



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 05:30 am BST

PDB ID : 1OHH  
Title : BOVINE MITOCHONDRIAL F1-ATPASE complexed with the inhibitor protein IF1  
Authors : Cabezon, E.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2003-05-27  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

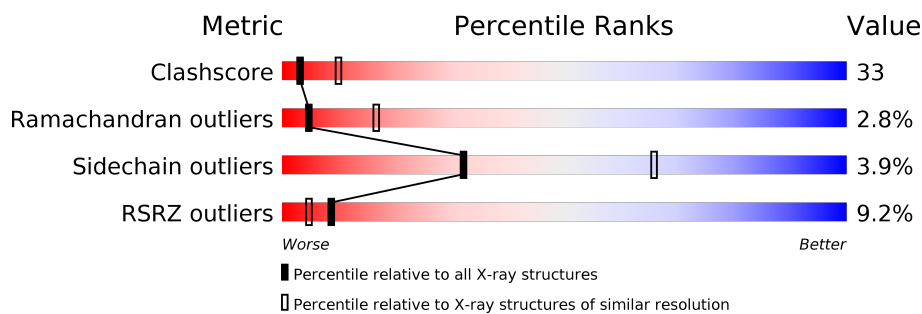
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	510	
1	1-B	510	
1	1-C	510	
1	2-A	510	
1	2-B	510	
1	2-C	510	
2	1-D	482	

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Mol	Chain	Length	Quality of chain
2	1-E	482	<div><div>18%</div><div><div></div><div></div><div></div></div><div>48%</div><div>45%</div><div><div></div><div></div></div></div>
2	1-F	482	<div><div>10%</div><div><div></div><div></div><div></div></div><div>49%</div><div>45%</div><div><div></div><div></div></div></div>
2	2-D	482	<div><div>9%</div><div><div></div><div></div><div></div></div><div>54%</div><div>39%</div><div><div></div><div></div></div></div>
2	2-E	482	<div><div>18%</div><div><div></div><div></div><div></div></div><div>48%</div><div>45%</div><div><div></div><div></div></div></div>
2	2-F	482	<div><div>10%</div><div><div></div><div></div><div></div></div><div>51%</div><div>43%</div><div><div></div><div></div></div></div>
3	1-G	272	<div><div>12%</div><div><div></div><div></div><div></div></div><div>18%</div><div>15%</div><div><div></div><div></div></div><div>65%</div></div>
3	2-G	272	<div><div>11%</div><div><div></div><div></div><div></div></div><div>22%</div><div>12%</div><div><div></div><div></div></div><div>65%</div></div>
4	1-H	84	<div><div>21%</div><div><div></div><div></div><div></div></div><div>11%</div><div>25%</div><div>8%</div><div>56%</div></div>
4	2-H	84	<div><div>27%</div><div><div></div><div></div><div></div></div><div>15%</div><div>33%</div><div><div></div><div></div></div><div>48%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 45703 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	1-A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	2-A	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	1-B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	2-B	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	1-C	488	Total	C	N	O	S	0	0	0
			3718	2341	656	709	12			
1	2-C	480	Total	C	N	O	S	0	0	0
			3661	2304	648	697	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 ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-D	469	Total	C	N	O	S	0	0	0
			3558	2254	605	688	11			
2	2-D	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	1-E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	2-E	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	1-F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2-F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

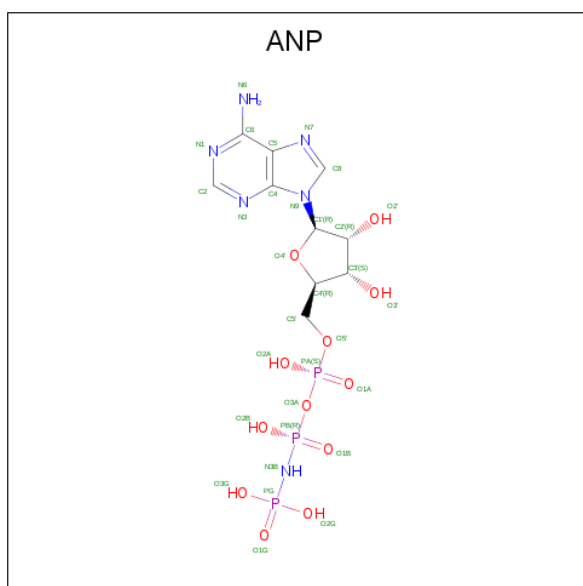
- Molecule 3 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1-G	94	Total	C	N	O	S	0	0	0
			709	437	130	136	6			
3	2-G	94	Total	C	N	O	S	0	0	0
			717	444	129	138	6			

- Molecule 4 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	1-H	37	Total	C	N	O	0	0	0
			283	167	59	57			
4	2-H	44	Total	C	N	O	0	0	0
			336	202	69	65			

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	2-A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	1-B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	2-B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	1-C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	2-C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	1-D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	2-D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	1-F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	2-F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

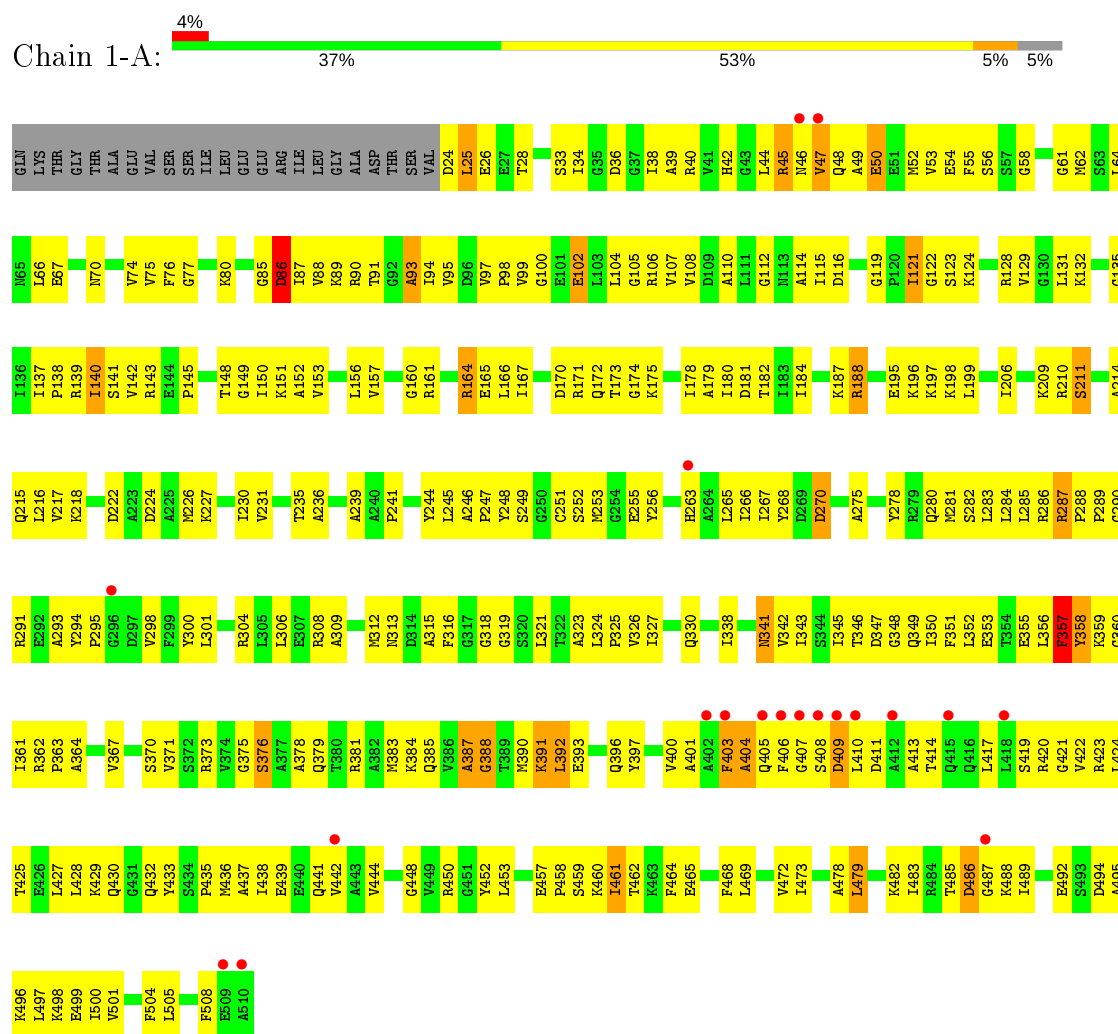
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1-D	1	Total	Mg	0	0
			1	1		
6	2-F	1	Total	Mg	0	0
			1	1		
6	1-B	1	Total	Mg	0	0
			1	1		
6	1-C	1	Total	Mg	0	0
			1	1		
6	2-D	1	Total	Mg	0	0
			1	1		
6	2-C	1	Total	Mg	0	0
			1	1		
6	1-A	1	Total	Mg	0	0
			1	1		
6	2-B	1	Total	Mg	0	0
			1	1		
6	2-A	1	Total	Mg	0	0
			1	1		
6	1-F	1	Total	Mg	0	0
			1	1		

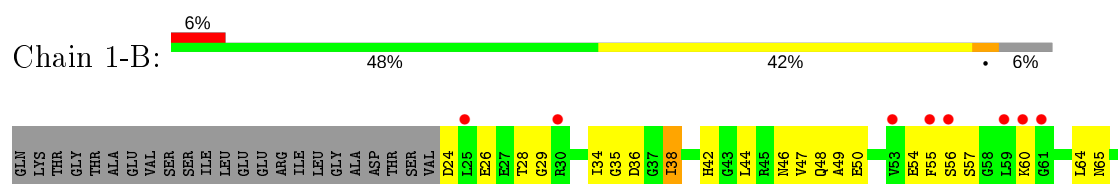
### 3 Residue-property plots

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

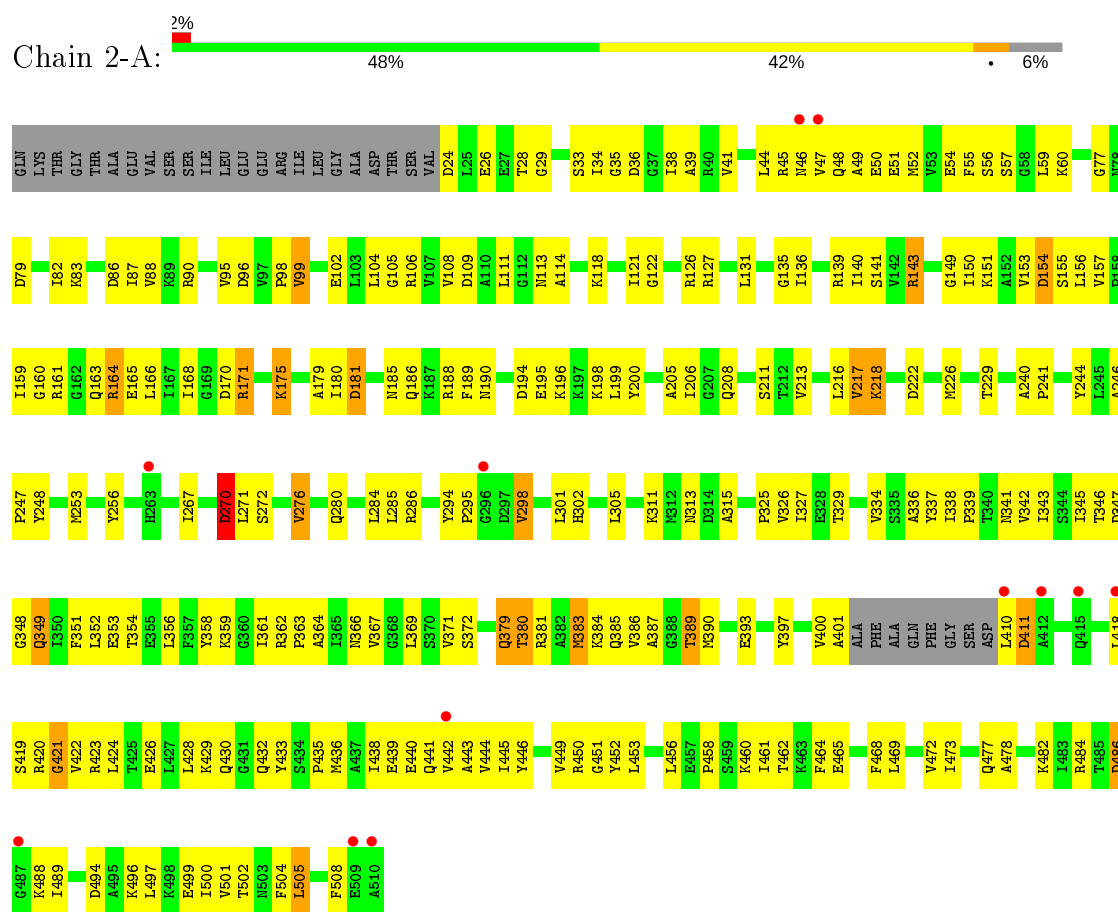


- Molecule 1: ATP synthase subunit alpha, mitochondrial

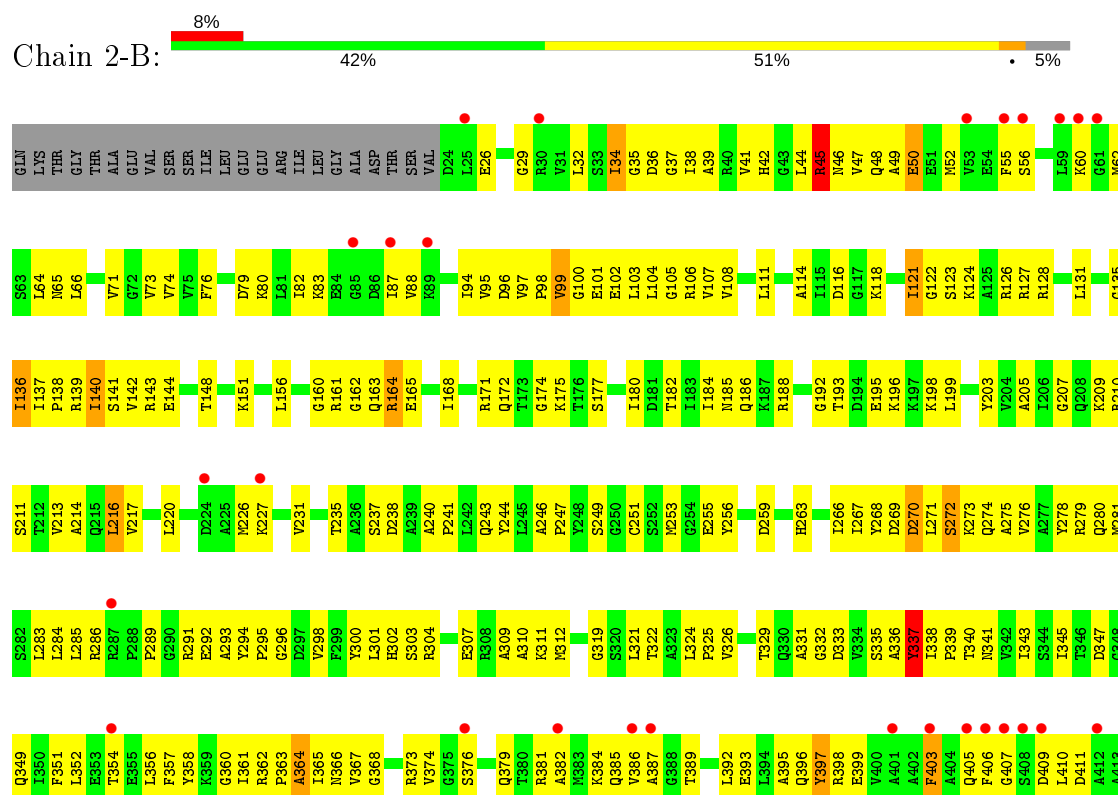


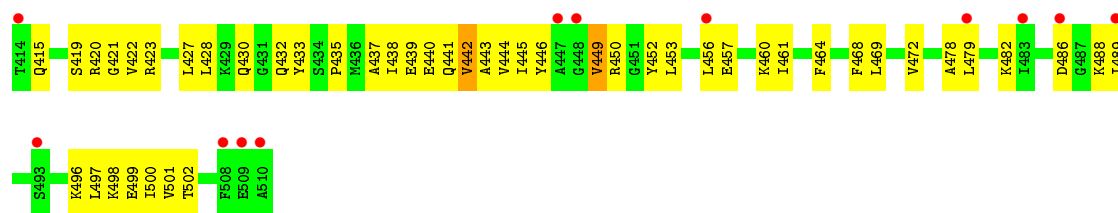




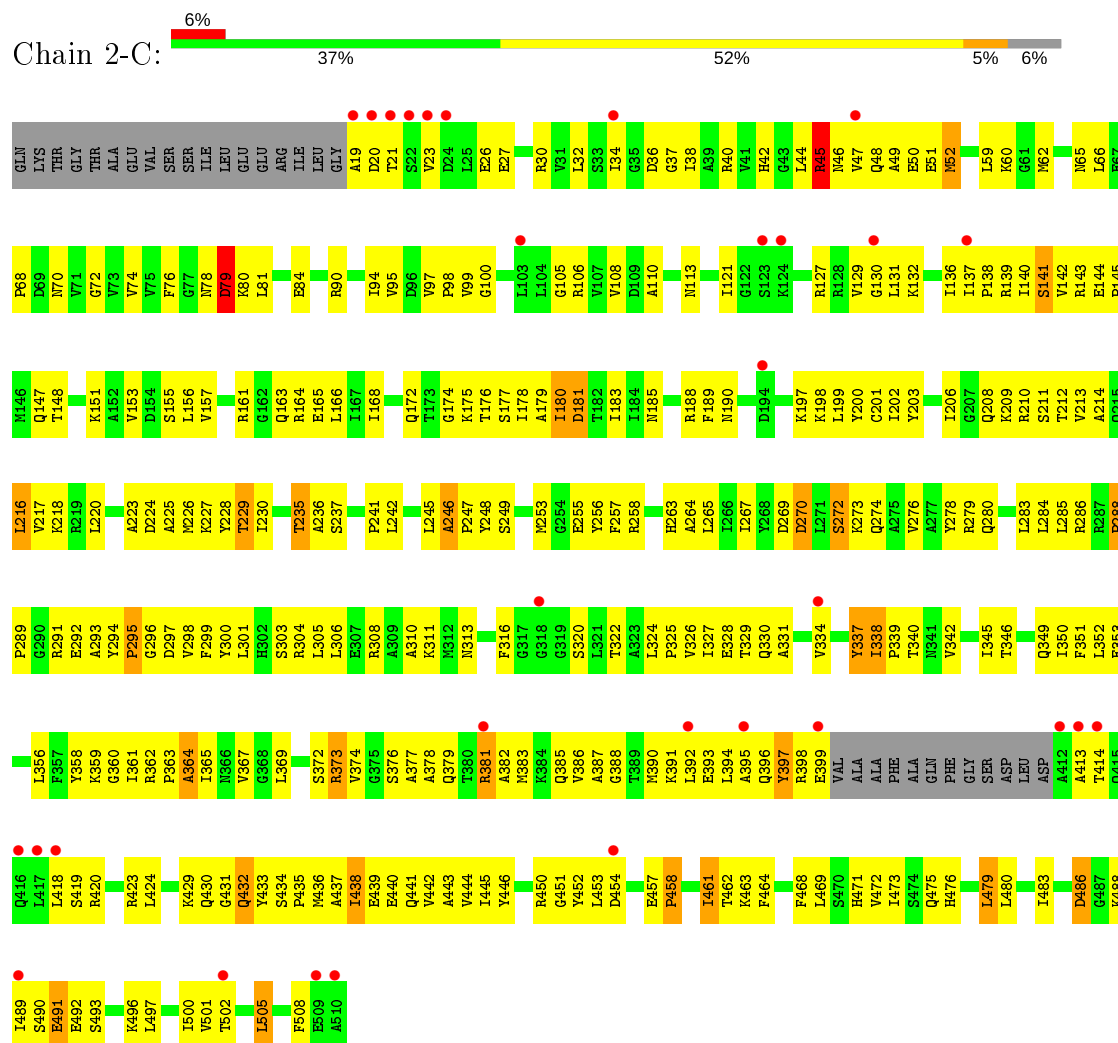


- Molecule 1: ATP synthase subunit alpha, mitochondrial

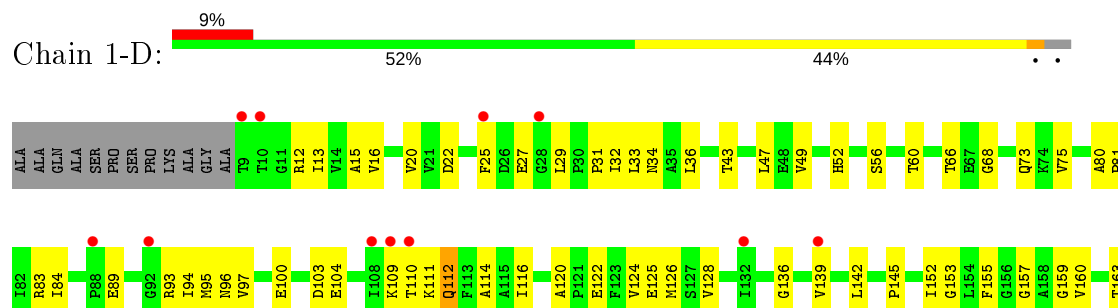


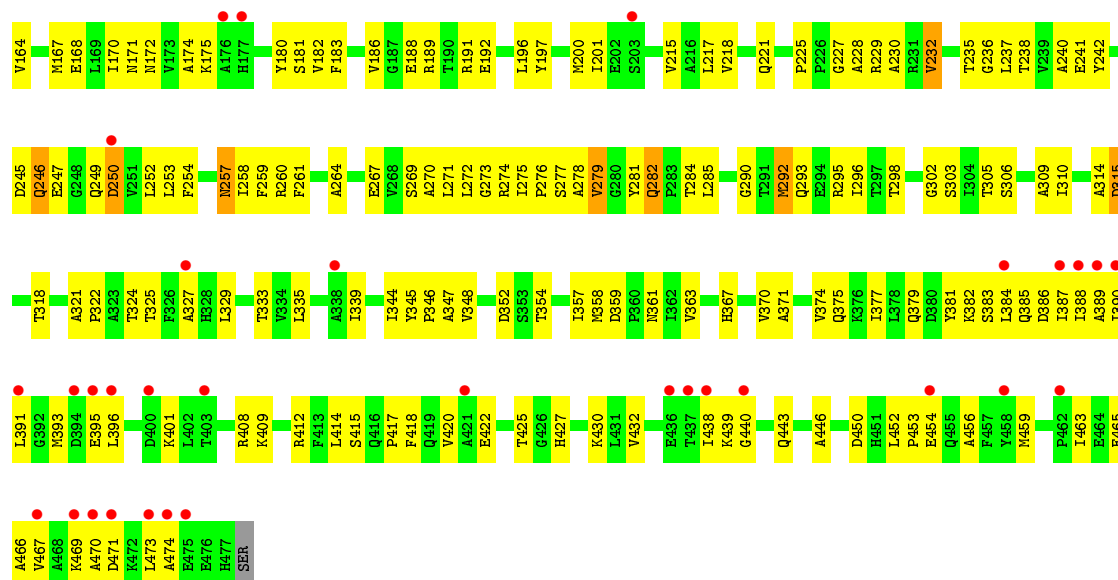


• Molecule 1: ATP synthase subunit alpha, mitochondrial

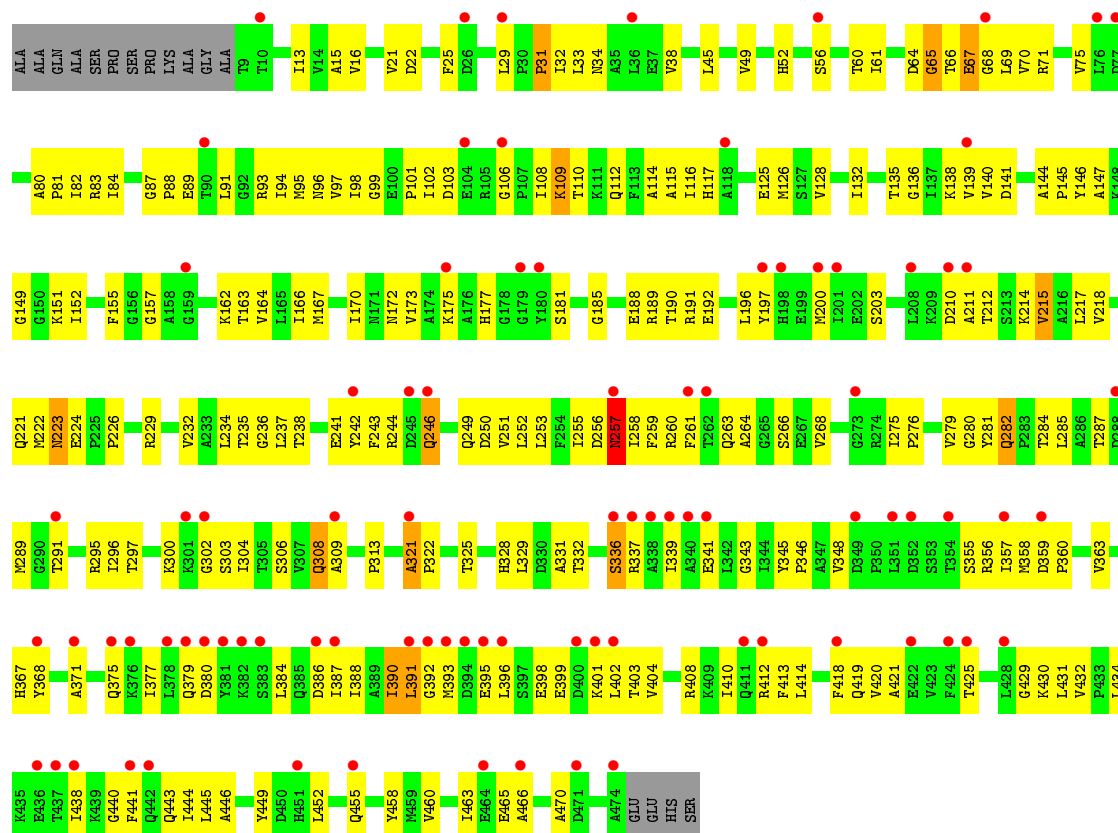


• Molecule 2: ATP synthase subunit beta, mitochondrial



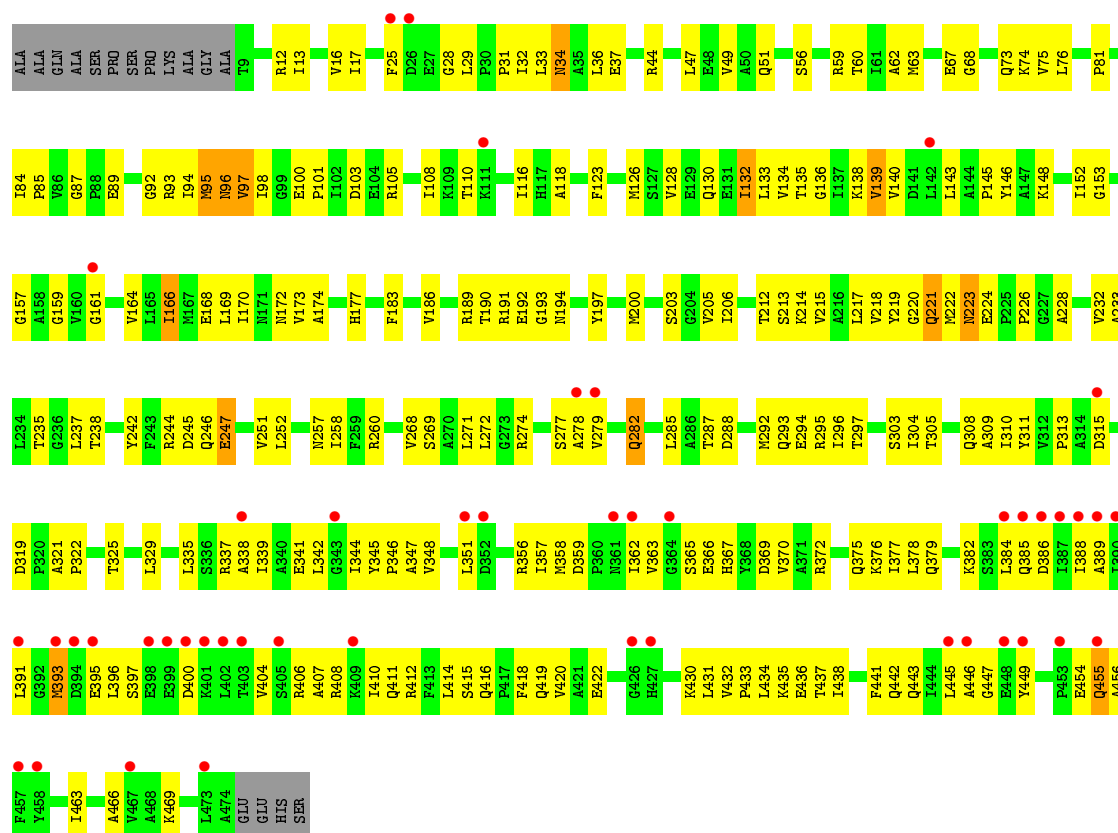


• Molecule 2: ATP synthase subunit beta, mitochondrial

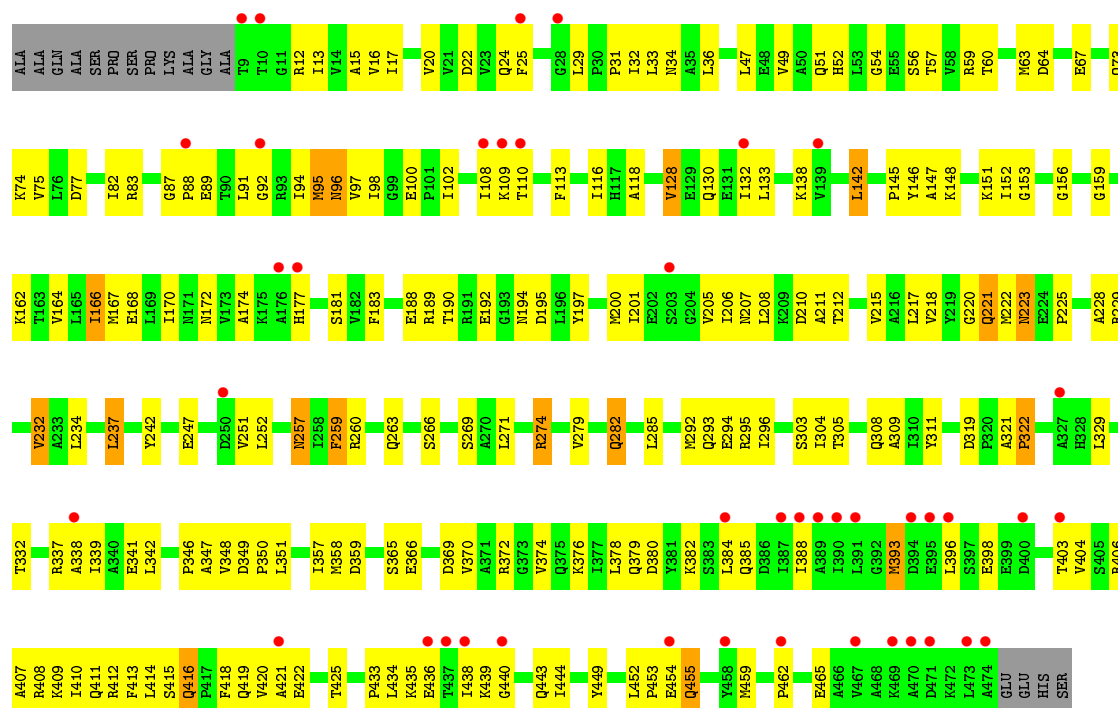


• Molecule 2: ATP synthase subunit beta, mitochondrial

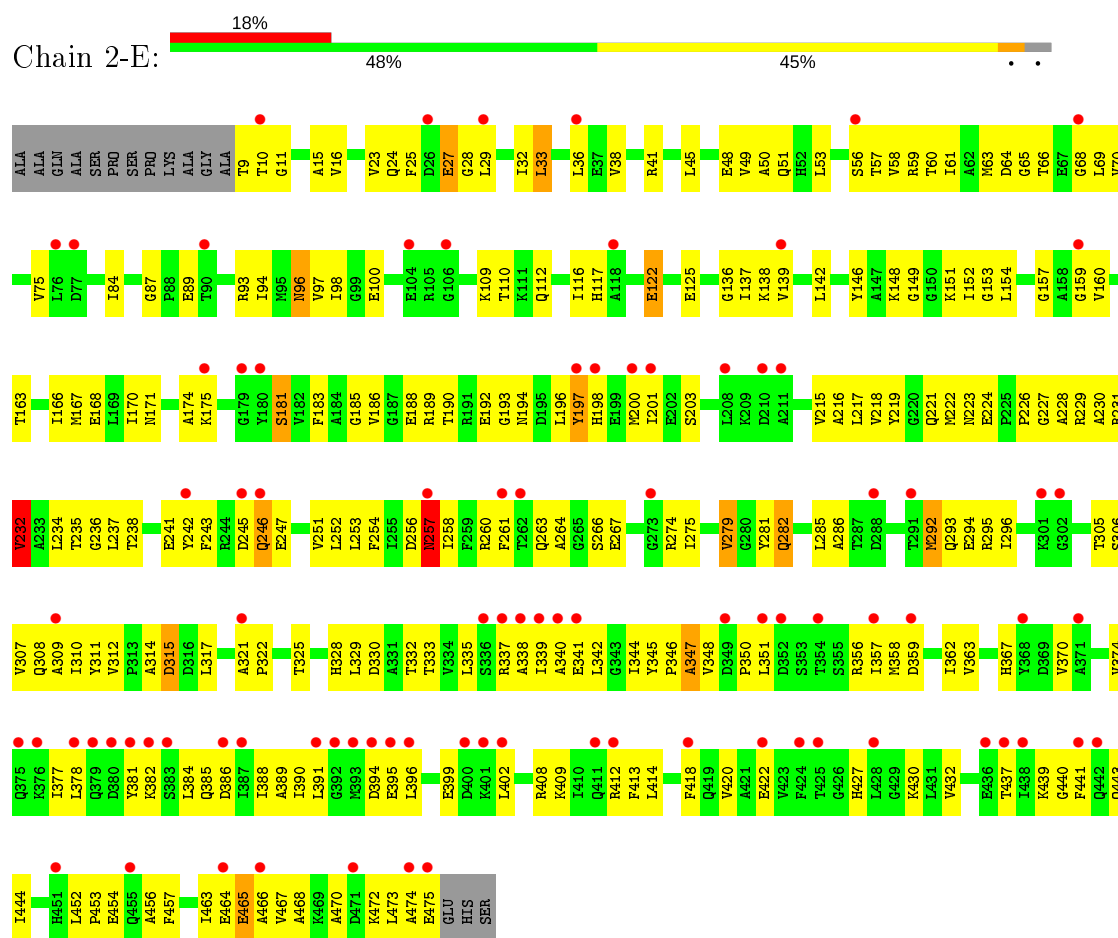




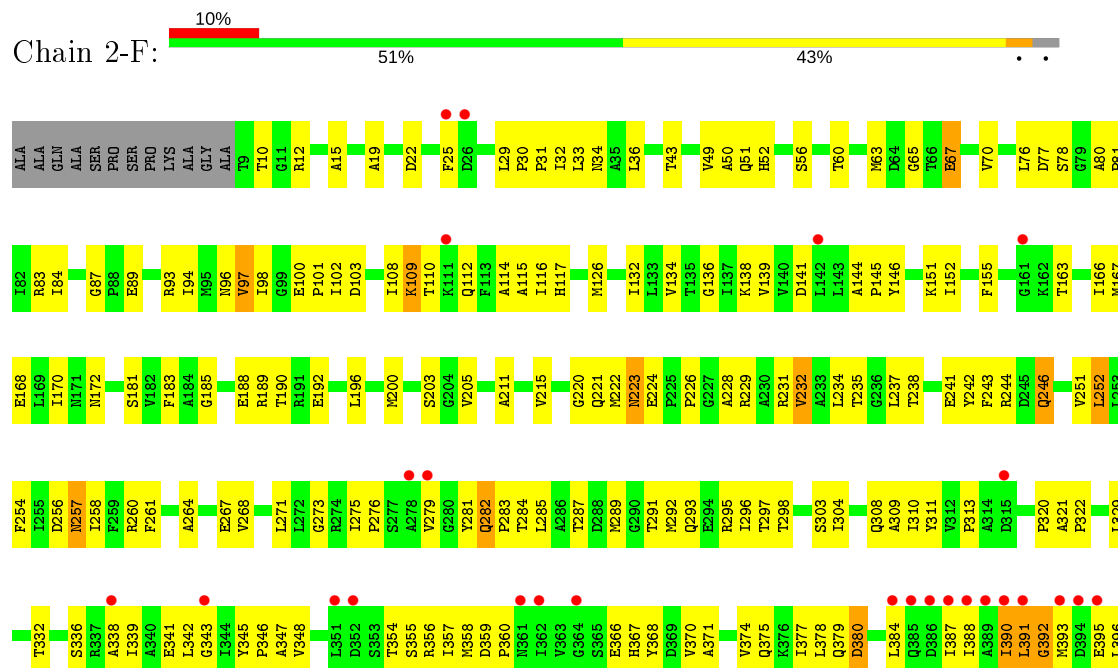
- Molecule 2: ATP synthase subunit beta, mitochondrial

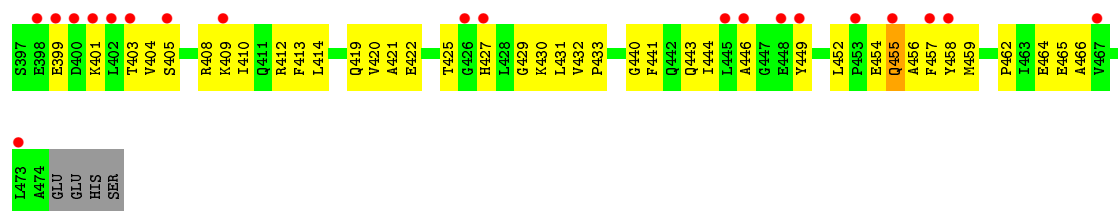


- Molecule 2: ATP synthase subunit beta, mitochondrial

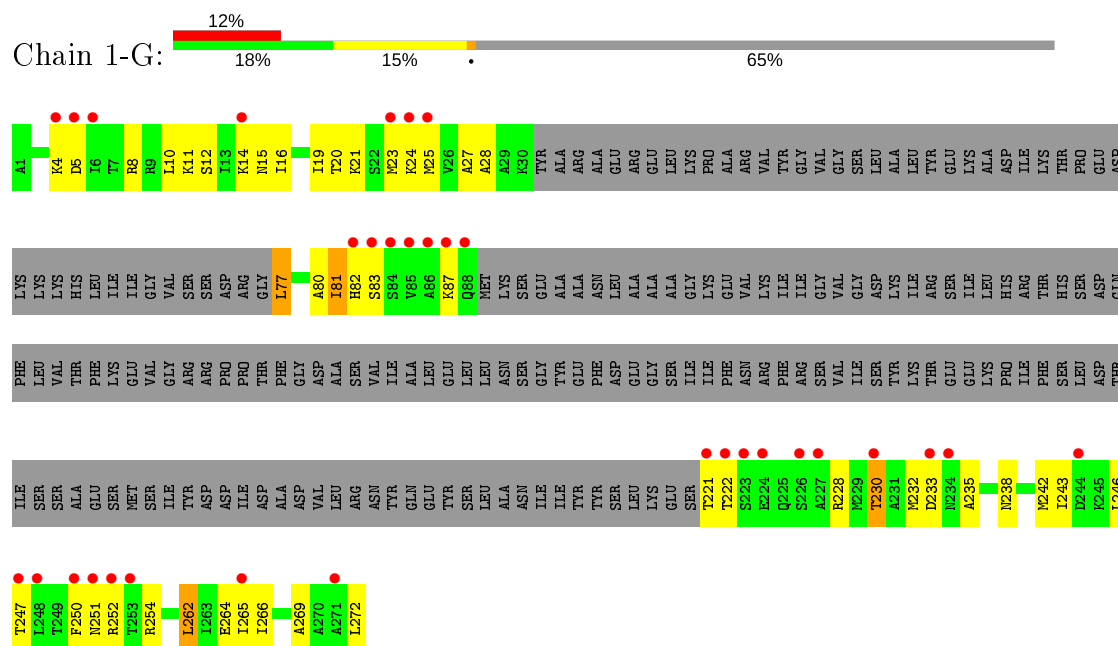


• Molecule 2: ATP synthase subunit beta, mitochondrial

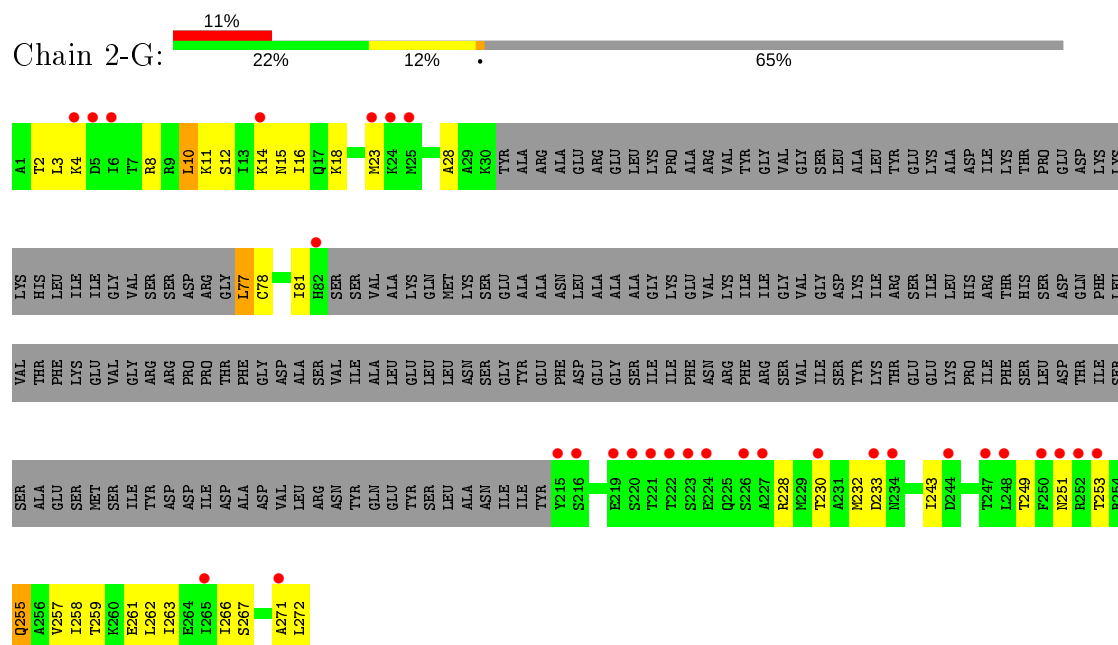




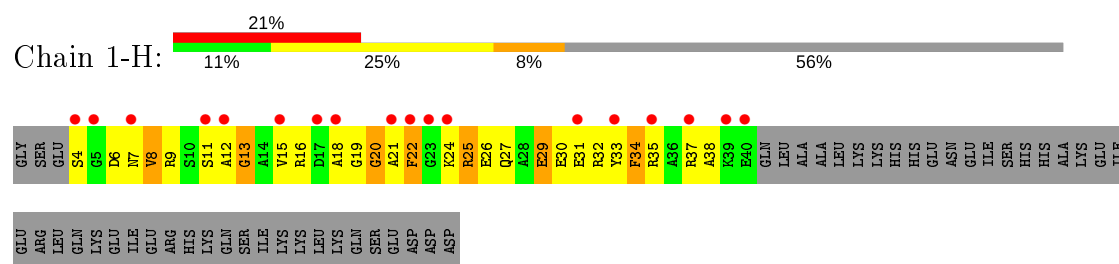
• Molecule 3: ATP synthase subunit gamma, mitochondrial



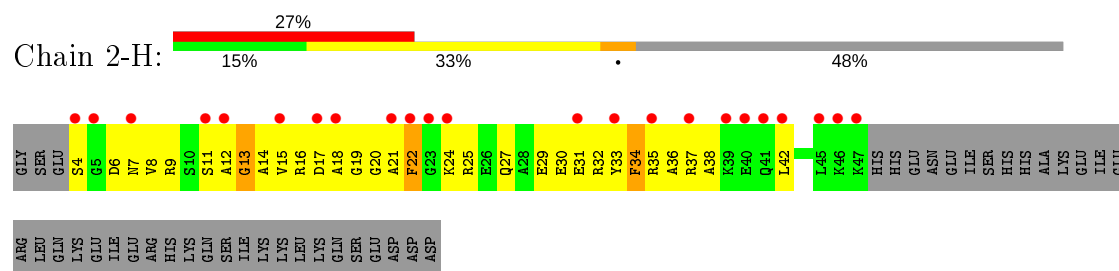
• Molecule 3: ATP synthase subunit gamma, mitochondrial



• Molecule 4: ATPase inhibitor, mitochondrial



- Molecule 4: ATPase inhibitor, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	272.30 Å   107.20 Å   152.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	39.50 – 2.80 39.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.50-2.80) 99.0 (39.48-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.81 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 ,   0.280 0.228 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.6	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 62.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	45703	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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	1-A	0.37	0/3766	0.65	0/5080
1	1-B	0.38	0/3704	0.67	0/4995
1	1-C	0.43	0/3767	0.71	0/5082
1	2-A	0.39	0/3704	0.66	0/4995
1	2-B	0.38	0/3766	0.65	0/5080
1	2-C	0.41	0/3709	0.65	0/5002
2	1-D	0.38	0/3616	0.65	0/4906
2	1-E	0.35	0/3587	0.63	0/4867
2	1-F	0.42	0/3587	0.71	0/4867
2	2-D	0.39	0/3587	0.66	0/4867
2	2-E	0.37	0/3596	0.64	0/4879
2	2-F	0.38	0/3587	0.65	0/4867
3	1-G	0.41	0/708	0.67	0/941
3	2-G	0.40	0/717	0.65	0/953
4	1-H	0.48	0/285	0.68	0/376
4	2-H	0.57	0/338	0.67	0/446
All	All	0.39	0/46024	0.66	0/62203

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	3715	0	3814	342	0
1	1-B	3656	0	3766	233	0
1	1-C	3718	0	3818	305	0
1	2-A	3656	0	3765	304	0
1	2-B	3715	0	3814	266	0
1	2-C	3661	0	3766	299	0
2	1-D	3558	0	3605	236	0
2	1-E	3530	0	3587	245	0
2	1-F	3530	0	3586	216	0
2	2-D	3530	0	3586	196	0
2	2-E	3539	0	3592	245	0
2	2-F	3530	0	3587	233	0
3	1-G	709	0	771	57	0
3	2-G	717	0	775	47	0
4	1-H	283	0	265	63	0
4	2-H	336	0	331	71	0
5	1-A	31	0	13	4	0
5	1-B	31	0	13	4	0
5	1-C	31	0	13	3	0
5	1-D	31	0	13	5	0
5	1-F	31	0	13	3	0
5	2-A	31	0	13	6	0
5	2-B	31	0	13	4	0
5	2-C	31	0	13	5	0
5	2-D	31	0	13	4	0
5	2-F	31	0	13	4	0
6	1-A	1	0	0	0	0
6	1-B	1	0	0	0	0
6	1-C	1	0	0	0	0
6	1-D	1	0	0	0	0
6	1-F	1	0	0	0	0
6	2-A	1	0	0	0	0
6	2-B	1	0	0	0	0
6	2-C	1	0	0	0	0
6	2-D	1	0	0	0	0
6	2-F	1	0	0	0	0
All	All	45703	0	46558	3080	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 33.

The worst 5 of 3080 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)
2:F:282:GLN:HE21	2:F:282:GLN:N	1.40	1.19
2:D:473:LEU:HB3	4:H:34:PHE:CZ	1.80	1.16
2:F:282:GLN:NE2	2:F:282:GLN:H	1.43	1.15
2:E:282:GLN:H	2:E:282:GLN:NE2	1.46	1.12
2:D:282:GLN:HE21	2:D:282:GLN:N	1.45	1.12

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	1-A	485/510 (95%)	398 (82%)	63 (13%)	24 (5%)	2	7
1	1-B	475/510 (93%)	408 (86%)	56 (12%)	11 (2%)	6	21
1	1-C	484/510 (95%)	411 (85%)	58 (12%)	15 (3%)	4	14
1	2-A	475/510 (93%)	416 (88%)	48 (10%)	11 (2%)	6	21
1	2-B	485/510 (95%)	413 (85%)	59 (12%)	13 (3%)	5	17
1	2-C	476/510 (93%)	390 (82%)	64 (13%)	22 (5%)	2	7
2	1-D	467/482 (97%)	411 (88%)	50 (11%)	6 (1%)	12	36
2	1-E	464/482 (96%)	396 (85%)	59 (13%)	9 (2%)	8	26
2	1-F	464/482 (96%)	400 (86%)	54 (12%)	10 (2%)	6	22
2	2-D	464/482 (96%)	408 (88%)	46 (10%)	10 (2%)	6	22
2	2-E	465/482 (96%)	400 (86%)	52 (11%)	13 (3%)	5	17
2	2-F	464/482 (96%)	400 (86%)	53 (11%)	11 (2%)	6	20
3	1-G	88/272 (32%)	78 (89%)	9 (10%)	1 (1%)	14	41
3	2-G	88/272 (32%)	76 (86%)	11 (12%)	1 (1%)	14	41
4	1-H	35/84 (42%)	20 (57%)	10 (29%)	5 (14%)	0	0
4	2-H	42/84 (50%)	30 (71%)	10 (24%)	2 (5%)	2	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5921/6664 (89%)	5055 (85%)	702 (12%)	164 (3%)	5 17

5 of 164 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	123	SER
1	1-A	141	SER
1	1-A	270	ASP
1	1-A	387	ALA
1	1-A	404	ALA

### 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	1-A	393/412 (95%)	379 (96%)	14 (4%)	35 69
1	1-B	388/412 (94%)	374 (96%)	14 (4%)	35 69
1	1-C	394/412 (96%)	375 (95%)	19 (5%)	25 58
1	2-A	388/412 (94%)	368 (95%)	20 (5%)	23 55
1	2-B	393/412 (95%)	373 (95%)	20 (5%)	24 55
1	2-C	389/412 (94%)	371 (95%)	18 (5%)	27 60
2	1-D	379/386 (98%)	369 (97%)	10 (3%)	46 79
2	1-E	376/386 (97%)	366 (97%)	10 (3%)	44 78
2	1-F	376/386 (97%)	363 (96%)	13 (4%)	36 70
2	2-D	376/386 (97%)	362 (96%)	14 (4%)	34 68
2	2-E	377/386 (98%)	368 (98%)	9 (2%)	49 81
2	2-F	376/386 (97%)	364 (97%)	12 (3%)	39 73
3	1-G	78/230 (34%)	75 (96%)	3 (4%)	33 67
3	2-G	79/230 (34%)	73 (92%)	6 (8%)	13 36
4	1-H	25/68 (37%)	23 (92%)	2 (8%)	12 34
4	2-H	30/68 (44%)	28 (93%)	2 (7%)	16 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4817/5384 (90%)	4631 (96%)	186 (4%)	32 66

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	1-H	34	PHE
1	2-A	505	LEU
2	2-F	246	GLN
1	2-A	86	ASP
1	2-A	270	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
2	1-F	385	GLN
1	2-A	466	ASN
2	2-F	246	GLN
2	1-F	443	GLN
1	2-A	48	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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
5	ANP	2-D	1478	6	29,33,33	1.54	6 (20%)	31,52,52	1.90	6 (19%)
5	ANP	1-A	1511	6	29,33,33	1.43	4 (13%)	31,52,52	1.38	4 (12%)
5	ANP	1-B	1511	6	29,33,33	1.48	5 (17%)	31,52,52	1.55	5 (16%)
5	ANP	2-F	1478	6	29,33,33	1.74	8 (27%)	31,52,52	1.73	6 (19%)
5	ANP	1-C	1511	6	29,33,33	1.35	3 (10%)	31,52,52	1.45	2 (6%)
5	ANP	2-B	1511	6	29,33,33	1.35	4 (13%)	31,52,52	1.19	3 (9%)
5	ANP	1-F	1478	6	29,33,33	1.59	6 (20%)	31,52,52	1.76	5 (16%)
5	ANP	1-D	1478	6	29,33,33	1.75	7 (24%)	31,52,52	1.80	8 (25%)
5	ANP	2-A	1511	6	29,33,33	1.57	5 (17%)	31,52,52	1.68	4 (12%)
5	ANP	2-C	1511	6	29,33,33	1.52	6 (20%)	31,52,52	1.66	3 (9%)

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
5	ANP	2-D	1478	6	-	8/14/38/38	0/3/3/3
5	ANP	1-A	1511	6	-	7/14/38/38	0/3/3/3
5	ANP	1-B	1511	6	-	7/14/38/38	0/3/3/3
5	ANP	2-F	1478	6	-	9/14/38/38	0/3/3/3
5	ANP	1-C	1511	6	-	7/14/38/38	0/3/3/3
5	ANP	2-B	1511	6	-	7/14/38/38	0/3/3/3
5	ANP	1-F	1478	6	-	9/14/38/38	0/3/3/3
5	ANP	1-D	1478	6	-	9/14/38/38	0/3/3/3
5	ANP	2-A	1511	6	-	7/14/38/38	0/3/3/3
5	ANP	2-C	1511	6	-	7/14/38/38	0/3/3/3

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2-F	1478	ANP	PG-O2G	-5.33	1.42	1.56
5	1-D	1478	ANP	PG-O2G	-5.05	1.43	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2-A	1511	ANP	PG-O2G	-4.48	1.44	1.56
5	1-C	1511	ANP	PG-O2G	-4.26	1.45	1.56
5	2-C	1511	ANP	PG-O1G	4.24	1.52	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2-D	1478	ANP	O1G-PG-N3B	-6.80	101.76	111.77
5	2-F	1478	ANP	O1G-PG-N3B	-6.45	102.27	111.77
5	1-F	1478	ANP	O1G-PG-N3B	-5.65	103.45	111.77
5	2-C	1511	ANP	O1G-PG-N3B	-5.49	103.68	111.77
5	2-A	1511	ANP	O1G-PG-N3B	-5.34	103.91	111.77

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	2-D	1478	ANP	PB-N3B-PG-O1G
5	2-D	1478	ANP	PG-N3B-PB-O1B
5	2-D	1478	ANP	PA-O3A-PB-O1B
5	2-D	1478	ANP	C5'-O5'-PA-O1A
5	2-D	1478	ANP	C5'-O5'-PA-O2A

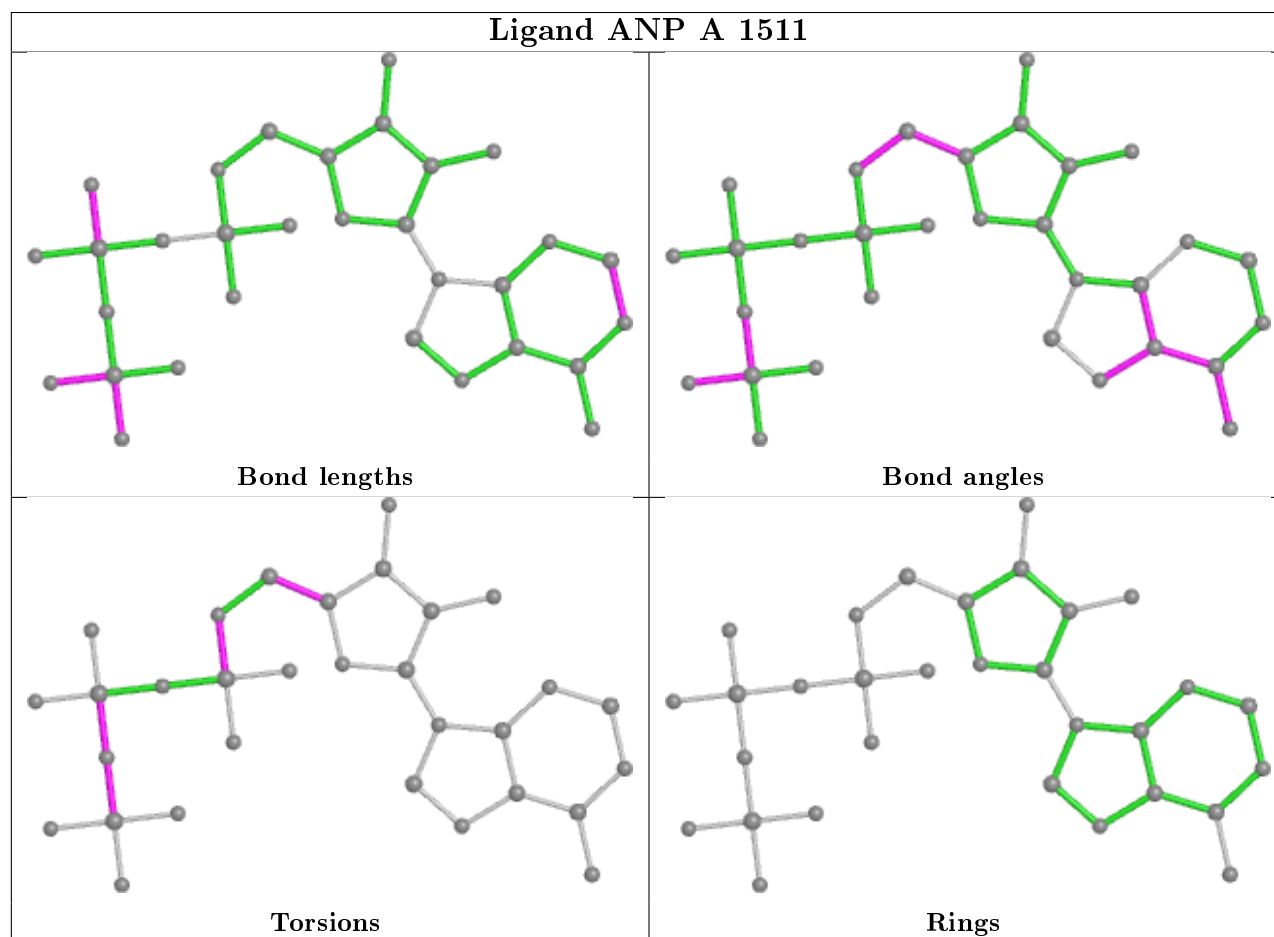
There are no ring outliers.

10 monomers are involved in 42 short contacts:

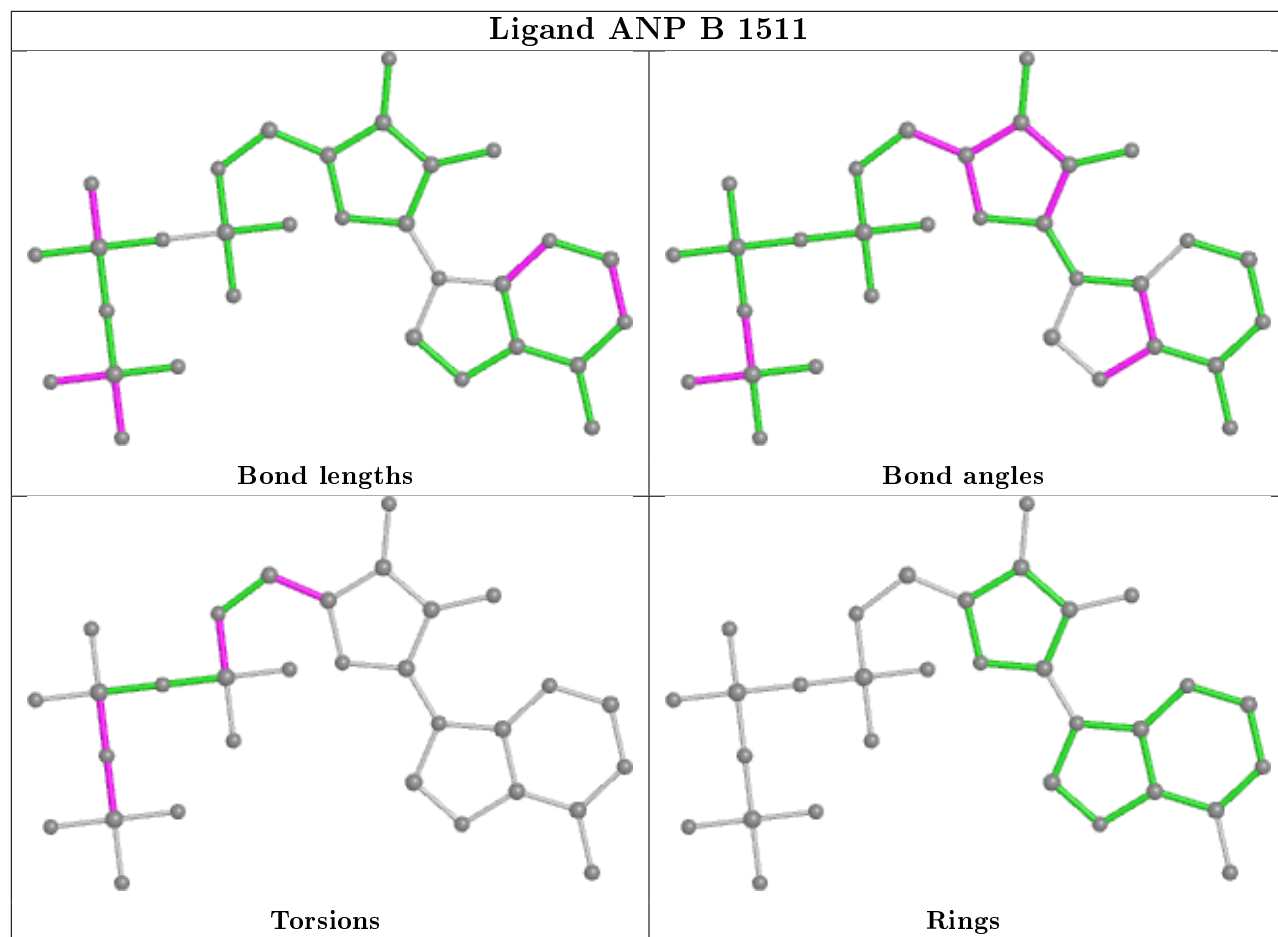
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	2-D	1478	ANP	4	0
5	1-A	1511	ANP	4	0
5	1-B	1511	ANP	4	0
5	2-F	1478	ANP	4	0
5	1-C	1511	ANP	3	0
5	2-B	1511	ANP	4	0
5	1-F	1478	ANP	3	0
5	1-D	1478	ANP	5	0
5	2-A	1511	ANP	6	0
5	2-C	1511	ANP	5	0

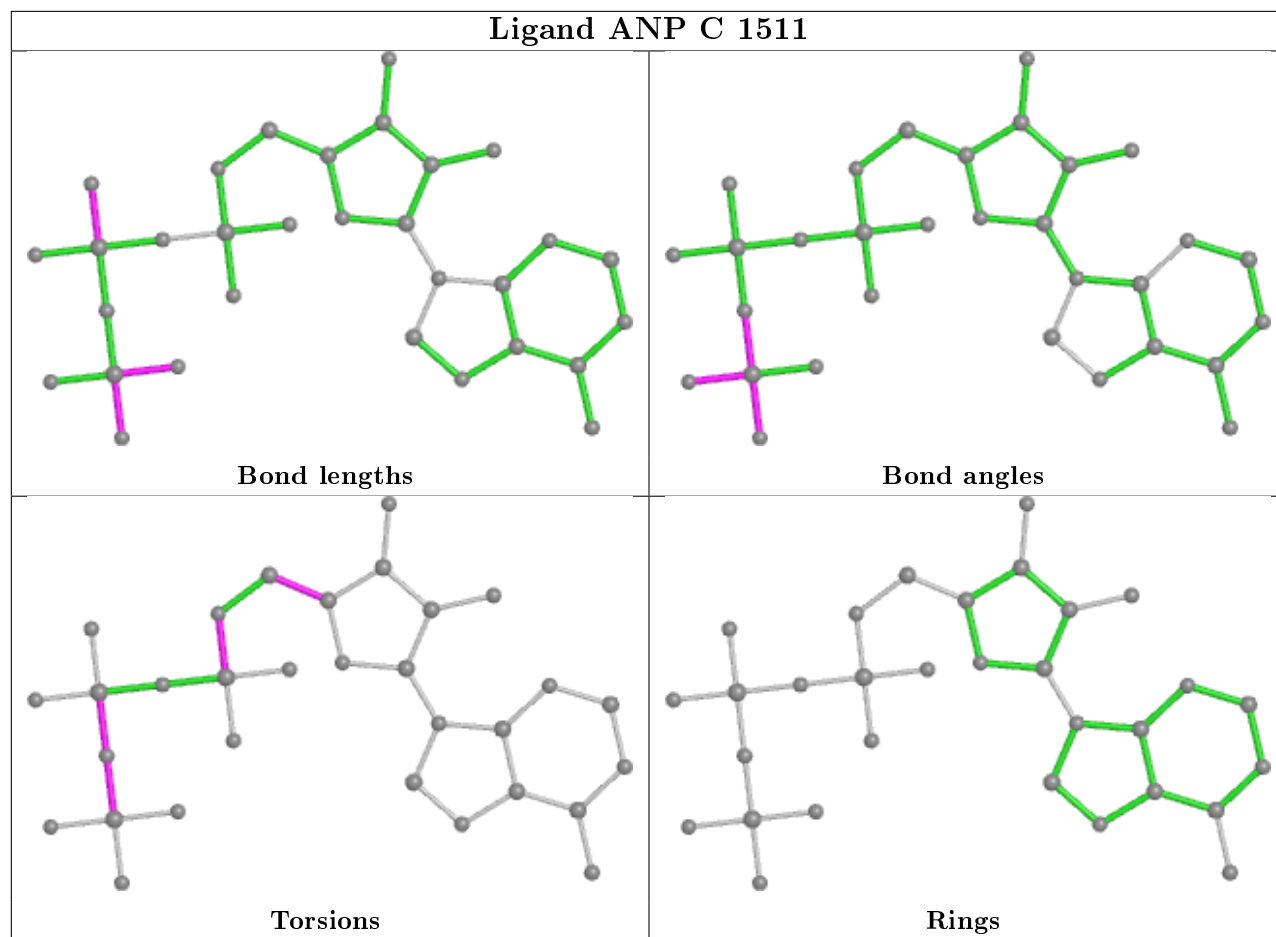
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

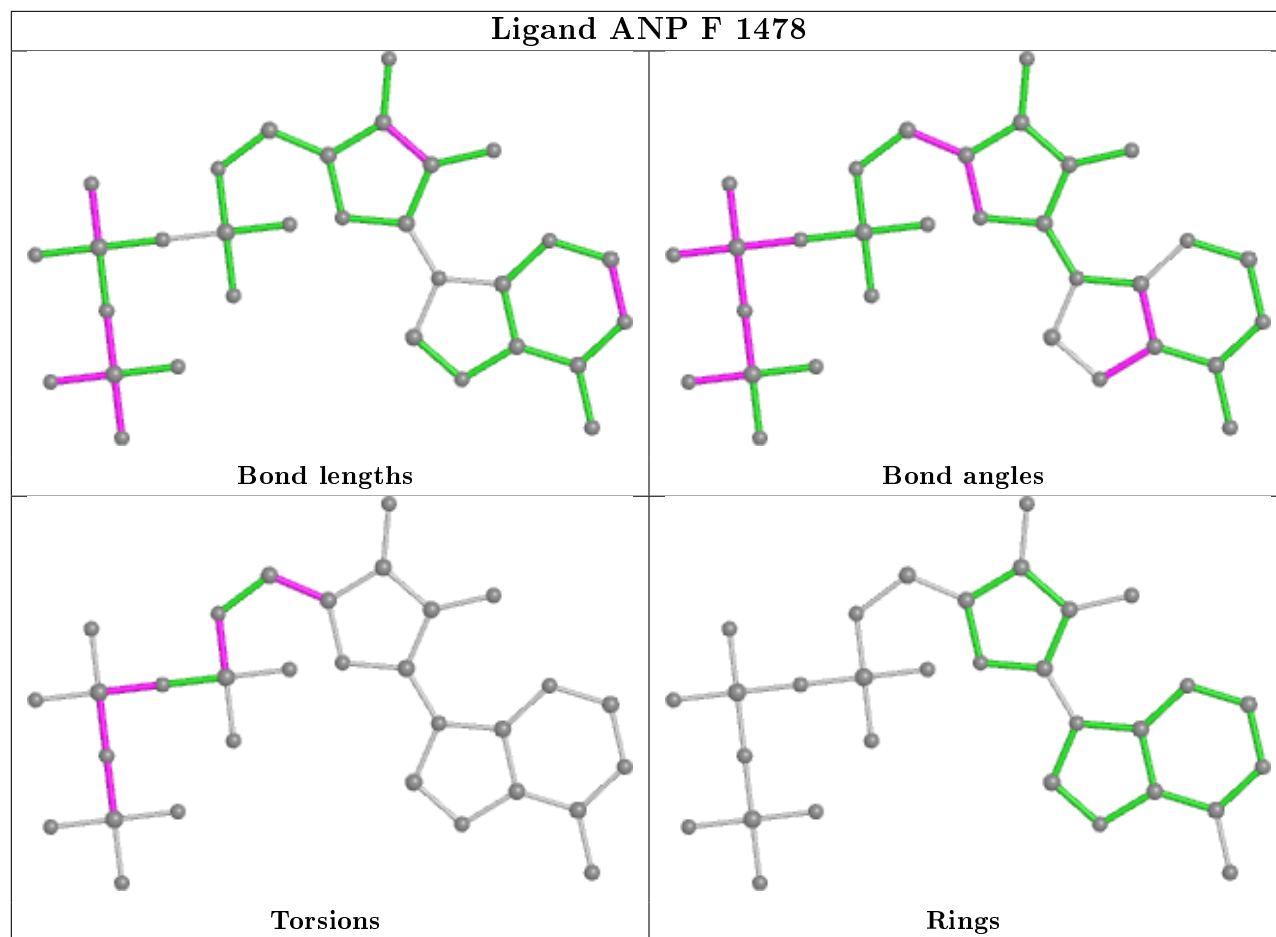
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

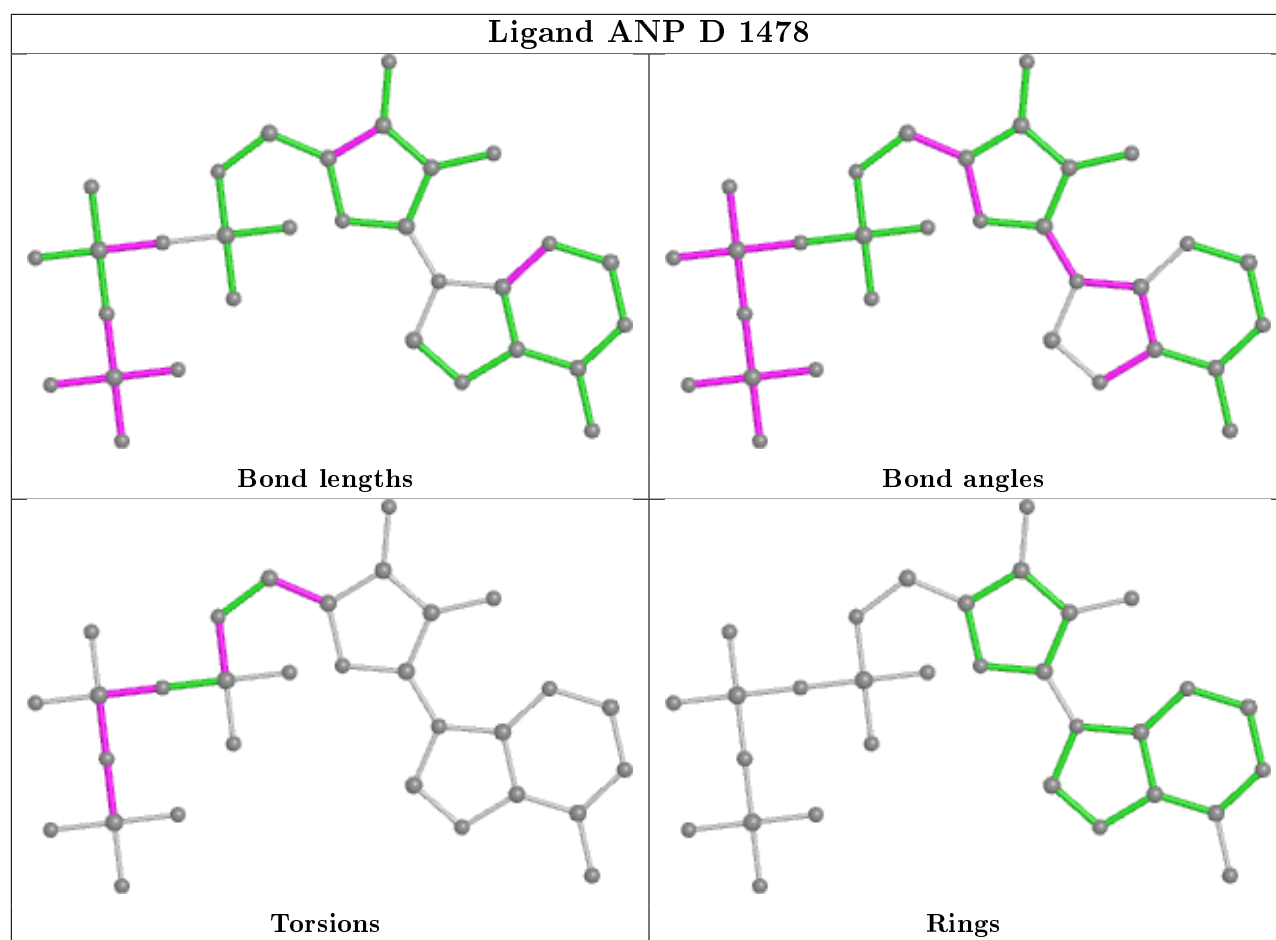












## 5.7 Other polymers [i](#)

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1-A	487/510 (95%)	-0.05	19 (3%) 39 29	33, 55, 103, 139	487 (100%)
1	1-B	479/510 (93%)	0.11	33 (6%) 16 10	38, 59, 88, 127	479 (100%)
1	1-C	488/510 (95%)	0.24	35 (7%) 15 8	37, 65, 99, 147	488 (100%)
1	2-A	479/510 (93%)	-0.14	12 (2%) 57 47	33, 55, 102, 139	479 (100%)
1	2-B	487/510 (95%)	0.15	39 (8%) 12 6	38, 59, 96, 128	487 (100%)
1	2-C	480/510 (94%)	0.19	31 (6%) 18 11	37, 65, 97, 130	480 (100%)
2	1-D	469/482 (97%)	0.41	43 (9%) 9 5	36, 56, 91, 117	469 (100%)
2	1-E	466/482 (96%)	0.83	88 (18%) 1 1	41, 65, 98, 111	466 (100%)
2	1-F	466/482 (96%)	0.43	46 (9%) 7 4	28, 60, 106, 135	466 (100%)
2	2-D	466/482 (96%)	0.40	42 (9%) 9 5	36, 56, 89, 112	466 (100%)
2	2-E	467/482 (96%)	0.84	89 (19%) 1 1	41, 65, 99, 111	467 (100%)
2	2-F	466/482 (96%)	0.43	46 (9%) 7 4	28, 60, 106, 135	466 (100%)
3	1-G	94/272 (34%)	1.83	32 (34%) 0 0	33, 71, 120, 123	94 (100%)
3	2-G	94/272 (34%)	1.78	30 (31%) 0 0	33, 71, 117, 123	94 (100%)
4	1-H	37/84 (44%)	2.39	18 (48%) 0 0	70, 90, 110, 115	37 (100%)
4	2-H	44/84 (52%)	2.53	23 (52%) 0 0	70, 93, 112, 118	44 (100%)
All	All	5969/6664 (89%)	0.39	626 (10%) 9 3	28, 61, 102, 147	5969 (100%)

The worst 5 of 626 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-C	414	THR	14.5
1	2-C	414	THR	14.5
2	1-F	394	ASP	14.1
2	2-F	394	ASP	14.1
2	1-F	391	LEU	13.2

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

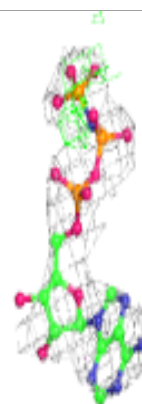
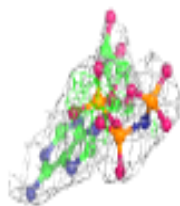
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	2-F	1479	1/1	0.76	0.35	62,62,62,62	1
6	MG	1-F	1479	1/1	0.76	0.35	44,44,44,44	1
5	ANP	2-F	1478	31/31	0.89	0.24	49,69,75,79	31
5	ANP	1-F	1478	31/31	0.89	0.24	33,52,59,61	31
6	MG	1-B	1512	1/1	0.90	0.55	57,57,57,57	1
6	MG	2-B	1512	1/1	0.90	0.55	45,45,45,45	1
6	MG	1-A	1512	1/1	0.92	0.47	39,39,39,39	1
6	MG	2-A	1512	1/1	0.92	0.47	41,41,41,41	1
6	MG	1-C	1512	1/1	0.94	0.42	46,46,46,46	1
6	MG	2-C	1512	1/1	0.94	0.42	44,44,44,44	1
5	ANP	1-C	1511	31/31	0.95	0.20	29,44,58,62	31
5	ANP	2-A	1511	31/31	0.95	0.19	40,59,70,76	31
5	ANP	2-C	1511	31/31	0.95	0.20	36,64,75,78	31
5	ANP	1-A	1511	31/31	0.95	0.19	39,57,65,70	31
6	MG	1-D	1479	1/1	0.96	0.39	60,60,60,60	1
6	MG	2-D	1479	1/1	0.96	0.39	47,47,47,47	1
5	ANP	1-D	1478	31/31	0.97	0.18	40,54,62,62	31
5	ANP	2-B	1511	31/31	0.97	0.16	40,54,61,67	31
5	ANP	2-D	1478	31/31	0.97	0.18	39,48,56,58	31
5	ANP	1-B	1511	31/31	0.97	0.16	41,68,80,81	31

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 F 1478:**

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

**Electron density around ANP C 1511:**

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

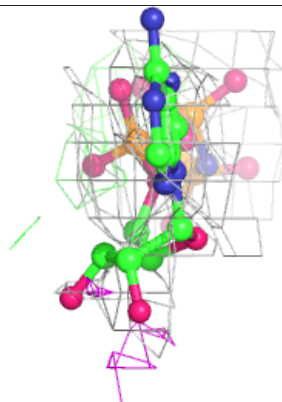
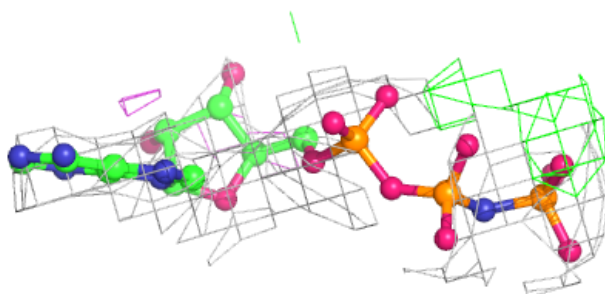
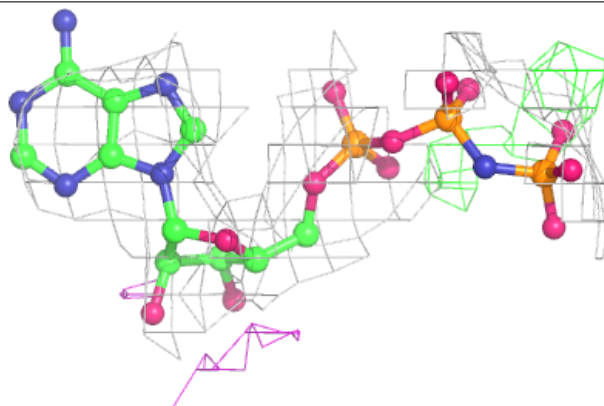


**Electron density around ANP A 1511:**

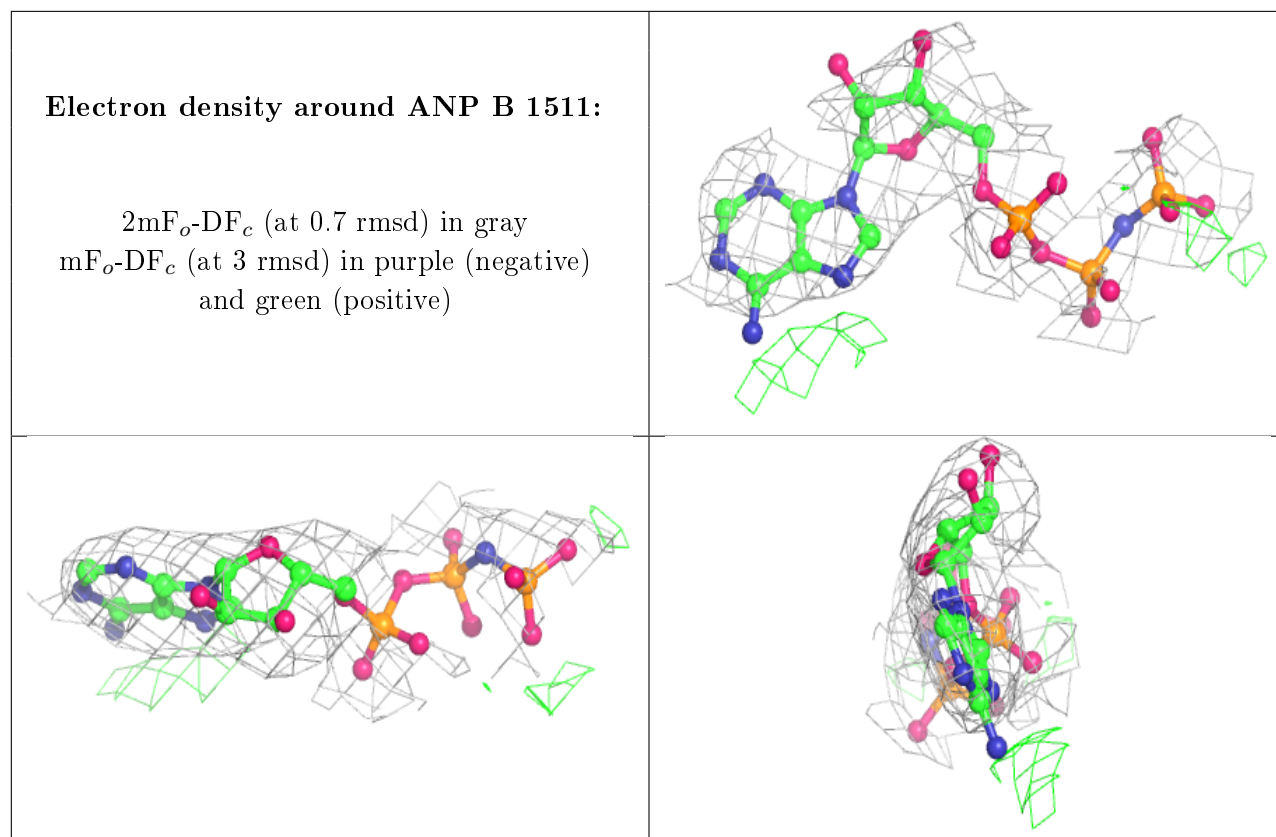
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ANP D 1478:**

$2mF_o-DF_c$  (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.