	388/412 (94%)	330 (85%)	58 (15%)	3	15
1	J	393/412 (95%)	332 (84%)	61 (16%)	2	14
1	K	389/412 (94%)	322 (83%)	67 (17%)	2	10
1	L	388/412 (94%)	326 (84%)	62 (16%)	2	13
2	D	377/386 (98%)	306 (81%)	71 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	376/386 (97%)	319 (85%)	57 (15%)	3	14
2	F	377/386 (98%)	314 (83%)	63 (17%)	2	11
2	M	377/386 (98%)	311 (82%)	66 (18%)	2	10
2	N	376/386 (97%)	325 (86%)	51 (14%)	3	18
2	O	376/386 (97%)	310 (82%)	66 (18%)	2	10
3	G	222/230 (96%)	182 (82%)	40 (18%)	2	9
3	P	222/230 (96%)	180 (81%)	42 (19%)	1	9
4	H	104/109 (95%)	92 (88%)	12 (12%)	5	24
4	Q	104/109 (95%)	92 (88%)	12 (12%)	5	24
5	I	38/41 (93%)	34 (90%)	4 (10%)	6	28
5	R	38/41 (93%)	33 (87%)	5 (13%)	4	19
6	S	146/158 (92%)	112 (77%)	34 (23%)	1	5
6	W	127/158 (80%)	99 (78%)	28 (22%)	1	6
7	T	81/100 (81%)	76 (94%)	5 (6%)	16	49
7	X	39/100 (39%)	37 (95%)	2 (5%)	21	54
8	U	26/100 (26%)	24 (92%)	2 (8%)	12	41
9	V	60/68 (88%)	53 (88%)	7 (12%)	5	23
9	Z	17/68 (25%)	16 (94%)	1 (6%)	18	50
All	All	5842/6300 (93%)	4892 (84%)	950 (16%)	2	12

5 of 950 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	208	GLN
6	S	79	SER
1	L	89	LYS
6	S	42	VAL
6	W	130	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	302	HIS
2	N	385	GLN
1	L	385	GLN

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Mol	Chain	Res	Type
2	M	419	GLN
2	O	96	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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
10	ANP	O	600	11	33,33,33	3.02	14 (42%)	45,52,52	2.11	15 (33%)
10	ANP	J	600	11	33,33,33	3.29	14 (42%)	45,52,52	2.29	16 (35%)
10	ANP	F	600	11	33,33,33	3.20	13 (39%)	45,52,52	2.04	14 (31%)
10	ANP	A	600	11	33,33,33	3.40	14 (42%)	45,52,52	2.06	13 (28%)
10	ANP	K	600	11	33,33,33	3.47	15 (45%)	45,52,52	2.06	13 (28%)
12	ADP	M	600	11	28,29,29	2.25	7 (25%)	43,45,45	1.88	10 (23%)
10	ANP	B	600	11	33,33,33	3.60	16 (48%)	45,52,52	2.15	15 (33%)
10	ANP	L	600	11	33,33,33	3.59	15 (45%)	45,52,52	2.08	16 (35%)
12	ADP	D	600	11	28,29,29	2.06	8 (28%)	43,45,45	2.15	15 (34%)
10	ANP	C	600	11	33,33,33	3.34	14 (42%)	45,52,52	2.15	17 (37%)

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
10	ANP	O	600	11	-	0/18/38/38	0/3/3/3
10	ANP	J	600	11	-	2/18/38/38	0/3/3/3
10	ANP	F	600	11	-	7/18/38/38	0/3/3/3
10	ANP	A	600	11	-	9/18/38/38	0/3/3/3
10	ANP	K	600	11	-	5/18/38/38	0/3/3/3
12	ADP	M	600	11	-	8/16/32/32	0/3/3/3
10	ANP	B	600	11	2/2/7/8	5/18/38/38	0/3/3/3
10	ANP	L	600	11	-	7/18/38/38	0/3/3/3
12	ADP	D	600	11	-	3/16/32/32	0/3/3/3
10	ANP	C	600	11	-	3/18/38/38	0/3/3/3

The worst 5 of 130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	600	ANP	PB-O1B	12.18	1.64	1.46
10	L	600	ANP	PB-O1B	12.16	1.64	1.46
10	C	600	ANP	PB-O1B	12.14	1.64	1.46
10	J	600	ANP	PB-O1B	12.02	1.64	1.46
10	B	600	ANP	PB-O1B	11.68	1.63	1.46

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	600	ANP	N3-C2-N1	-5.98	119.53	128.58
10	C	600	ANP	N3-C2-N1	-5.98	119.54	128.58
12	D	600	ADP	C5-C4-N3	-5.96	118.51	126.72
10	J	600	ANP	C5-C4-N3	-5.80	118.74	126.72
10	F	600	ANP	C5-C4-N3	-5.77	118.78	126.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	600	ANP	C3'
10	B	600	ANP	C4'

5 of 49 torsion outliers are listed below:

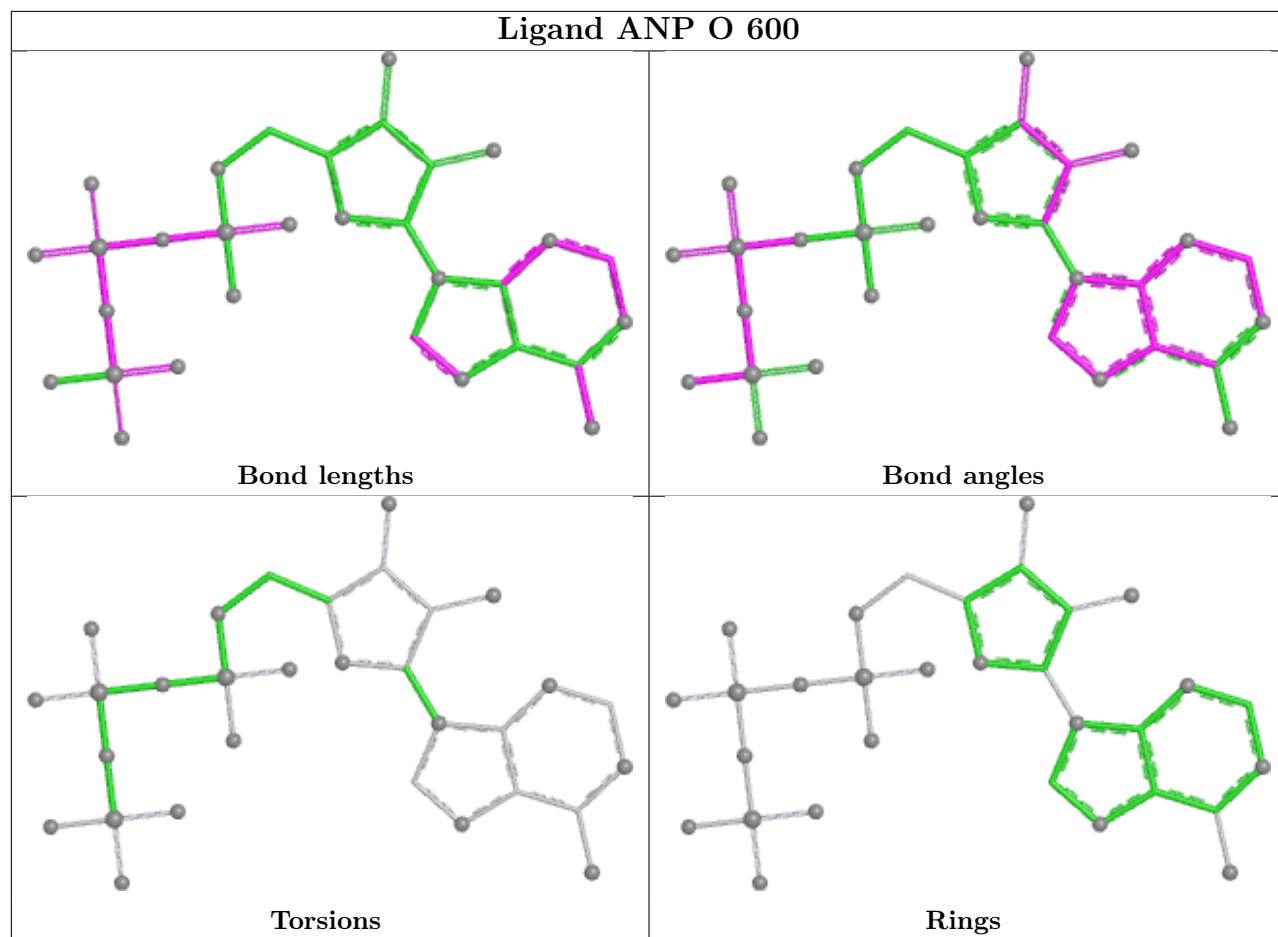
Mol	Chain	Res	Type	Atoms
10	A	600	ANP	PG-N3B-PB-O1B
10	A	600	ANP	C5'-O5'-PA-O1A
10	A	600	ANP	C5'-O5'-PA-O2A
10	A	600	ANP	C5'-O5'-PA-O3A
10	A	600	ANP	O4'-C4'-C5'-O5'

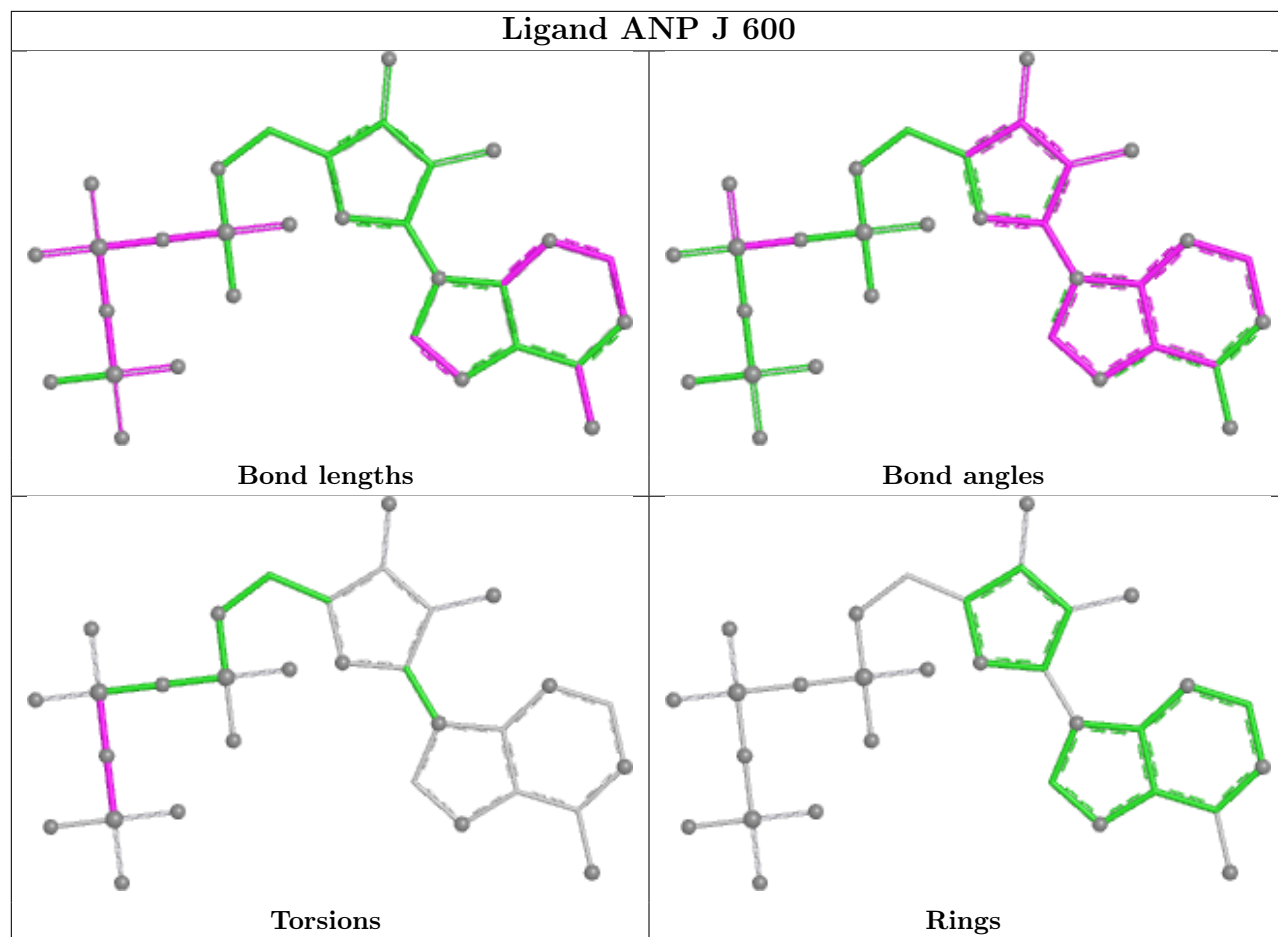
There are no ring outliers.

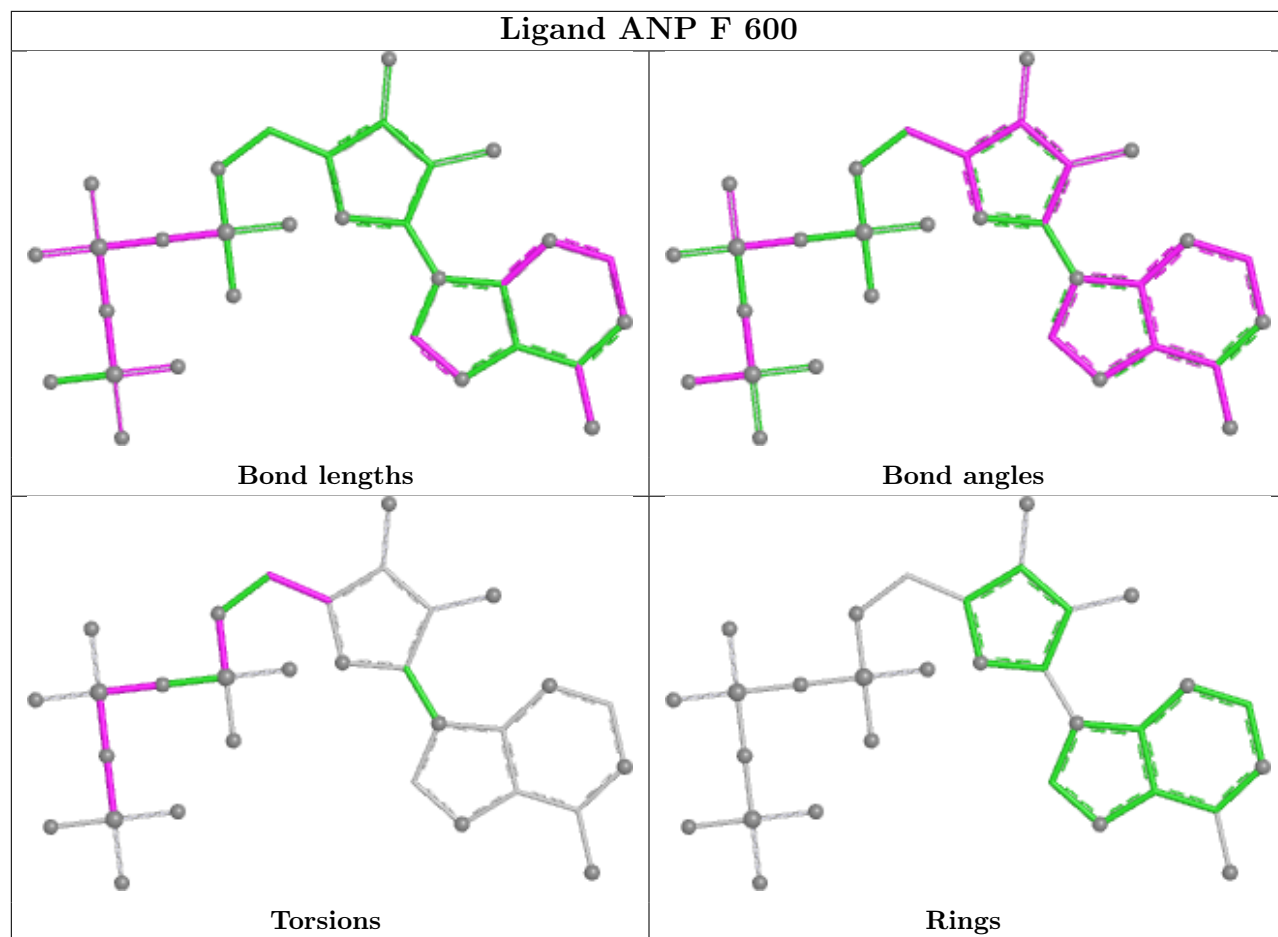
9 monomers are involved in 32 short contacts:

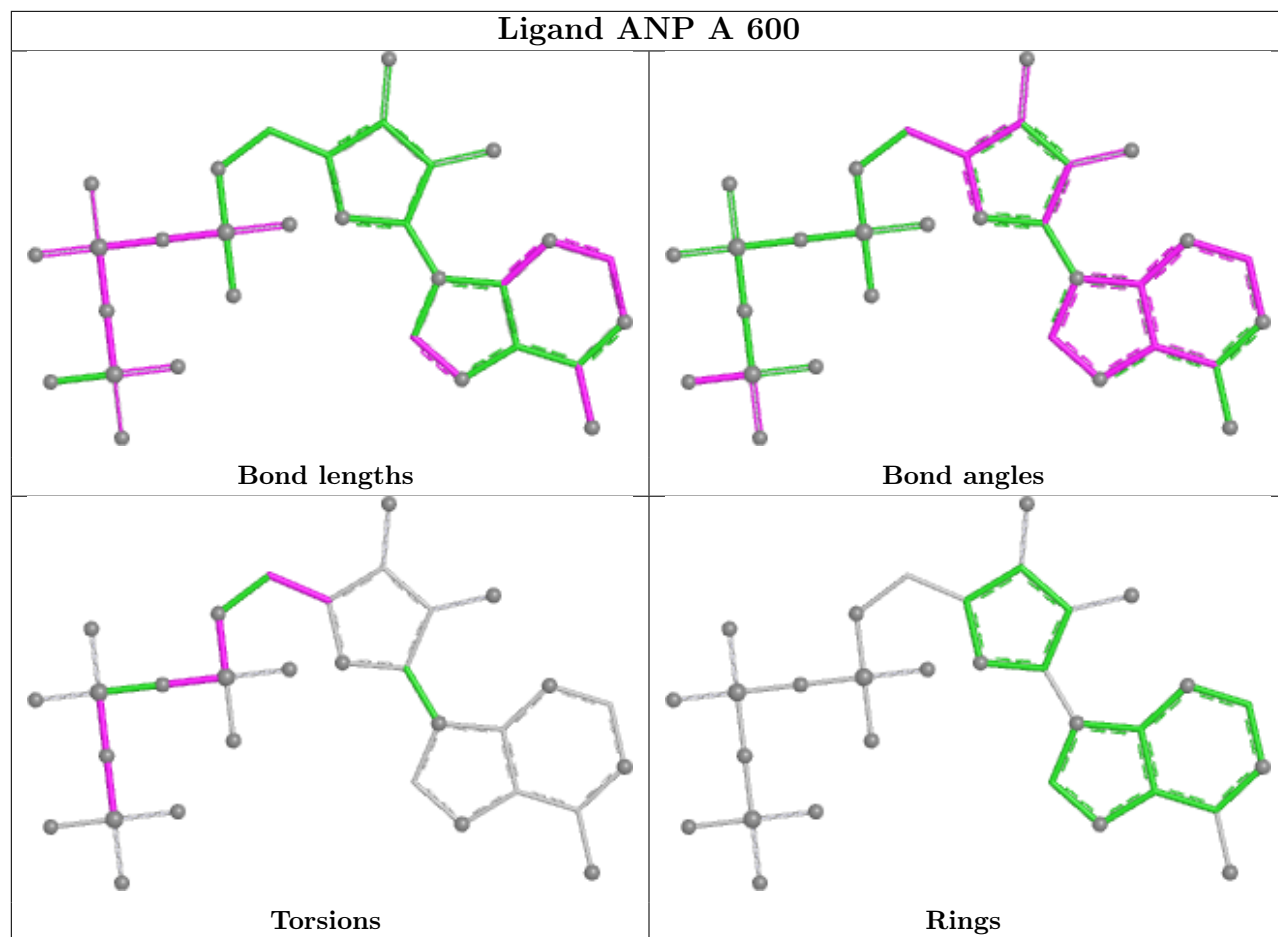
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	O	600	ANP	5	0
10	J	600	ANP	2	0
10	F	600	ANP	9	0
10	A	600	ANP	2	0
10	K	600	ANP	4	0
12	M	600	ADP	4	0
10	B	600	ANP	1	0
10	L	600	ANP	2	0
12	D	600	ADP	3	0

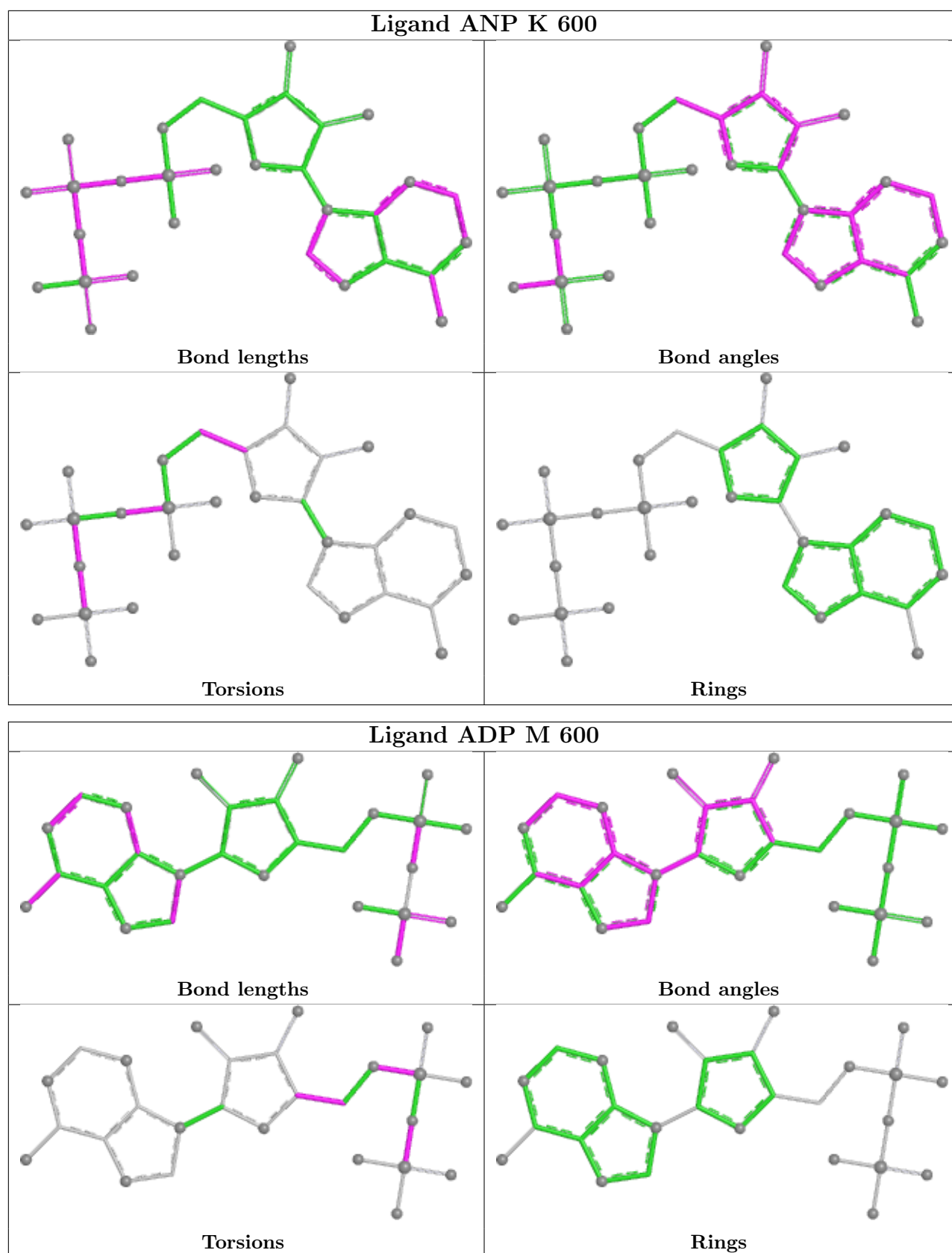
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

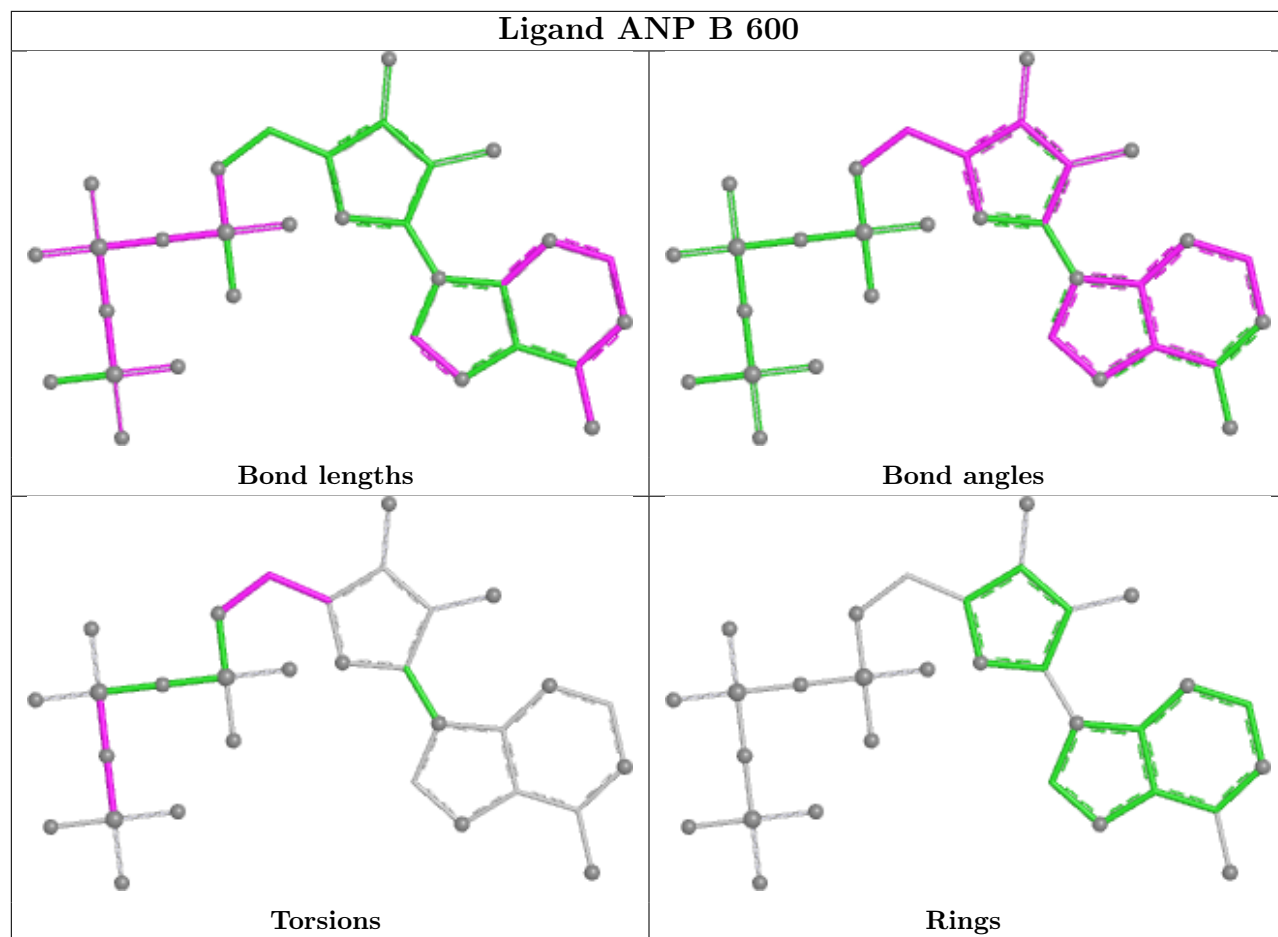


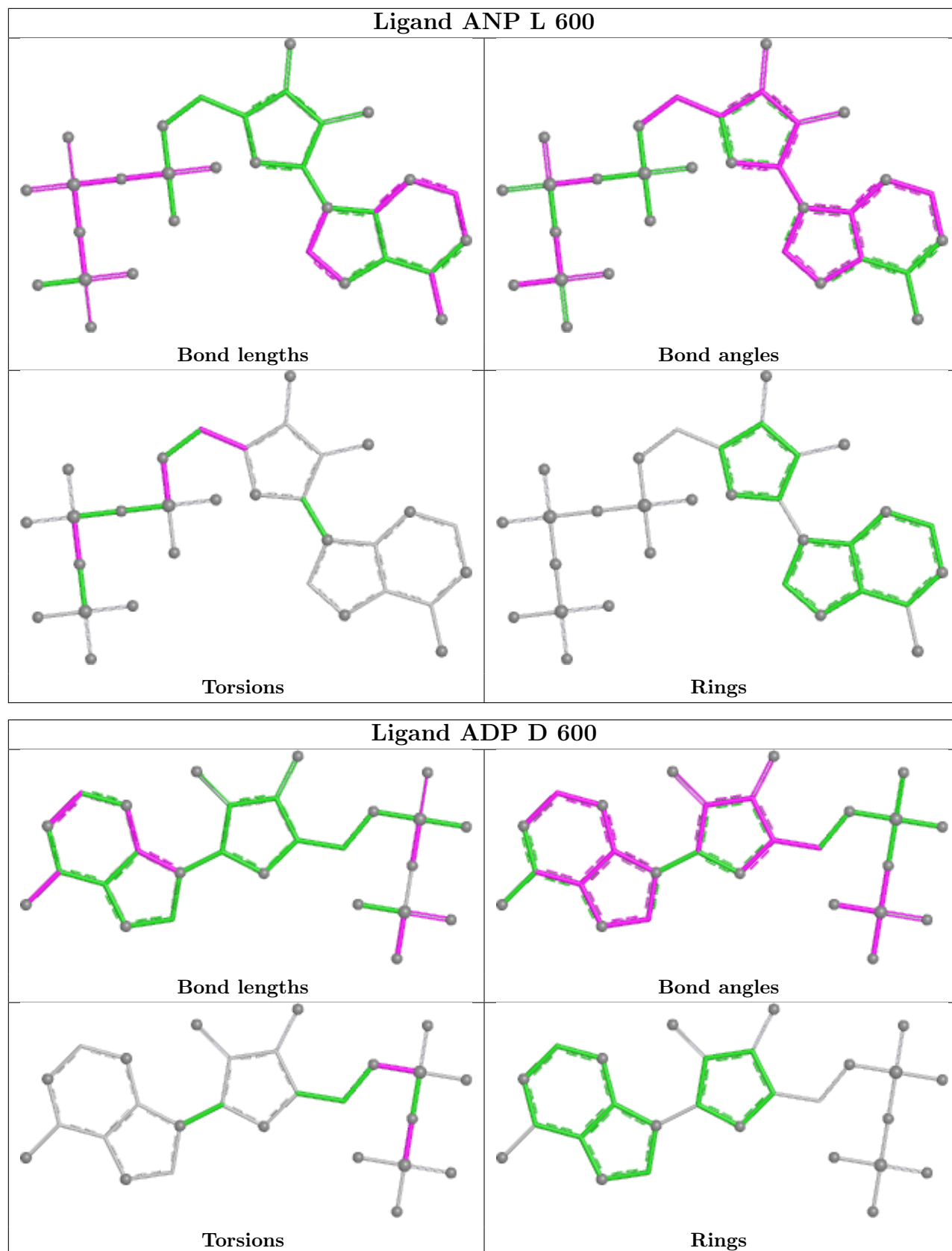


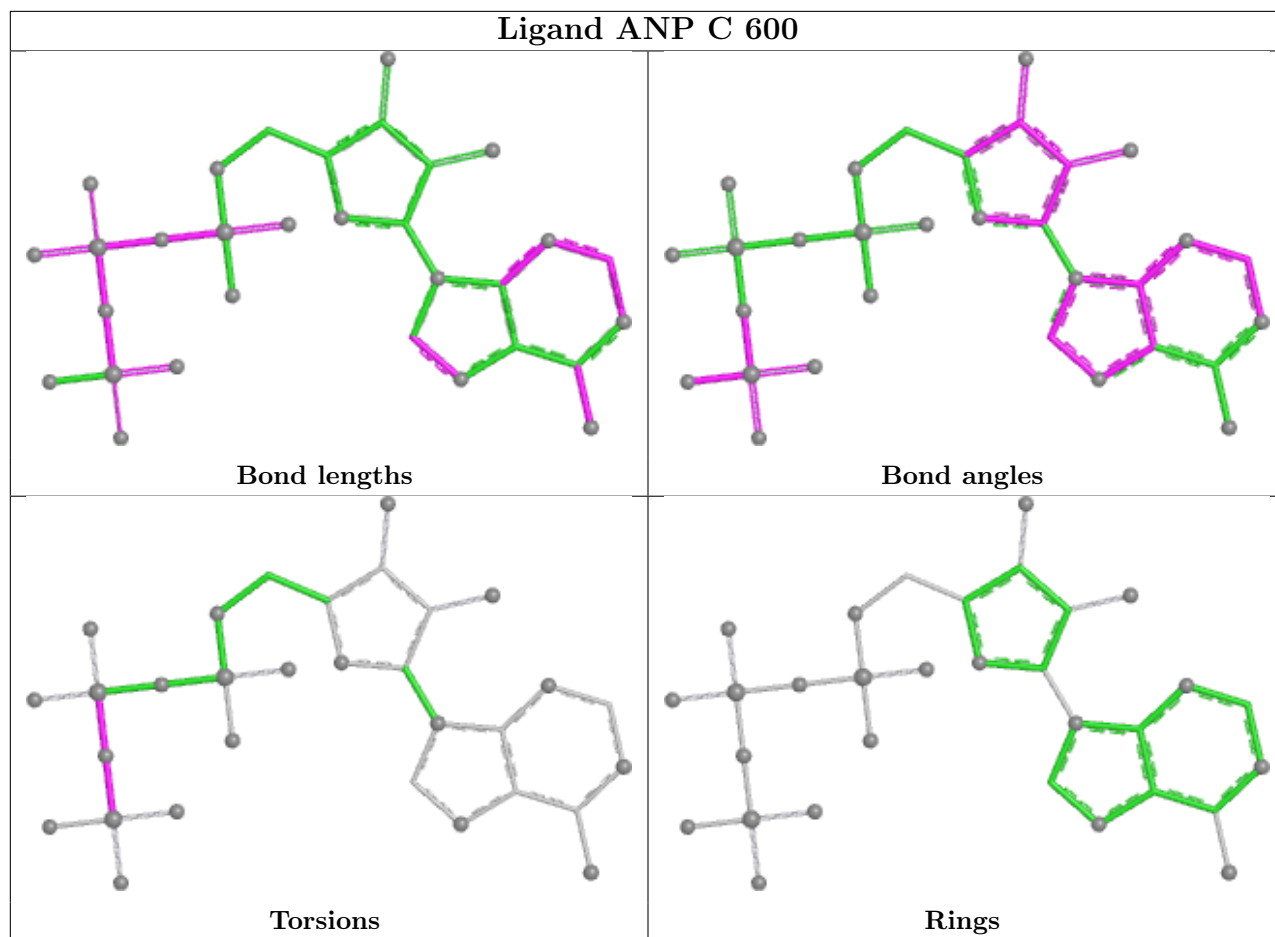












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	191:ASP	C	192:GLY	N	1.93

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	510/510 (100%)	-0.48	3 (0%) 85 73	32, 60, 113, 179	0
1	B	480/510 (94%)	-0.62	0 100 100	34, 59, 91, 147	0
1	C	484/510 (94%)	-0.04	2 (0%) 88 79	50, 86, 171, 227	0
1	J	487/510 (95%)	-0.38	2 (0%) 88 79	32, 62, 98, 132	0
1	K	480/510 (94%)	-0.55	0 100 100	33, 59, 95, 144	0
1	L	481/510 (94%)	0.13	9 (1%) 66 46	51, 87, 170, 227	0
2	D	467/482 (96%)	-0.26	1 (0%) 91 85	46, 79, 126, 169	0
2	E	466/482 (96%)	-0.53	2 (0%) 88 79	30, 64, 113, 174	0
2	F	466/482 (96%)	-0.44	0 100 100	35, 71, 105, 130	1 (0%)
2	M	467/482 (96%)	-0.10	4 (0%) 81 64	46, 82, 127, 168	0
2	N	466/482 (96%)	-0.47	2 (0%) 88 79	31, 65, 119, 173	0
2	O	466/482 (96%)	-0.37	0 100 100	40, 71, 106, 139	0
3	G	260/272 (95%)	0.44	22 (8%) 16 11	33, 119, 237, 251	0
3	P	260/272 (95%)	0.47	27 (10%) 11 8	34, 118, 236, 252	0
4	H	131/146 (89%)	1.08	20 (15%) 5 4	117, 199, 238, 252	0
4	Q	131/146 (89%)	1.33	24 (18%) 3 3	123, 201, 239, 254	0
5	I	47/50 (94%)	1.01	8 (17%) 4 3	125, 193, 238, 252	0
5	R	47/50 (94%)	0.90	3 (6%) 25 16	124, 195, 239, 251	0
6	S	161/190 (84%)	0.69	13 (8%) 18 11	113, 159, 188, 206	0
6	W	142/190 (74%)	0.63	8 (5%) 30 19	115, 157, 191, 203	0
7	T	82/116 (70%)	0.82	8 (9%) 13 9	165, 233, 275, 288	0
7	X	38/116 (32%)	0.86	1 (2%) 57 37	164, 217, 238, 239	0
8	U	28/118 (23%)	0.60	0 100 100	195, 232, 254, 261	0
9	V	64/76 (84%)	0.73	4 (6%) 26 17	157, 221, 291, 302	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
9	Z	17/76 (22%)	0.89	0 100 100	175, 211, 230, 238	0
All	All	7128/7770 (91%)	-0.13	163 (2%) 61 41	30, 76, 216, 302	1 (0%)

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	180	SER	7.9
4	Q	80	GLY	6.7
4	H	55	LEU	5.7
4	Q	93	LEU	5.4
4	Q	58	LEU	5.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

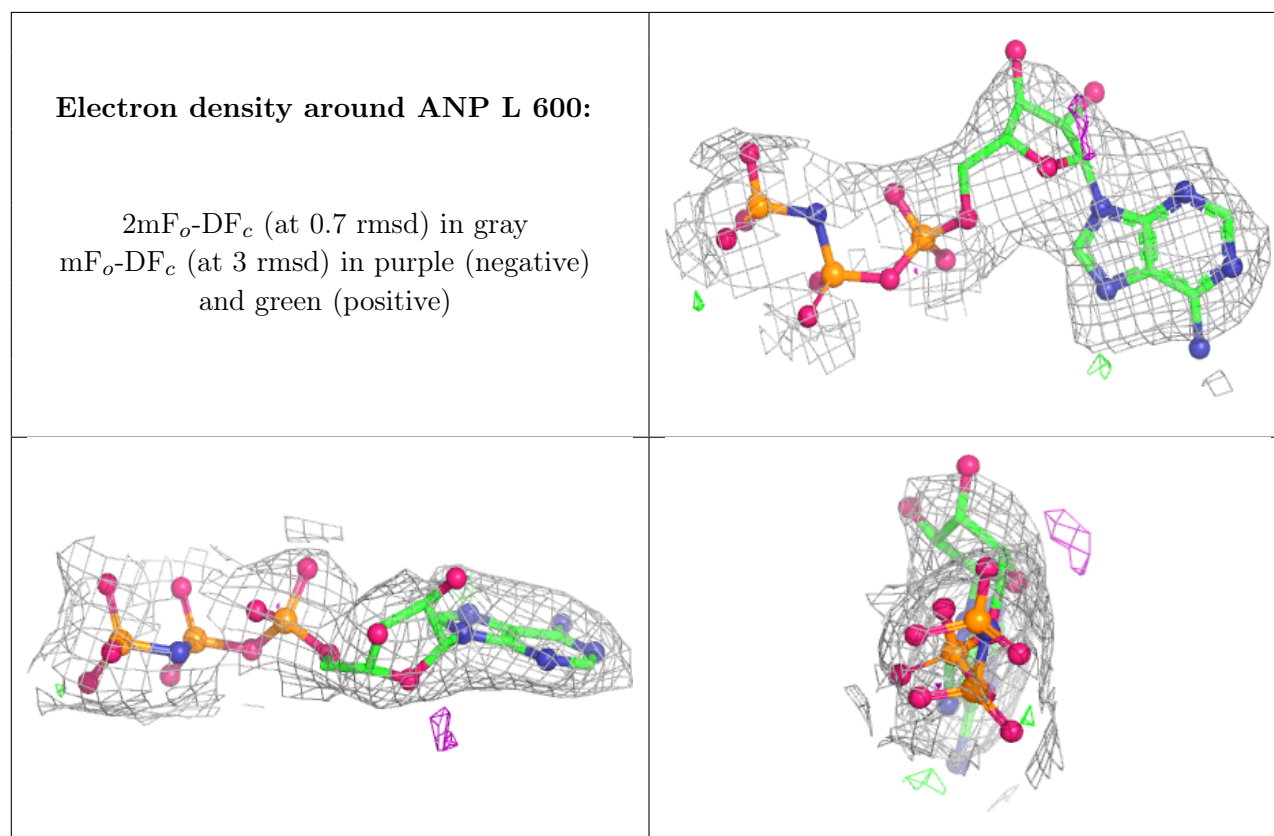
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	MG	J	601	1/1	0.87	0.12	81,81,81,81	0
11	MG	B	601	1/1	0.90	0.09	84,84,84,84	0
10	ANP	L	600	31/31	0.91	0.09	54,91,101,115	0
11	MG	L	601	1/1	0.91	0.10	81,81,81,81	0
12	ADP	M	600	27/27	0.92	0.10	46,66,79,86	0
11	MG	O	601	1/1	0.93	0.13	51,51,51,51	0
11	MG	D	601	1/1	0.94	0.17	66,66,66,66	0
12	ADP	D	600	27/27	0.94	0.08	53,70,80,84	0
11	MG	M	601	1/1	0.94	0.16	64,64,64,64	0
10	ANP	J	600	31/31	0.95	0.07	50,70,85,95	0
10	ANP	C	600	31/31	0.95	0.07	78,98,114,115	0

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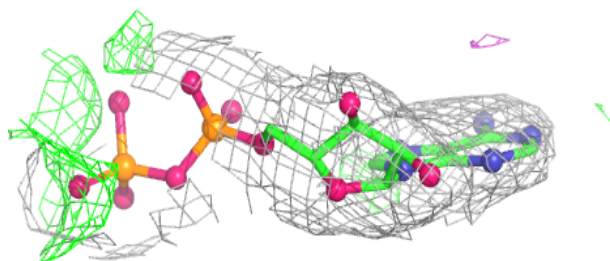
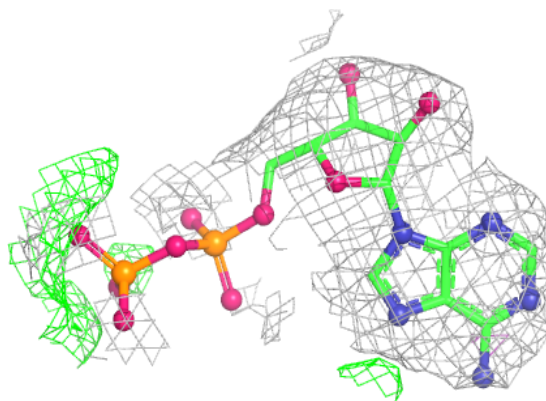
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	ANP	B	600	31/31	0.96	0.08	44,92,104,109	0
11	MG	F	601	1/1	0.96	0.11	52,52,52,52	0
11	MG	A	601	1/1	0.96	0.09	49,49,49,49	0
10	ANP	K	600	31/31	0.96	0.08	40,95,115,117	0
10	ANP	F	600	31/31	0.97	0.06	41,52,63,78	0
10	ANP	A	600	31/31	0.97	0.05	51,64,82,93	0
11	MG	K	601	1/1	0.97	0.06	65,65,65,65	0
10	ANP	O	600	31/31	0.97	0.05	44,55,67,81	0
11	MG	C	601	1/1	0.98	0.03	76,76,76,76	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.

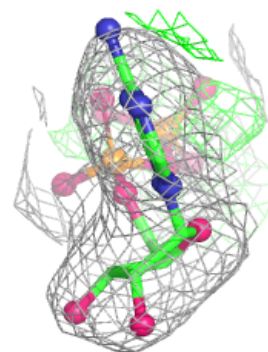
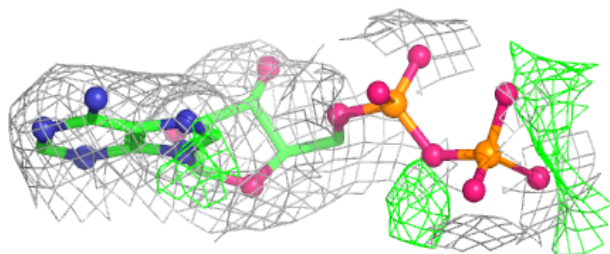
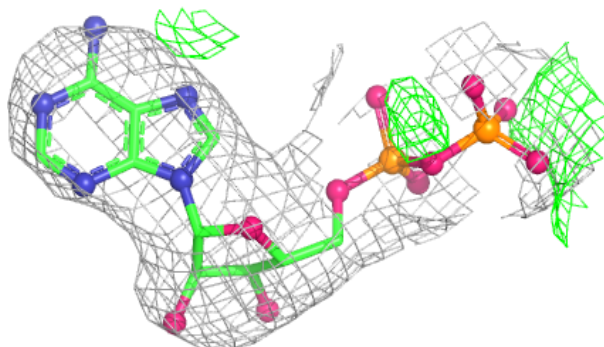


Electron density around ADP M 600:

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

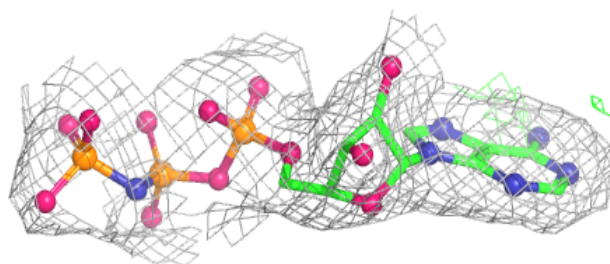
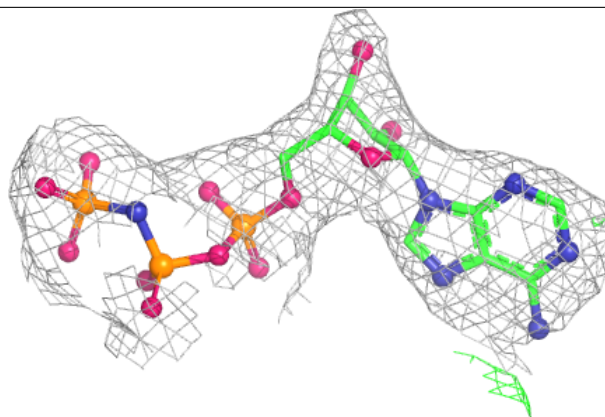
**Electron density around ADP D 600:**

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

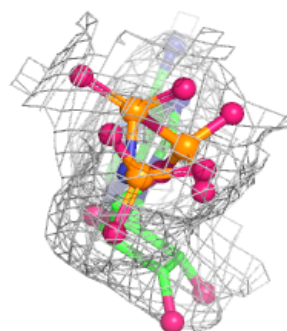
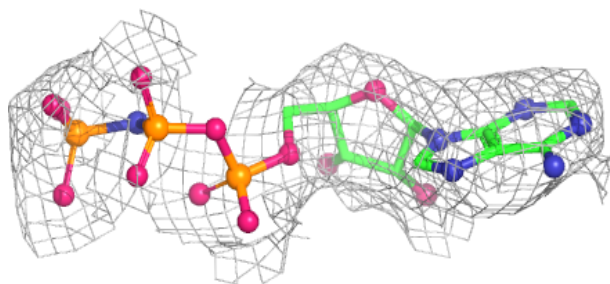
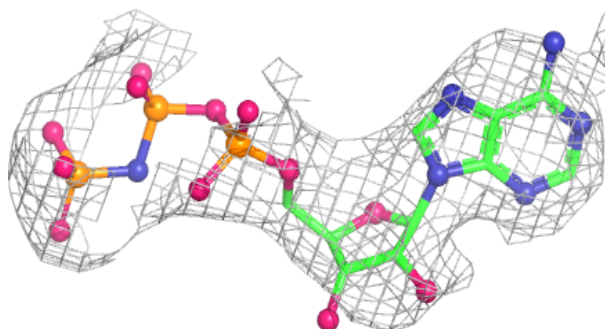


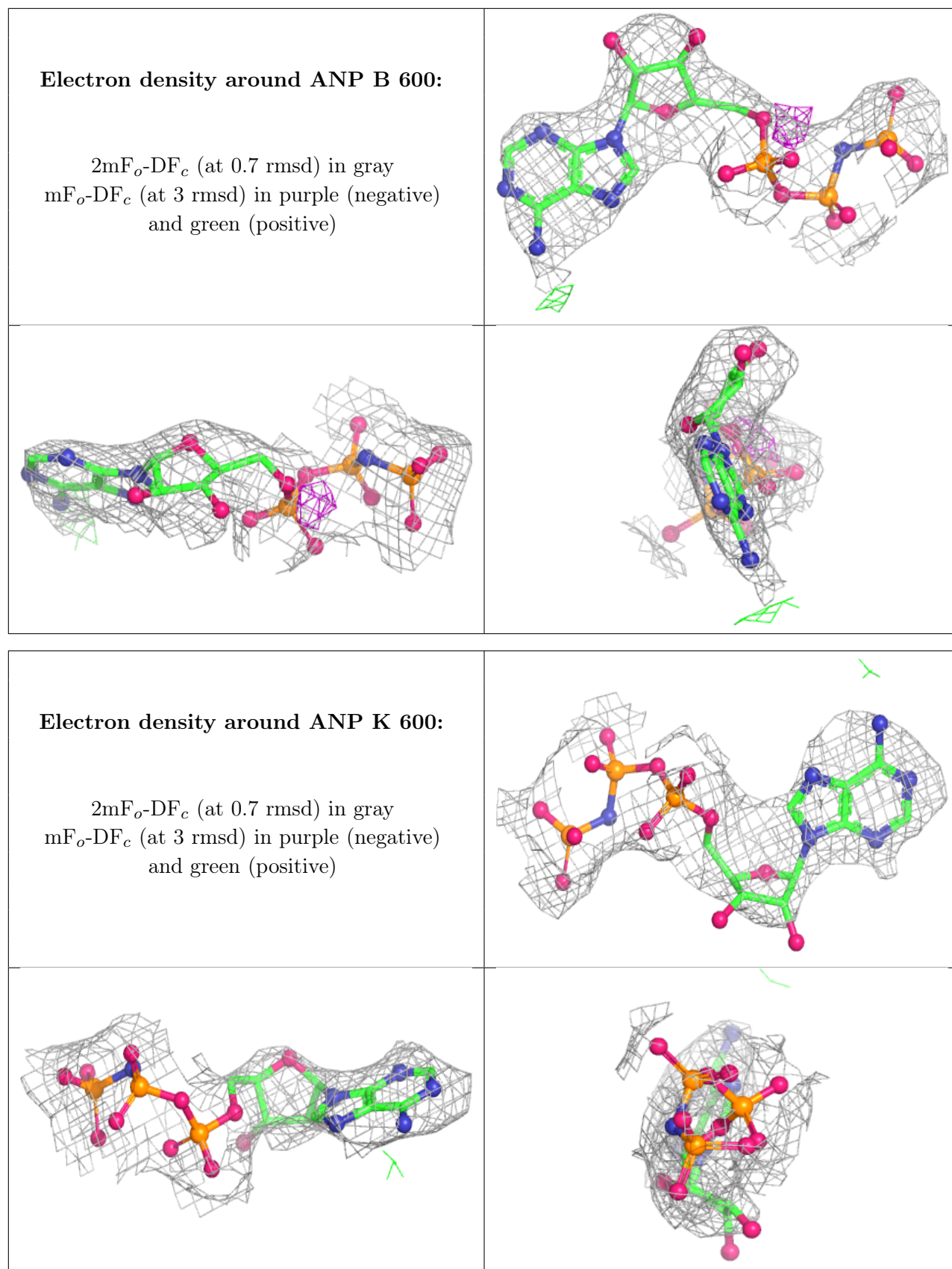
Electron density around ANP J 600:

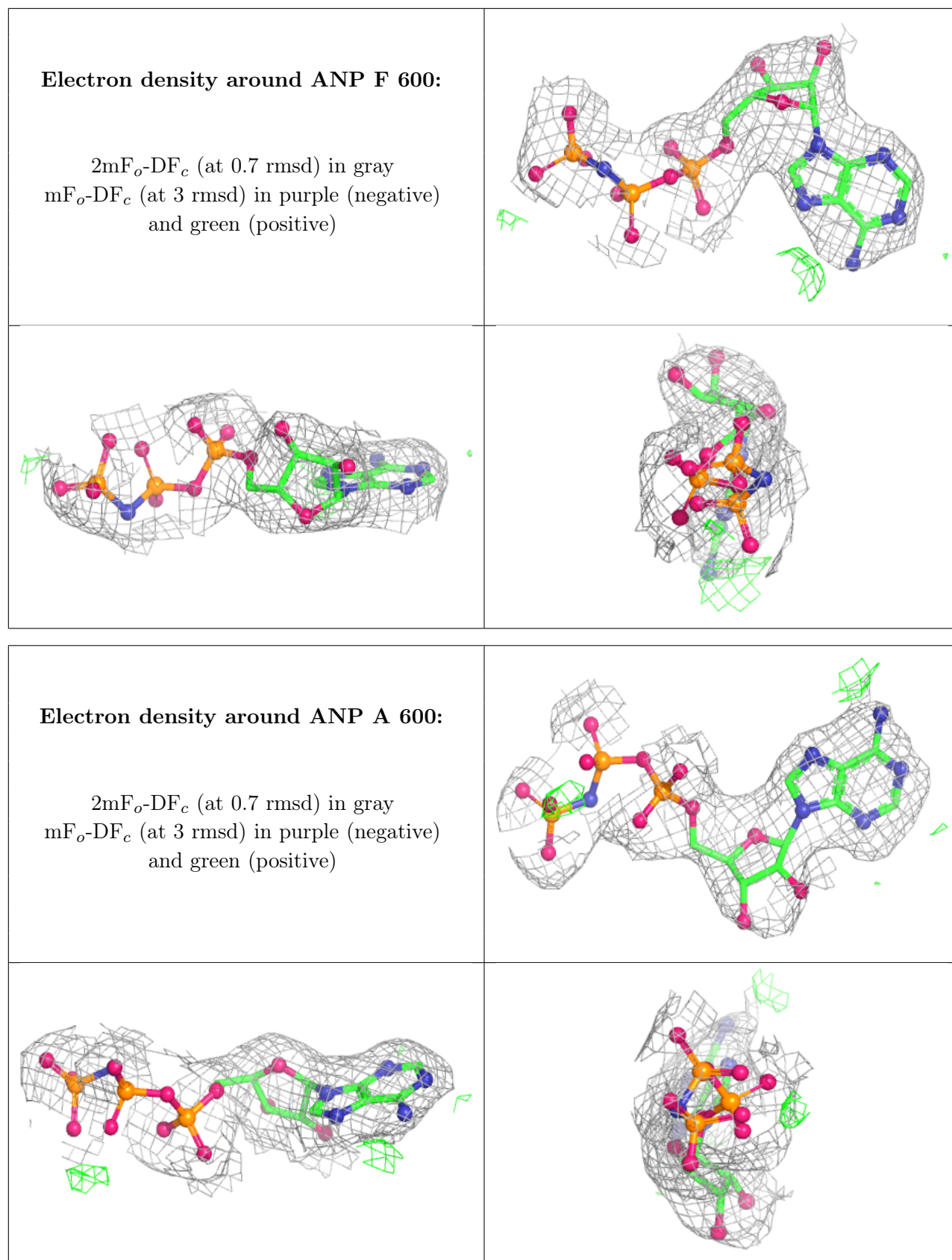
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

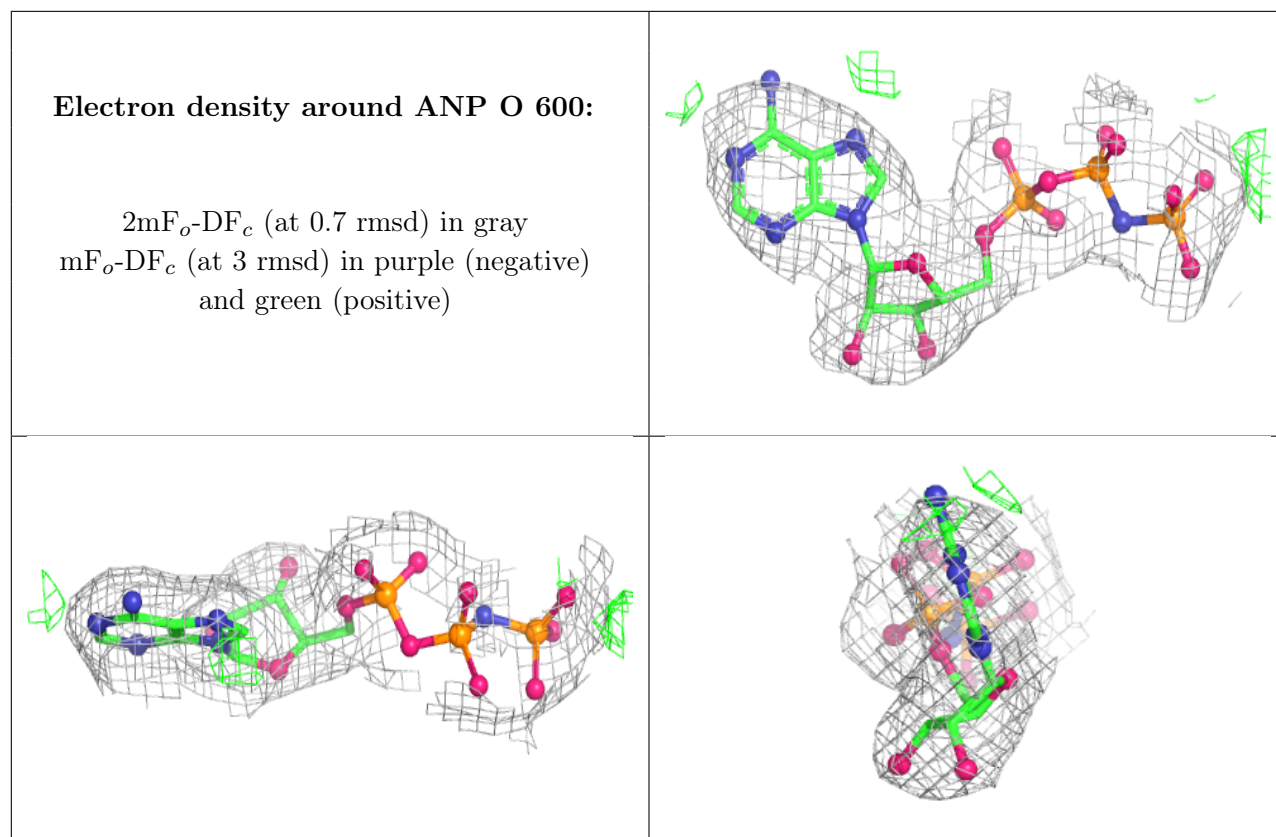
**Electron density around ANP C 600:**

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









6.5 Other polymers [i](#)

There are no such residues in this entry.