



## wwPDB EM Validation Summary Report ⓘ

May 11, 2024 – 03:03 pm BST

PDB ID : 6RE9  
EMDB ID : EMD-4846  
Title : Cryo-EM structure of Polytomella F-ATP synthase, Rotary substate 2D, monomer-masked refinement  
Authors : Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.  
Deposited on : 2019-04-12  
Resolution : 3.90 Å(reported)

This is a wwPDB EM 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/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>.

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

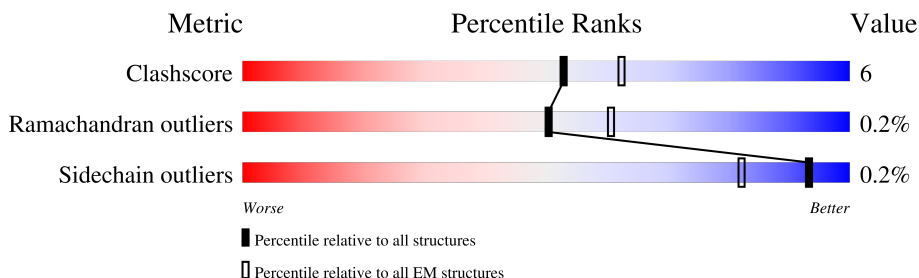
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	0	82	<div> <div>30%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
2	1	618	<div> <div>24%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>
3	2	441	<div> <div>40%</div> <div>85%</div> <div>15%</div> </div>
4	3	325	<div> <div>30%</div> <div>65%</div> <div>11%</div> <div>25%</div> </div>
5	4	294	<div> <div>32%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
6	5	123	<div> <div>9%</div> <div>92%</div> <div>8%</div> </div>
7	6	151	<div> <div>18%</div> <div>75%</div> <div>7%</div> <div>18%</div> </div>
8	7	190	<div> <div>28%</div> <div>78%</div> <div>14%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
9	8	89	
10	9	97	
11	A	127	
11	B	127	
11	C	127	
11	D	127	
11	E	127	
11	F	127	
11	G	127	
11	H	127	
11	I	127	
11	J	127	
12	M	327	
13	P	229	
14	Q	74	
15	R	199	
16	S	317	
17	T	562	
17	U	562	
17	V	562	
18	X	574	
18	Y	574	
18	Z	574	

## 2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 53720 atoms, of which 0 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 ASA-10: Polytomella F-ATP synthase associated subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	81	Total	C	N	O	S	0	0
			607	388	107	110	2		

- Molecule 2 is a protein called ATP synthase associated protein ASA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	595	Total	C	N	O	S	0	0
			4661	2958	798	900	5		

- Molecule 3 is a protein called ASA-2: Polytomella F-ATP synthase associated subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	2	441	Total	C	N	O	0	0
			3163	2020	532	611		

- Molecule 4 is a protein called Mitochondrial F1F0 ATP synthase associated 32 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	245	Total	C	N	O	S	0	0
			1874	1204	299	370	1		

- Molecule 5 is a protein called Mitochondrial ATP synthase associated protein ASA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	290	Total	C	N	O	S	0	0
			2177	1385	356	434	2		

- Molecule 6 is a protein called Mitochondrial F1F0 ATP synthase associated 14 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	123	Total	C	N	O	S	0	0
			986	640	172	170	4		

- Molecule 7 is a protein called Mitochondrial ATP synthase subunit ASA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	124	Total	C	N	O	S	0	0
			926	599	154	172	1		

- Molecule 8 is a protein called Mitochondrial ATP synthase associated protein ASA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	176	Total	C	N	O	S	0	0
			1347	860	227	259	1		

- Molecule 9 is a protein called Mitochondrial ATP synthase subunit ASA8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	88	Total	C	N	O	0	0
			692	456	115	121		

- Molecule 10 is a protein called ASA-9: Polytomella F-ATP synthase associated subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	97	Total	C	N	O	S	0	0
			776	514	124	132	6		

- Molecule 11 is a protein called Mitochondrial ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	B	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	C	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	D	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	E	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	F	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	G	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	H	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	J	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

- Molecule 12 is a protein called Mitochondrial ATP synthase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	217	Total	C	N	O	S	0	0
			1640	1077	267	288	8		

- Molecule 13 is a protein called Mitochondrial ATP synthase subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	193	Total	C	N	O	S	0	0
			1532	988	250	290	4		

- Molecule 14 is a protein called epsilon: Polytomella F-ATP synthase epsilon subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	72	Total	C	N	O	S	0	0
			561	358	102	99	2		

- Molecule 15 is a protein called Mitochondrial ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	177	Total	C	N	O	S	0	0
			1303	833	213	256	1		

- Molecule 16 is a protein called ATP synthase gamma chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	277	Total	C	N	O	S	0	0
			2130	1327	377	416	10		

- Molecule 17 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	523	Total	C	N	O	S	0	0
			3979	2537	703	728	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	523	Total	C	N	O	S	0	0
			3978	2537	702	728	11		
17	V	520	Total	C	N	O	S	0	0
			3961	2527	700	723	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	266	ARG	LYS	conflict	UNP A0ZW40
U	266	ARG	LYS	conflict	UNP A0ZW40
V	266	ARG	LYS	conflict	UNP A0ZW40

- Molecule 18 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	538	Total	C	N	O	S	0	0
			4087	2568	692	814	13		
18	Y	520	Total	C	N	O	S	0	0
			3952	2484	669	786	13		
18	Z	539	Total	C	N	O	S	0	0
			4095	2572	693	817	13		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	350	ALA	GLY	conflict	UNP A0ZW41
X	387	LEU	ARG	conflict	UNP A0ZW41
Y	350	ALA	GLY	conflict	UNP A0ZW41
Y	387	LEU	ARG	conflict	UNP A0ZW41
Z	350	ALA	GLY	conflict	UNP A0ZW41
Z	387	LEU	ARG	conflict	UNP A0ZW41

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	M	1	Total	Zn	0
			1	1	

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: 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
20	T	1	Total 31	C 10	N 5	O 13	P 3	0
20	U	1	Total 31	C 10	N 5	O 13	P 3	0
20	V	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
21	T	1	Total Mg 1 1	0
21	U	1	Total Mg 1 1	0
21	V	1	Total Mg 1 1	0
21	Y	1	Total Mg 1 1	0
21	Z	1	Total Mg 1 1	0

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



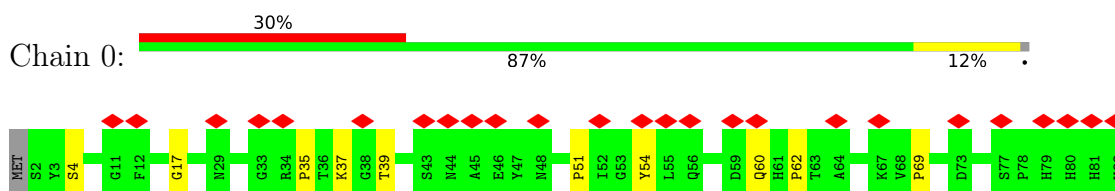


Mol	Chain	Residues	Atoms					AltConf
22	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	
22	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	

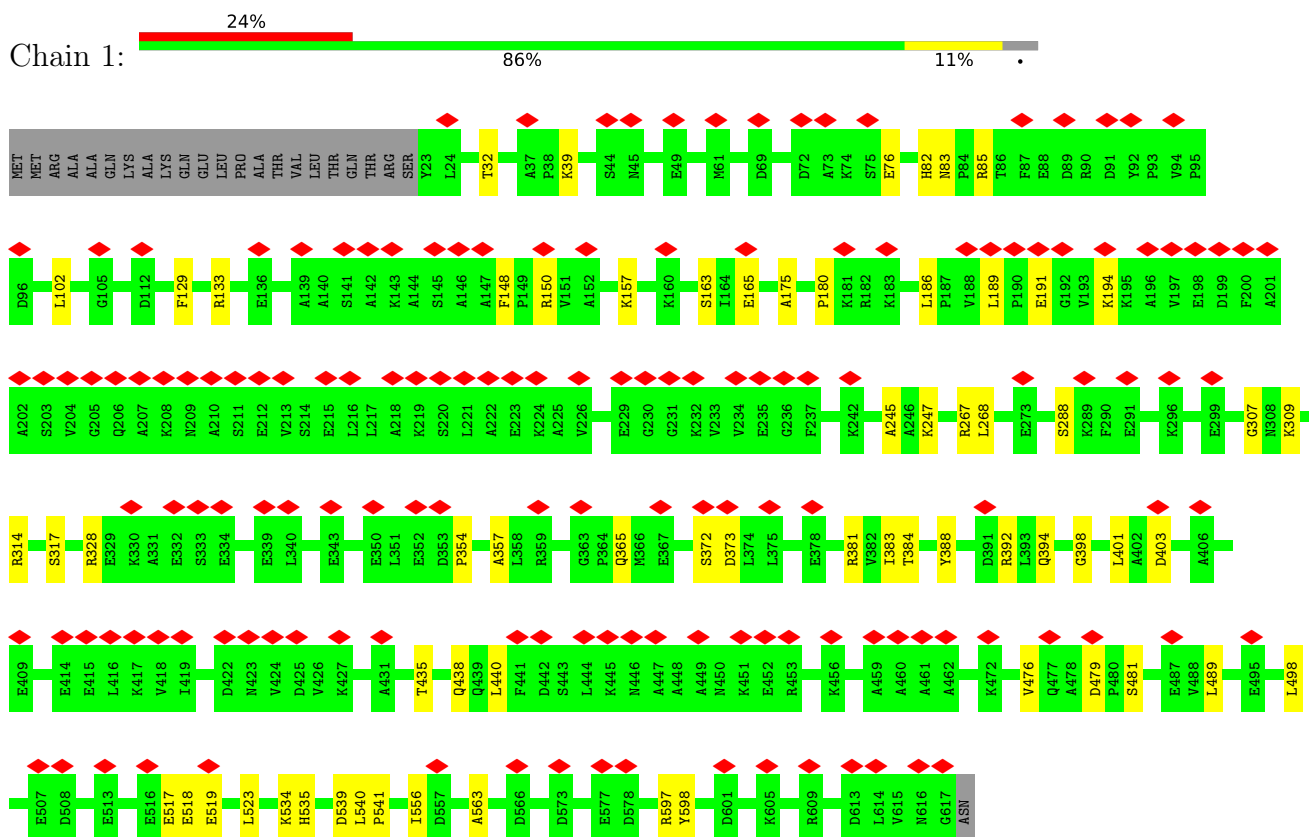
### 3 Residue-property plots [i](#)

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.

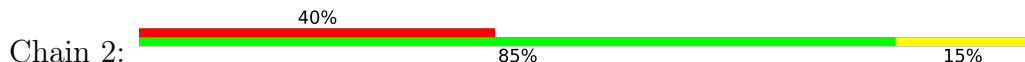
- Molecule 1: ASA-10: *Polytomella* F-ATP synthase associated subunit 10

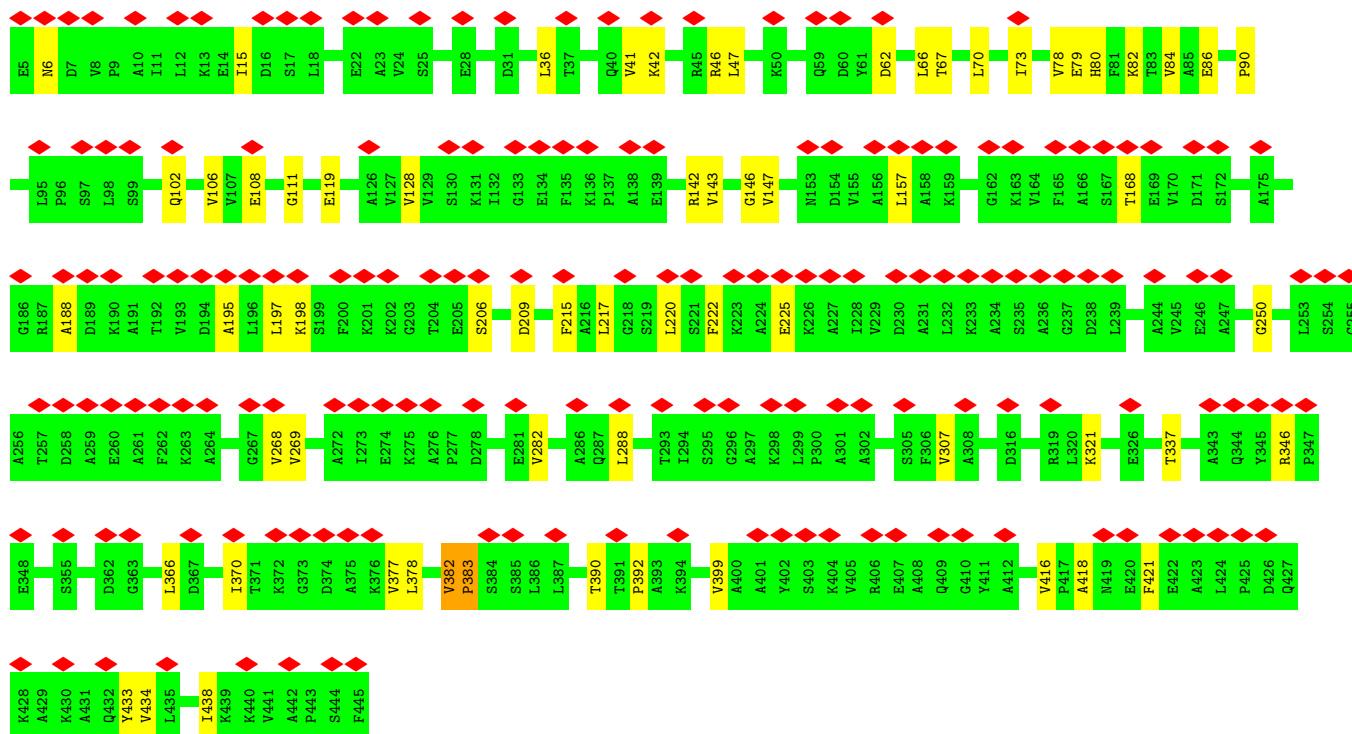


- Molecule 2: ATP synthase associated protein ASA1

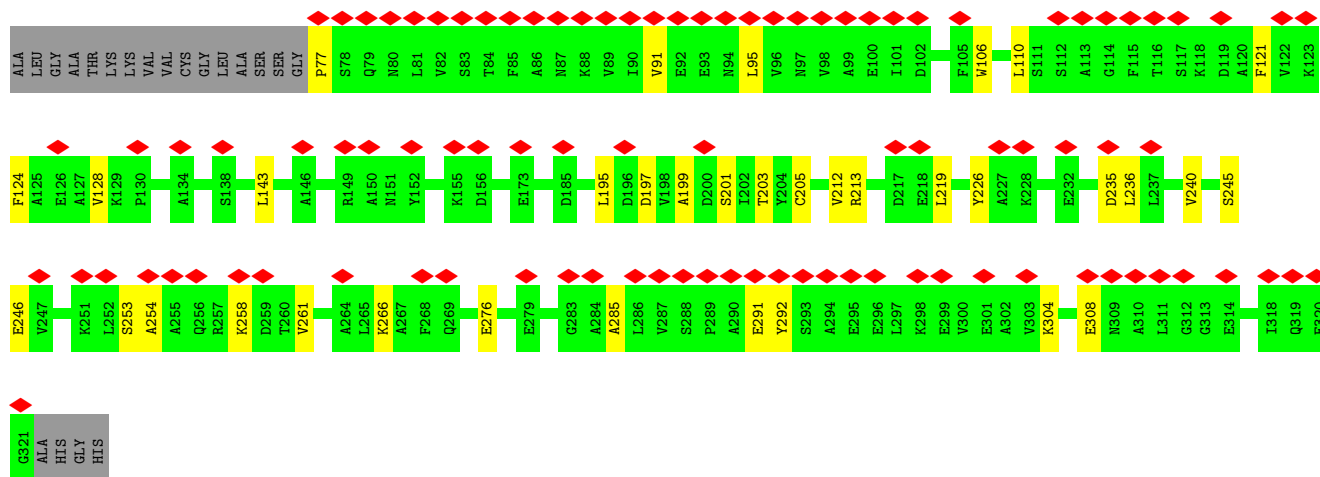
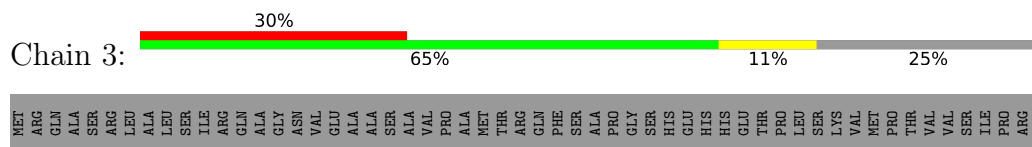


- Molecule 3: ASA-2: *Polytomella* F-ATP synthase associated subunit 2

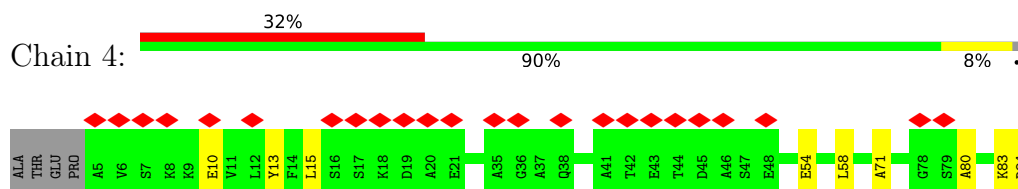


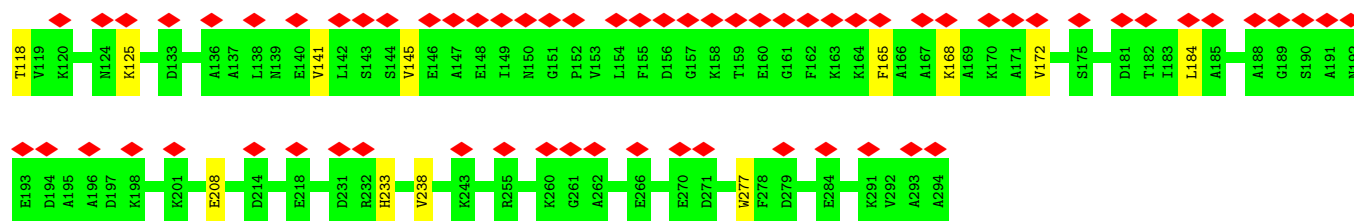


• Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein

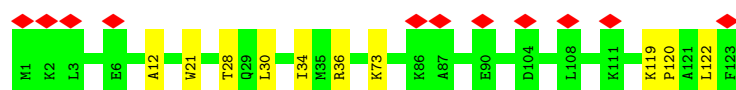
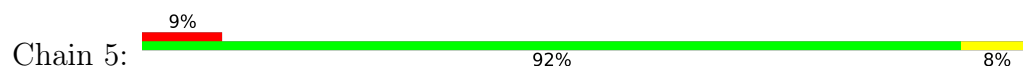


• Molecule 5: Mitochondrial ATP synthase associated protein ASA4

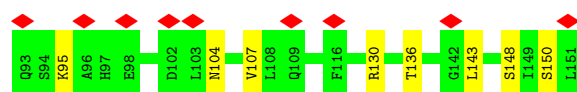
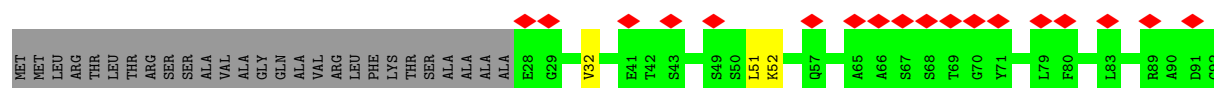
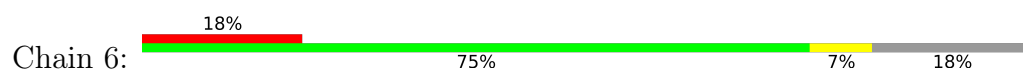




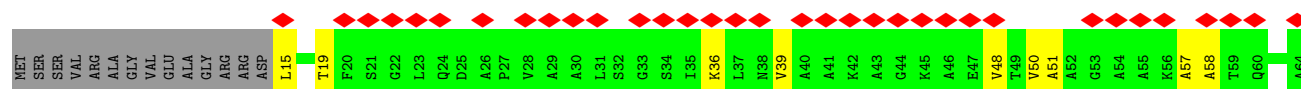
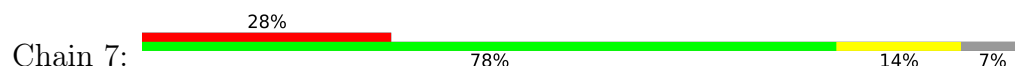
- Molecule 6: Mitochondrial F1F0 ATP synthase associated 14 kDa protein



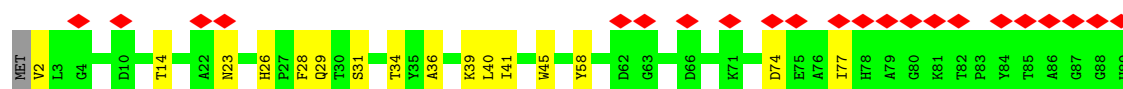
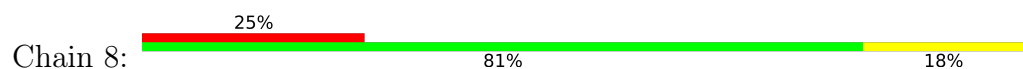
- Molecule 7: Mitochondrial ATP synthase subunit ASA6



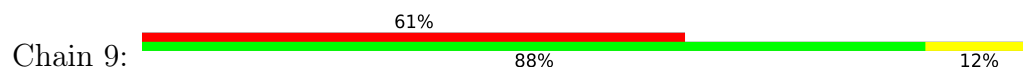
- Molecule 8: Mitochondrial ATP synthase associated protein ASA7

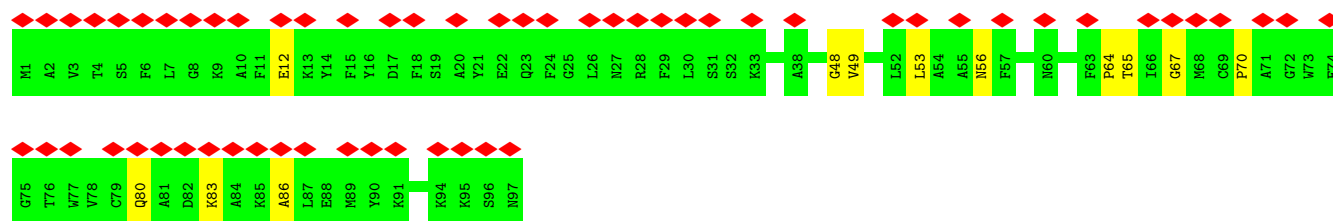


- Molecule 9: Mitochondrial ATP synthase subunit ASA8

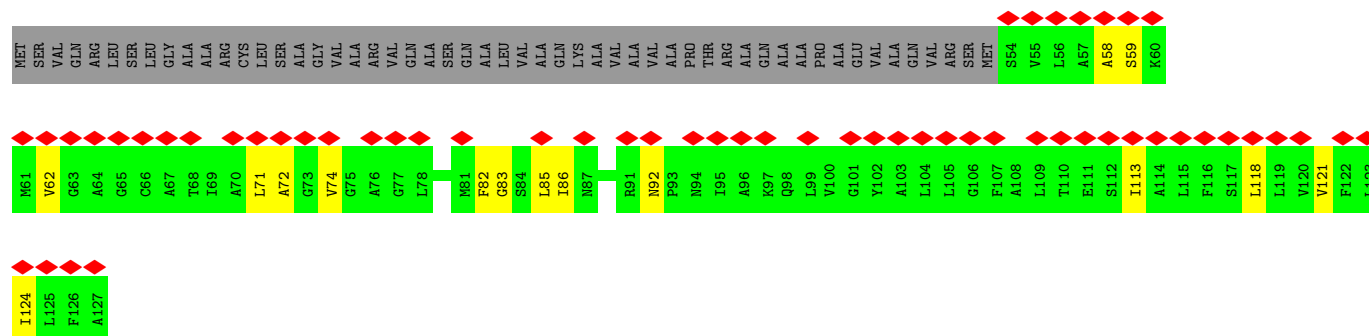


- Molecule 10: ASA-9: Polytomella F-ATP synthase associated subunit 9

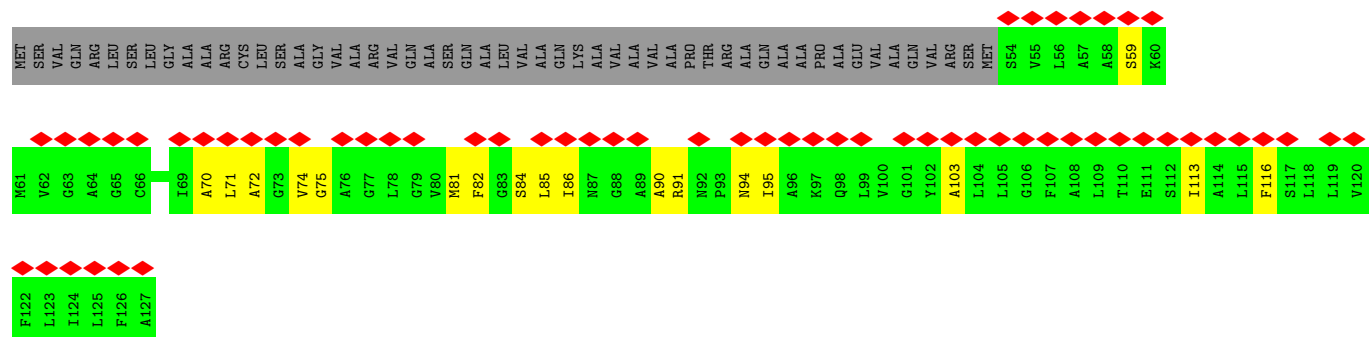
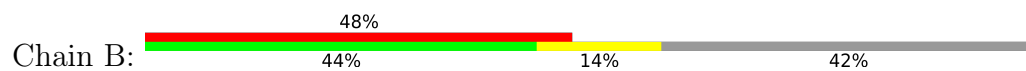




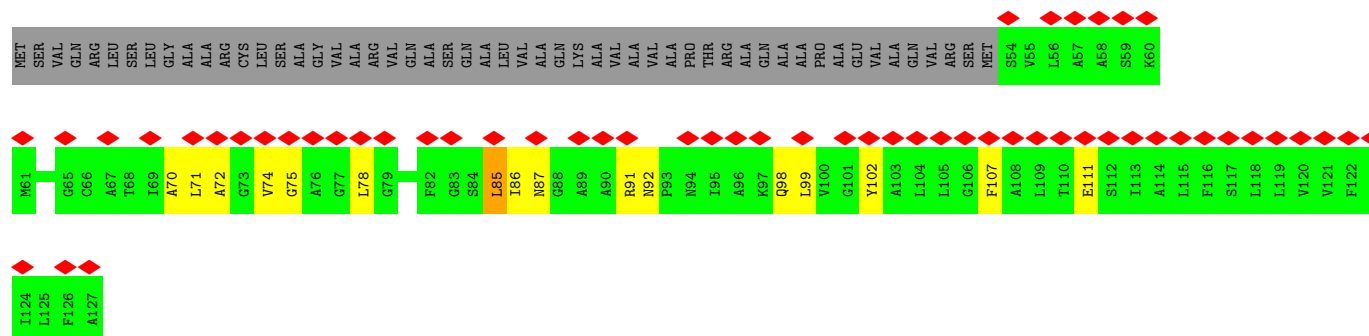
• Molecule 11: Mitochondrial ATP synthase subunit c



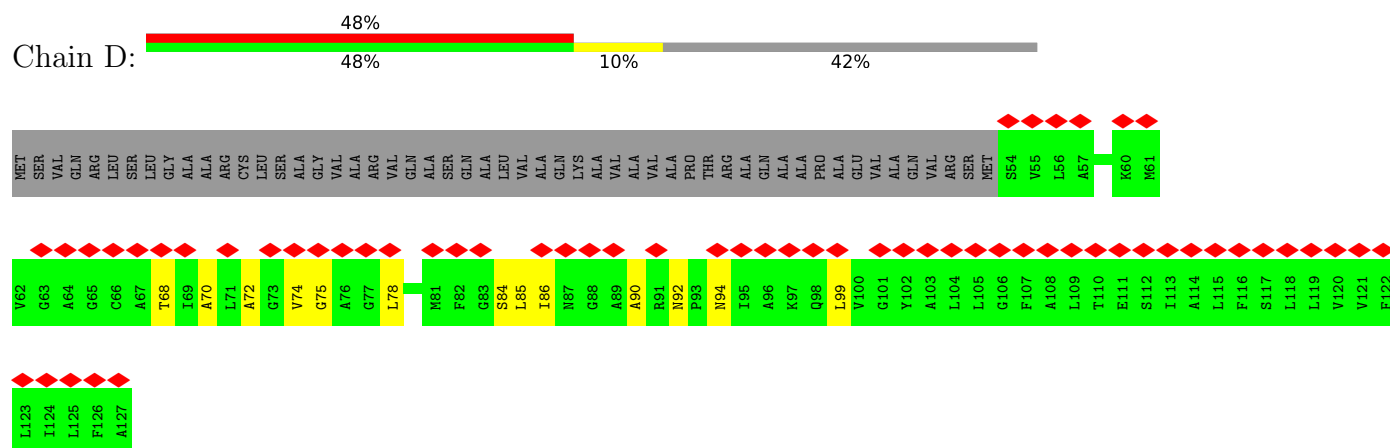
• Molecule 11: Mitochondrial ATP synthase subunit c



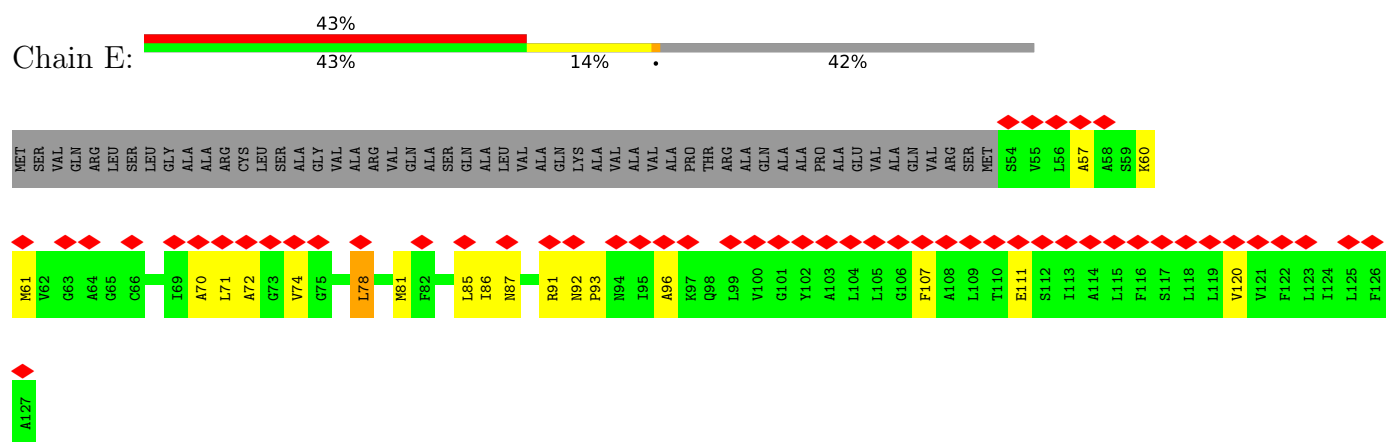
• Molecule 11: Mitochondrial ATP synthase subunit c



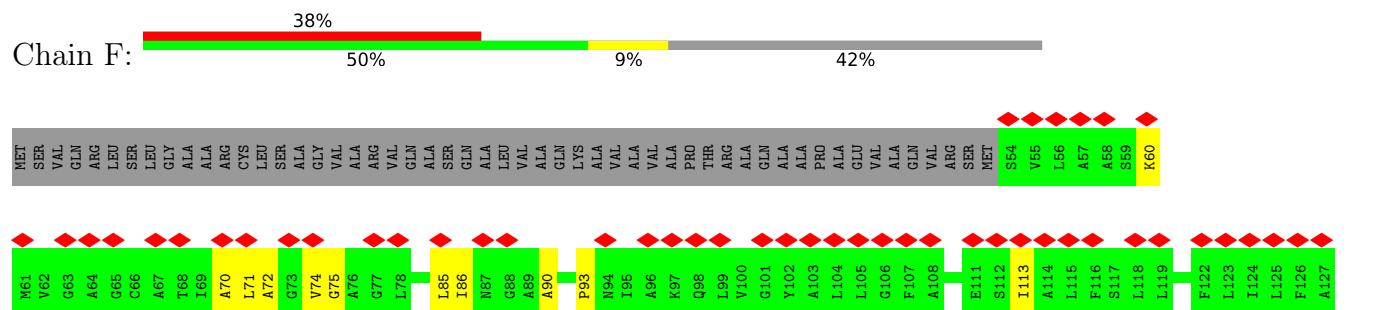
## • Molecule 11: Mitochondrial ATP synthase subunit c



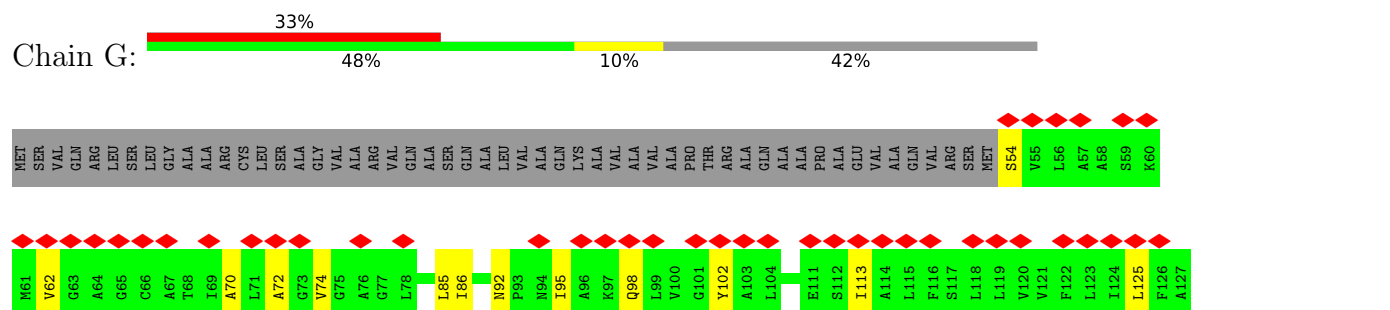
## • Molecule 11: Mitochondrial ATP synthase subunit c



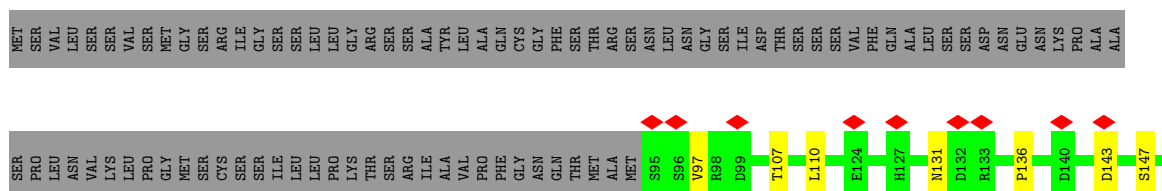
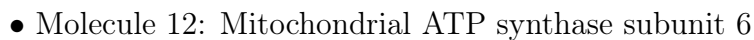
## • Molecule 11: Mitochondrial ATP synthase subunit c

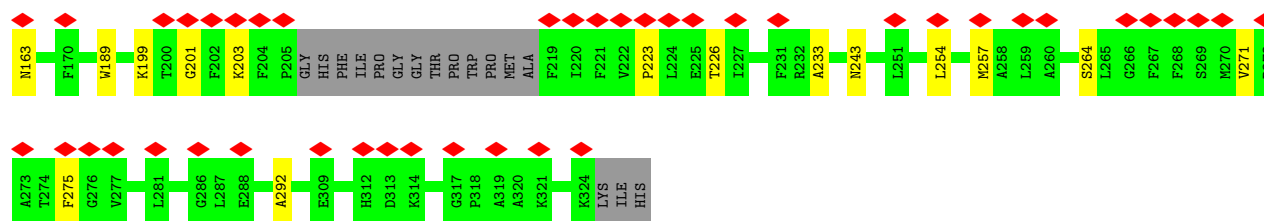


## • Molecule 11: Mitochondrial ATP synthase subunit c

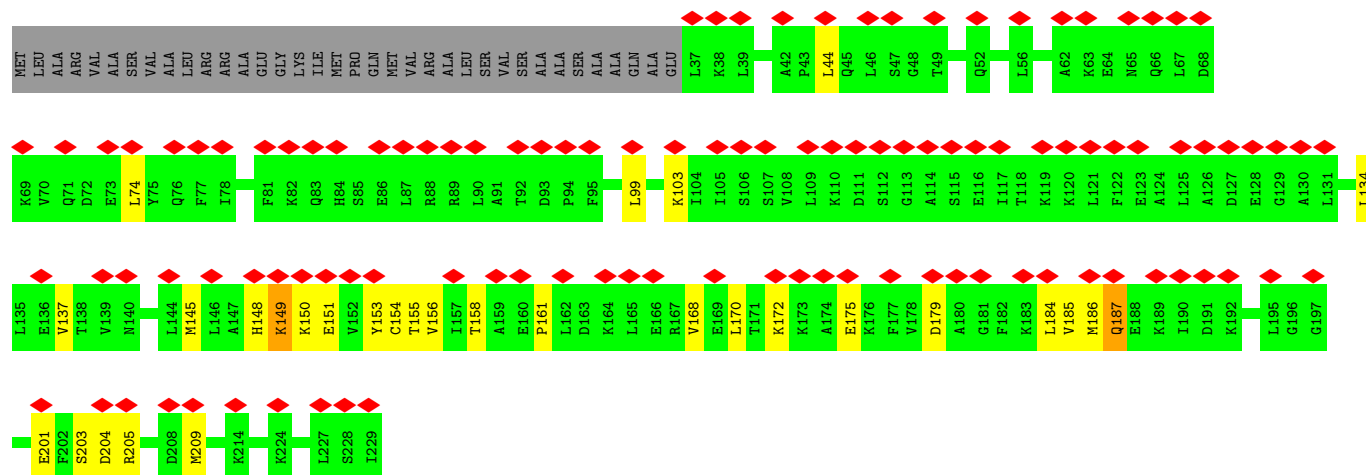


## Chain H:

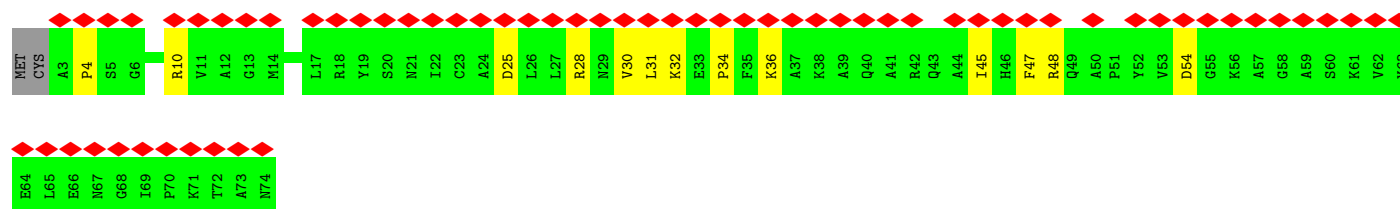
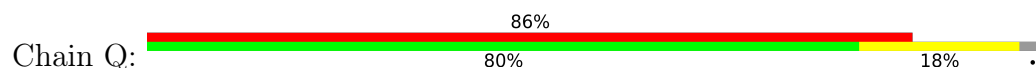




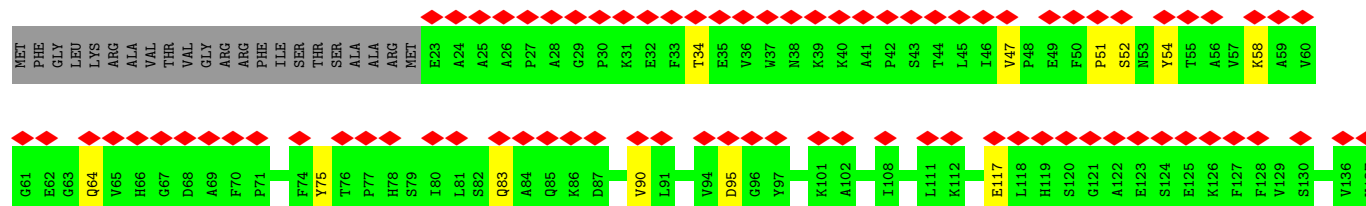
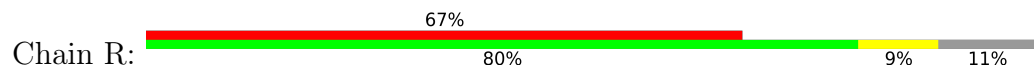
• Molecule 13: Mitochondrial ATP synthase subunit OSCP



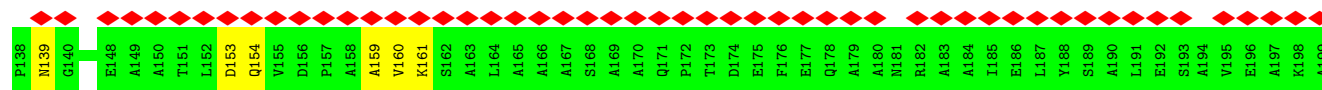
• Molecule 14: epsilon: Polytomella F-ATP synthase epsilon subunit



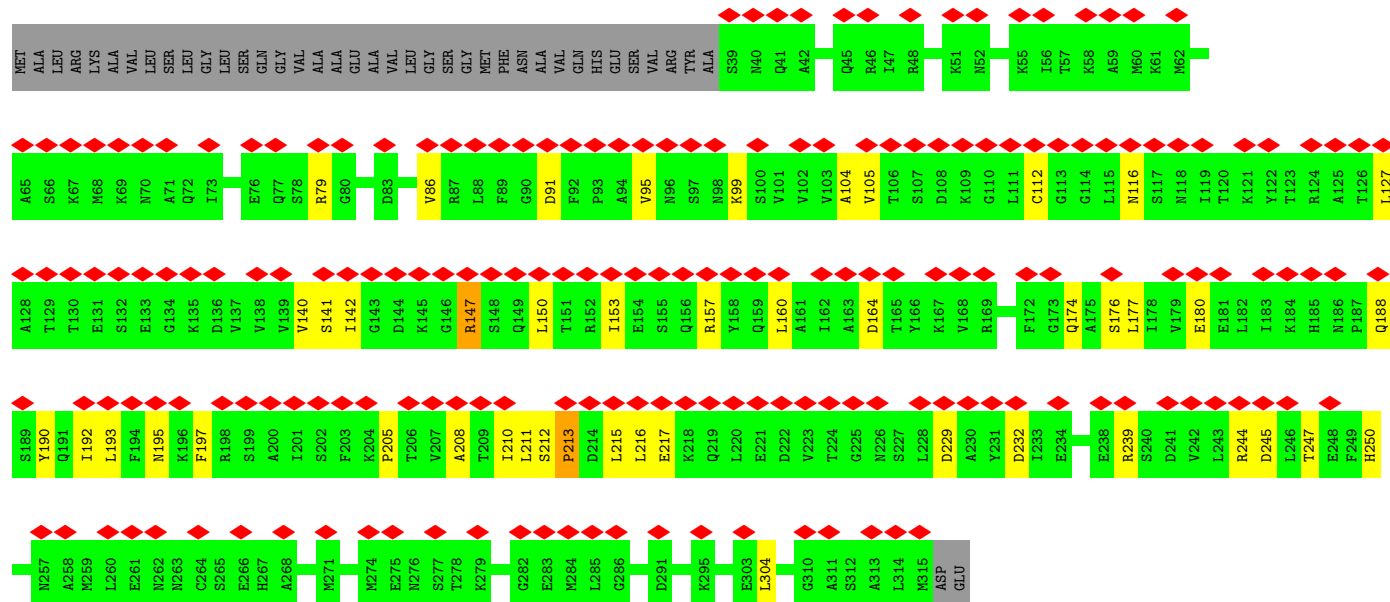
• Molecule 15: Mitochondrial ATP synthase subunit delta



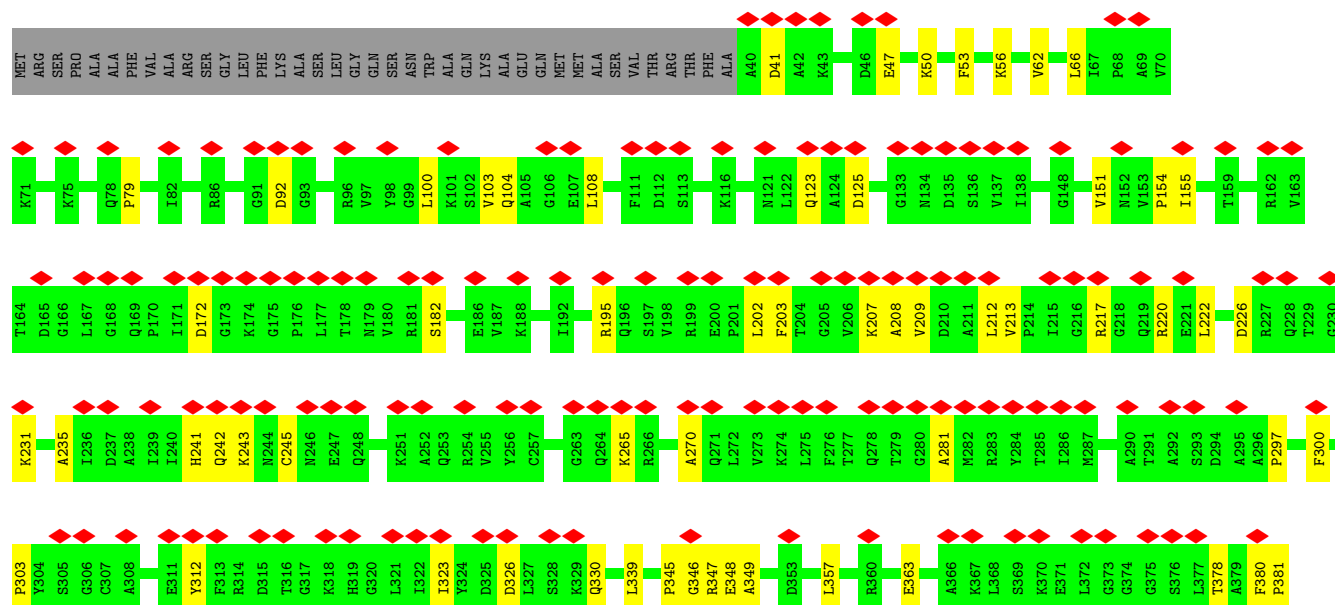
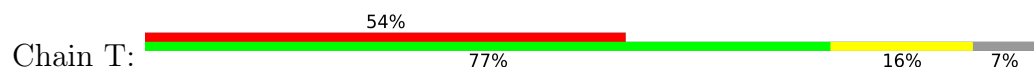


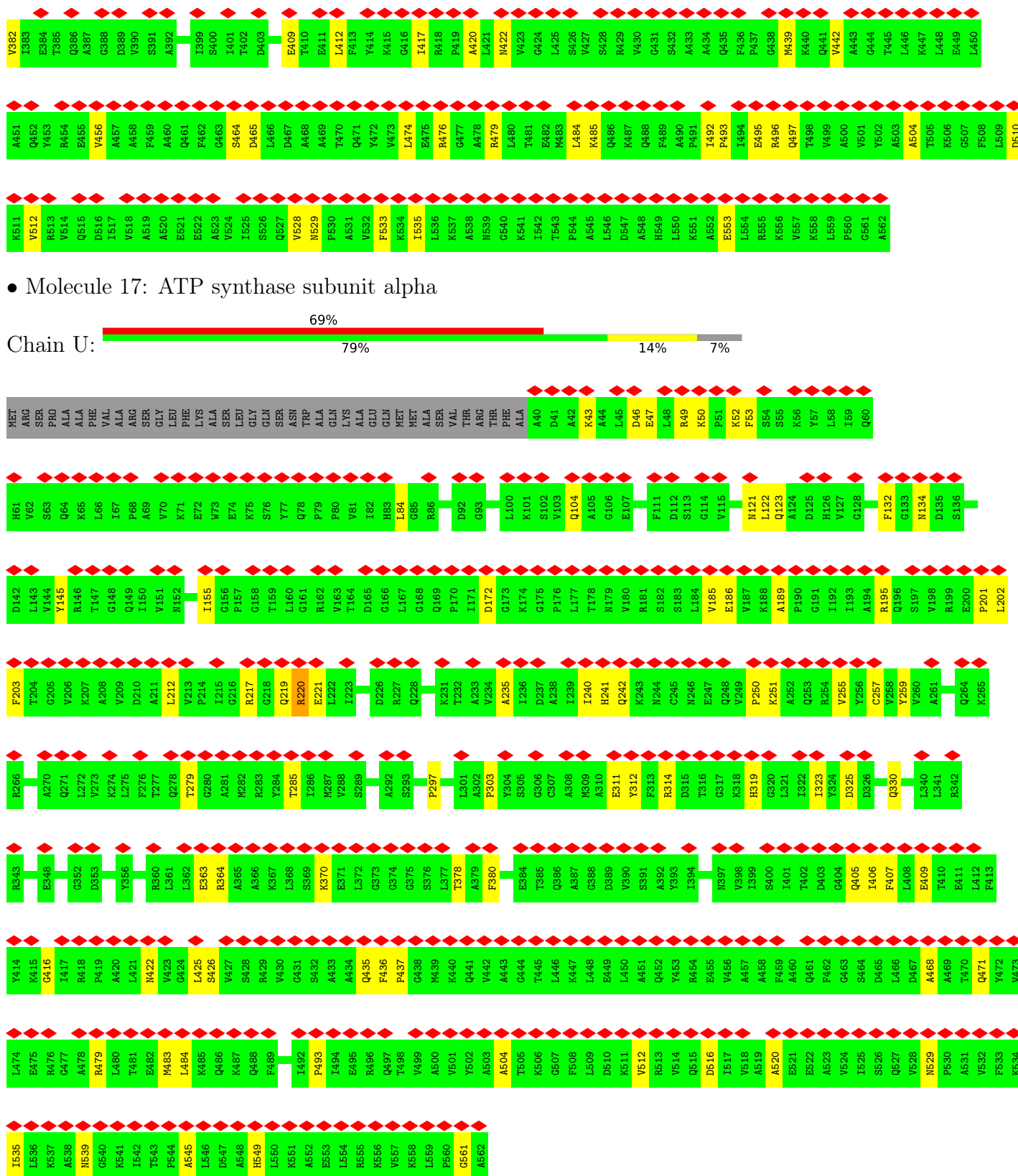


• Molecule 16: ATP synthase gamma chain, mitochondrial

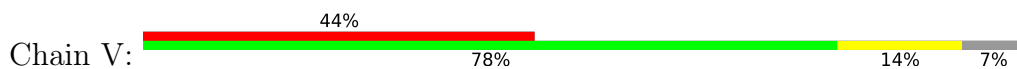


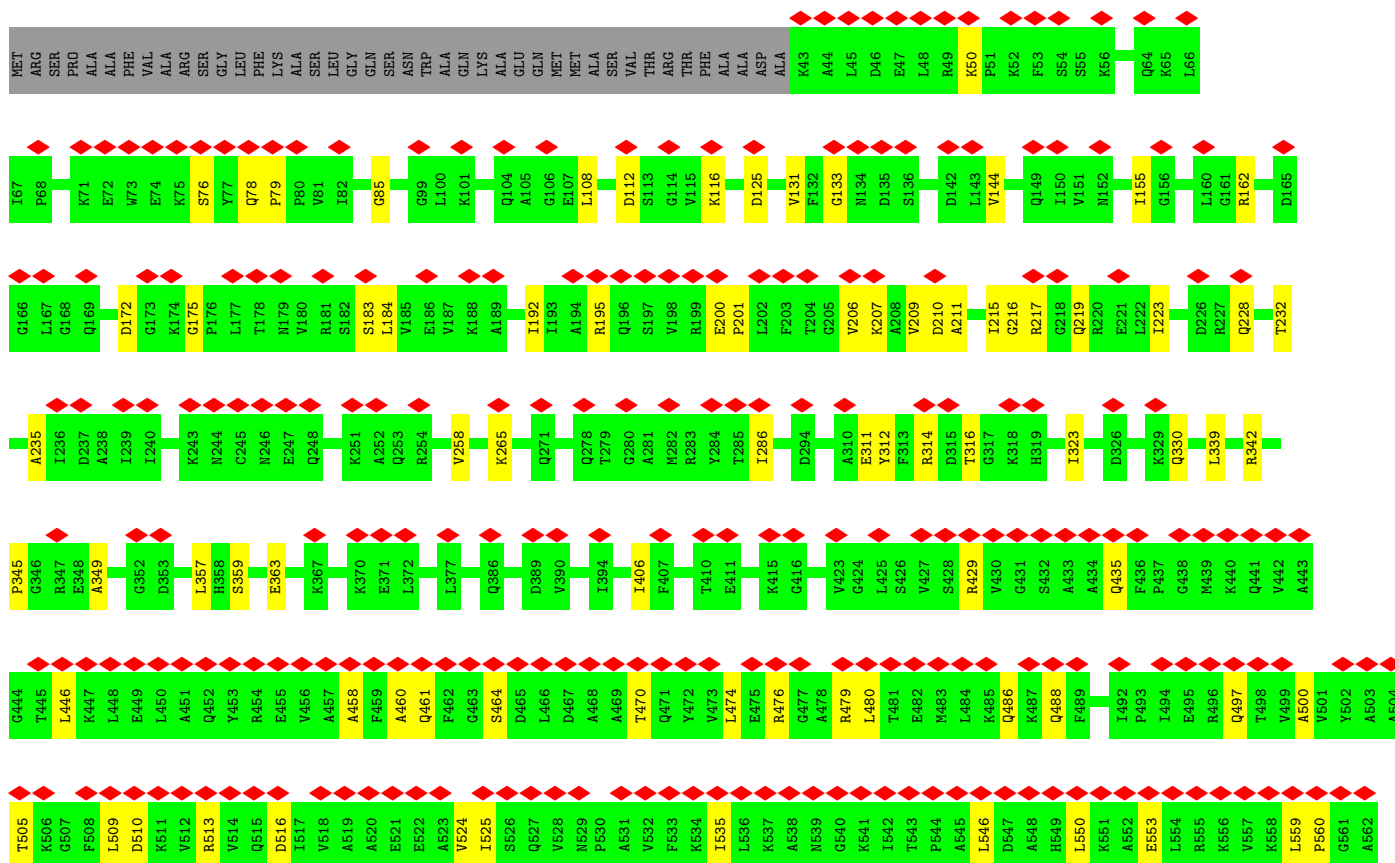
• Molecule 17: ATP synthase subunit alpha



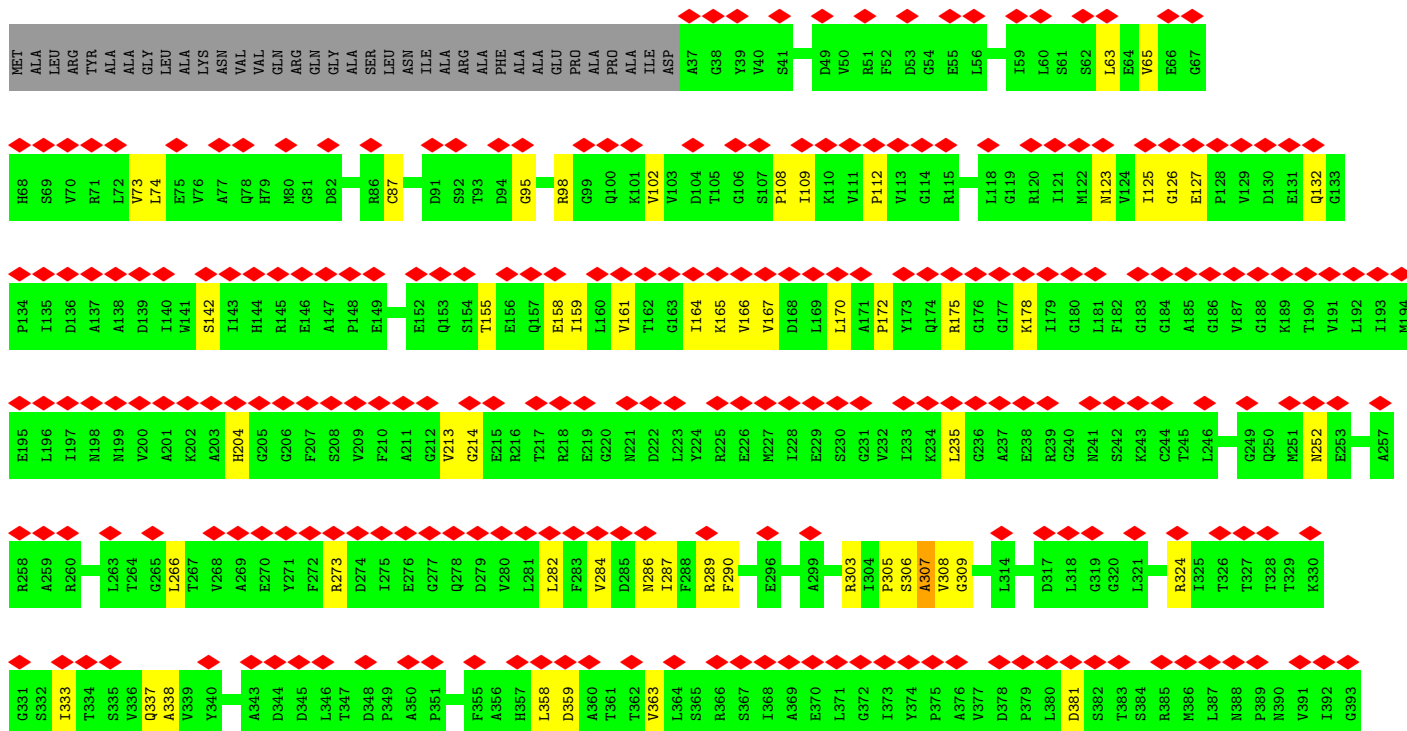
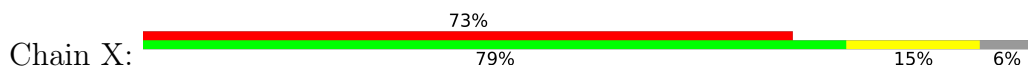


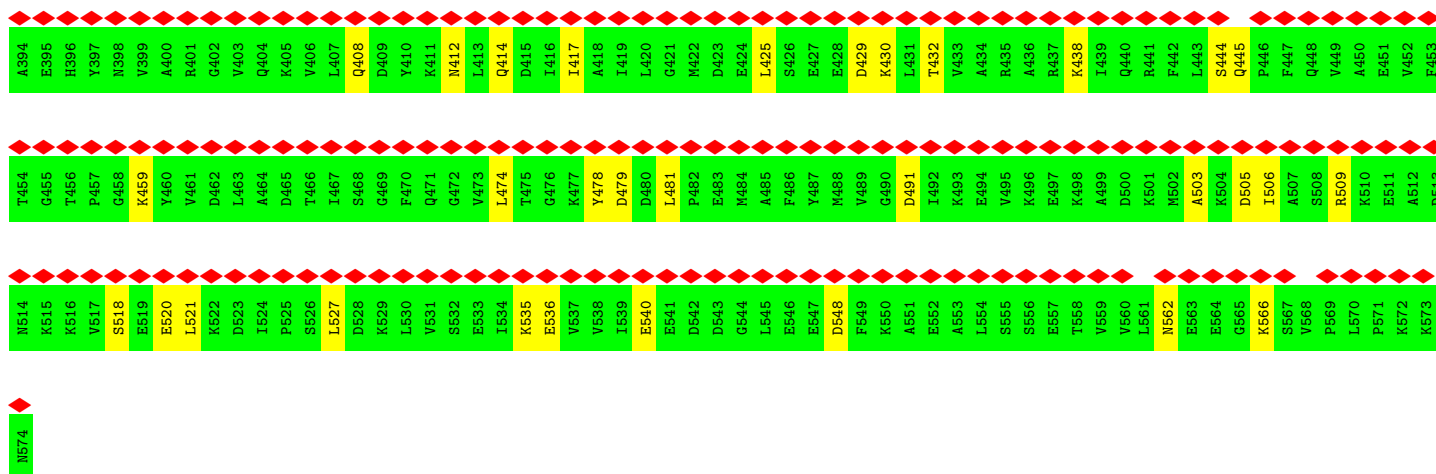
• Molecule 17: ATP synthase subunit alpha



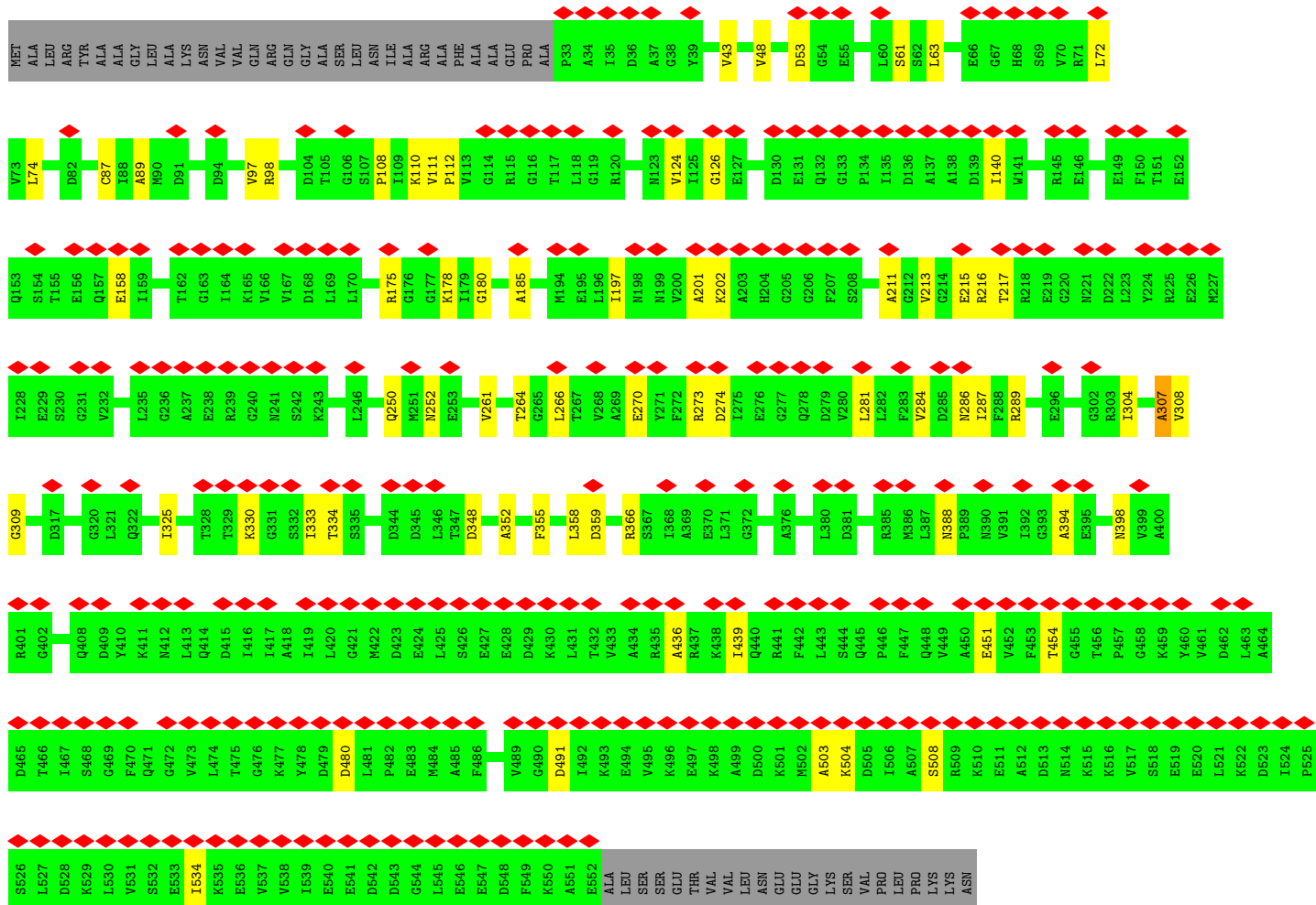
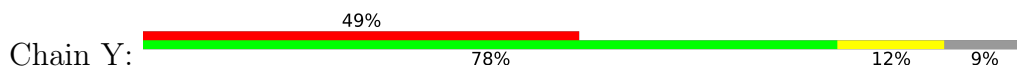


• Molecule 18: ATP synthase subunit beta




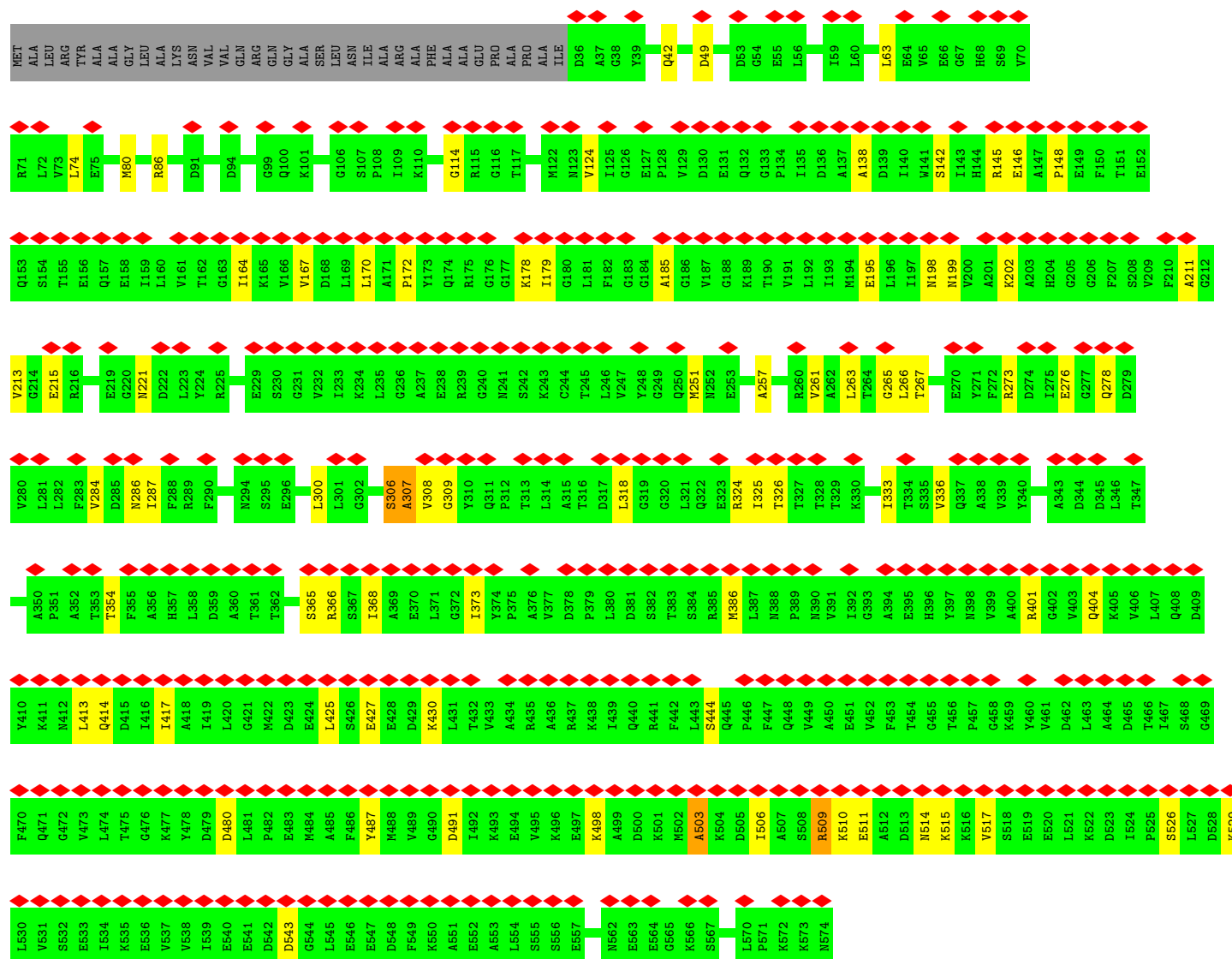


• Molecule 18: ATP synthase subunit beta



• Molecule 18: ATP synthase subunit beta

Chain Z: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16363	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 ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.151	Depositor
Minimum map value	-0.083	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	505.44, 505.44, 505.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0	0.30	0/628	0.45	0/856
2	1	0.30	0/4750	0.47	1/6434 (0.0%)
3	2	0.29	0/3212	0.51	0/4371
4	3	0.31	0/1911	0.50	1/2601 (0.0%)
5	4	0.30	0/2216	0.46	0/3000
6	5	0.32	0/1011	0.56	0/1376
7	6	0.30	0/946	0.49	0/1287
8	7	0.32	0/1374	0.49	0/1865
9	8	0.31	0/715	0.51	0/974
10	9	0.30	0/802	0.50	0/1084
11	A	0.28	0/520	0.53	0/704
11	B	0.28	0/520	0.59	0/704
11	C	0.28	0/519	0.57	1/701 (0.1%)
11	D	0.28	0/520	0.49	0/704
11	E	0.28	0/520	0.53	0/704
11	F	0.30	0/520	0.52	0/704
11	G	0.29	0/520	0.49	0/704
11	H	0.31	0/520	0.48	0/704
11	I	0.28	0/520	0.54	0/704
11	J	0.29	0/520	0.56	0/704
12	M	0.33	0/1683	0.56	0/2295
13	P	0.32	0/1553	0.55	1/2093 (0.0%)
14	Q	0.30	0/574	0.49	0/774
15	R	0.31	0/1336	0.51	0/1827
16	S	0.30	0/2153	0.50	0/2901
17	T	0.34	0/4048	0.53	0/5481
17	U	0.33	0/4047	0.53	0/5479
17	V	0.34	0/4030	0.52	0/5456
18	X	0.34	0/4147	0.53	0/5619
18	Y	0.34	0/4011	0.52	0/5435
18	Z	0.33	0/4155	0.55	2/5630 (0.0%)
All	All	0.32	0/54501	0.52	6/73875 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	5	0	1
18	X	0	1
18	Y	0	2
18	Z	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Z	543	ASP	CB-CG-OD1	6.62	124.26	118.30
4	3	77	PRO	N-CA-CB	5.92	110.40	103.30
13	P	44	LEU	CA-CB-CG	5.73	128.49	115.30
18	Z	413	LEU	CA-CB-CG	5.63	128.26	115.30
2	1	388	TYR	C-N-CA	5.29	134.92	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	5	119	LYS	Peptide
18	X	307	ALA	Peptide
18	Y	307	ALA	Peptide
18	Y	503	ALA	Mainchain
18	Z	503	ALA	Mainchain

## 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	0	607	0	584	7	0
2	1	4661	0	4695	42	0
3	2	3163	0	3262	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	1874	0	1826	22	0
5	4	2177	0	2169	19	0
6	5	986	0	1021	9	0
7	6	926	0	941	10	0
8	7	1347	0	1345	22	0
9	8	692	0	694	13	0
10	9	776	0	757	10	0
11	A	514	0	554	12	0
11	B	514	0	554	17	0
11	C	514	0	553	16	0
11	D	514	0	554	13	0
11	E	514	0	554	16	0
11	F	514	0	554	11	0
11	G	514	0	554	13	0
11	H	514	0	554	14	0
11	I	514	0	554	11	0
11	J	514	0	554	13	0
12	M	1640	0	1665	18	0
13	P	1532	0	1603	28	0
14	Q	561	0	565	11	0
15	R	1303	0	1266	13	0
16	S	2130	0	2180	30	0
17	T	3979	0	4119	56	0
17	U	3978	0	4116	53	0
17	V	3961	0	4105	51	0
18	X	4087	0	4110	54	0
18	Y	3952	0	3964	45	0
18	Z	4095	0	4114	50	0
19	M	1	0	0	0	0
20	T	31	0	12	0	0
20	U	31	0	12	0	0
20	V	31	0	12	2	0
21	T	1	0	0	0	0
21	U	1	0	0	0	0
21	V	1	0	0	0	0
21	Y	1	0	0	0	0
21	Z	1	0	0	0	0
22	Y	27	0	12	0	0
22	Z	27	0	12	1	0
All	All	53720	0	54700	609	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 6.

The worst 5 of 609 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)
18:Z:514:ASN:O	18:Z:517:VAL:HG22	1.18	1.28
13:P:184:LEU:HD12	13:P:184:LEU:O	1.48	1.10
18:Z:514:ASN:O	18:Z:517:VAL:CG2	1.99	1.10
13:P:154:CYS:SG	13:P:185:VAL:O	2.33	0.86
3:2:82:LYS:O	3:2:86:GLU:HB2	1.78	0.83

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 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	0	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
2	1	593/618 (96%)	576 (97%)	17 (3%)	0	100	100
3	2	439/441 (100%)	424 (97%)	14 (3%)	1 (0%)	47	79
4	3	243/325 (75%)	236 (97%)	7 (3%)	0	100	100
5	4	288/294 (98%)	276 (96%)	12 (4%)	0	100	100
6	5	121/123 (98%)	111 (92%)	9 (7%)	1 (1%)	19	57
7	6	122/151 (81%)	110 (90%)	12 (10%)	0	100	100
8	7	174/190 (92%)	169 (97%)	5 (3%)	0	100	100
9	8	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
10	9	95/97 (98%)	82 (86%)	13 (14%)	0	100	100
11	A	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	B	72/127 (57%)	72 (100%)	0	0	100	100
11	C	71/127 (56%)	71 (100%)	0	0	100	100
11	D	72/127 (57%)	72 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	E	72/127 (57%)	72 (100%)	0	0	100	100
11	F	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	G	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	H	72/127 (57%)	72 (100%)	0	0	100	100
11	I	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	J	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
12	M	213/327 (65%)	208 (98%)	5 (2%)	0	100	100
13	P	191/229 (83%)	178 (93%)	12 (6%)	1 (0%)	29	67
14	Q	70/74 (95%)	67 (96%)	3 (4%)	0	100	100
15	R	175/199 (88%)	167 (95%)	8 (5%)	0	100	100
16	S	275/317 (87%)	262 (95%)	12 (4%)	1 (0%)	34	71
17	T	521/562 (93%)	501 (96%)	19 (4%)	1 (0%)	47	79
17	U	521/562 (93%)	493 (95%)	28 (5%)	0	100	100
17	V	518/562 (92%)	499 (96%)	19 (4%)	0	100	100
18	X	536/574 (93%)	510 (95%)	24 (4%)	2 (0%)	34	71
18	Y	518/574 (90%)	484 (93%)	33 (6%)	1 (0%)	47	79
18	Z	537/574 (94%)	499 (93%)	34 (6%)	4 (1%)	22	60
All	All	7034/8234 (85%)	6718 (96%)	304 (4%)	12 (0%)	50	79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	X	308	VAL
18	Y	308	VAL
18	Z	308	VAL
13	P	149	LYS
18	Z	307	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 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	0	63/64 (98%)	63 (100%)	0	100	100
2	1	493/512 (96%)	493 (100%)	0	100	100
3	2	312/312 (100%)	310 (99%)	2 (1%)	86	91
4	3	195/258 (76%)	195 (100%)	0	100	100
5	4	220/223 (99%)	220 (100%)	0	100	100
6	5	107/107 (100%)	107 (100%)	0	100	100
7	6	96/115 (84%)	96 (100%)	0	100	100
8	7	140/150 (93%)	140 (100%)	0	100	100
9	8	71/72 (99%)	71 (100%)	0	100	100
10	9	79/79 (100%)	79 (100%)	0	100	100
11	A	50/86 (58%)	50 (100%)	0	100	100
11	B	50/86 (58%)	50 (100%)	0	100	100
11	C	50/86 (58%)	50 (100%)	0	100	100
11	D	50/86 (58%)	50 (100%)	0	100	100
11	E	50/86 (58%)	49 (98%)	1 (2%)	55	74
11	F	50/86 (58%)	50 (100%)	0	100	100
11	G	50/86 (58%)	50 (100%)	0	100	100
11	H	50/86 (58%)	50 (100%)	0	100	100
11	I	50/86 (58%)	50 (100%)	0	100	100
11	J	50/86 (58%)	50 (100%)	0	100	100
12	M	178/272 (65%)	178 (100%)	0	100	100
13	P	171/196 (87%)	169 (99%)	2 (1%)	71	83
14	Q	56/58 (97%)	56 (100%)	0	100	100
15	R	134/151 (89%)	134 (100%)	0	100	100
16	S	235/265 (89%)	234 (100%)	1 (0%)	91	94
17	T	419/448 (94%)	418 (100%)	1 (0%)	93	96
17	U	419/448 (94%)	416 (99%)	3 (1%)	84	90
17	V	418/448 (93%)	417 (100%)	1 (0%)	93	96
18	X	446/469 (95%)	446 (100%)	0	100	100
18	Y	429/469 (92%)	429 (100%)	0	100	100
18	Z	447/469 (95%)	446 (100%)	1 (0%)	93	96
All	All	5628/6445 (87%)	5616 (100%)	12 (0%)	93	96

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	U	53	PHE
17	U	220	ARG
18	Z	509	ARG
17	U	479	ARG
13	P	158	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
17	V	242	GLN
18	Y	408	GLN
17	V	264	GLN
18	X	199	ASN
11	H	98	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	ADP	Y	601	21	24,29,29	0.96	1 (4%)	29,45,45	1.52	4 (13%)
22	ADP	Z	601	21	24,29,29	0.97	1 (4%)	29,45,45	1.34	4 (13%)
20	ATP	T	1001	21	26,33,33	0.91	1 (3%)	31,52,52	1.51	5 (16%)
20	ATP	V	1001	21	26,33,33	0.91	1 (3%)	31,52,52	1.58	5 (16%)
20	ATP	U	1001	21	26,33,33	0.89	1 (3%)	31,52,52	1.59	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	ADP	Y	601	21	-	5/12/32/32	0/3/3/3
22	ADP	Z	601	21	-	3/12/32/32	0/3/3/3
20	ATP	T	1001	21	-	0/18/38/38	0/3/3/3
20	ATP	V	1001	21	-	5/18/38/38	0/3/3/3
20	ATP	U	1001	21	-	2/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	601	ADP	C5-C4	2.47	1.47	1.40
22	Y	601	ADP	C5-C4	2.31	1.47	1.40
20	T	1001	ATP	C5-C4	2.27	1.46	1.40
20	V	1001	ATP	C5-C4	2.26	1.46	1.40
20	U	1001	ATP	C5-C4	2.21	1.46	1.40

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	V	1001	ATP	PA-O3A-PB	-4.38	117.80	132.83
20	U	1001	ATP	PB-O3B-PG	-4.07	118.86	132.83
20	U	1001	ATP	PA-O3A-PB	-3.98	119.16	132.83
20	T	1001	ATP	PB-O3B-PG	-3.78	119.84	132.83
22	Y	601	ADP	C3'-C2'-C1'	3.73	106.60	100.98

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

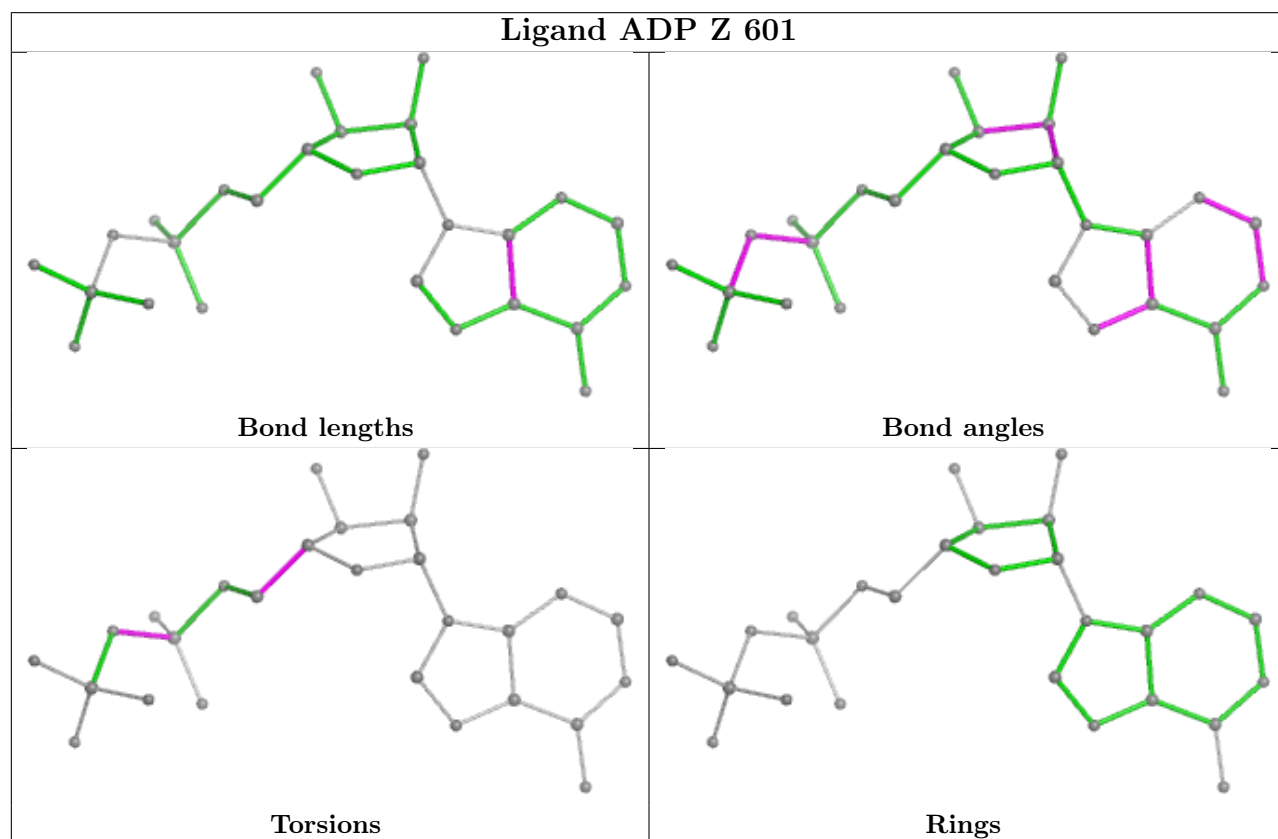
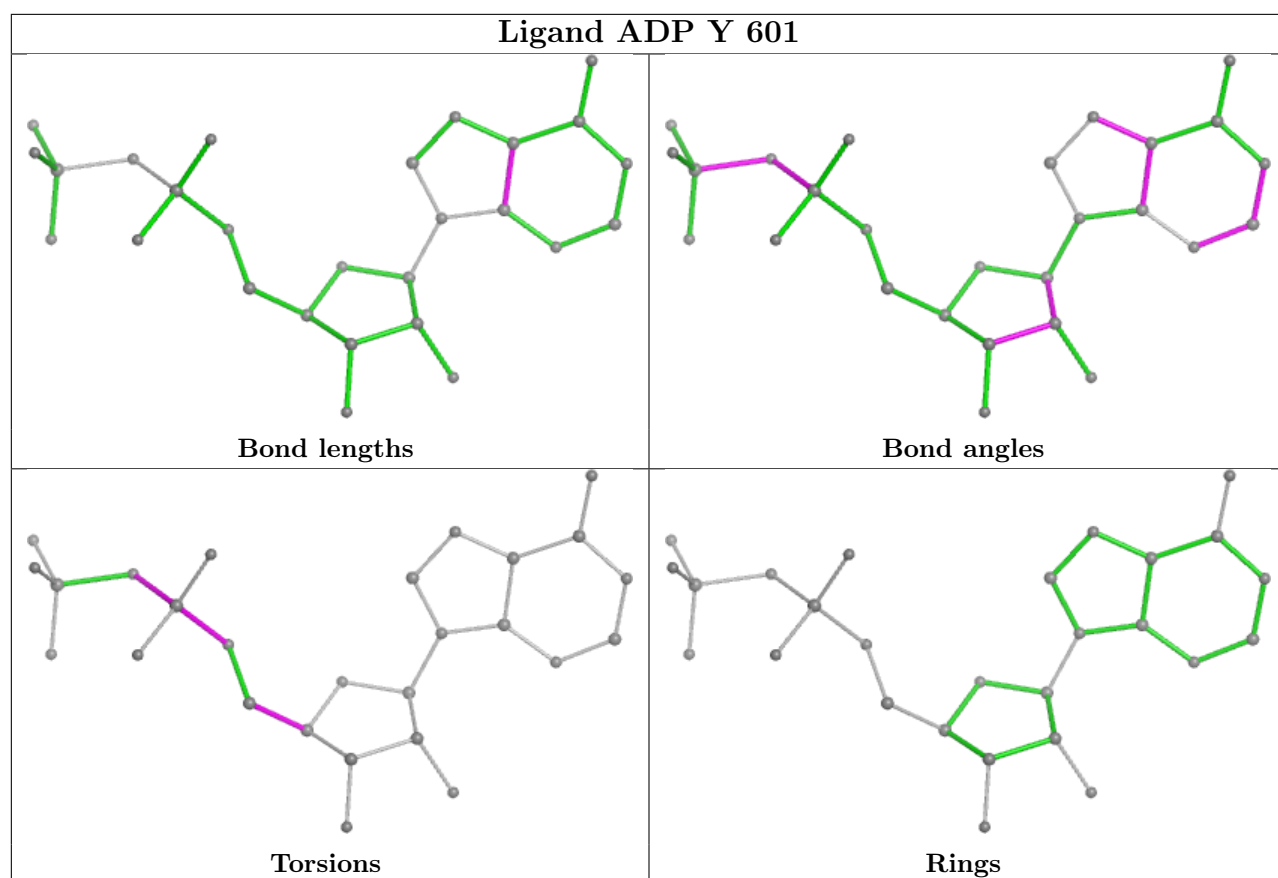
Mol	Chain	Res	Type	Atoms
20	V	1001	ATP	C5'-O5'-PA-O3A
22	Y	601	ADP	C5'-O5'-PA-O3A
22	Y	601	ADP	O4'-C4'-C5'-O5'
22	Y	601	ADP	C3'-C4'-C5'-O5'
22	Z	601	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

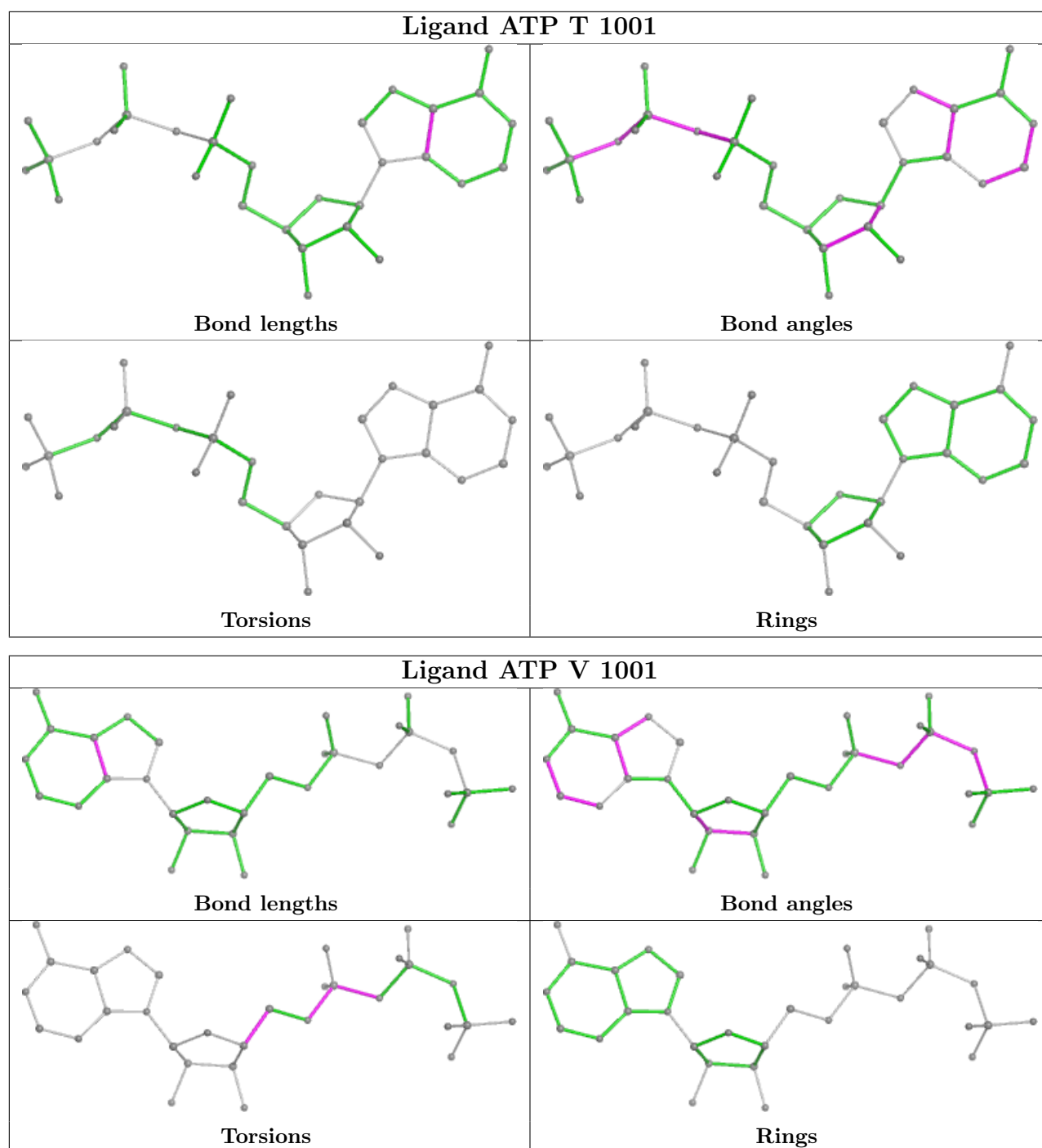
2 monomers are involved in 3 short contacts:

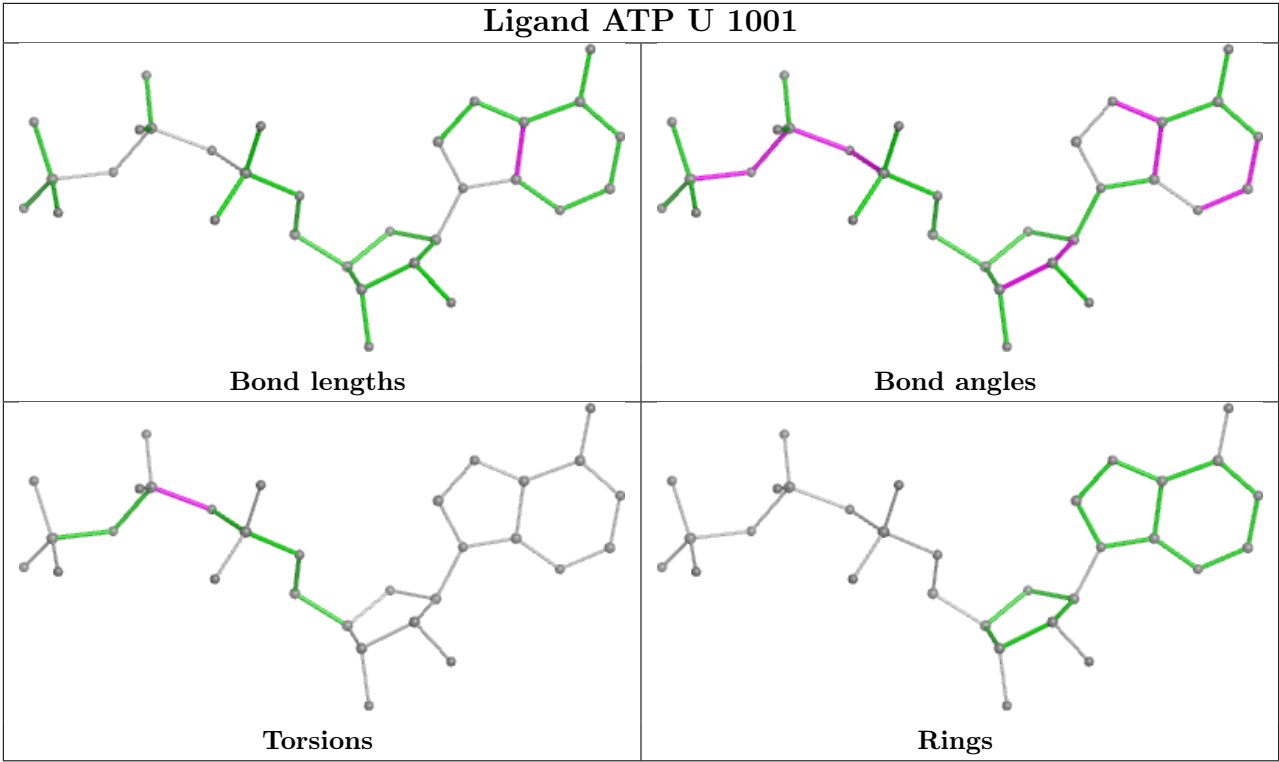
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	Z	601	ADP	1	0
20	V	1001	ATP	2	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	126:PHE	C	127:ALA	N	3.68

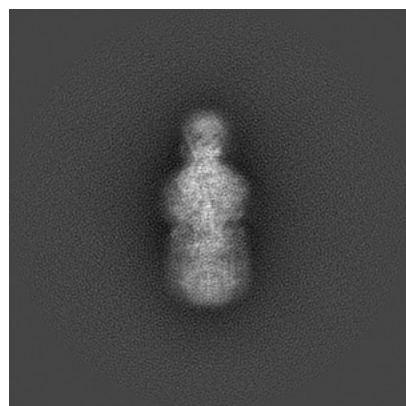
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4846. These allow visual inspection of the internal detail of the map and identification of artifacts.

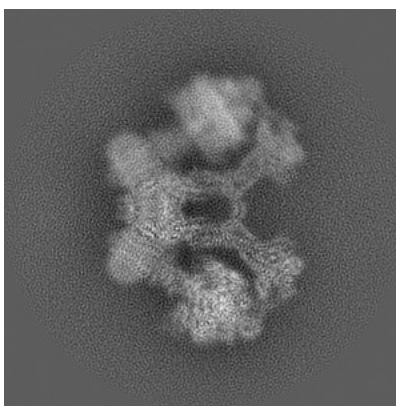
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

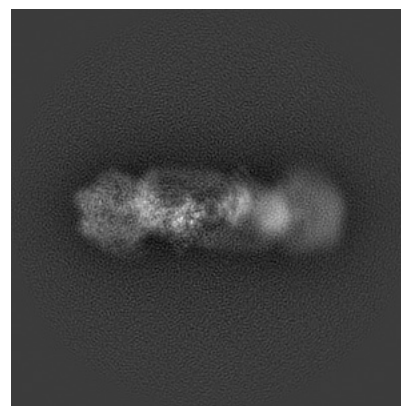
#### 6.1.1 Primary map



X

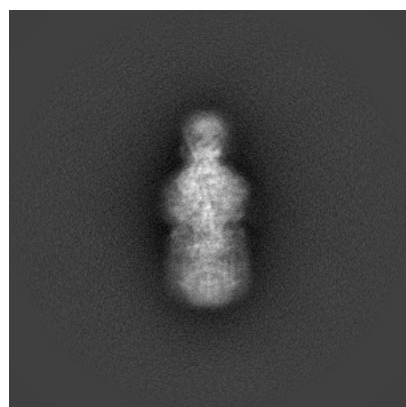


Y

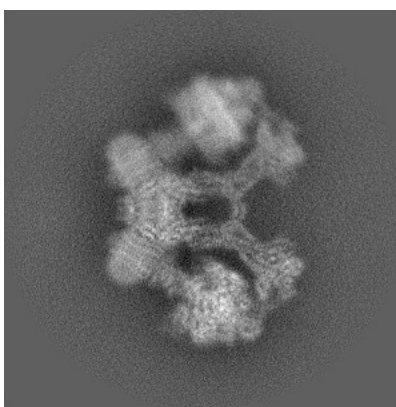


Z

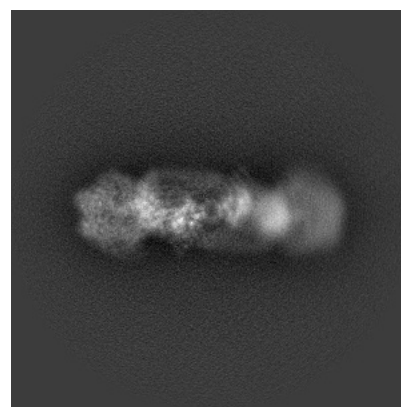
#### 6.1.2 Raw map



X



Y

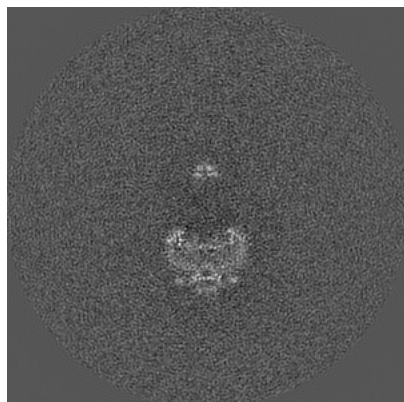


Z

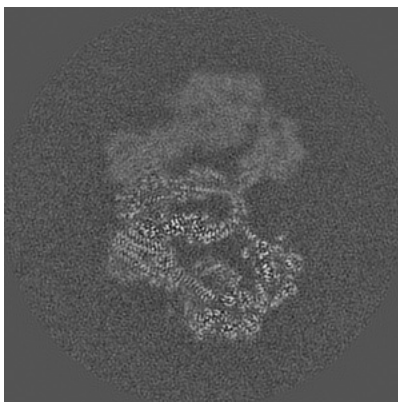
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

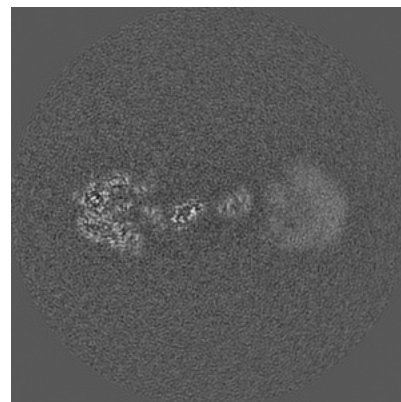
### 6.2.1 Primary map



X Index: 240

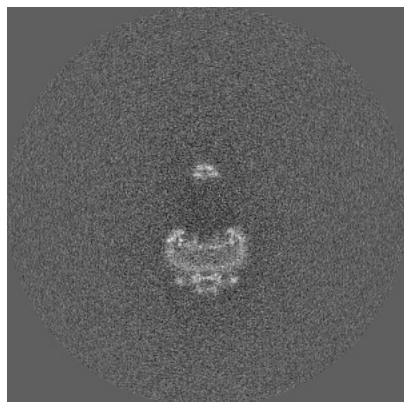


Y Index: 240

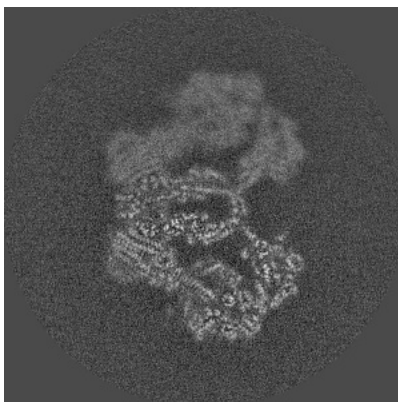


Z Index: 240

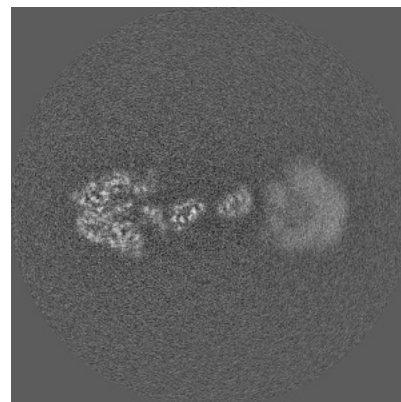
### 6.2.2 Raw map



X Index: 240



Y Index: 240

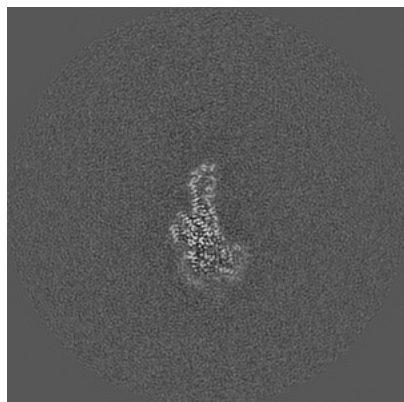


Z Index: 240

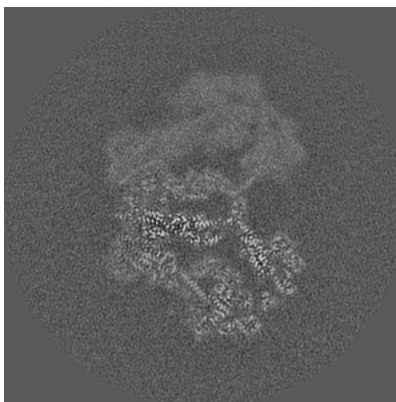
The images above show central slices of the map in three orthogonal directions.

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

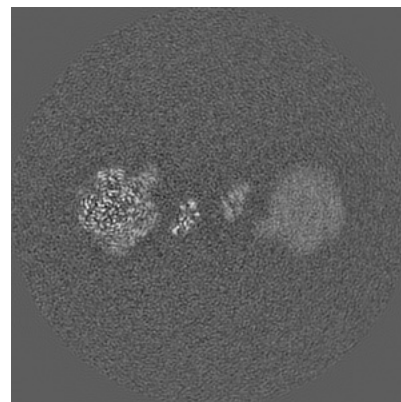
### 6.3.1 Primary map



X Index: 216



Y Index: 235

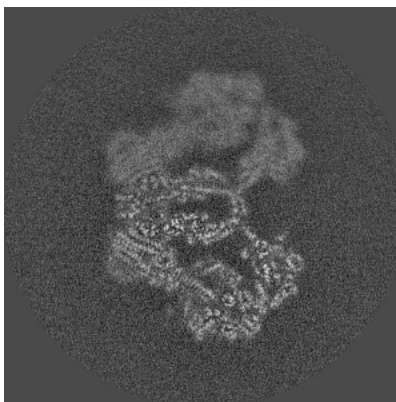


Z Index: 262

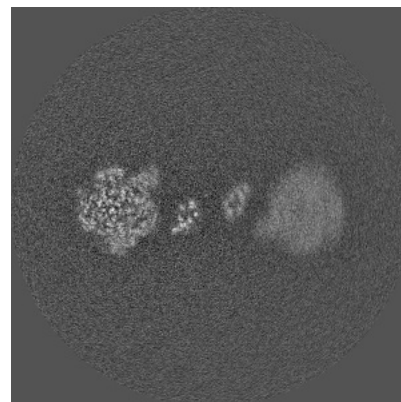
### 6.3.2 Raw map



X Index: 216



Y Index: 240



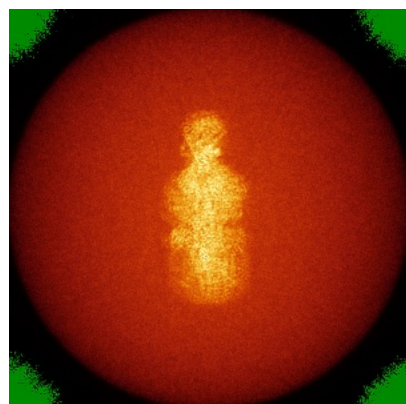
Z Index: 261

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

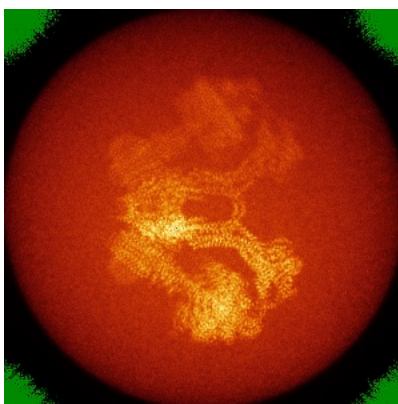


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

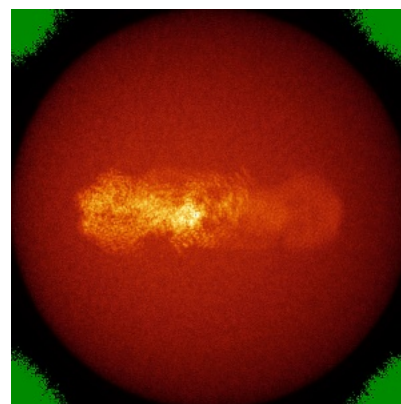
### 6.4.1 Primary map



X

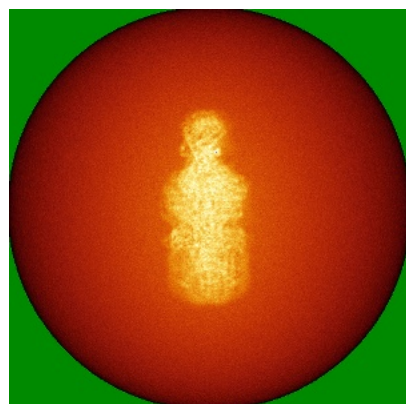


Y

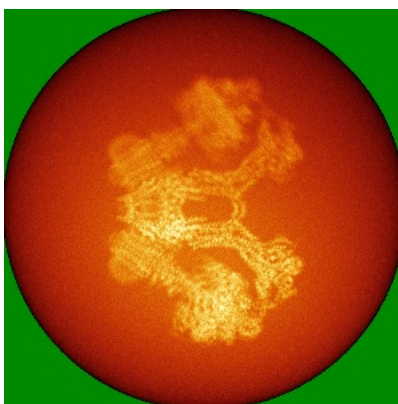


Z

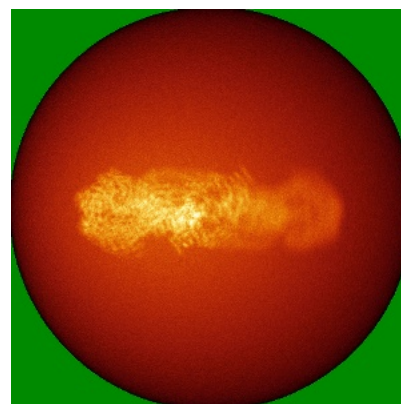
### 6.4.2 Raw map



X



Y

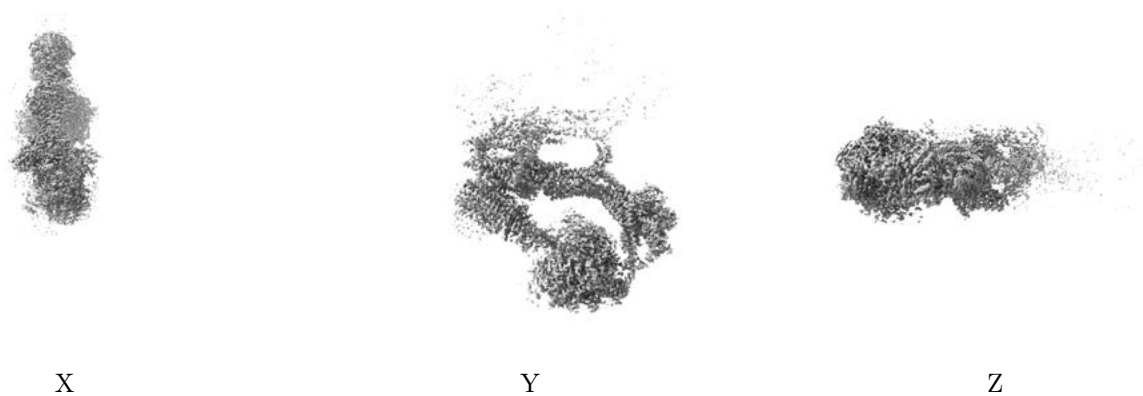


Z

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.

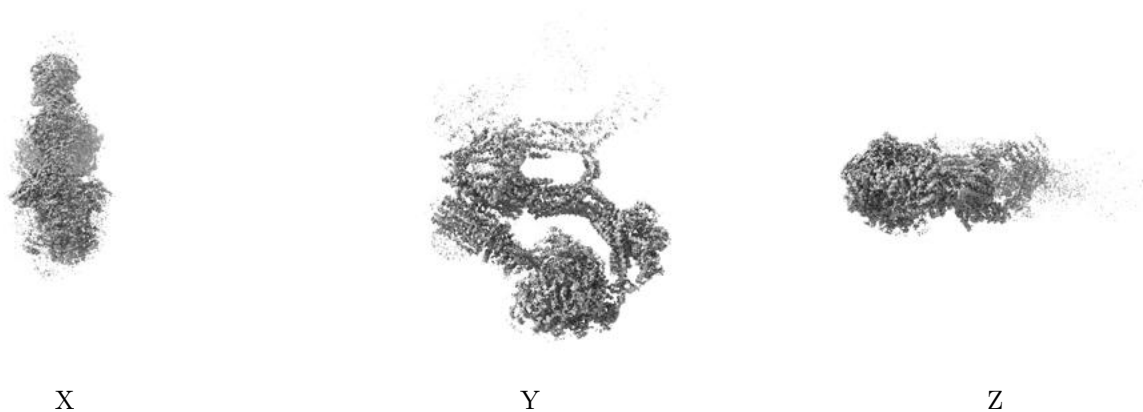
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

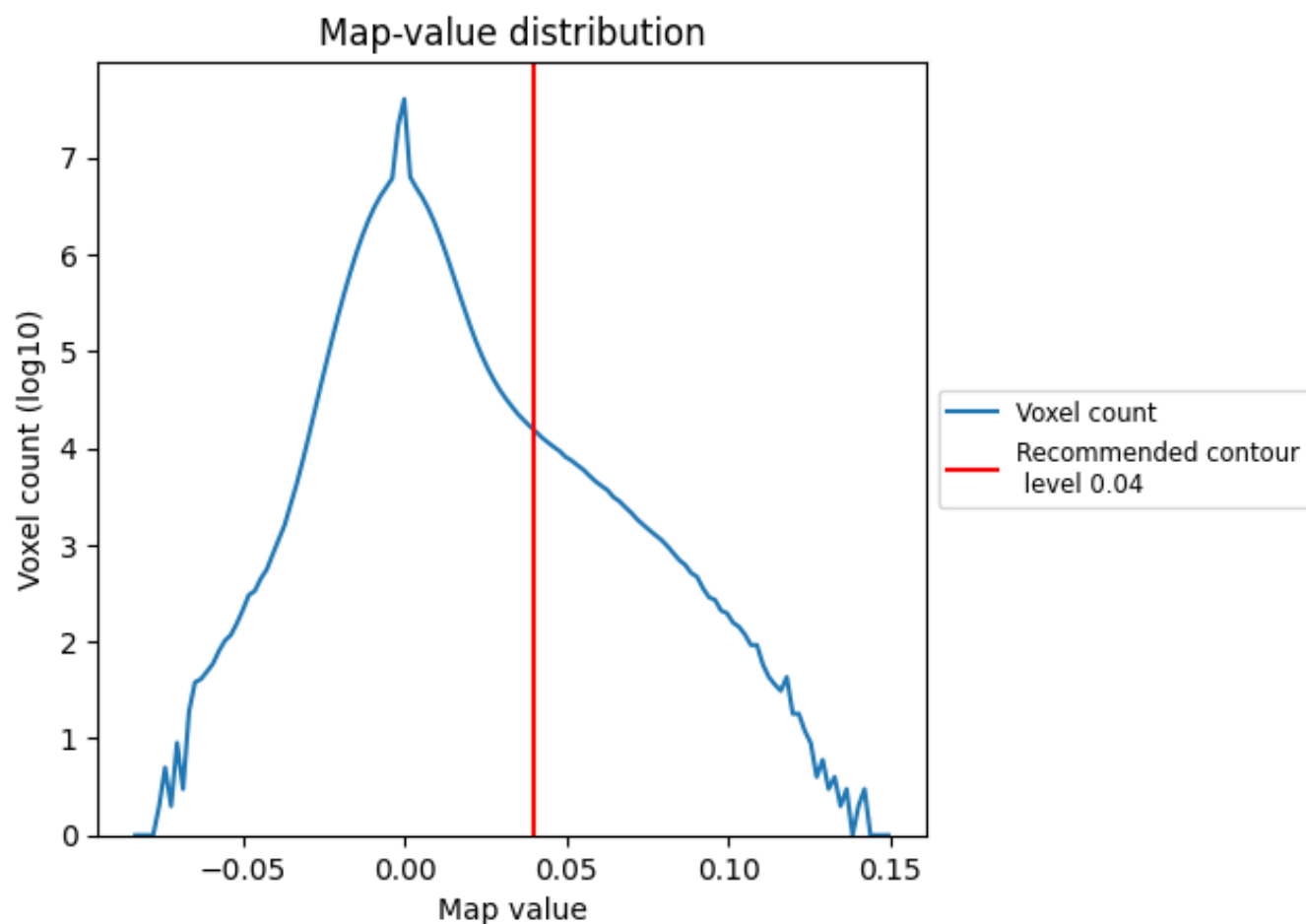
## 6.6 Mask visualisation [i](#)

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.

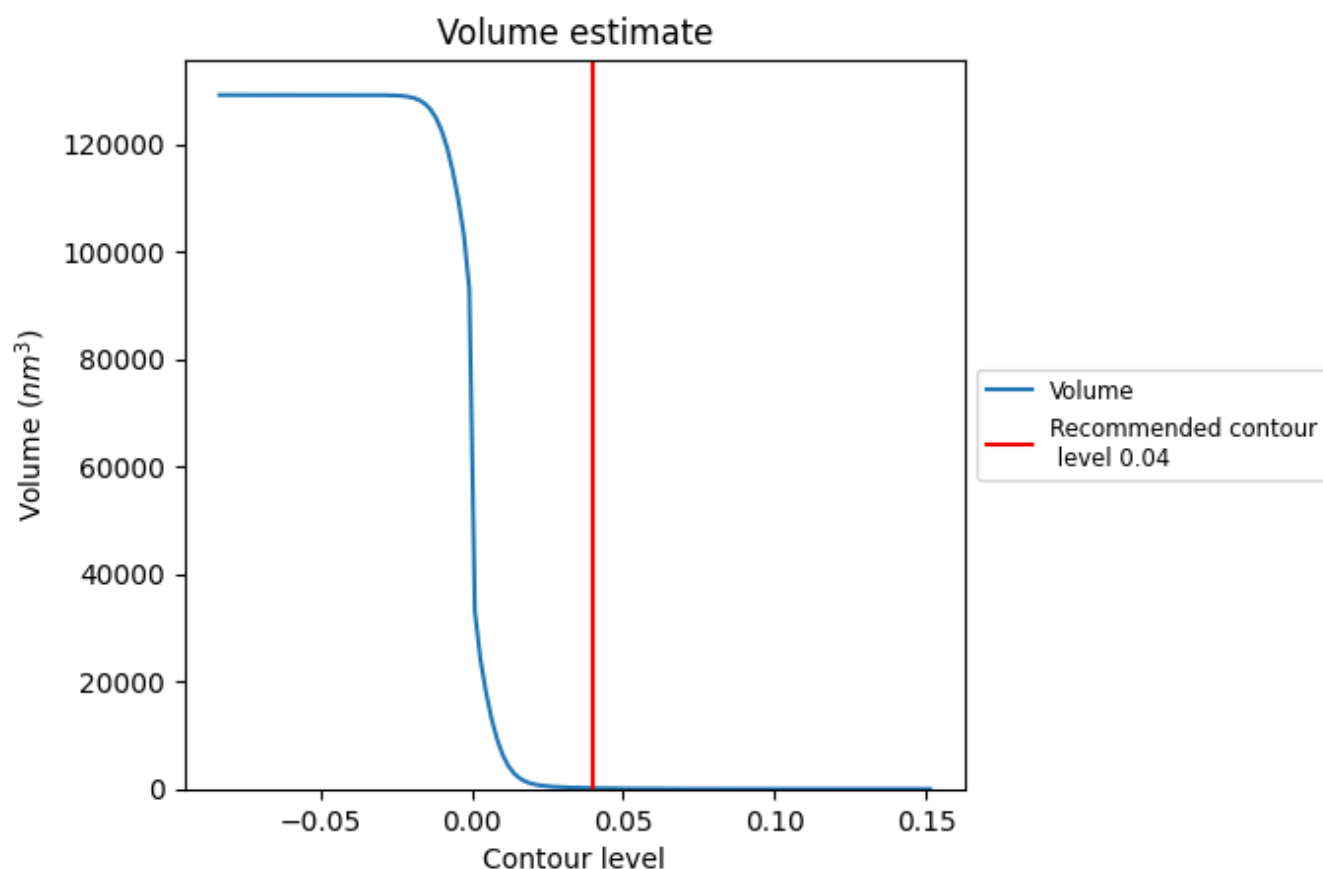
### 7.1 Map-value distribution [i](#)



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.



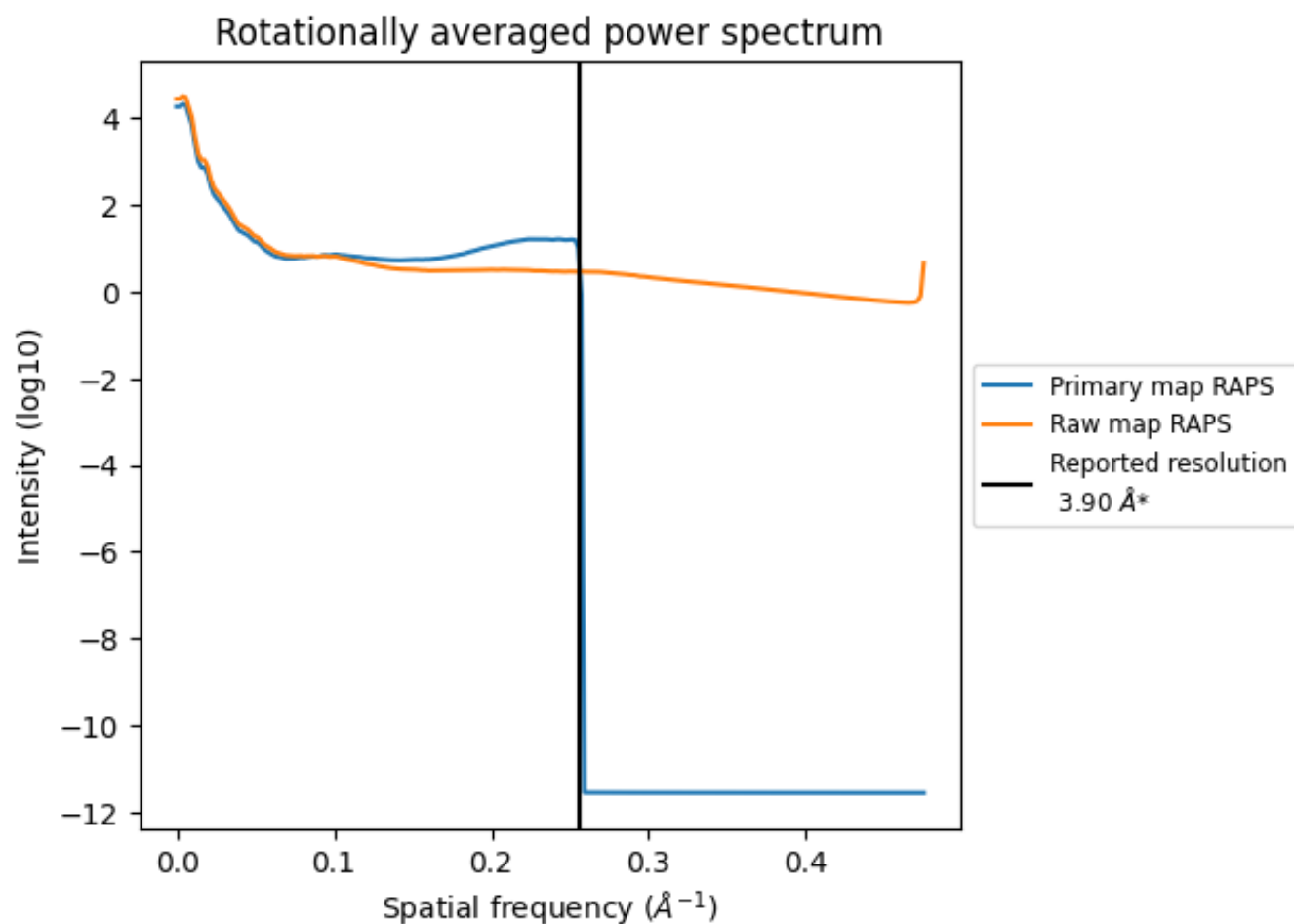
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm<sup>3</sup>; this corresponds to an approximate mass of 139 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 ⓘ

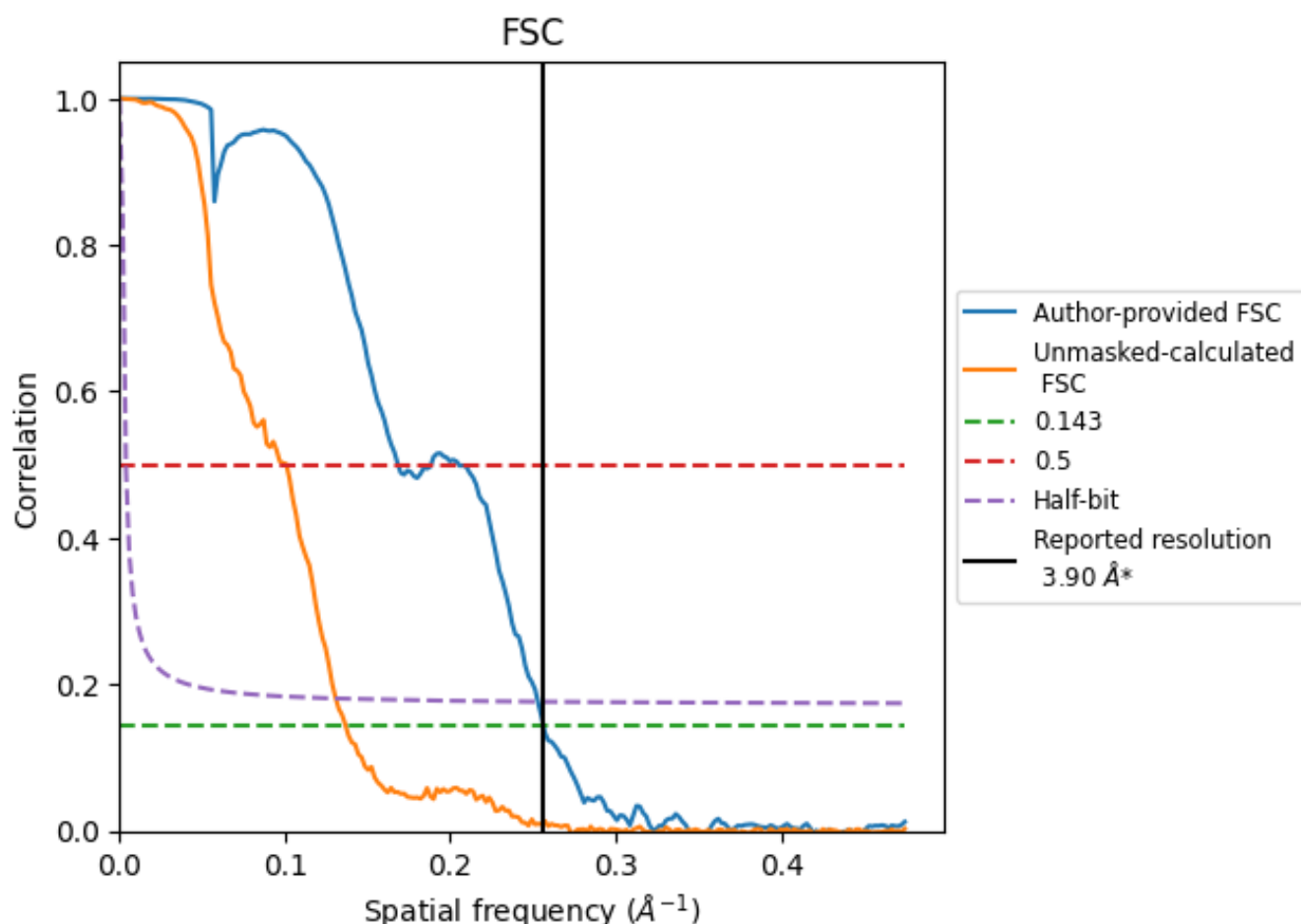


\*Reported resolution corresponds to spatial frequency of  $0.256 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.256  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

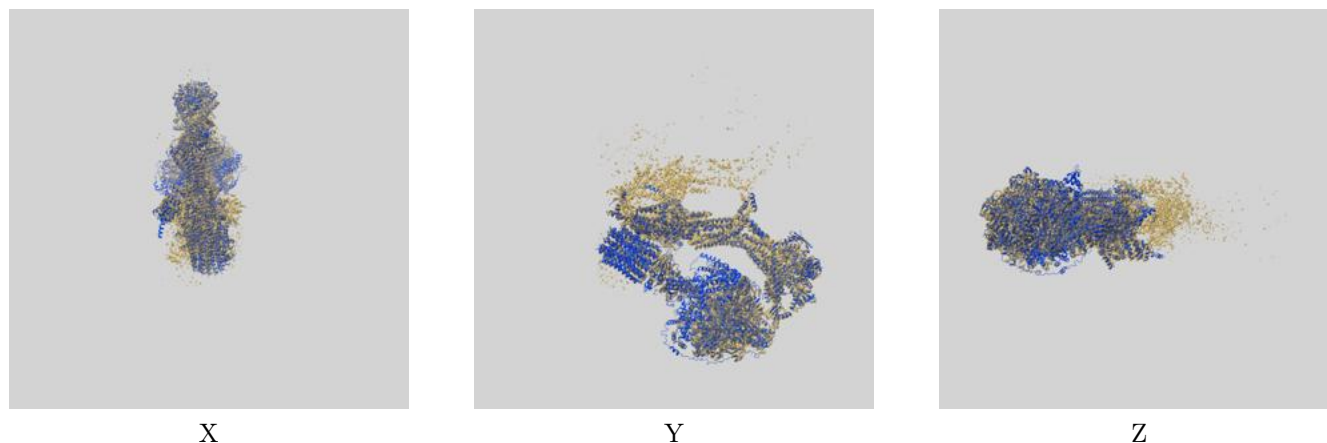
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.90	5.94	3.95
Unmasked-calculated*	7.31	9.90	7.65

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.31 differs from the reported value 3.9 by more than 10 %

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

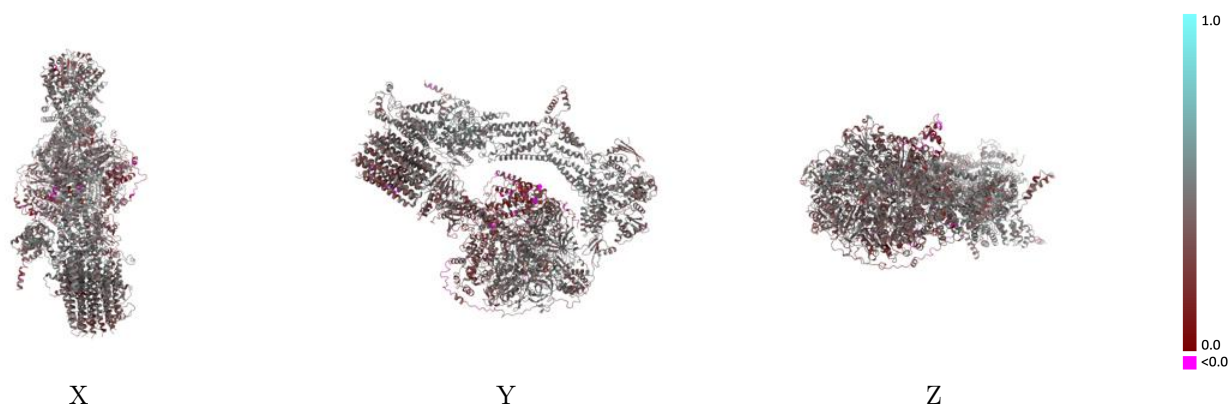
This section contains information regarding the fit between EMDB map EMD-4846 and PDB model 6RE9. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



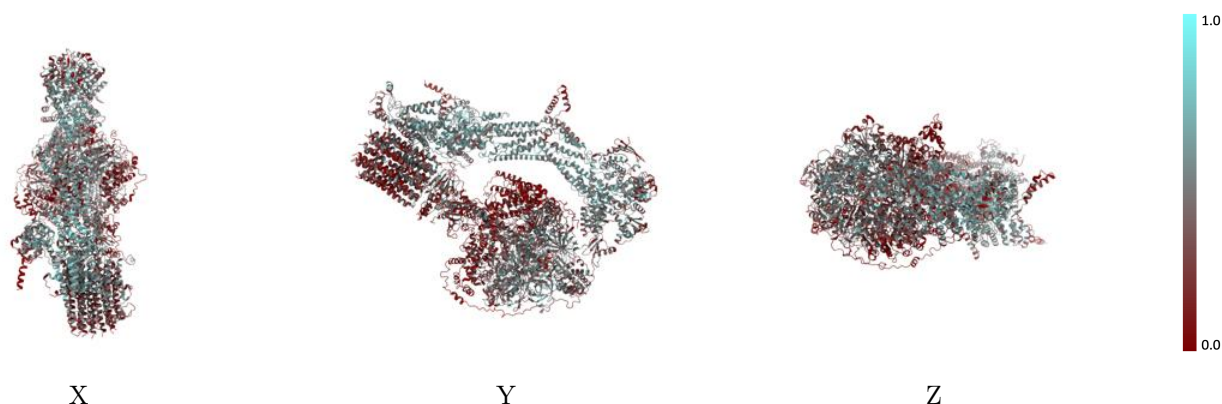
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



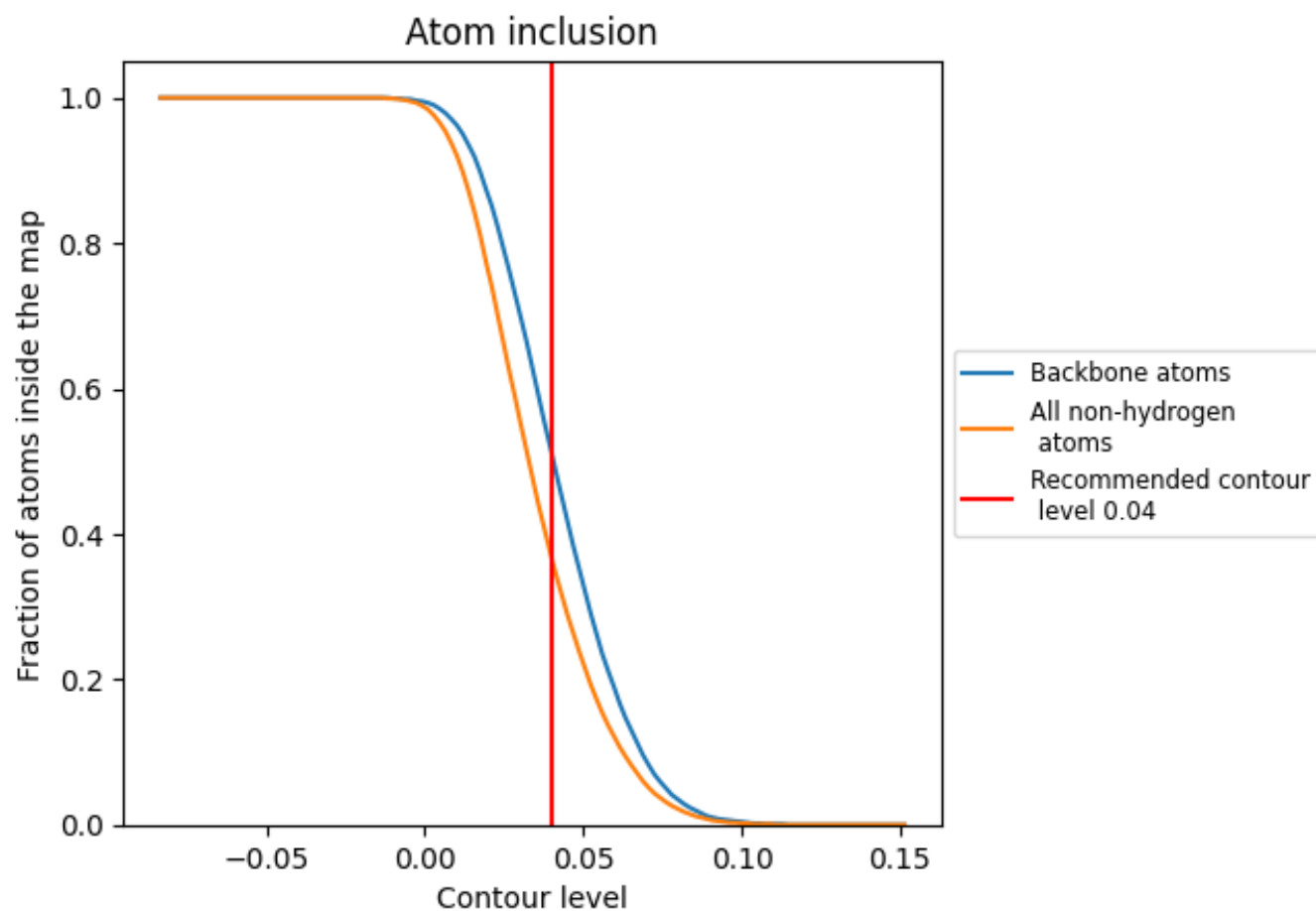
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 37% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3670	 0.3900
0	 0.4740	 0.4470
1	 0.5340	 0.4580
2	 0.4380	 0.4210
3	 0.4370	 0.4230
4	 0.4820	 0.4410
5	 0.6140	 0.4790
6	 0.5360	 0.4690
7	 0.5290	 0.4450
8	 0.5560	 0.4700
9	 0.3680	 0.4070
A	 0.2310	 0.3620
B	 0.2660	 0.3440
C	 0.2780	 0.3440
D	 0.2330	 0.3590
E	 0.2640	 0.3880
F	 0.3370	 0.4030
G	 0.3910	 0.4190
H	 0.4010	 0.4240
I	 0.3030	 0.4110
J	 0.2520	 0.3830
M	 0.5170	 0.4580
P	 0.3660	 0.3990
Q	 0.1960	 0.3340
R	 0.2280	 0.3520
S	 0.3050	 0.3520
T	 0.3370	 0.3670
U	 0.2570	 0.3280
V	 0.3940	 0.4020
X	 0.2120	 0.3120
Y	 0.3530	 0.3750
Z	 0.2460	 0.3420

