



## Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 09:46 pm BST

PDB ID : 6ZQN / pdb\_00006zqn  
EMDB ID : EMD-11369  
Title : bovine ATP synthase monomer state 3 (combined)  
Authors : Spikes, T.E.; Montgomery, M.G.; Walker, J.E.  
Deposited on : 2020-07-10  
Resolution : 4.00 Å (reported)  
Based on initial models : 2V7Q, 2CLY

This is a Full wwPDB EM Validation 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/EMValidationReportHelp>  
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:

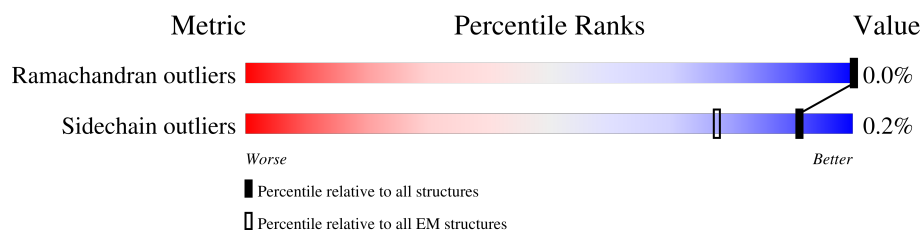
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	 98%
1	B	510	 98%
1	C	510	 95% 5%
2	D	482	 97%
2	E	482	 97%
2	F	482	 97%
3	G	273	 100%
4	H	146	 90% 10%
5	I	50	 94% 6%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	J	66	 14% 71% 29%
7	K	75	 7% 99%
7	L	75	 99%
7	M	75	 100%
7	N	75	 100%
7	O	75	 99%
7	P	75	 96%
7	Q	75	 99%
7	R	75	 100%
8	S	190	 5% 98%
9	8	66	 62% 38%
10	a	226	 100%
11	d	160	 96%
12	f	87	 95% 5%
13	g	102	 77% 23%
14	j	60	 80% 20%
15	b	214	 97%
16	h	76	 11% 80% 18%
17	k	57	 5% 63% 37%
18	e	70	 11% 80% 20%

## 2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 81277 atoms, of which 41197 are hydrogens and 0 are deuteriums.

In the tables below, 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						AltConf	Trace
1	A	501	Total	C	H	N	O	S	0	0
			7741	2405	3923	673	728	12		
1	B	502	Total	C	H	N	O	S	0	0
			7760	2408	3935	674	731	12		
1	C	483	Total	C	H	N	O	S	0	0
			7488	2329	3798	652	697	12		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	GLN	variant	UNP P19483
A	481	GLY	SER	microheterogeneity	UNP P19483
B	1	GLU	GLN	variant	UNP P19483
B	481	GLY	SER	microheterogeneity	UNP P19483
C	1	GLU	GLN	variant	UNP P19483
C	481	GLY	SER	microheterogeneity	UNP P19483

- Molecule 2 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	469	Total	C	H	N	O	S	0	0
			7163	2254	3605	605	688	11		
2	E	467	Total	C	H	N	O	S	0	0
			7132	2243	3593	601	684	11		
2	F	467	Total	C	H	N	O	S	0	0
			7131	2243	3592	601	684	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	272	Total	C	H	N	O	S	0	0
			4300	1330	2185	368	409	8		

- Molecule 4 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	H	131	Total	C	H	N	O	S	0	0
			1940	609	970	163	196	2		

- Molecule 5 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	47	Total	C	H	N	O	S	0	0
			764	237	395	66	64	2		

- Molecule 6 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	J	47	Total	C	H	N	O		0	0
			731	224	361	76	70			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	61	HIS	-	expression tag	UNP P01096
J	62	HIS	-	expression tag	UNP P01096
J	63	HIS	-	expression tag	UNP P01096
J	64	HIS	-	expression tag	UNP P01096
J	65	HIS	-	expression tag	UNP P01096
J	66	HIS	-	expression tag	UNP P01096

- Molecule 7 is a protein called ATP synthase F(0) complex subunit C2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	K	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		
7	L	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		
7	M	75	Total	C	H	N	O	S	0	0
			1095	356	558	83	94	4		
7	N	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		
7	P	74	Total	C	H	N	O	S	0	0
			1079	351	550	82	93	3		
7	R	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms						AltConf	Trace
7	O	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		
7	Q	75	Total	C	H	N	O	S	0	0
			1096	356	559	83	94	4		

- Molecule 8 is a protein called ATP synthase subunit O, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	S	187	Total	C	H	N	O	S	0	0
			2989	915	1551	248	266	9		

- Molecule 9 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	8	41	Total	C	H	N	O	S	0	0
			696	231	352	52	58	3		

- Molecule 10 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	a	226	Total	C	H	N	O	S	0	0
			3611	1155	1870	276	298	12		

- Molecule 11 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	d	155	Total	C	H	N	O	S	0	0
			2549	821	1276	207	242	3		

- Molecule 12 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	f	83	Total	C	H	N	O	S	0	0
			1411	456	718	120	114	3		

- Molecule 13 is a protein called ATP synthase subunit g, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	g	79	Total	C	H	N	O	S	0	0
			1291	420	662	100	108	1		

- Molecule 14 is a protein called ATP synthase subunit ATP5MPL, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	j	48	Total	C	H	N	O	S	0	0
			828	267	428	66	65	2		

- Molecule 15 is a protein called ATP synthase F(0) complex subunit B1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	b	209	Total	C	H	N	O	S	0	0
			3456	1095	1755	292	308	6		

- Molecule 16 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	h	62	Total	C	H	N	O	S	0	0
			1009	326	495	87	99	2		

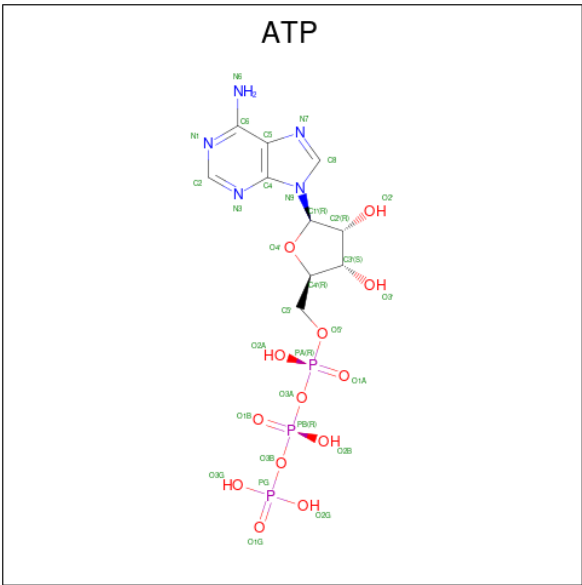
- Molecule 17 is a protein called ATP synthase membrane subunit DAPIT, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	k	36	Total	C	H	N	O	S	0	0
			596	192	307	47	48	2		

- Molecule 18 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	e	56	Total	C	H	N	O	S	0	0
			951	295	487	87	81	1		

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



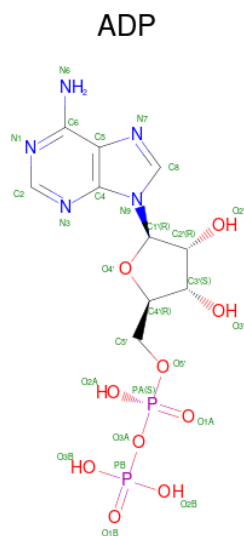
Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
19	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
19	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

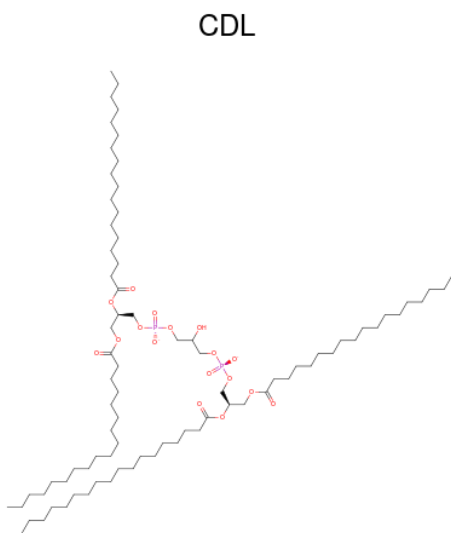
- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).





Mol	Chain	Residues	Atoms						AltConf
21	D	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
21	E	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
21	F	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula:  $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$ ).



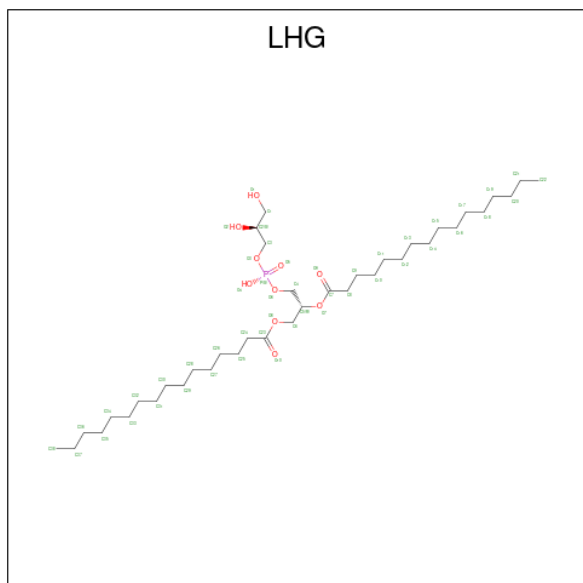
Mol	Chain	Residues	Atoms					AltConf
22	f	1	Total	C	H	O	P	0
			185	65	101	17	2	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	H	O	P	0
			171	59	93	17	2	
22	b	1	Total	C	H	O	P	0
			190	64	107	17	2	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms					AltConf
23	f	1	Total	C	H	O	P	0
			87	28	48	10	1	
23	f	1	Total	C	H	O	P	0
			123	38	74	10	1	

- Molecule 24 is water.

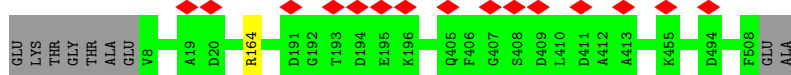
Mol	Chain	Residues	Atoms		AltConf
24	A	3	Total	O	0
			3	3	
24	B	3	Total	O	0
			3	3	
24	C	3	Total	O	0
			3	3	
24	D	4	Total	O	0
			4	4	
24	F	4	Total	O	0
			4	4	

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

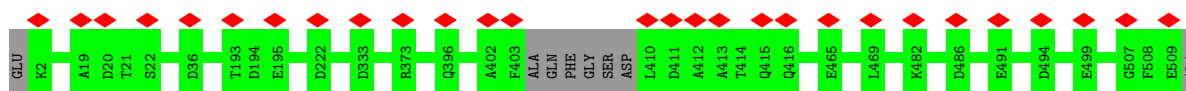
- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain A:  98%



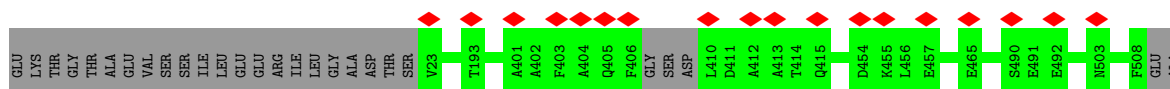
- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain B:  98%



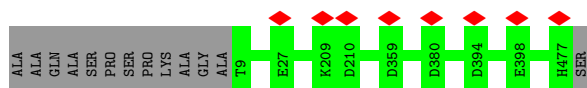
- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain C:  95%



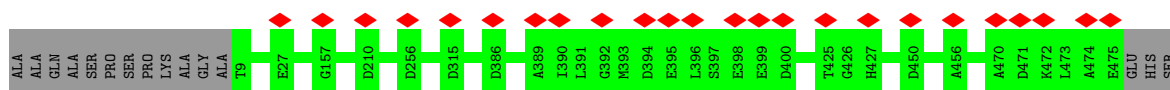
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain D:  97%

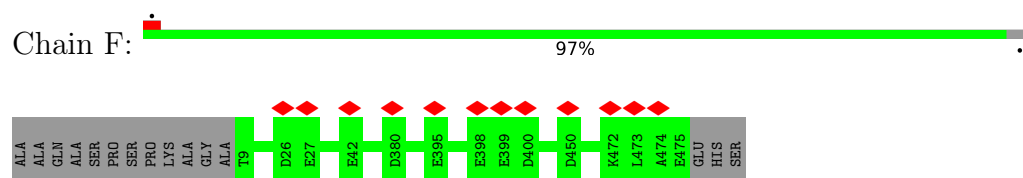


- Molecule 2: ATP synthase subunit beta, mitochondrial

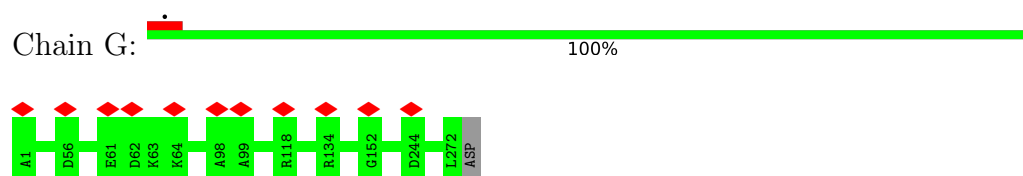
Chain E:  97%



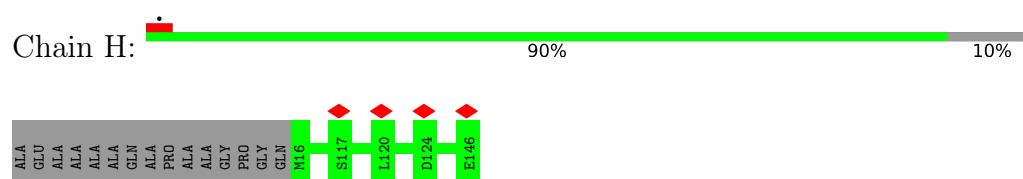
- Molecule 2: ATP synthase subunit beta, mitochondrial



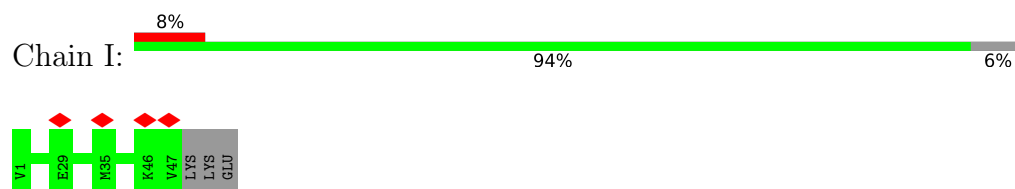
- Molecule 3: ATP synthase subunit gamma, mitochondrial



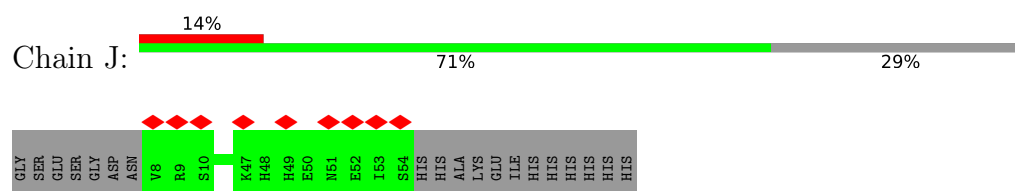
- Molecule 4: ATP synthase subunit delta, mitochondrial



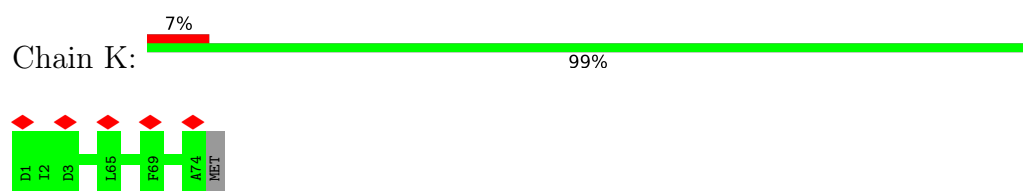
- Molecule 5: ATP synthase subunit epsilon, mitochondrial



- Molecule 6: ATPase inhibitor, mitochondrial



- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial



- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial





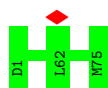
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial

Chain M: 100%

There are no outlier residues recorded for this chain.

- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial

Chain N: 100%



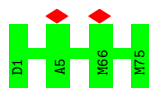
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial

Chain P: 96%



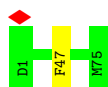
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial

Chain R: 100%



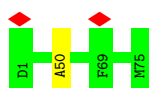
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial

Chain O: 99%



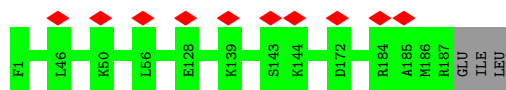
- Molecule 7: ATP synthase F(0) complex subunit C2, mitochondrial

Chain Q: 99%

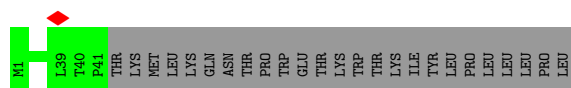


- Molecule 8: ATP synthase subunit O, mitochondrial

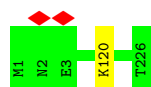
Chain S: 5%



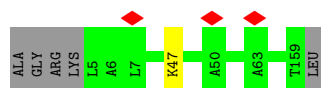
- Molecule 9: ATP synthase protein 8



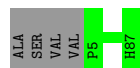
- Molecule 10: ATP synthase subunit a



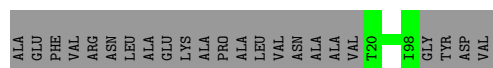
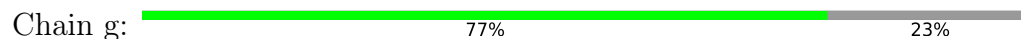
- Molecule 11: ATP synthase subunit d, mitochondrial



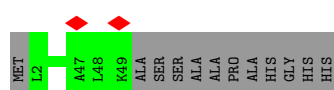
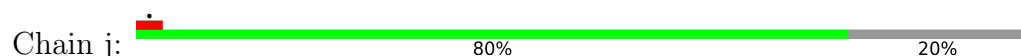
- Molecule 12: ATP synthase subunit f, mitochondrial



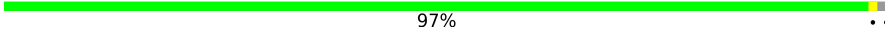
- Molecule 13: ATP synthase subunit g, mitochondrial

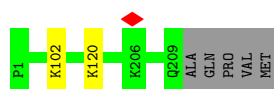


- Molecule 14: ATP synthase subunit ATP5MPL, mitochondrial




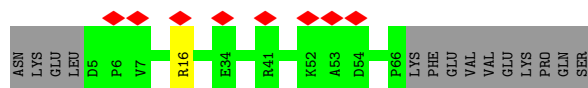
- Molecule 15: ATP synthase F(0) complex subunit B1, mitochondrial

Chain b:  97% ..



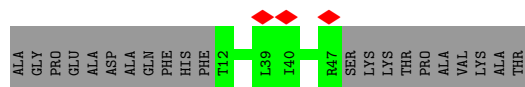
- Molecule 16: ATP synthase-coupling factor 6, mitochondrial

Chain h:  11% 80% 18%




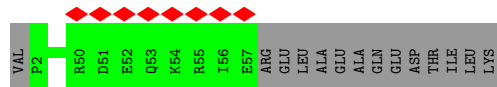
- Molecule 17: ATP synthase membrane subunit DAPIT, mitochondrial

Chain k:  5% 63% 37%



- Molecule 18: ATP synthase subunit e, mitochondrial

Chain e:  11% 80% 20%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61458	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	4.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	45.029	Depositor
Minimum map value	-26.424	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.103	Depositor
Recommended contour level	7.92	Depositor
Map size (Å)	524.0, 524.0, 524.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor



## 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: LHG, ADP, CDL, MG, ATP, M3L

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	0.40	0/3869	0.47	0/5220
1	B	0.41	0/3874	0.47	0/5225
1	C	0.41	0/3740	0.47	0/5044
2	D	0.41	0/3616	0.47	0/4906
2	E	0.39	0/3596	0.47	0/4879
2	F	0.41	0/3596	0.47	0/4879
3	G	0.38	0/2141	0.46	0/2876
4	H	0.41	0/982	0.51	0/1337
5	I	0.44	0/374	0.49	0/501
6	J	0.38	0/374	0.48	0/495
7	K	0.44	0/526	0.50	0/711
7	L	0.43	0/526	0.51	0/711
7	M	0.42	0/534	0.53	0/721
7	N	0.36	0/534	0.53	0/721
7	O	0.46	0/534	0.62	0/721
7	P	0.64	1/526 (0.2%)	0.65	0/711
7	Q	0.38	0/534	0.66	1/721 (0.1%)
7	R	0.44	0/534	0.53	0/721
8	S	0.32	0/1455	0.45	0/1957
9	8	0.50	0/355	0.53	0/483
10	a	0.39	0/1779	0.50	0/2433
11	d	0.31	0/1304	0.42	0/1768
12	f	0.43	0/711	0.45	0/952
13	g	0.32	0/646	0.51	0/879
14	j	0.33	0/410	0.42	0/552
15	b	0.33	0/1733	0.44	0/2334
16	h	0.33	0/526	0.49	0/707
17	k	0.29	0/294	0.41	0/395
18	e	0.35	0/472	0.52	0/628
All	All	0.40	1/40095 (0.0%)	0.48	1/54188 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	47	PHE	C-O	-8.79	1.06	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	50	ALA	N-CA-CB	5.72	118.11	110.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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 PDB entries followed by that with respect to all EM entries.

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	499/510 (98%)	450 (90%)	49 (10%)	0	100	100
1	B	498/510 (98%)	453 (91%)	45 (9%)	0	100	100
1	C	479/510 (94%)	423 (88%)	56 (12%)	0	100	100
2	D	467/482 (97%)	430 (92%)	37 (8%)	0	100	100
2	E	465/482 (96%)	423 (91%)	42 (9%)	0	100	100
2	F	465/482 (96%)	420 (90%)	45 (10%)	0	100	100
3	G	270/273 (99%)	255 (94%)	15 (6%)	0	100	100
4	H	129/146 (88%)	115 (89%)	14 (11%)	0	100	100
5	I	45/50 (90%)	45 (100%)	0	0	100	100
6	J	45/66 (68%)	41 (91%)	4 (9%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	K	71/75 (95%)	66 (93%)	5 (7%)	0	100	100
7	L	71/75 (95%)	70 (99%)	1 (1%)	0	100	100
7	M	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
7	N	72/75 (96%)	67 (93%)	5 (7%)	0	100	100
7	O	72/75 (96%)	70 (97%)	2 (3%)	0	100	100
7	P	71/75 (95%)	67 (94%)	3 (4%)	1 (1%)	9	40
7	Q	72/75 (96%)	69 (96%)	3 (4%)	0	100	100
7	R	72/75 (96%)	66 (92%)	6 (8%)	0	100	100
8	S	185/190 (97%)	173 (94%)	12 (6%)	0	100	100
9	8	39/66 (59%)	33 (85%)	6 (15%)	0	100	100
10	a	224/226 (99%)	195 (87%)	29 (13%)	0	100	100
11	d	153/160 (96%)	136 (89%)	17 (11%)	0	100	100
12	f	81/87 (93%)	71 (88%)	10 (12%)	0	100	100
13	g	77/102 (76%)	70 (91%)	7 (9%)	0	100	100
14	j	46/60 (77%)	44 (96%)	2 (4%)	0	100	100
15	b	207/214 (97%)	197 (95%)	10 (5%)	0	100	100
16	h	60/76 (79%)	53 (88%)	7 (12%)	0	100	100
17	k	34/57 (60%)	34 (100%)	0	0	100	100
18	e	54/70 (77%)	53 (98%)	1 (2%)	0	100	100
All	All	5095/5419 (94%)	4655 (91%)	439 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	P	44	GLN

### 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 PDB entries followed by that with respect to all EM entries.

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	406/412 (98%)	405 (100%)	1 (0%)	92	93
1	B	407/412 (99%)	407 (100%)	0	100	100
1	C	391/412 (95%)	391 (100%)	0	100	100
2	D	379/386 (98%)	379 (100%)	0	100	100
2	E	377/386 (98%)	377 (100%)	0	100	100
2	F	377/386 (98%)	377 (100%)	0	100	100
3	G	230/231 (100%)	230 (100%)	0	100	100
4	H	104/109 (95%)	104 (100%)	0	100	100
5	I	38/41 (93%)	38 (100%)	0	100	100
6	J	34/50 (68%)	34 (100%)	0	100	100
7	K	49/50 (98%)	49 (100%)	0	100	100
7	L	49/50 (98%)	49 (100%)	0	100	100
7	M	50/50 (100%)	50 (100%)	0	100	100
7	N	50/50 (100%)	50 (100%)	0	100	100
7	O	50/50 (100%)	49 (98%)	1 (2%)	50	68
7	P	49/50 (98%)	49 (100%)	0	100	100
7	Q	50/50 (100%)	50 (100%)	0	100	100
7	R	50/50 (100%)	50 (100%)	0	100	100
8	S	162/165 (98%)	162 (100%)	0	100	100
9	8	41/66 (62%)	41 (100%)	0	100	100
10	a	200/200 (100%)	199 (100%)	1 (0%)	86	89
11	d	139/142 (98%)	138 (99%)	1 (1%)	81	86
12	f	72/75 (96%)	72 (100%)	0	100	100
13	g	67/83 (81%)	67 (100%)	0	100	100
14	j	42/49 (86%)	42 (100%)	0	100	100
15	b	186/190 (98%)	184 (99%)	2 (1%)	70	80
16	h	56/70 (80%)	55 (98%)	1 (2%)	54	71
17	k	31/46 (67%)	31 (100%)	0	100	100
18	e	47/59 (80%)	47 (100%)	0	100	100
All	All	4183/4370 (96%)	4176 (100%)	7 (0%)	91	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
7	O	47	PHE
10	a	120	LYS
11	d	47	LYS
15	b	102	LYS
15	b	120	LYS
16	h	16	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
7	N	44	GLN
8	S	112	HIS
9	8	35	HIS
9	8	36	ASN
13	g	57	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	M3L	Q	43	7	10,11,12	0.50	0	9,14,16	0.50	0
7	M3L	N	43	7	10,11,12	0.40	0	9,14,16	0.55	0
7	M3L	R	43	7	10,11,12	0.48	0	9,14,16	0.62	0
7	M3L	O	43	7	10,11,12	0.38	0	9,14,16	0.65	0
7	M3L	P	43	7	10,11,12	0.45	0	9,14,16	0.45	0
7	M3L	M	43	7	10,11,12	0.55	0	9,14,16	0.48	0
7	M3L	L	43	7	10,11,12	0.45	0	9,14,16	0.74	0
7	M3L	K	43	7	10,11,12	0.48	0	9,14,16	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	M3L	Q	43	7	-	1/9/10/12	-
7	M3L	N	43	7	-	1/9/10/12	-
7	M3L	R	43	7	-	1/9/10/12	-
7	M3L	O	43	7	-	3/9/10/12	-
7	M3L	P	43	7	-	1/9/10/12	-
7	M3L	M	43	7	-	2/9/10/12	-
7	M3L	L	43	7	-	1/9/10/12	-
7	M3L	K	43	7	-	1/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	43	M3L	N-CA-CB-CG
7	O	43	M3L	N-CA-CB-CG
7	O	43	M3L	O-C-CA-CB
7	R	43	M3L	CG-CD-CE-NZ
7	L	43	M3L	CG-CD-CE-NZ
7	K	43	M3L	CE-CD-CG-CB
7	O	43	M3L	CE-CD-CG-CB
7	N	43	M3L	CG-CD-CE-NZ
7	P	43	M3L	CE-CD-CG-CB
7	M	43	M3L	C-CA-CB-CG
7	Q	43	M3L	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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
22	CDL	b	302	-	82,82,99	0.98	6 (7%)	88,94,111	1.16	5 (5%)
22	CDL	f	101	-	83,83,99	0.98	7 (8%)	89,95,111	1.11	4 (4%)
22	CDL	b	301	-	77,77,99	1.00	6 (7%)	83,89,111	1.12	4 (4%)
21	ADP	F	600	20	24,29,29	0.93	1 (4%)	29,45,45	1.57	4 (13%)
23	LHG	f	102	-	38,38,48	0.70	1 (2%)	41,44,54	1.32	5 (12%)
21	ADP	E	600	-	24,29,29	0.94	1 (4%)	29,45,45	1.55	4 (13%)
23	LHG	f	103	-	48,48,48	0.62	1 (2%)	51,54,54	1.22	4 (7%)
21	ADP	D	600	20	24,29,29	0.95	1 (4%)	29,45,45	1.61	4 (13%)
19	ATP	C	600	20	26,33,33	0.93	1 (3%)	31,52,52	1.62	5 (16%)
19	ATP	B	600	20	26,33,33	0.91	1 (3%)	31,52,52	1.61	4 (12%)
19	ATP	A	600	20	26,33,33	0.90	1 (3%)	31,52,52	1.72	5 (16%)

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
22	CDL	b	302	-	-	34/93/93/110	-
22	CDL	f	101	-	-	41/94/94/110	-
22	CDL	b	301	-	-	41/88/88/110	-
21	ADP	F	600	20	-	5/12/32/32	0/3/3/3
23	LHG	f	102	-	-	14/43/43/53	-
21	ADP	E	600	-	-	5/12/32/32	0/3/3/3
23	LHG	f	103	-	-	17/53/53/53	-
21	ADP	D	600	20	-	2/12/32/32	0/3/3/3
19	ATP	C	600	20	-	4/18/38/38	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ATP	B	600	20	-	1/18/38/38	0/3/3/3
19	ATP	A	600	20	-	0/18/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	301	CDL	OA6-CA4	-2.76	1.39	1.46
22	b	302	CDL	OA6-CA4	-2.75	1.39	1.46
22	f	101	CDL	OB8-CB7	2.70	1.41	1.33
22	f	101	CDL	OA6-CA4	-2.67	1.39	1.46
22	f	101	CDL	OB6-CB4	-2.64	1.40	1.46
22	b	302	CDL	OB8-CB7	2.62	1.41	1.33
22	b	301	CDL	OB8-CB7	2.61	1.41	1.33
22	b	302	CDL	OB6-CB4	-2.54	1.40	1.46
22	b	301	CDL	OB6-CB4	-2.50	1.40	1.46
22	b	301	CDL	OB6-CB5	2.44	1.41	1.34
22	b	302	CDL	OA8-CA7	2.36	1.40	1.33
22	b	302	CDL	OB6-CB5	2.34	1.40	1.34
23	f	102	LHG	O7-C5	-2.32	1.40	1.46
22	f	101	CDL	OB6-CB5	2.32	1.40	1.34
22	f	101	CDL	OA8-CA7	2.30	1.40	1.33
21	E	600	ADP	C5-C4	2.26	1.46	1.40
22	b	301	CDL	OA8-CA6	-2.25	1.40	1.45
22	f	101	CDL	OA8-CA6	-2.25	1.40	1.45
23	f	103	LHG	O7-C5	-2.21	1.41	1.46
22	b	301	CDL	OA8-CA7	2.19	1.39	1.33
21	D	600	ADP	C5-C4	2.13	1.46	1.40
22	b	302	CDL	OA8-CA6	-2.10	1.40	1.45
21	F	600	ADP	C5-C4	2.09	1.46	1.40
22	f	101	CDL	OA6-CA5	2.08	1.40	1.34
19	C	600	ATP	C5-C4	2.08	1.46	1.40
19	A	600	ATP	C5-C4	2.06	1.46	1.40
19	B	600	ATP	C5-C4	2.06	1.46	1.40

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	600	ATP	PB-O3B-PG	-4.64	116.89	132.83
19	A	600	ATP	PB-O3B-PG	-4.45	117.57	132.83
23	f	102	LHG	O4-P-O5	4.31	133.57	112.24
23	f	103	LHG	O4-P-O5	4.23	133.16	112.24
22	b	302	CDL	OA6-CA5-C11	4.20	120.56	111.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	600	ATP	PB-O3B-PG	-4.16	118.53	132.83
22	b	302	CDL	OB6-CB5-C51	4.11	120.35	111.50
21	D	600	ADP	PA-O3A-PB	-4.08	118.82	132.83
22	b	301	CDL	OB6-CB5-C51	4.00	120.12	111.50
22	f	101	CDL	OA6-CA5-C11	3.98	120.09	111.50
19	A	600	ATP	PA-O3A-PB	-3.97	119.21	132.83
19	B	600	ATP	PA-O3A-PB	-3.94	119.32	132.83
22	f	101	CDL	OB6-CB5-C51	3.93	119.97	111.50
22	b	301	CDL	OA6-CA5-C11	3.88	119.86	111.50
21	D	600	ADP	C3'-C2'-C1'	3.81	106.71	100.98
19	A	600	ATP	N3-C2-N1	-3.81	122.73	128.68
21	E	600	ADP	PA-O3A-PB	-3.74	119.99	132.83
19	B	600	ATP	N3-C2-N1	-3.71	122.89	128.68
21	F	600	ADP	C3'-C2'-C1'	3.68	106.52	100.98
21	F	600	ADP	PA-O3A-PB	-3.67	120.23	132.83
21	E	600	ADP	N3-C2-N1	-3.63	123.01	128.68
21	F	600	ADP	N3-C2-N1	-3.60	123.06	128.68
21	D	600	ADP	N3-C2-N1	-3.56	123.11	128.68
21	E	600	ADP	C3'-C2'-C1'	3.54	106.31	100.98
19	C	600	ATP	N3-C2-N1	-3.48	123.24	128.68
19	A	600	ATP	C3'-C2'-C1'	3.23	105.84	100.98
19	C	600	ATP	C3'-C2'-C1'	3.02	105.53	100.98
19	C	600	ATP	PA-O3A-PB	-2.85	123.03	132.83
21	E	600	ADP	C4-C5-N7	-2.79	106.50	109.40
21	F	600	ADP	C4-C5-N7	-2.77	106.51	109.40
22	b	302	CDL	OA8-CA7-C31	2.74	120.52	111.91
22	b	302	CDL	OB8-CB7-C71	2.69	120.36	111.91
23	f	103	LHG	O8-C23-C24	2.66	120.27	111.91
21	D	600	ADP	C4-C5-N7	-2.66	106.63	109.40
22	f	101	CDL	OA8-CA7-C31	2.60	120.08	111.91
23	f	102	LHG	O8-C23-C24	2.59	120.05	111.91
22	b	301	CDL	OA8-CA7-C31	2.57	119.96	111.91
23	f	102	LHG	C11-C10-C9	-2.51	101.67	114.42
19	C	600	ATP	C4-C5-N7	-2.46	106.84	109.40
22	f	101	CDL	OB8-CB7-C71	2.44	119.56	111.91
22	b	301	CDL	OB8-CB7-C71	2.40	119.44	111.91
19	B	600	ATP	C4-C5-N7	-2.36	106.94	109.40
23	f	103	LHG	C11-C10-C9	-2.31	102.71	114.42
22	b	302	CDL	CA4-OA6-CA5	-2.19	112.40	117.79
19	A	600	ATP	C4-C5-N7	-2.18	107.13	109.40
23	f	102	LHG	C27-C26-C25	-2.16	103.46	114.42
23	f	102	LHG	C18-C17-C16	-2.09	103.82	114.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	f	103	LHG	C20-C19-C18	-2.03	104.10	114.42

There are no chirality outliers.

All (164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	C	600	ATP	C5'-O5'-PA-O1A
21	D	600	ADP	C5'-O5'-PA-O3A
21	E	600	ADP	PB-O3A-PA-O5'
21	E	600	ADP	C5'-O5'-PA-O1A
21	F	600	ADP	C5'-O5'-PA-O1A
21	F	600	ADP	C5'-O5'-PA-O2A
21	F	600	ADP	O4'-C4'-C5'-O5'
22	f	101	CDL	CB2-OB2-PB2-OB3
22	b	301	CDL	C11-CA5-OA6-CA4
22	b	301	CDL	CB2-OB2-PB2-OB3
22	b	301	CDL	CB2-OB2-PB2-OB4
22	b	301	CDL	CB3-OB5-PB2-OB3
22	b	301	CDL	OB5-CB3-CB4-OB6
22	b	301	CDL	C51-CB5-OB6-CB4
22	b	302	CDL	C1-CA2-OA2-PA1
22	b	302	CDL	CA2-OA2-PA1-OA3
22	b	302	CDL	CA2-OA2-PA1-OA4
22	b	302	CDL	CB2-OB2-PB2-OB3
22	b	302	CDL	CB2-OB2-PB2-OB4
22	b	302	CDL	CB3-OB5-PB2-OB2
22	b	302	CDL	CB3-OB5-PB2-OB3
22	b	302	CDL	CB3-OB5-PB2-OB4
23	f	102	LHG	C3-O3-P-O4
23	f	103	LHG	C1-C2-C3-O3
22	b	301	CDL	OA7-CA5-OA6-CA4
22	b	301	CDL	OB7-CB5-OB6-CB4
22	f	101	CDL	C31-CA7-OA8-CA6
22	b	301	CDL	O1-C1-CA2-OA2
23	f	103	LHG	O2-C2-C3-O3
22	f	101	CDL	C1-CB2-OB2-PB2
22	f	101	CDL	OA9-CA7-OA8-CA6
22	b	302	CDL	CA5-C11-C12-C13
23	f	103	LHG	C7-C8-C9-C10
21	F	600	ADP	C3'-C4'-C5'-O5'
22	b	301	CDL	C1-CA2-OA2-PA1
22	b	301	CDL	CB5-C51-C52-C53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	f	101	CDL	CA5-C11-C12-C13
22	f	101	CDL	CB5-C51-C52-C53
22	b	301	CDL	CA2-OA2-PA1-OA5
22	b	301	CDL	CB2-OB2-PB2-OB5
22	b	301	CDL	CB3-OB5-PB2-OB2
22	b	302	CDL	CA2-OA2-PA1-OA5
22	b	302	CDL	CB2-OB2-PB2-OB5
23	f	102	LHG	C3-O3-P-O6
22	b	301	CDL	CB2-C1-CA2-OA2
22	b	301	CDL	C19-C20-C21-C22
22	b	301	CDL	C21-C22-C23-C24
22	f	101	CDL	C75-C76-C77-C78
23	f	103	LHG	C28-C29-C30-C31
22	b	302	CDL	CB4-CB3-OB5-PB2
23	f	102	LHG	C7-C8-C9-C10
22	b	301	CDL	C40-C41-C42-C43
23	f	102	LHG	O1-C1-C2-C3
23	f	103	LHG	O1-C1-C2-C3
22	b	302	CDL	C11-CA5-OA6-CA4
22	f	101	CDL	C71-C72-C73-C74
22	b	301	CDL	C37-C38-C39-C40
22	b	302	CDL	C60-C61-C62-C63
22	b	302	CDL	C13-C14-C15-C16
22	f	101	CDL	C73-C74-C75-C76
22	b	302	CDL	OA7-CA5-OA6-CA4
22	b	302	CDL	C73-C74-C75-C76
22	b	302	CDL	C54-C55-C56-C57
23	f	102	LHG	C13-C14-C15-C16
23	f	103	LHG	C31-C32-C33-C34
23	f	103	LHG	C5-C4-O6-P
22	f	101	CDL	C54-C55-C56-C57
22	f	101	CDL	OB5-CB3-CB4-CB6
22	b	301	CDL	C71-C72-C73-C74
22	b	302	CDL	C71-C72-C73-C74
22	f	101	CDL	C12-C13-C14-C15
22	f	101	CDL	CA7-C31-C32-C33
23	f	102	LHG	C27-C28-C29-C30
22	b	301	CDL	C17-C18-C19-C20
22	b	302	CDL	OB6-CB4-CB6-OB8
22	f	101	CDL	C71-CB7-OB8-CB6
22	b	301	CDL	OB5-CB3-CB4-CB6
23	f	103	LHG	C14-C15-C16-C17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	b	302	CDL	C11-C12-C13-C14
23	f	102	LHG	C4-C5-C6-O8
22	f	101	CDL	C13-C14-C15-C16
22	b	302	CDL	C16-C17-C18-C19
22	f	101	CDL	C74-C75-C76-C77
22	b	302	CDL	C53-C54-C55-C56
22	f	101	CDL	OB9-CB7-OB8-CB6
23	f	103	LHG	O6-C4-C5-C6
23	f	103	LHG	C15-C16-C17-C18
23	f	103	LHG	C13-C14-C15-C16
23	f	103	LHG	O6-C4-C5-O7
22	f	101	CDL	C52-C53-C54-C55
19	C	600	ATP	C5'-O5'-PA-O3A
21	E	600	ADP	C5'-O5'-PA-O3A
21	F	600	ADP	C5'-O5'-PA-O3A
22	f	101	CDL	OB7-CB5-OB6-CB4
22	b	302	CDL	C51-C52-C53-C54
22	f	101	CDL	CA2-OA2-PA1-OA5
23	f	102	LHG	C2-C3-O3-P
19	C	600	ATP	C5'-O5'-PA-O2A
21	D	600	ADP	C5'-O5'-PA-O1A
22	f	101	CDL	CA3-OA5-PA1-OA3
22	b	301	CDL	CA2-OA2-PA1-OA3
22	b	301	CDL	CA2-OA2-PA1-OA4
22	b	301	CDL	CA3-OA5-PA1-OA4
22	f	101	CDL	C56-C57-C58-C59
22	f	101	CDL	C77-C78-C79-C80
22	f	101	CDL	OB5-CB3-CB4-OB6
22	b	302	CDL	OB5-CB3-CB4-OB6
22	f	101	CDL	C51-CB5-OB6-CB4
23	f	102	LHG	O7-C5-C6-O8
23	f	102	LHG	O1-C1-C2-O2
22	b	301	CDL	C73-C74-C75-C76
23	f	103	LHG	C32-C33-C34-C35
23	f	103	LHG	O10-C23-O8-C6
23	f	103	LHG	C11-C12-C13-C14
22	b	301	CDL	C13-C14-C15-C16
22	f	101	CDL	CB3-OB5-PB2-OB2
22	b	302	CDL	CA3-OA5-PA1-OA2
22	b	301	CDL	C72-C73-C74-C75
22	b	301	CDL	CA3-CA4-CA6-OA8
22	b	302	CDL	CB3-CB4-CB6-OB8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
22	b	301	CDL	C52-C53-C54-C55
22	f	101	CDL	CA4-CA3-OA5-PA1
22	b	301	CDL	C1-CB2-OB2-PB2
22	f	101	CDL	C1-CA2-OA2-PA1
22	b	301	CDL	CA5-C11-C12-C13
22	f	101	CDL	C39-C40-C41-C42
19	C	600	ATP	PB-O3B-PG-O1G
22	f	101	CDL	CA4-CA6-OA8-CA7
23	f	103	LHG	C34-C35-C36-C37
22	b	302	CDL	OB5-CB3-CB4-CB6
22	f	101	CDL	C14-C15-C16-C17
22	b	301	CDL	C31-CA7-OA8-CA6
22	f	101	CDL	C53-C54-C55-C56
22	f	101	CDL	C31-C32-C33-C34
22	b	301	CDL	OA9-CA7-OA8-CA6
22	b	301	CDL	CB3-CB4-CB6-OB8
22	f	101	CDL	C60-C61-C62-C63
22	f	101	CDL	C76-C77-C78-C79
22	b	302	CDL	C12-C11-CA5-OA6
23	f	102	LHG	C16-C17-C18-C19
22	b	302	CDL	C59-C60-C61-C62
22	f	101	CDL	CB2-OB2-PB2-OB5
22	b	301	CDL	C31-C32-C33-C34
22	f	101	CDL	OA7-CA5-OA6-CA4
22	f	101	CDL	C16-C17-C18-C19
23	f	102	LHG	C10-C11-C12-C13
21	E	600	ADP	O4'-C4'-C5'-O5'
19	B	600	ATP	C5'-O5'-PA-O3A
22	f	101	CDL	C11-C12-C13-C14
22	b	302	CDL	C33-C34-C35-C36
22	b	301	CDL	C53-C54-C55-C56
22	b	301	CDL	CA2-C1-CB2-OB2
23	f	102	LHG	C1-C2-C3-O3
23	f	102	LHG	C24-C25-C26-C27
22	b	301	CDL	CA4-CA3-OA5-PA1
21	E	600	ADP	C5'-O5'-PA-O2A
23	f	103	LHG	C29-C30-C31-C32
22	b	301	CDL	CB4-CB6-OB8-CB7
22	b	302	CDL	CB6-CB4-OB6-CB5
22	f	101	CDL	C12-C11-CA5-OA6
22	f	101	CDL	C12-C11-CA5-OA7
22	b	302	CDL	C72-C71-CB7-OB8

*Continued on next page...*

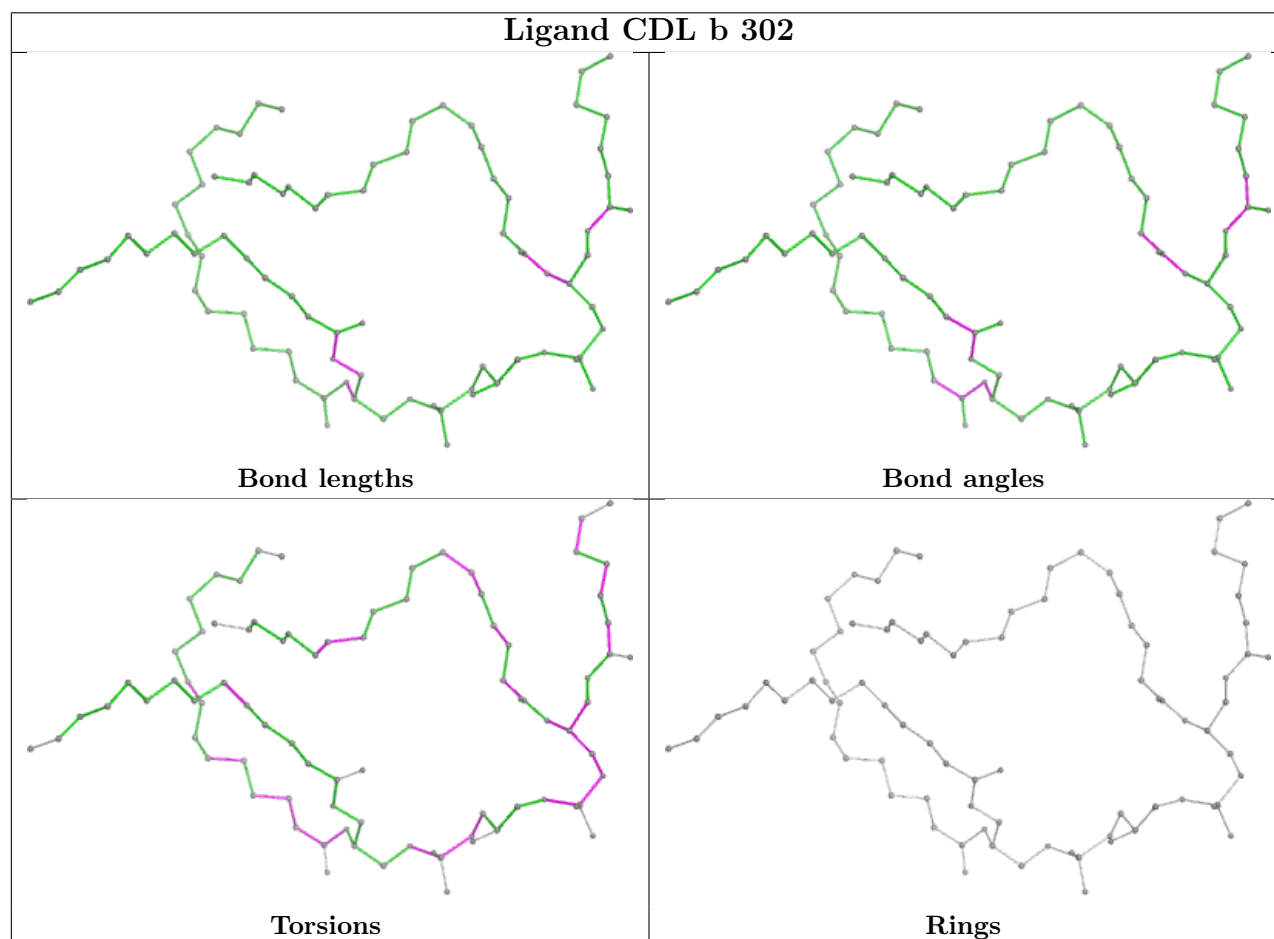
*Continued from previous page...*

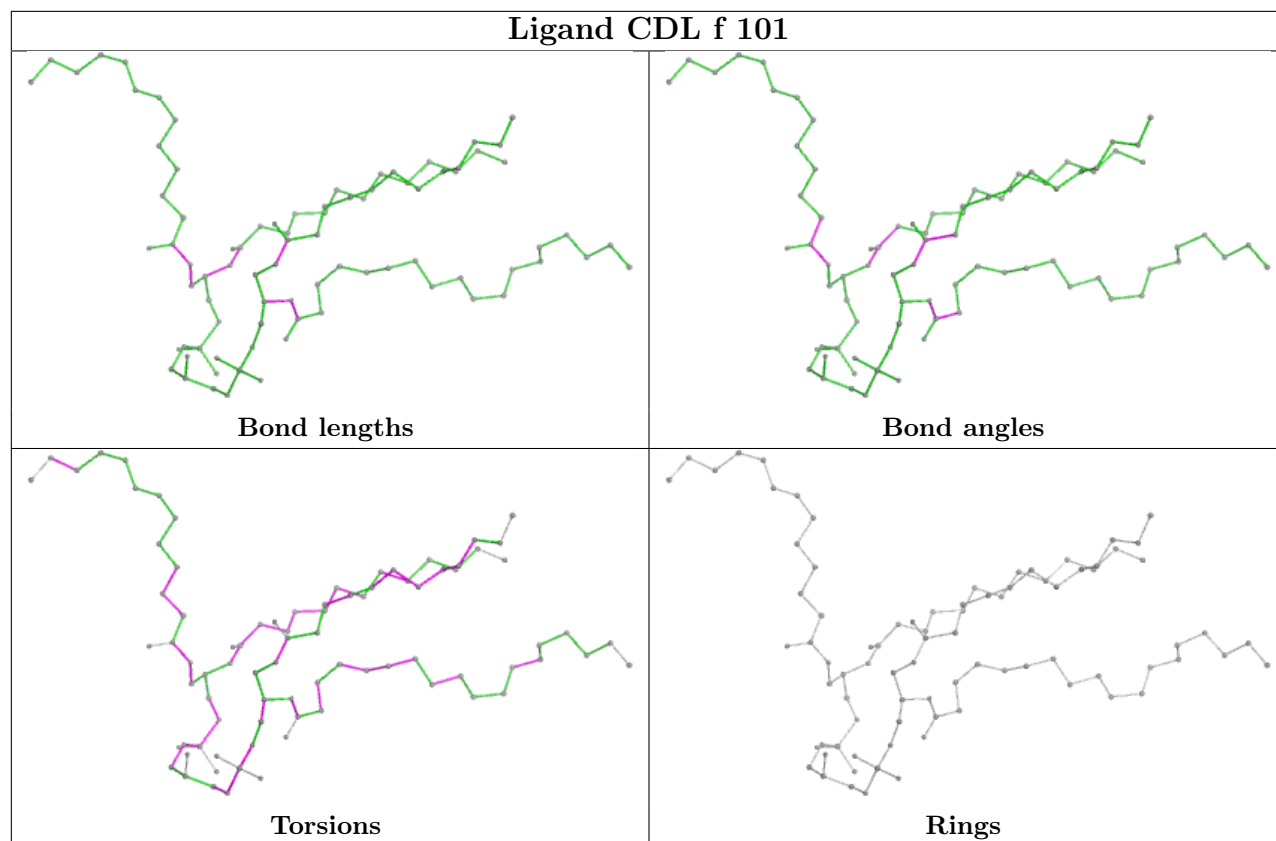
Mol	Chain	Res	Type	Atoms
22	b	301	CDL	C35-C36-C37-C38
22	b	302	CDL	C52-C51-CB5-OB6

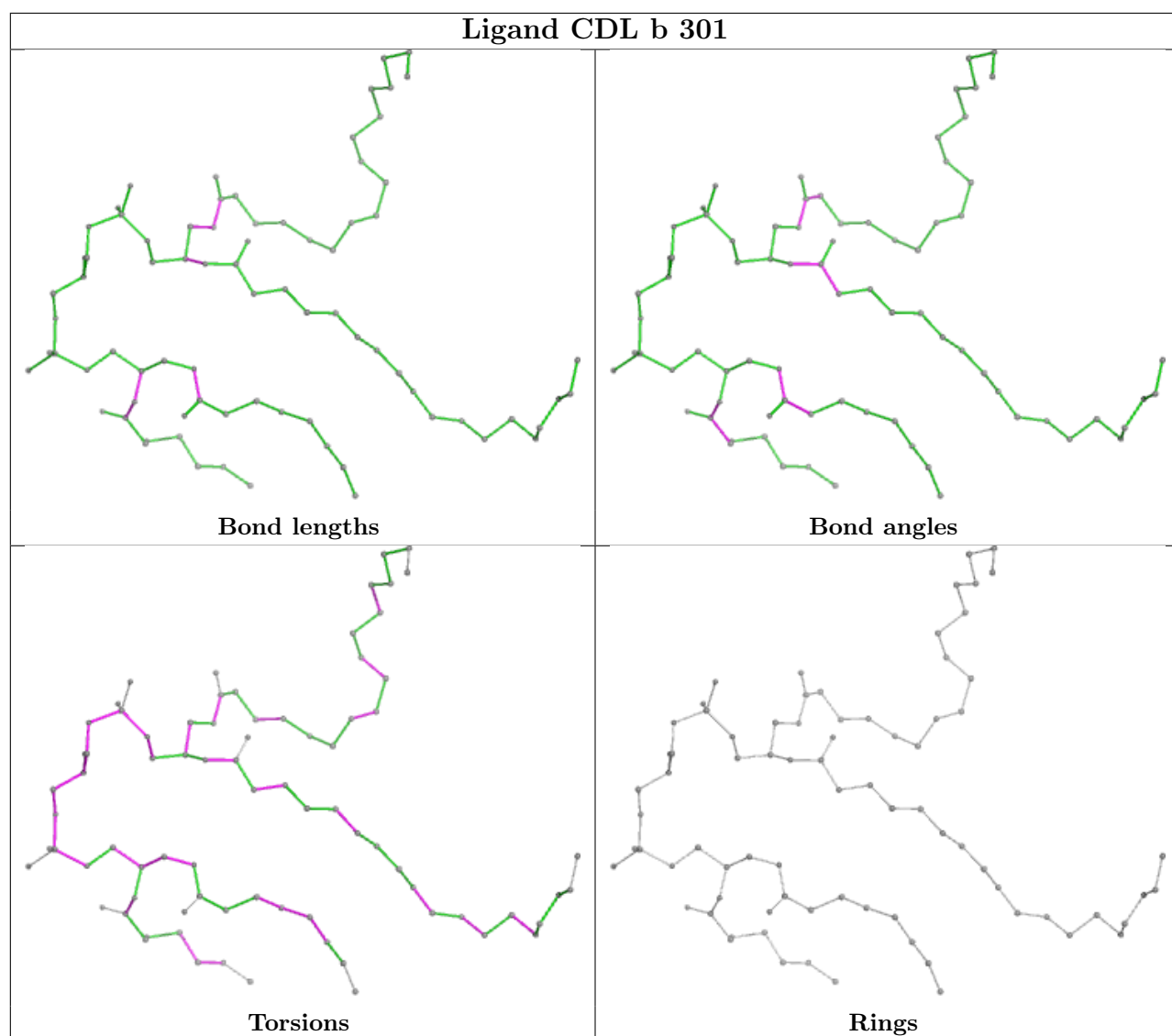
There are no ring outliers.

No monomer is involved in short contacts.

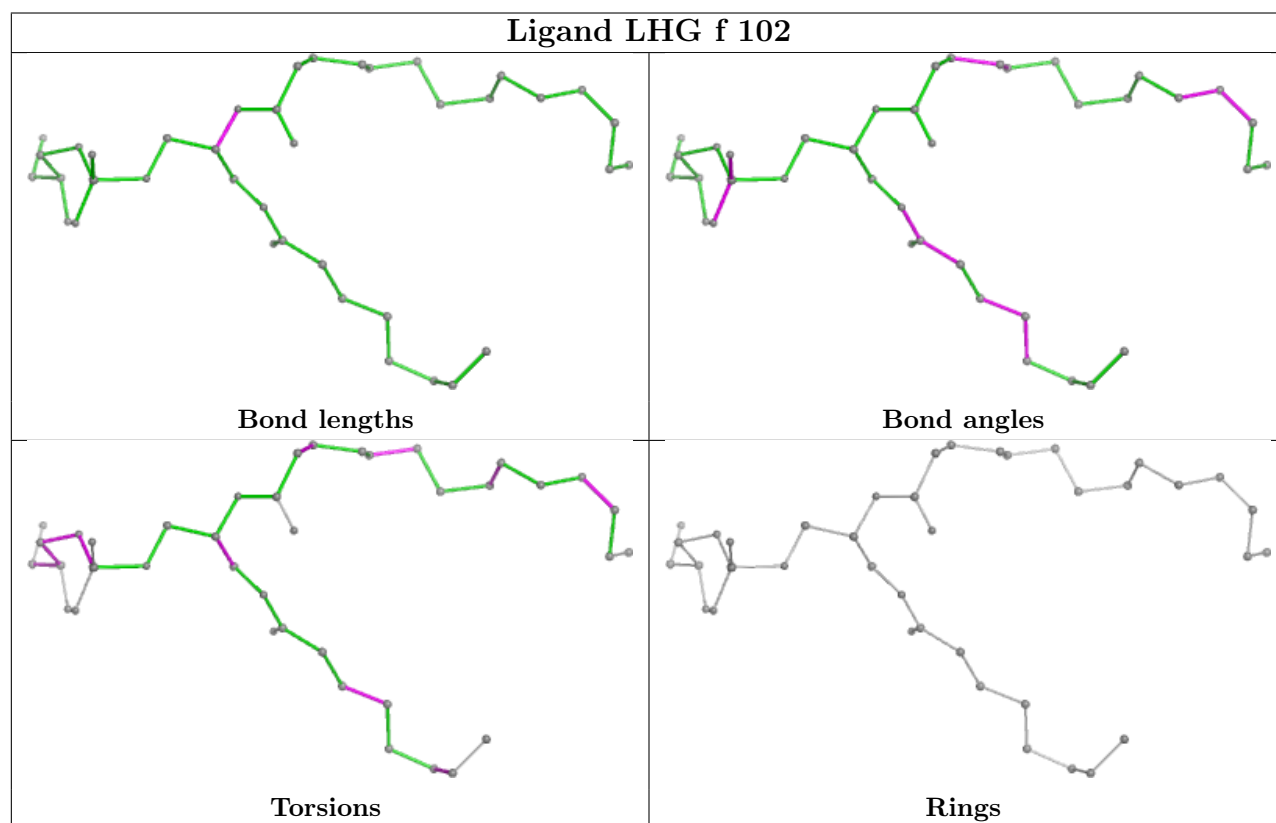
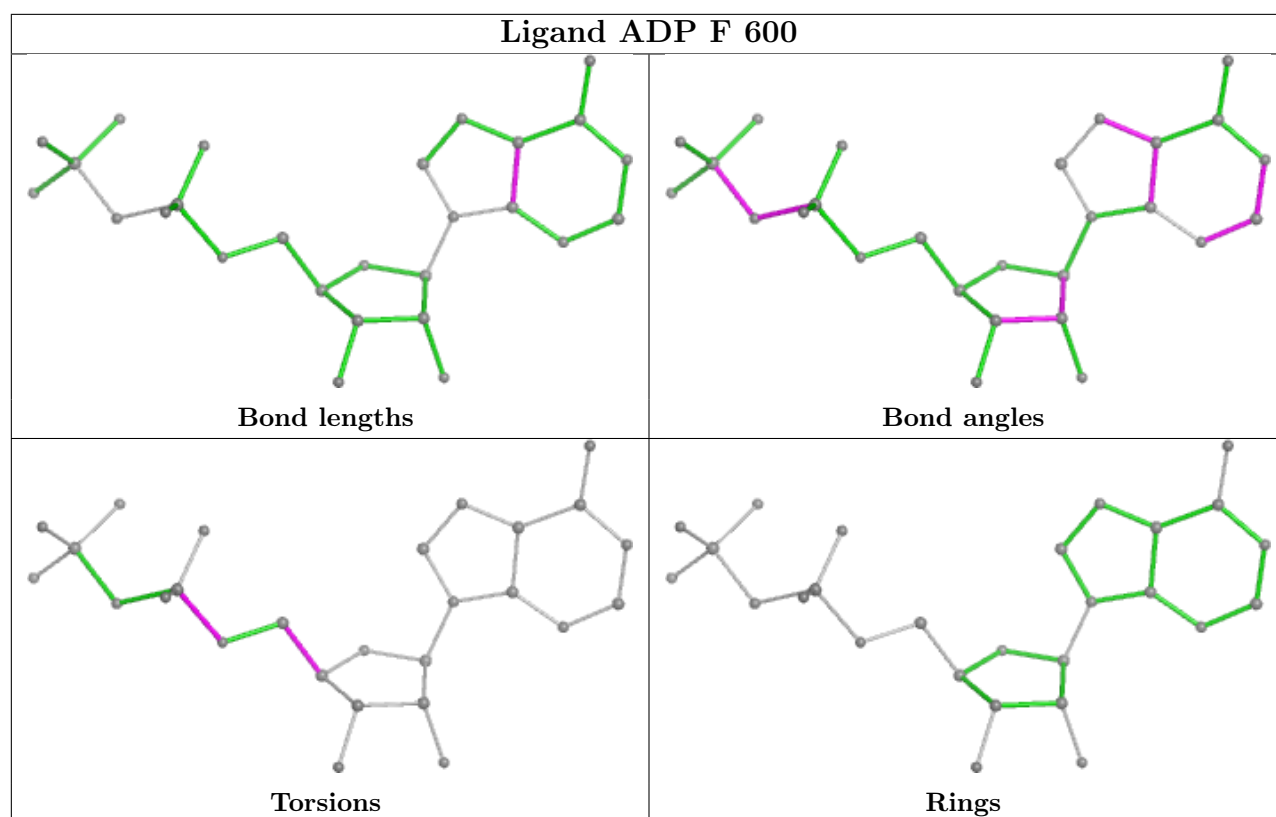
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

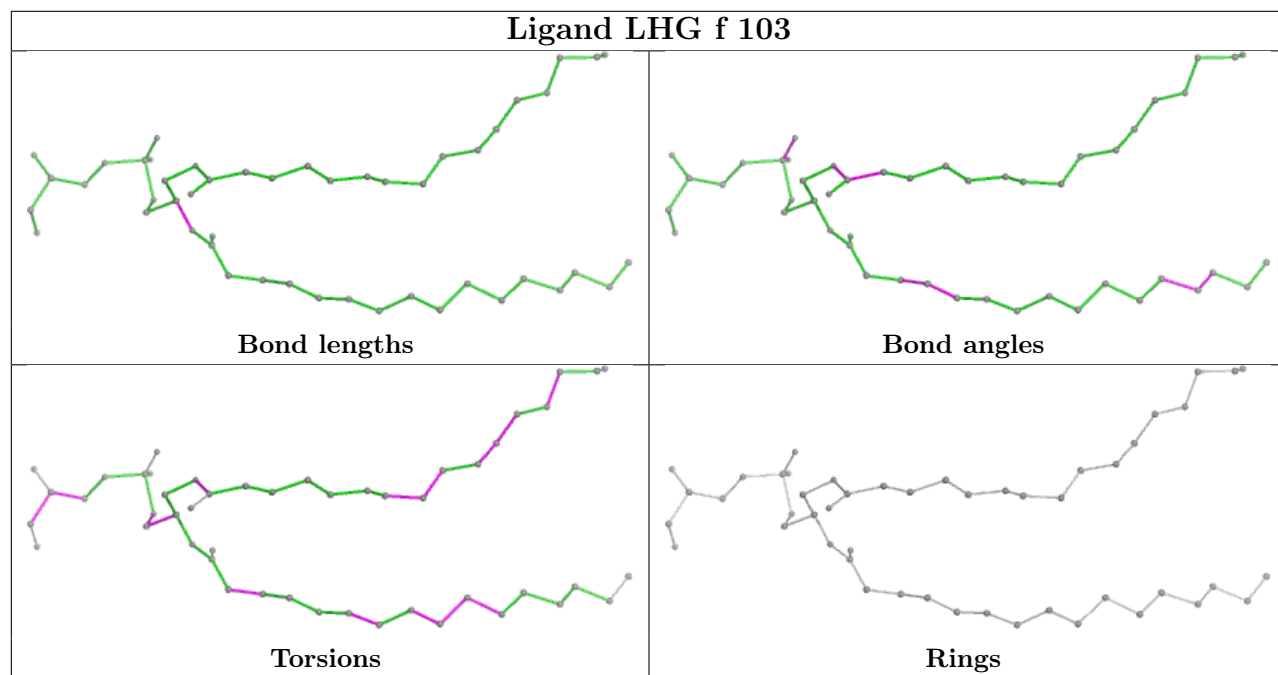
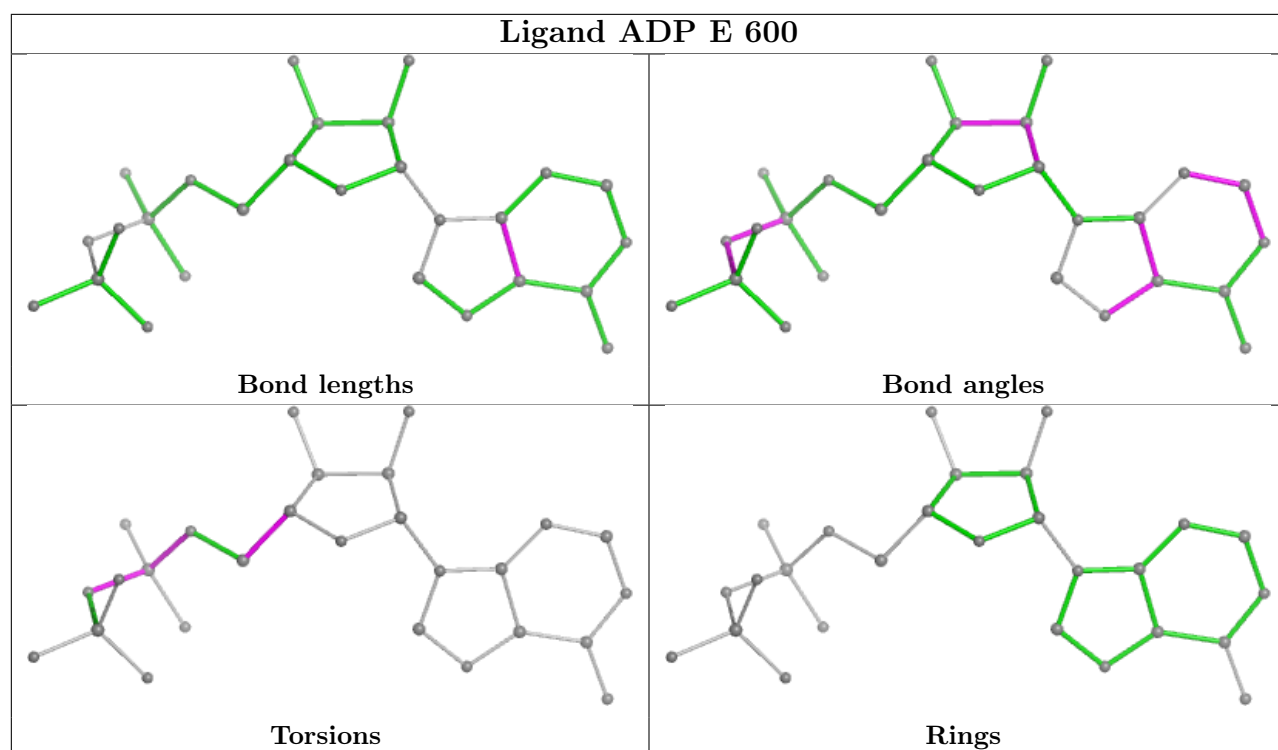


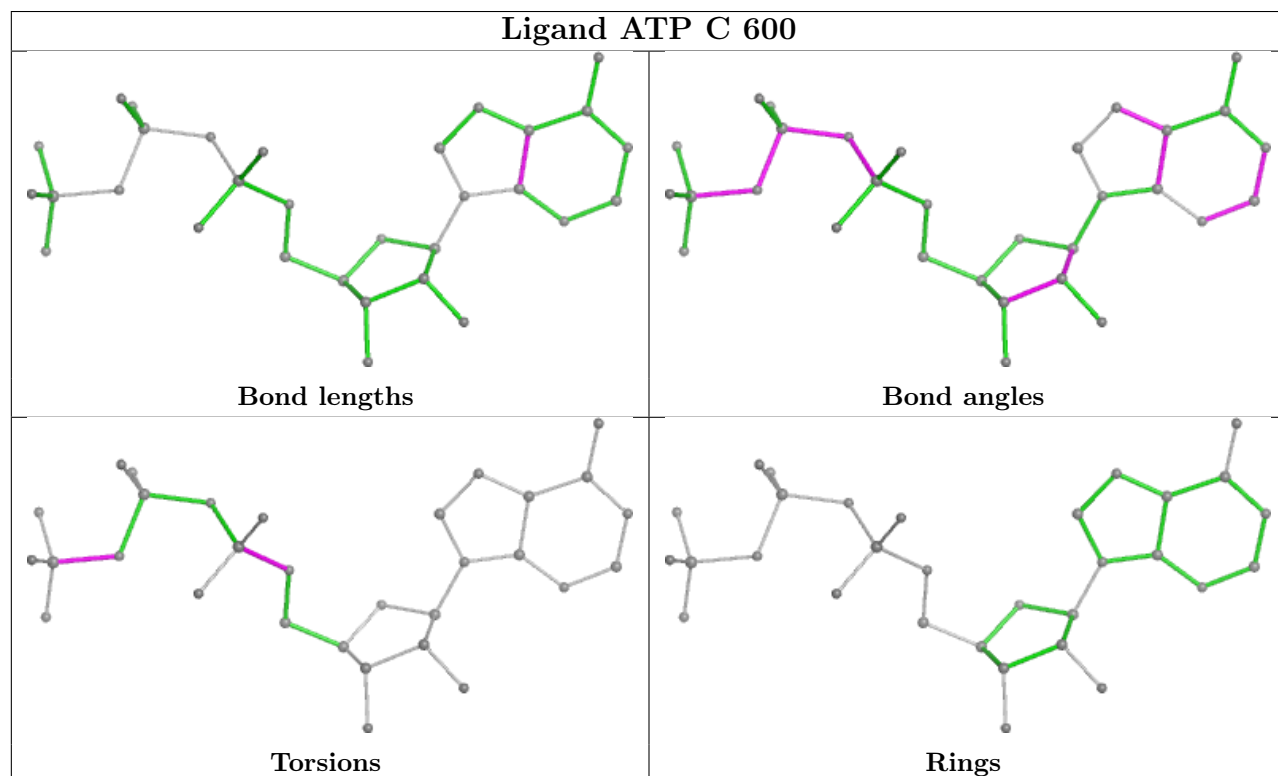
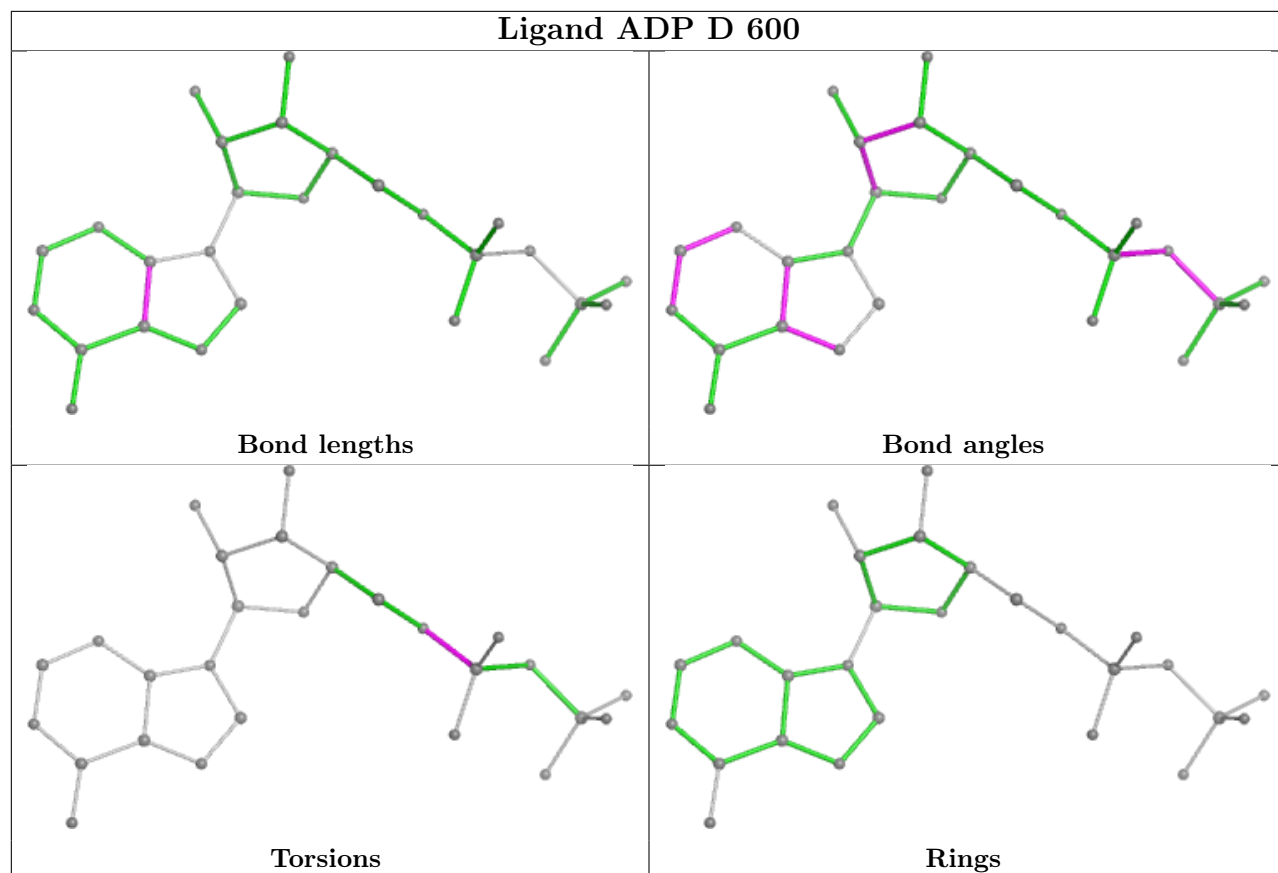


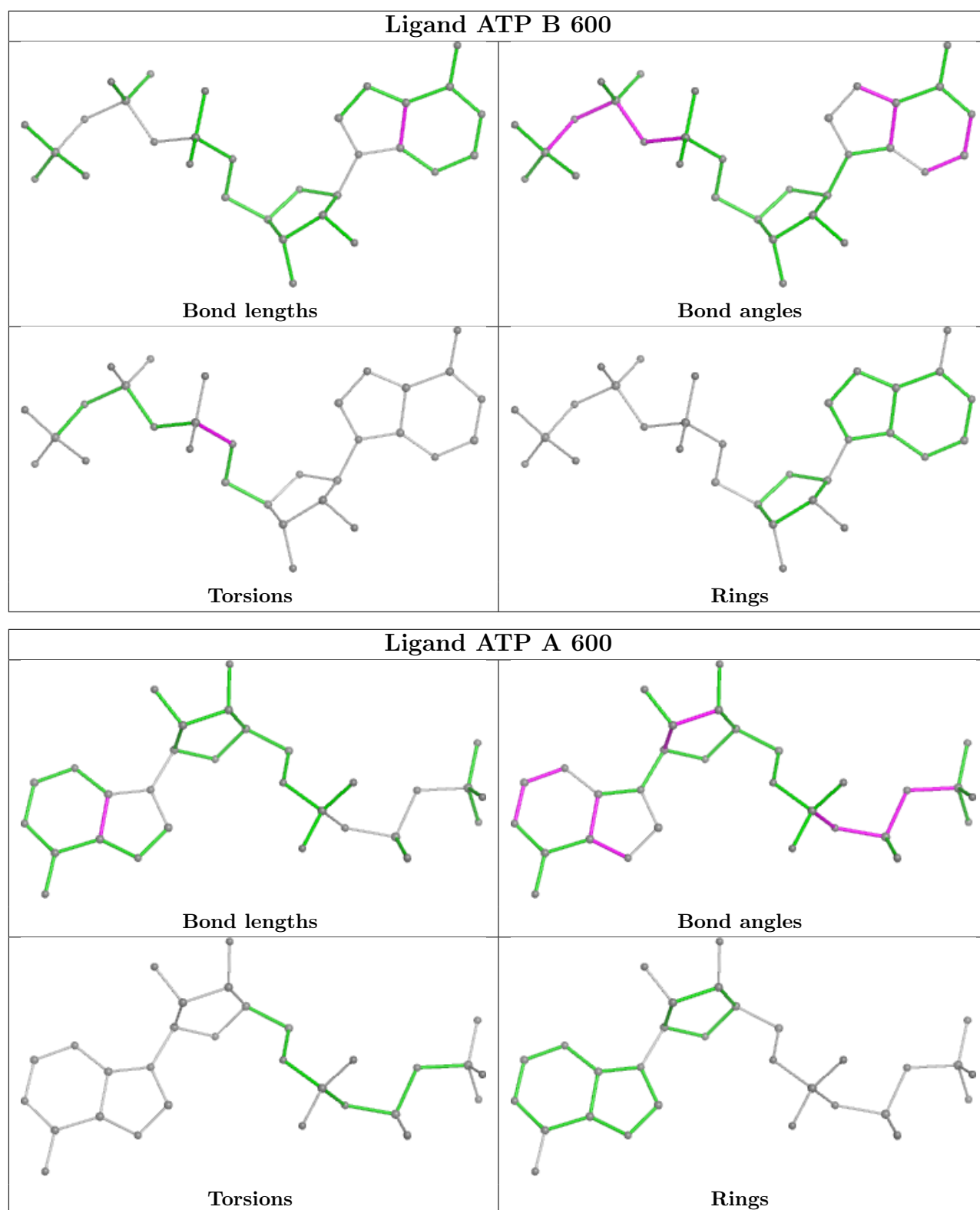












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

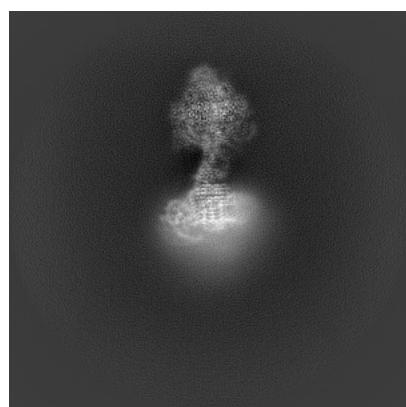
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11369. These allow visual inspection of the internal detail of the map and identification of artifacts.

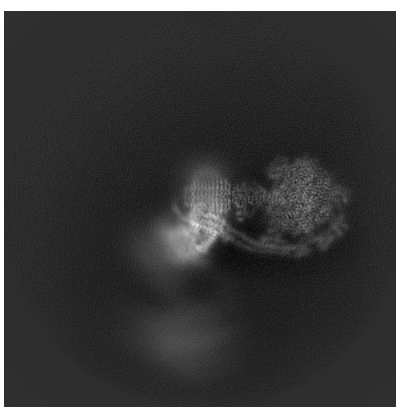
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

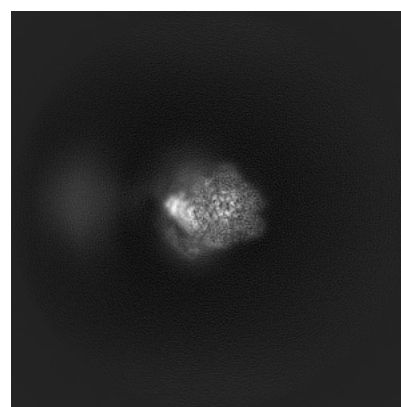
#### 6.1.1 Primary map



X



Y

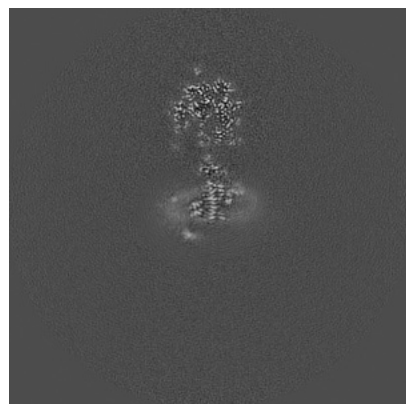


Z

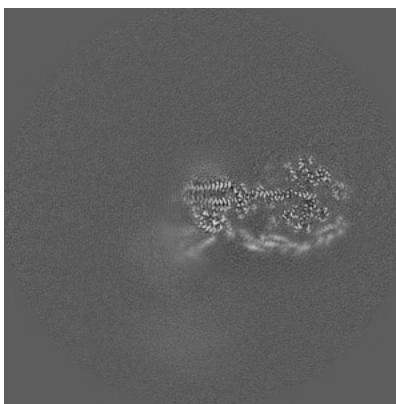
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

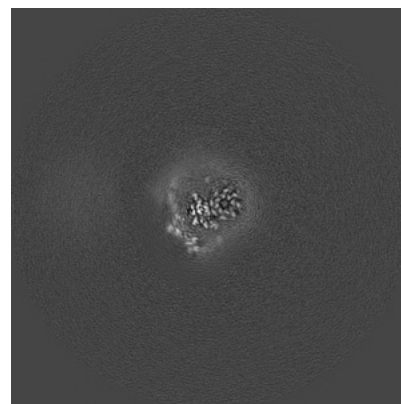
#### 6.2.1 Primary map



X Index: 250



Y Index: 250

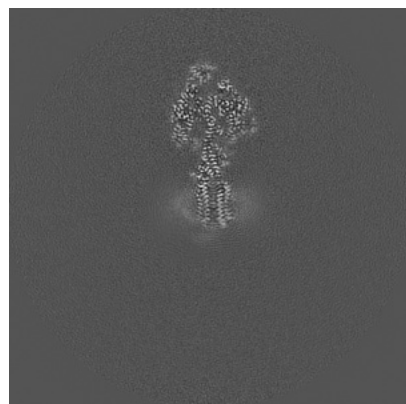


Z Index: 250

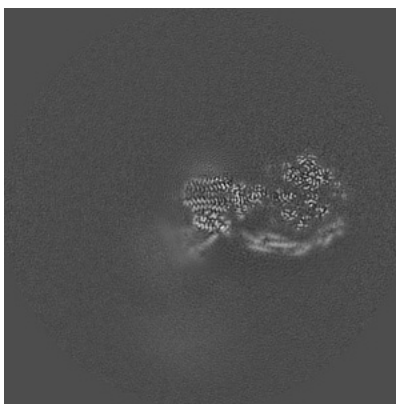
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

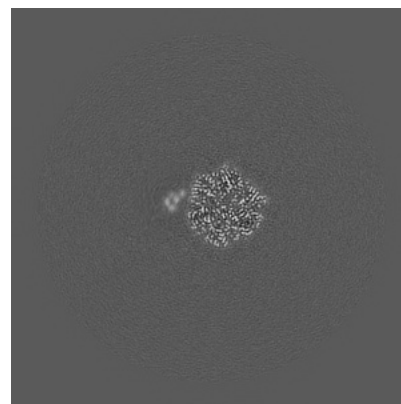
### 6.3.1 Primary map



X Index: 264



Y Index: 253

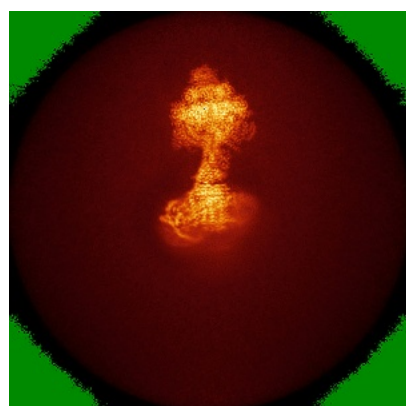


Z Index: 375

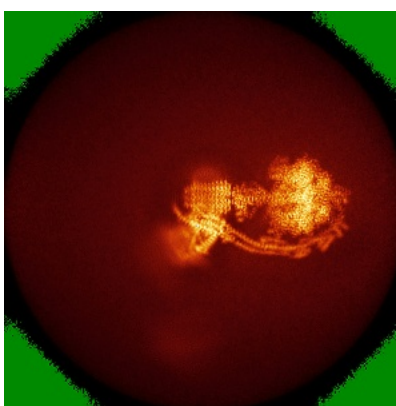
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

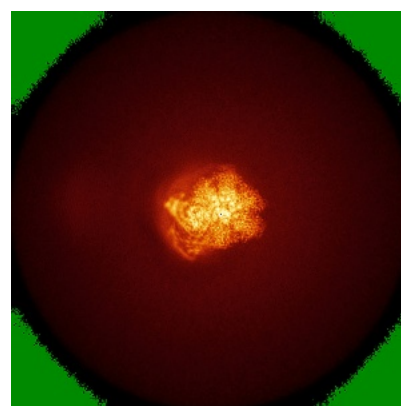
### 6.4.1 Primary map



X



Y



Z

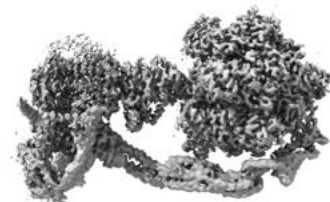
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

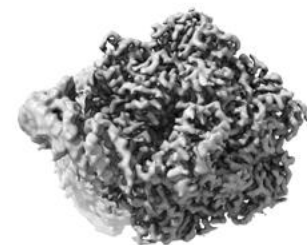
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.92. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

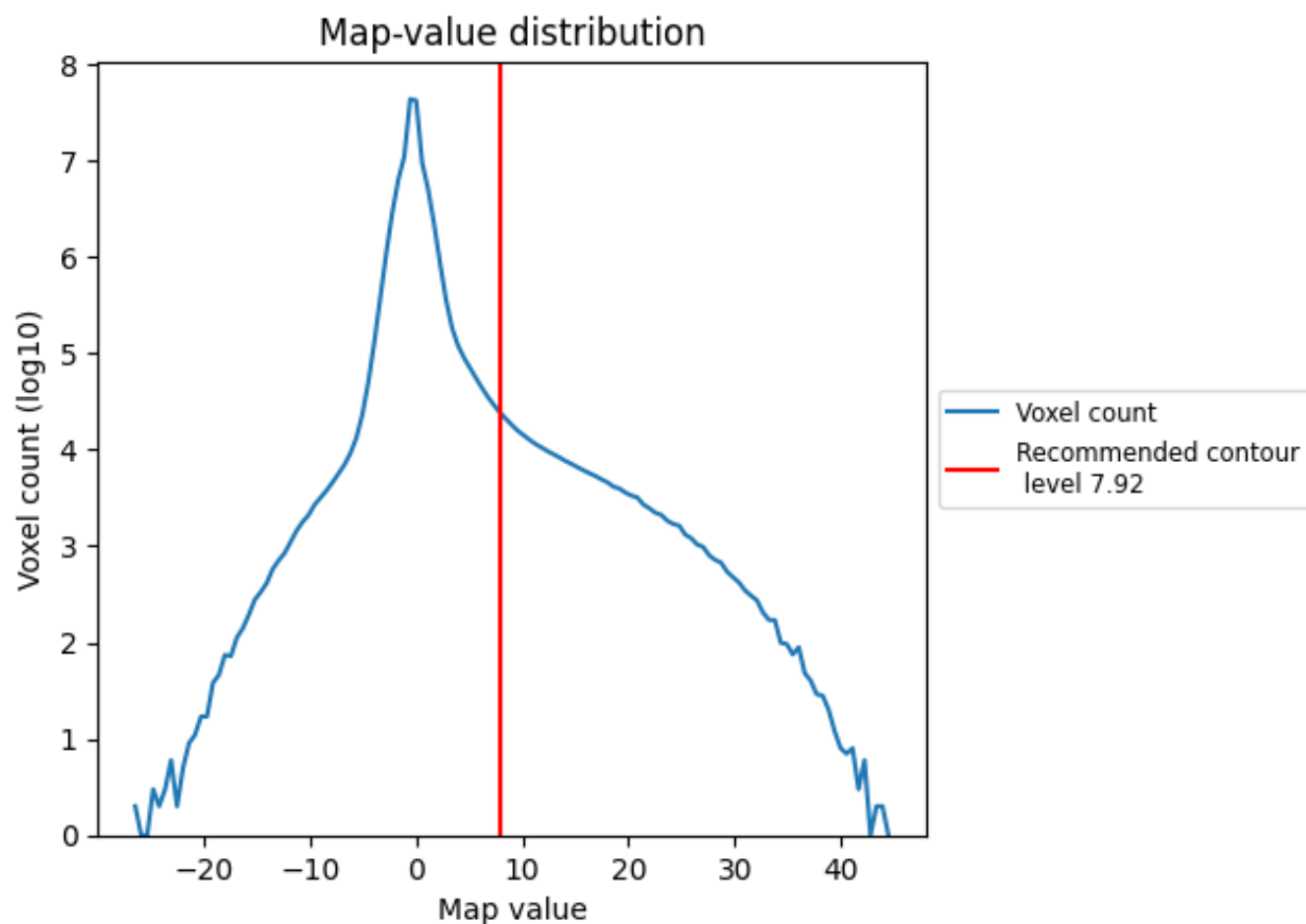
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

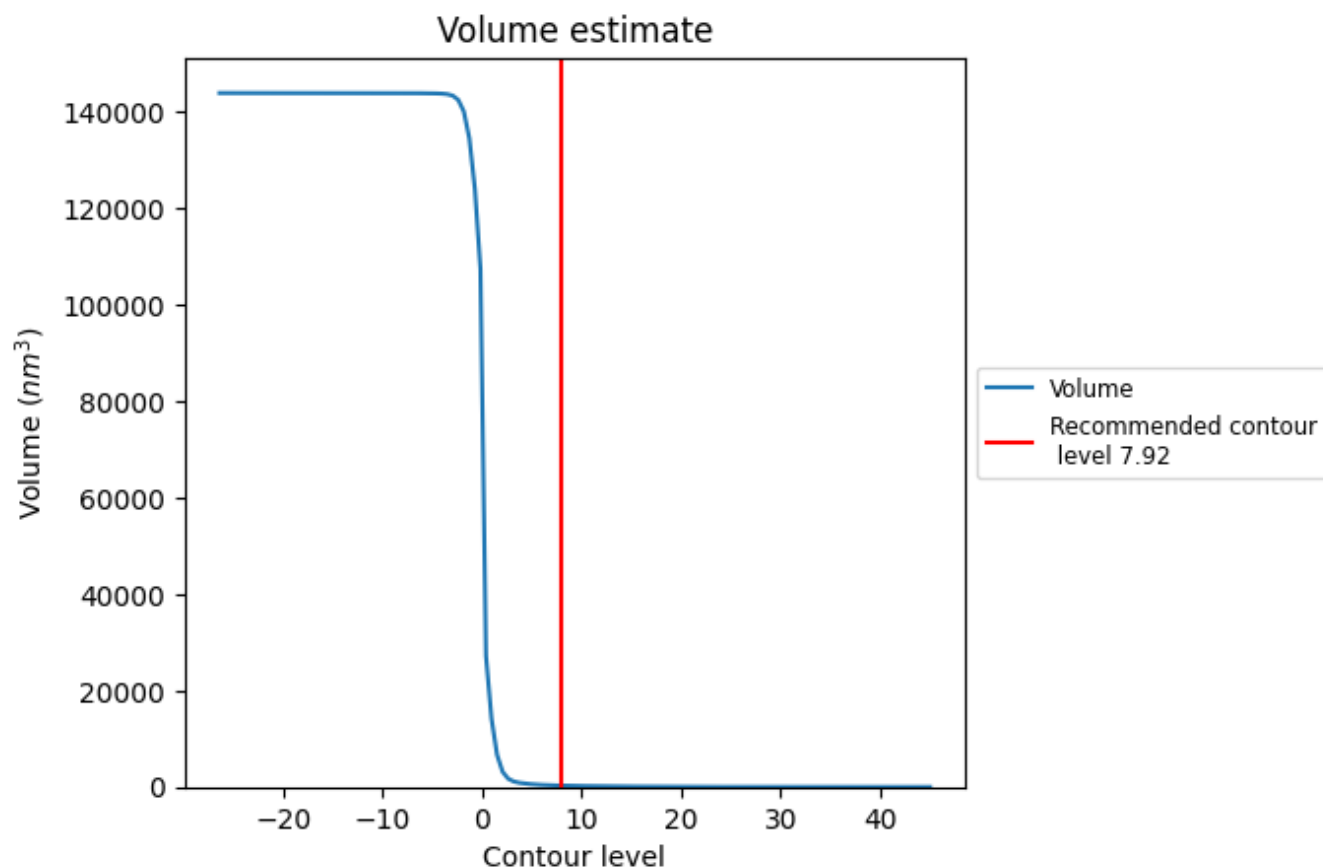
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

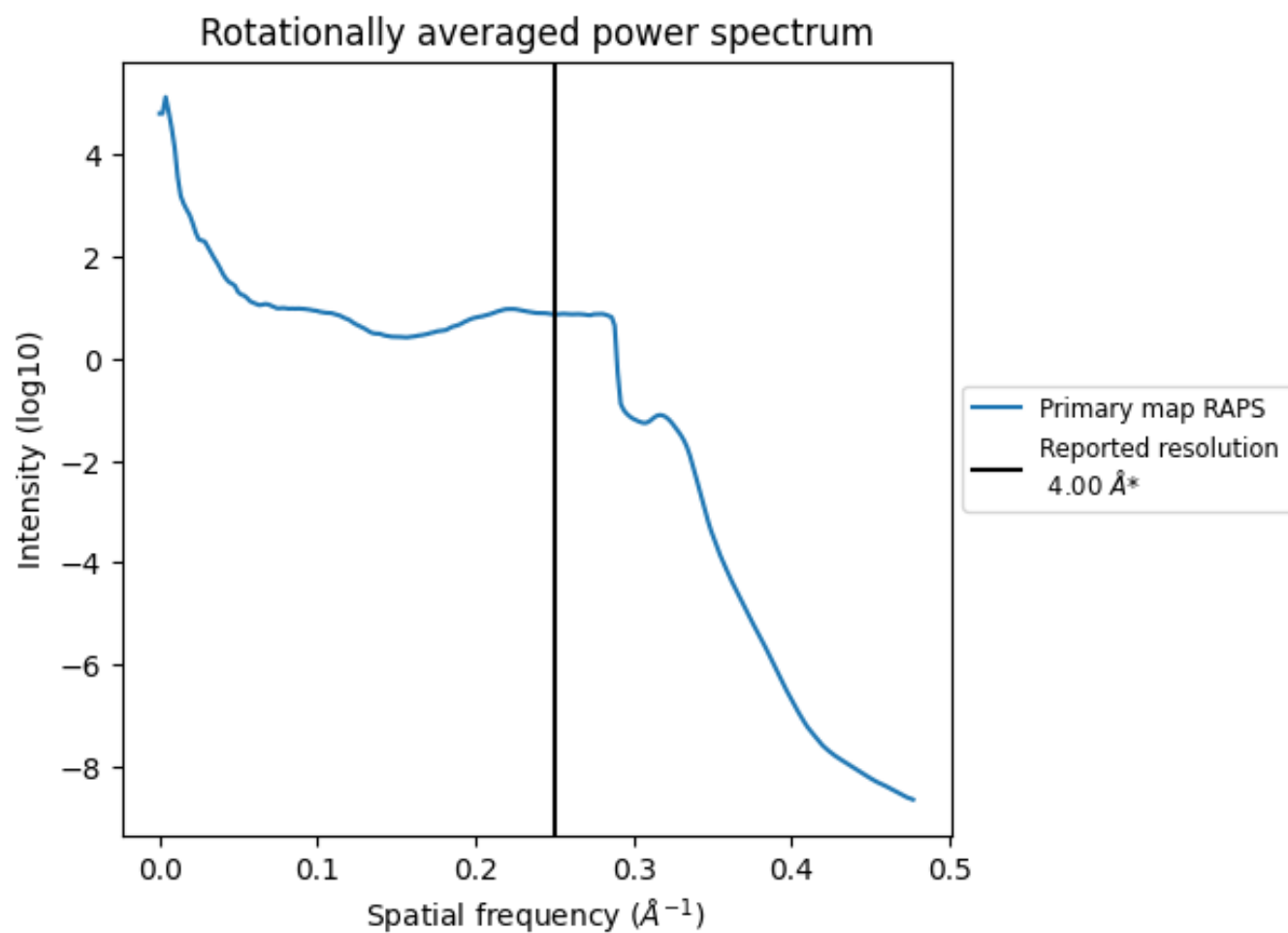
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 281 nm<sup>3</sup>; this corresponds to an approximate mass of 254 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

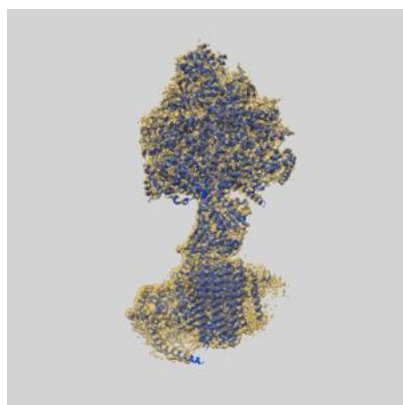
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

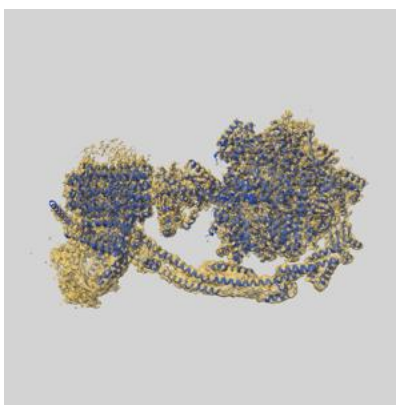
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11369 and PDB model 6ZQN. Per-residue inclusion information can be found in section 3 on page 11.

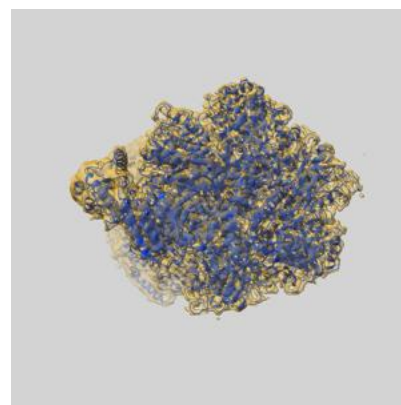
### 9.1 Map-model overlay [i](#)



X



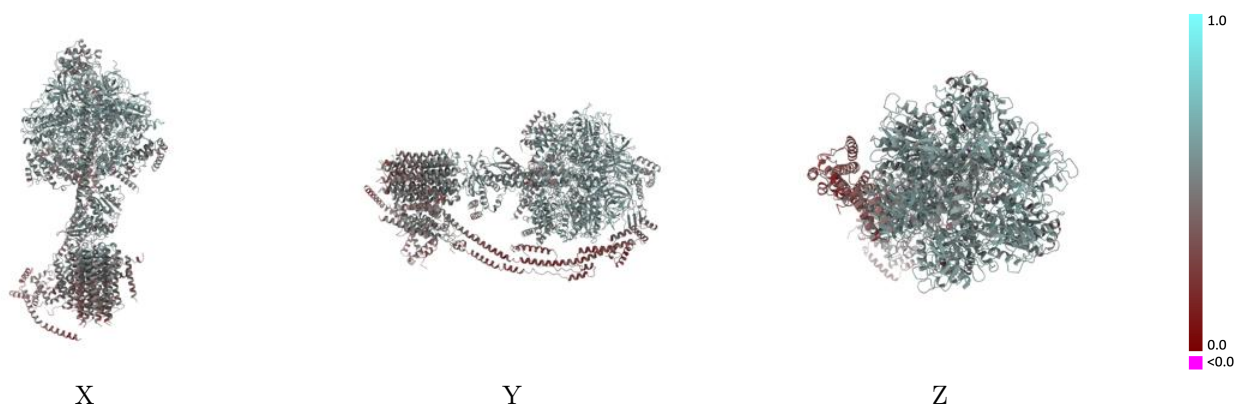
Y



Z

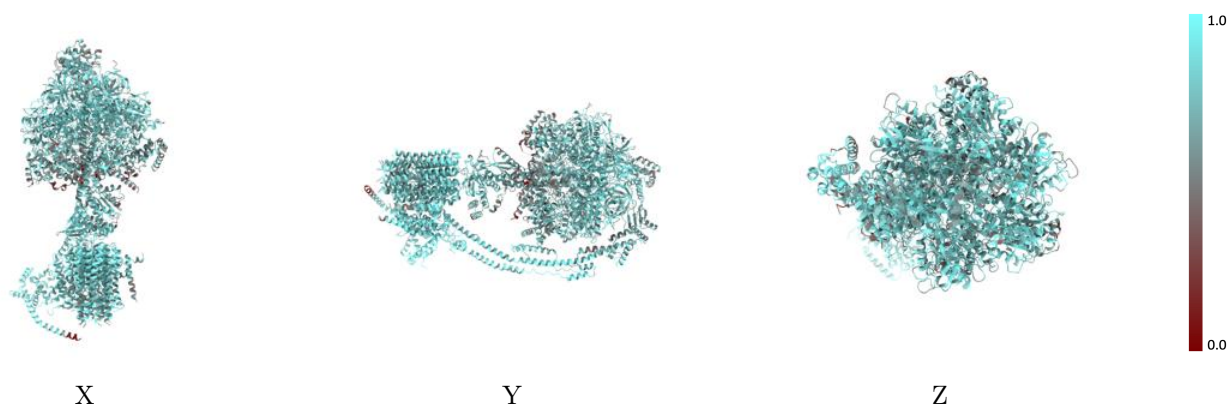
The images above show the 3D surface view of the map at the recommended contour level 7.92 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



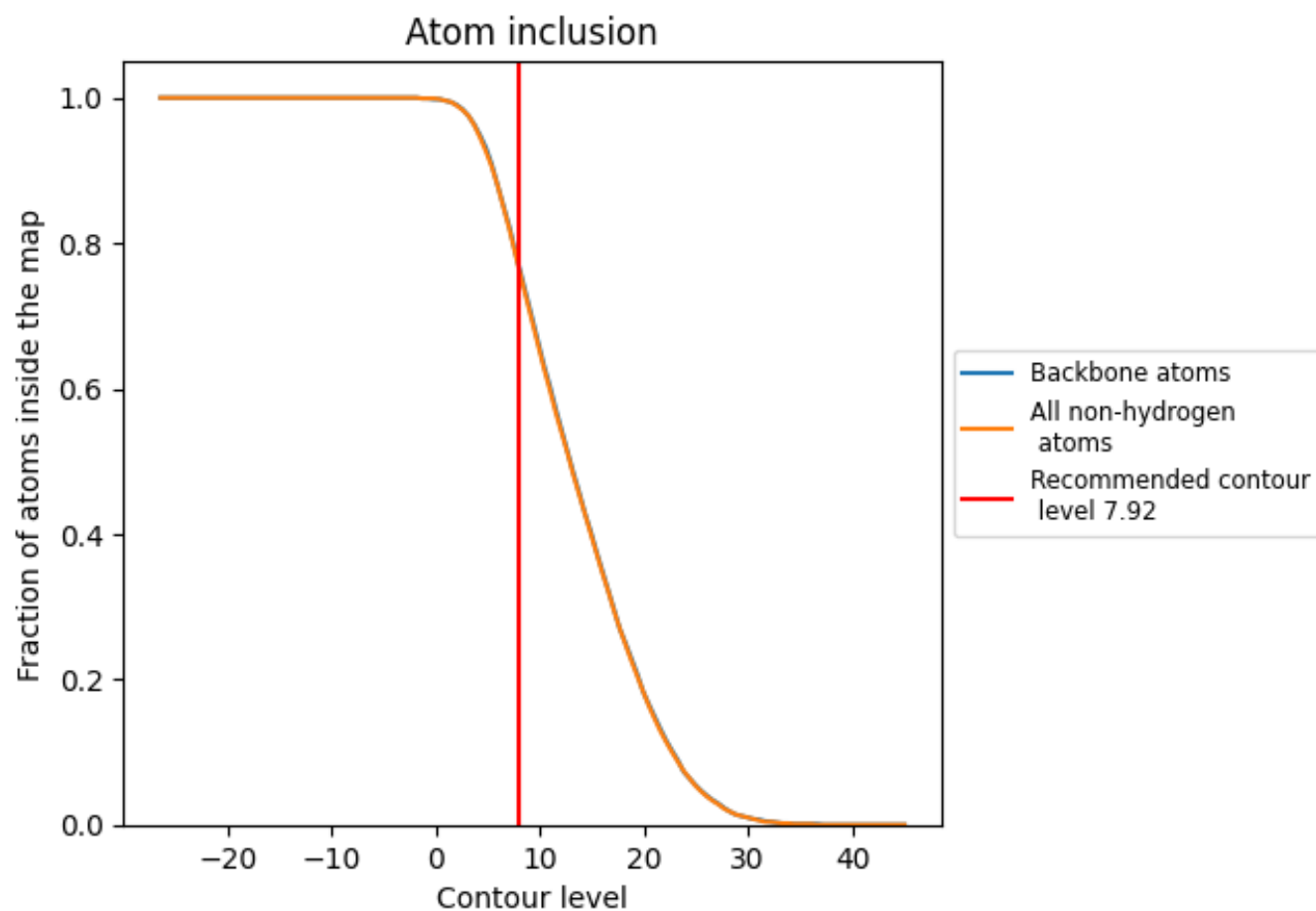
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7.92).





























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (7.92) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.5020
8	 0.8860	 0.4780
A	 0.7730	 0.5470
B	 0.7510	 0.5480
C	 0.7510	 0.5460
D	 0.7740	 0.5570
E	 0.7410	 0.5470
F	 0.7730	 0.5560
G	 0.7190	 0.5290
H	 0.7940	 0.5060
I	 0.7240	 0.5290
J	 0.5830	 0.4990
K	 0.7850	 0.4510
L	 0.8090	 0.4640
M	 0.8090	 0.4660
N	 0.8160	 0.4710
O	 0.7900	 0.4680
P	 0.8110	 0.4750
Q	 0.7360	 0.4010
R	 0.7820	 0.4600
S	 0.6810	 0.4950
a	 0.8680	 0.4630
b	 0.8390	 0.3740
d	 0.8630	 0.3290
e	 0.7730	 0.3650
f	 0.8730	 0.4560
g	 0.9030	 0.3370
h	 0.7020	 0.2740
j	 0.8360	 0.3930
k	 0.7080	 0.3970

