



Full wwPDB EM Validation Report ⓘ

Jun 17, 2024 – 11:28 AM EDT

PDB ID : 9BRB
EMDB ID : EMD-44355
Title : Synaptic Vesicle V-ATPase with synaptophysin and SidK, State 1
Authors : Coupland, C.E.; Rubinstein, J.L.
Deposited on : 2024-05-11
Resolution : 3.60 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

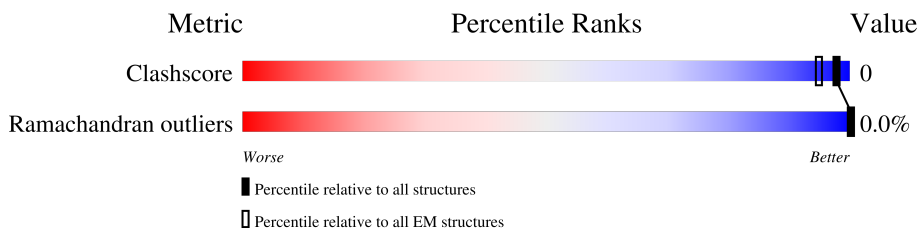
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 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

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 ≥ 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	647	92% 7%
1	B	647	93% 7%
1	C	647	93% 7%
2	D	511	90% 10%
2	E	511	89% 10%
2	F	511	88% 10%
3	G	382	97% ..
4	H	247	87% 13%
5	I	226	24% 100%

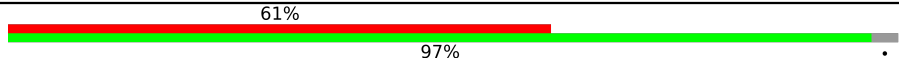

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	J	226	12% 99%
5	K	226	13% 99%
6	L	119	14% 92% 8%
7	M	118	41% 97%
7	N	118	28% 94%
7	O	118	34% 96%
8	P	463	26% 44% 56%
9	Q	573	47% 53%
9	R	573	46% 54%
9	S	573	46% 54%
10	T	463	92% 93% 7%
11	U	307	69% 69% 30%
12	a	838	81% 92% 8%
13	b	205	65% 99%
14	d	351	41% 100%
15	e	81	96% 99%
16	f	94	90% 91% 9%
17	g	155	86% 97%
17	h	155	89% 97%
17	i	155	81% 97%
17	j	155	74% 97%
17	k	155	82% 97%
17	l	155	85% 97%
17	m	155	85% 97%
17	n	155	77% 97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	o	155	 <p>61% 97%</p>
18	p	350	 <p>11% 15% 85%</p>

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 46437 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 H(+)-transporting two-sector ATPase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	600	2950	1750	600	600	0	0
1	B	600	2950	1750	600	600	0	0
1	C	600	2950	1750	600	600	0	0

- Molecule 2 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	459	2261	1343	459	459	0	0
2	E	459	2261	1343	459	459	0	0
2	F	459	2261	1343	459	459	0	0

- Molecule 3 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	G	375	1864	1114	375	375	0	0

- Molecule 4 is a protein called ATPase H⁺-transporting V1 subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	H	214	1061	633	214	214	0	0

- Molecule 5 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	225	Total	C	N	O	0	0
			1117	667	225	225		
5	J	223	Total	C	N	O	0	0
			1107	661	223	223		
5	K	224	Total	C	N	O	0	0
			1112	664	224	224		

- Molecule 6 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	110	Total	C	N	O	0	0
			542	322	110	110		

- Molecule 7 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	114	Total	C	N	O	0	0
			565	337	114	114		
7	N	113	Total	C	N	O	0	0
			560	334	113	113		
7	O	113	Total	C	N	O	0	0
			560	334	113	113		

- Molecule 8 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	204	Total	C	N	O	0	0
			1009	601	204	204		

- Molecule 9 is a protein called Type IV secretion protein Dot.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	267	Total	C	N	O	0	0
			1325	791	267	267		
9	R	263	Total	C	N	O	0	0
			1306	780	263	263		
9	S	264	Total	C	N	O	0	0
			1310	782	264	264		

- Molecule 10 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	T	430	2136	1276	430	430	0	0

- Molecule 11 is a protein called Synaptophysin.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	U	214	1055	627	214	214	0	0

- Molecule 12 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	a	772	3817	2273	772	772	0	0

- Molecule 13 is a protein called ATPase, H⁺ transporting, V0 subunit B (Predicted), isoform CRA_a.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	b	203	989	583	203	203	0	0

- Molecule 14 is a protein called V-type proton ATPase subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	d	350	1734	1034	350	350	0	0

- Molecule 15 is a protein called V-type proton ATPase subunit e 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	e	80	394	234	80	80	0	0

- Molecule 16 is a protein called Rnasek protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	f	86	422	250	86	86	0	0

- Molecule 17 is a protein called V-type proton ATPase 16 kDa proteolipid subunit c.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	150	Total 729	C 429	N 150	O 150	0	0
17	h	150	Total 729	C 429	N 150	O 150	0	0
17	i	150	Total 729	C 429	N 150	O 150	0	0
17	j	150	Total 729	C 429	N 150	O 150	0	0
17	k	150	Total 729	C 429	N 150	O 150	0	0
17	l	150	Total 729	C 429	N 150	O 150	0	0
17	m	150	Total 729	C 429	N 150	O 150	0	0
17	n	150	Total 729	C 429	N 150	O 150	0	0
17	o	150	Total 729	C 429	N 150	O 150	0	0

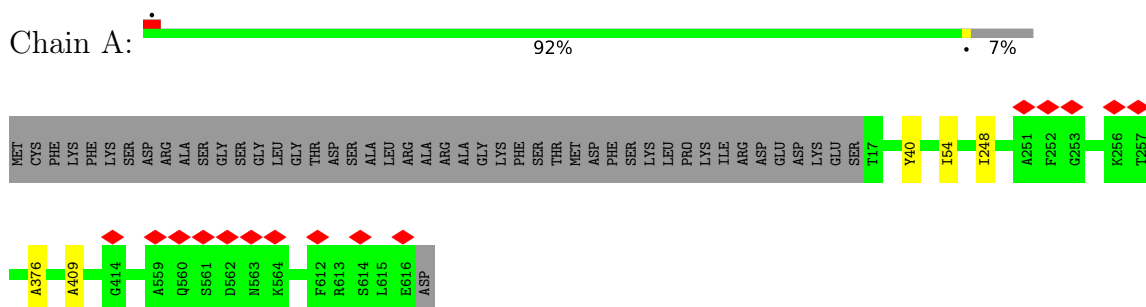
- Molecule 18 is a protein called Renin receptor.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	p	52	Total 258	C 154	N 52	O 52	0	0

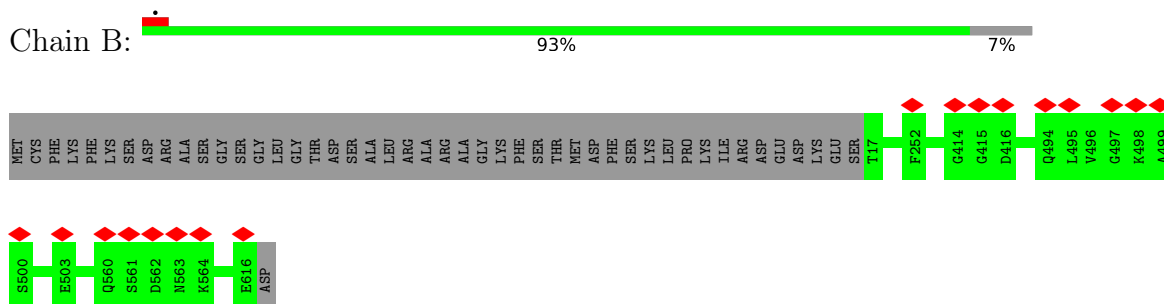
3 Residue-property plots

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.

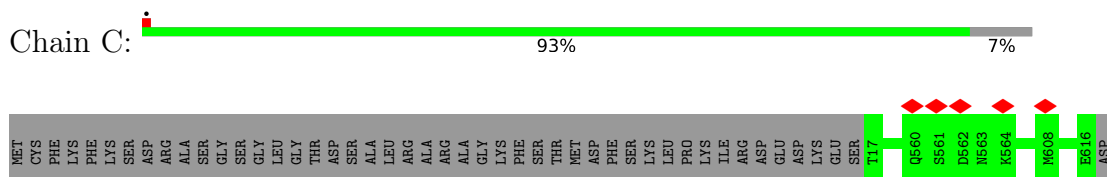
- Molecule 1: H(+)-transporting two-sector ATPase



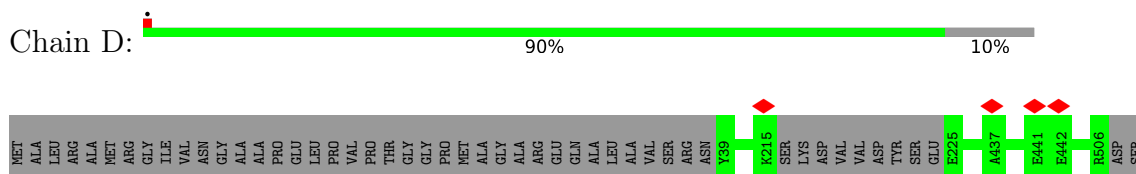
- Molecule 1: H(+)-transporting two-sector ATPase



- Molecule 1: H(+)-transporting two-sector ATPase




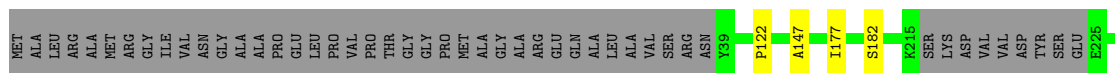
- Molecule 2: V-type proton ATPase subunit B, brain isoform



ALA
LYS
HIS


- Molecule 2: V-type proton ATPase subunit B, brain isoform

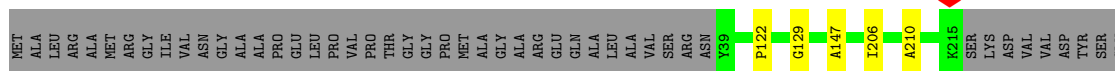
Chain E:  89% 10%



E309
R506
ASP
SER
ALA
LYS
HIS

- Molecule 2: V-type proton ATPase subunit B, brain isoform

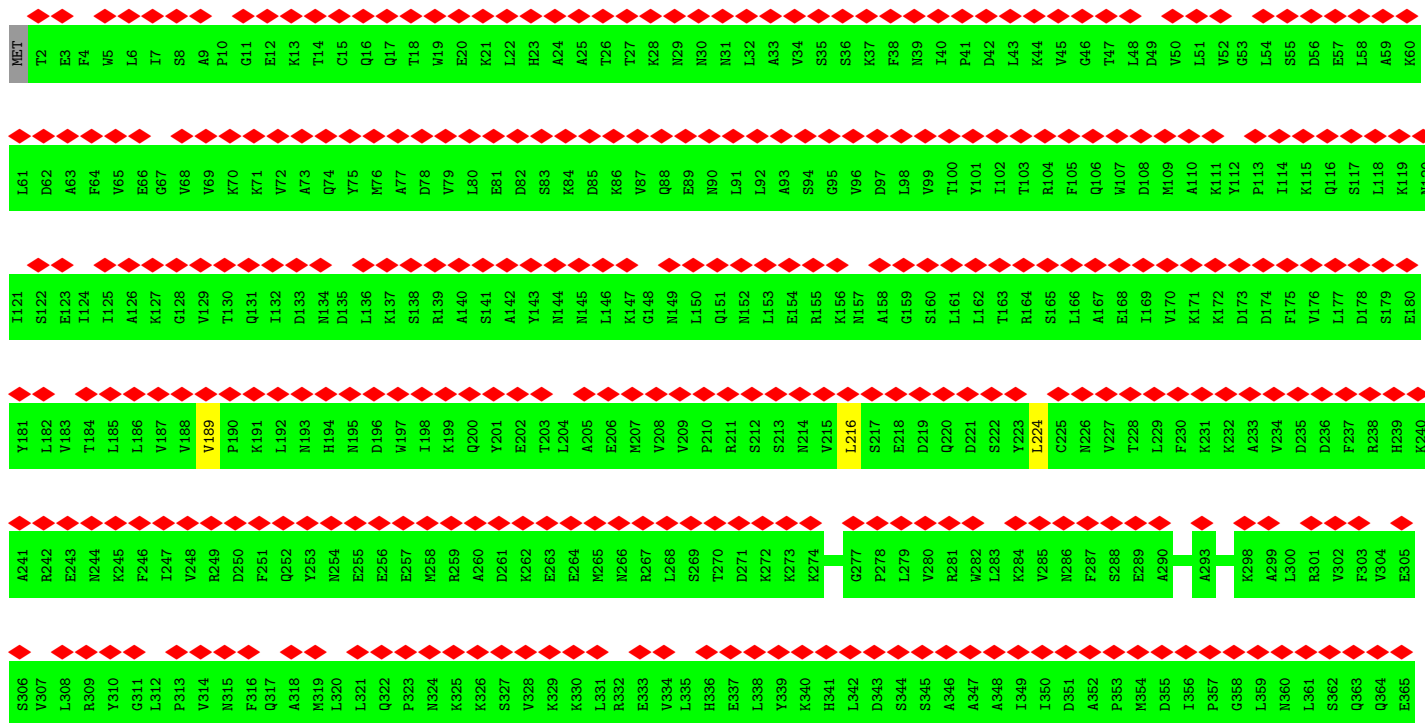
Chain F:  88% 10%

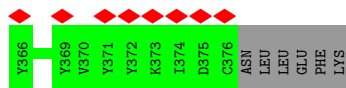


E225
A228
V257
V293
R506
ASP
SER
ALA
LYS
HIS

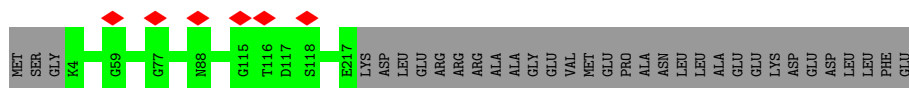
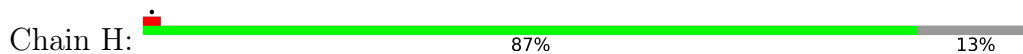
- Molecule 3: V-type proton ATPase subunit C 1

Chain G:  89% 97%

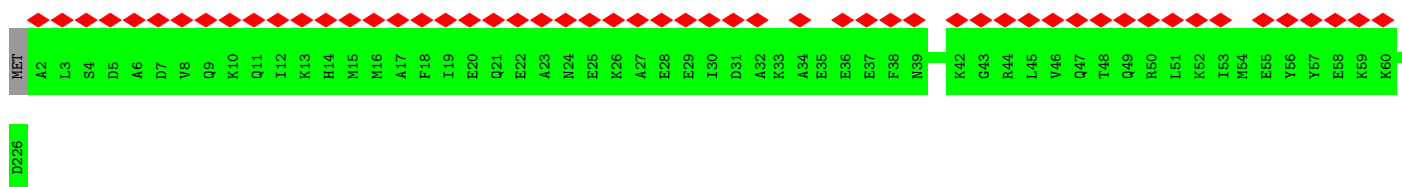




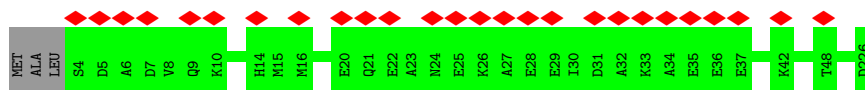
- Molecule 4: ATPase H⁺-transporting V1 subunit D



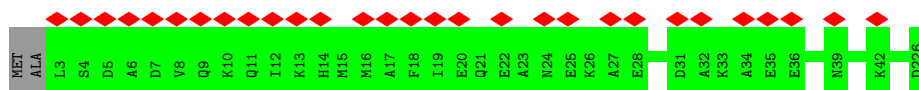
- Molecule 5: V-type proton ATPase subunit E 1



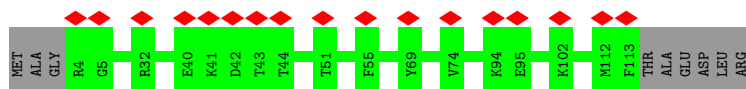
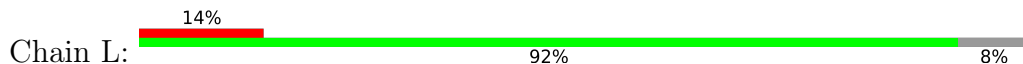
- Molecule 5: V-type proton ATPase subunit E 1



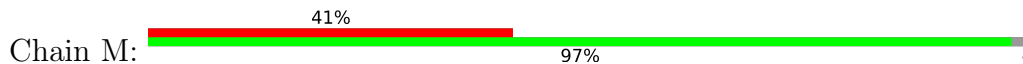
- Molecule 5: V-type proton ATPase subunit E 1



- Molecule 6: V-type proton ATPase subunit F

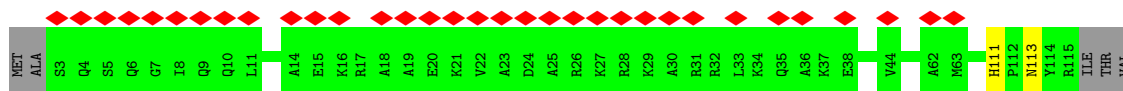
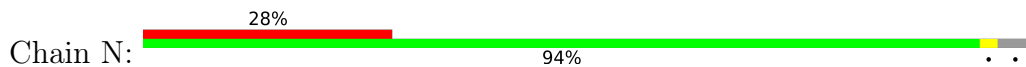


- Molecule 7: V-type proton ATPase subunit G

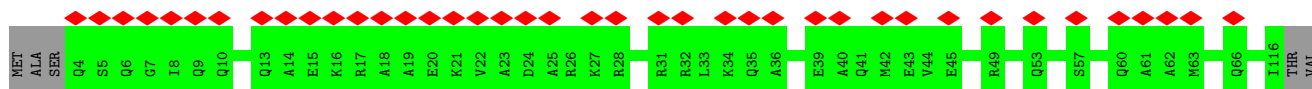




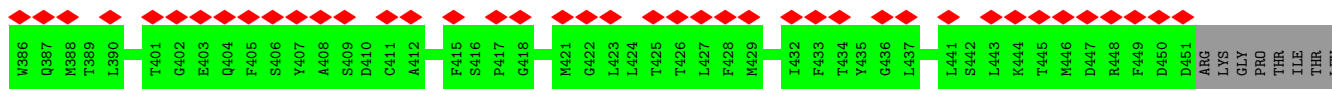
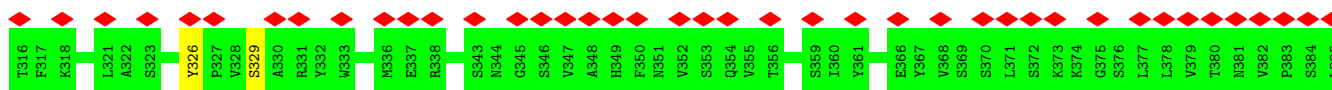
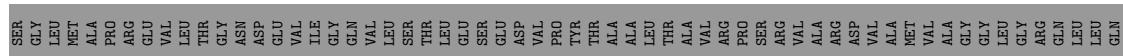
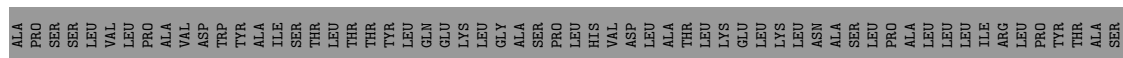
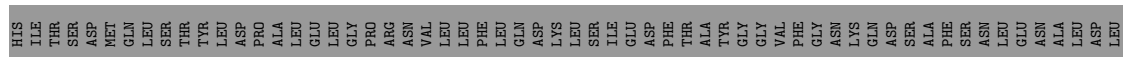
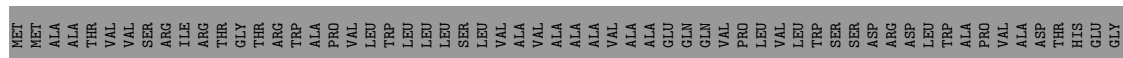
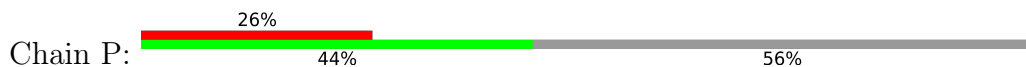
• Molecule 7: V-type proton ATPase subunit G



• Molecule 7: V-type proton ATPase subunit G

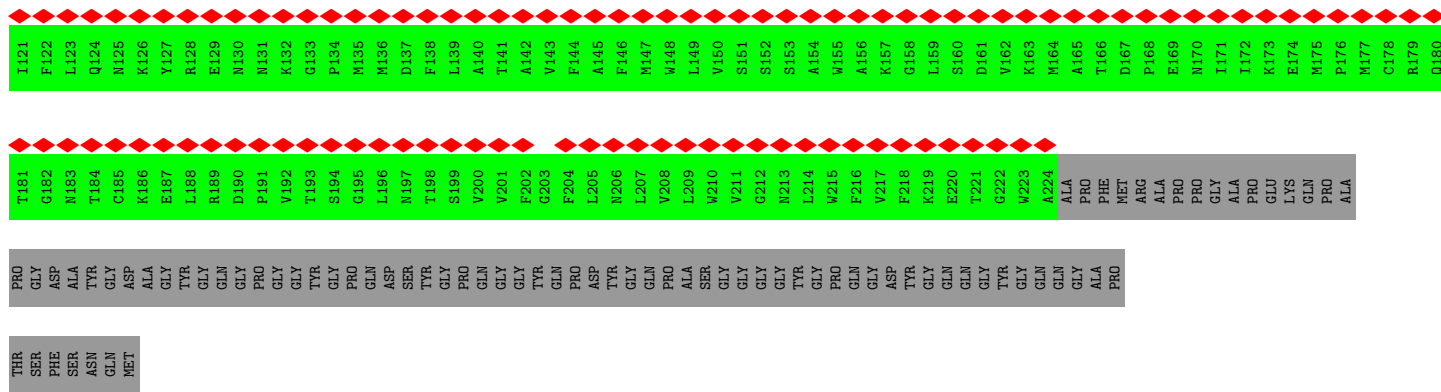


• Molecule 8: V-type proton ATPase subunit S1

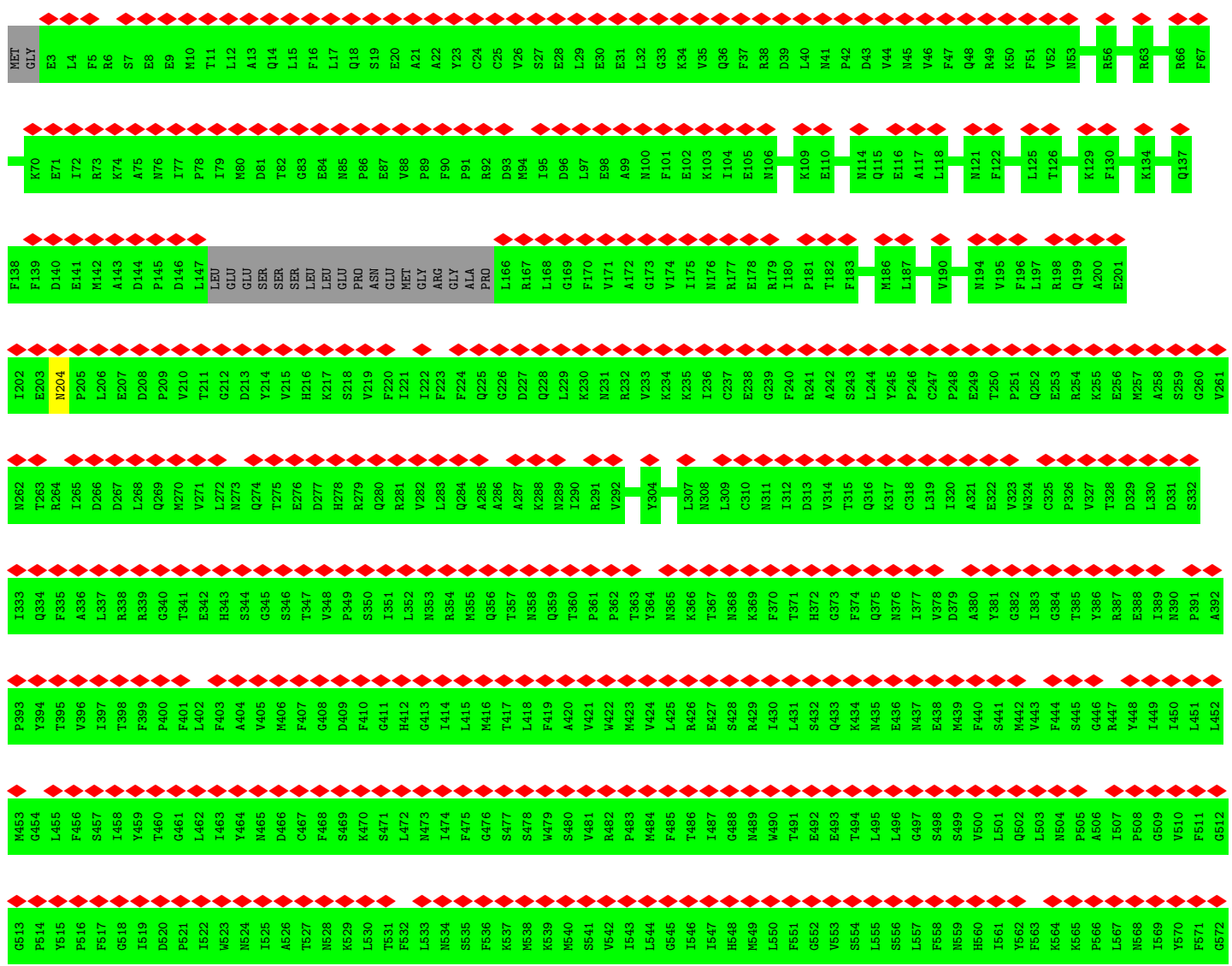
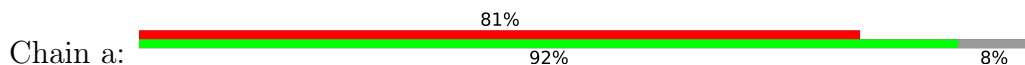


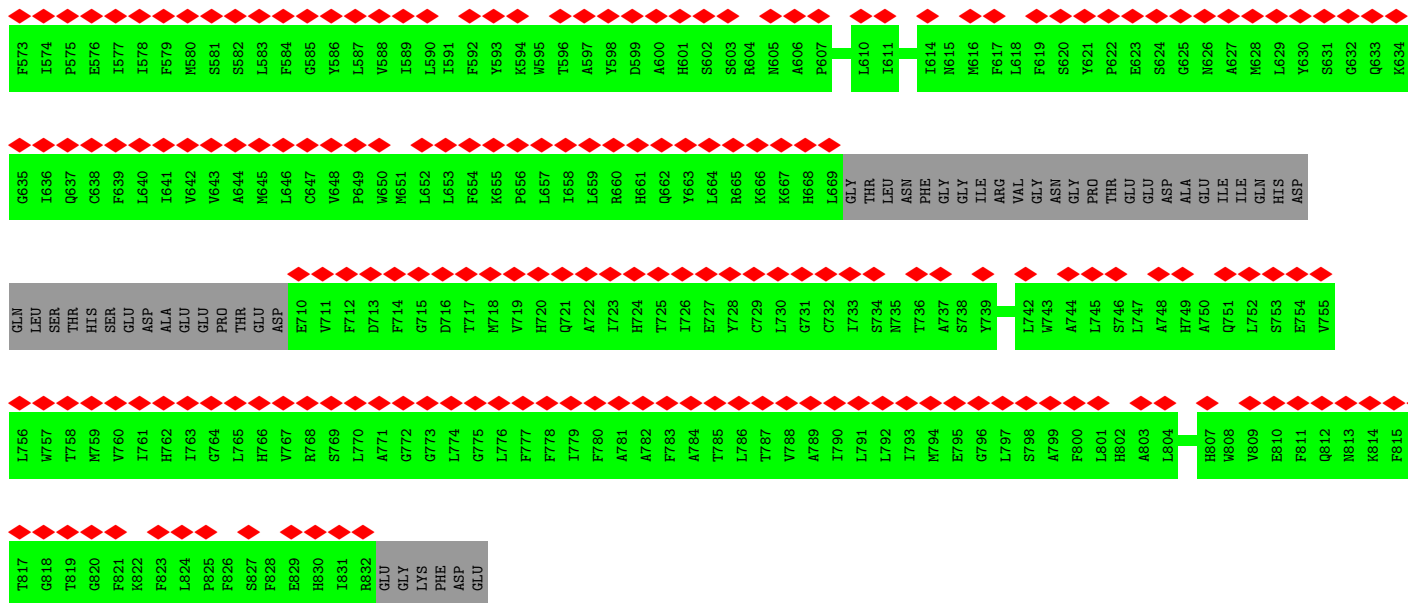
• Molecule 9: Type IV secretion protein Dot



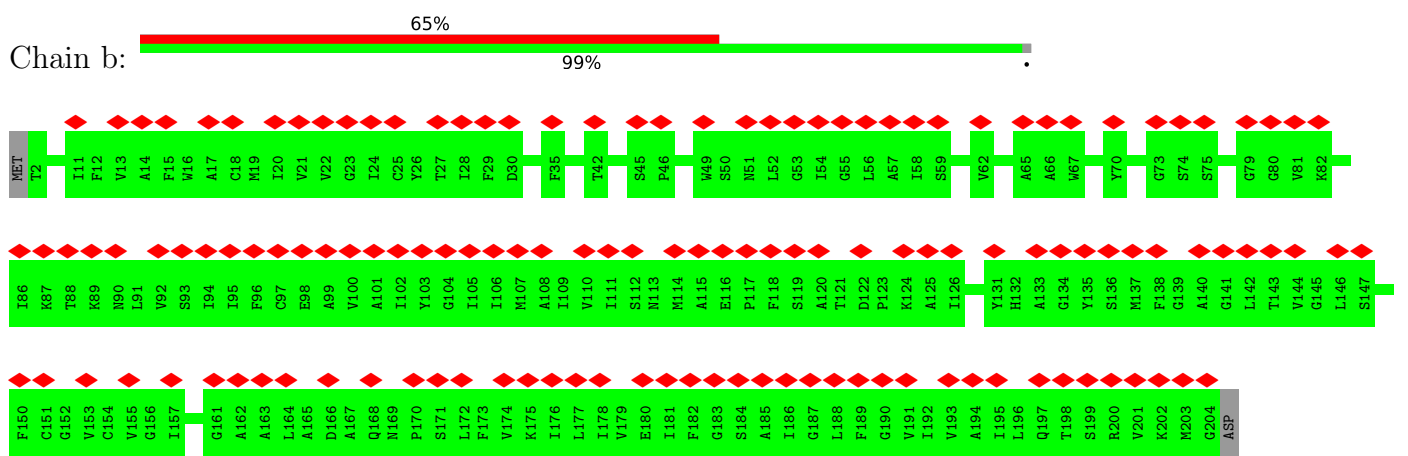


• Molecule 12: V-type proton ATPase 116 kDa subunit a isoform 1

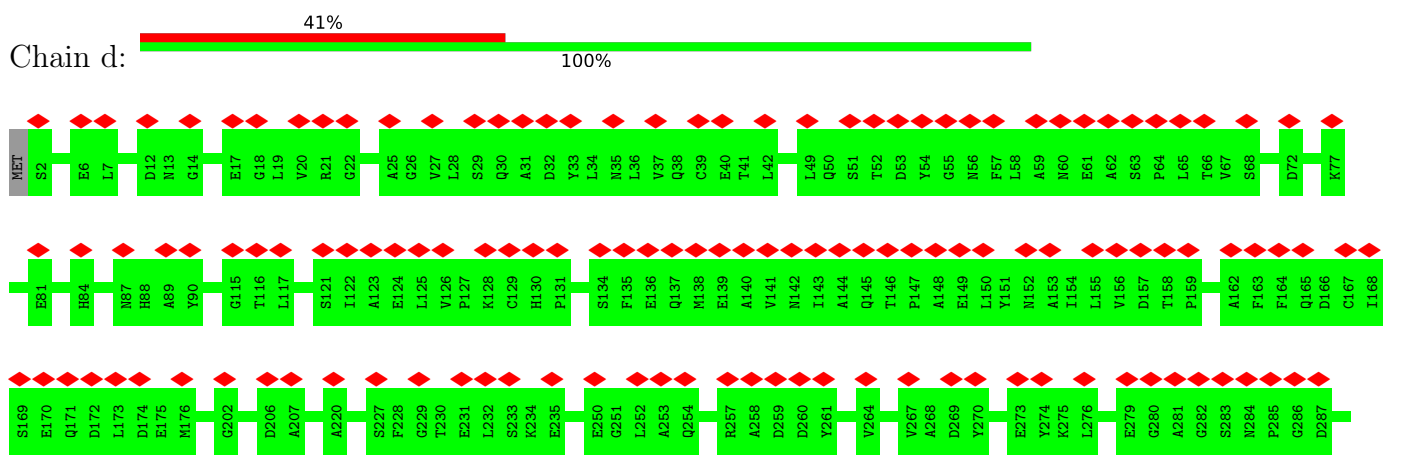


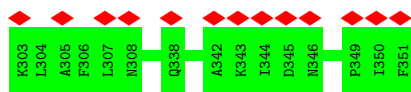


• Molecule 13: ATPase, H+ transporting, V0 subunit B (Predicted), isoform CRA_a

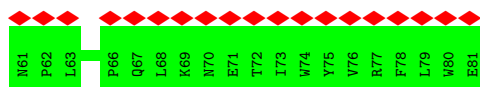
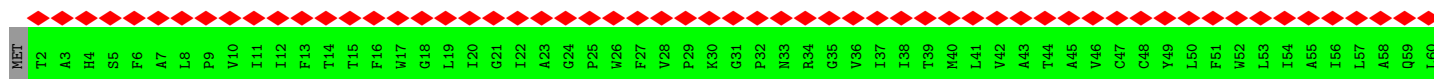


• Molecule 14: V-type proton ATPase subunit

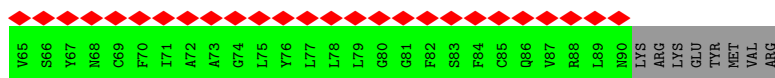
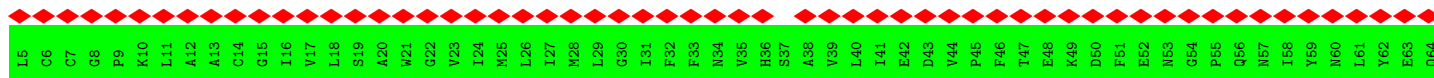
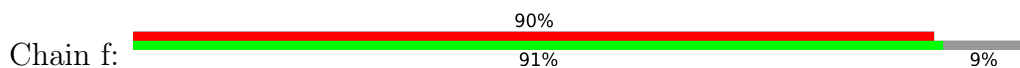




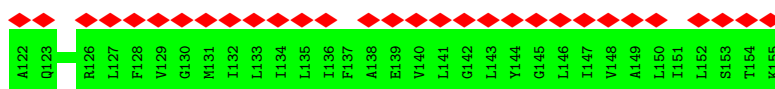
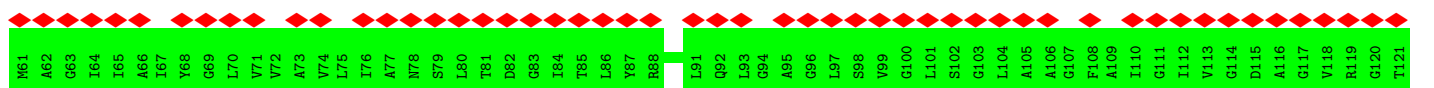
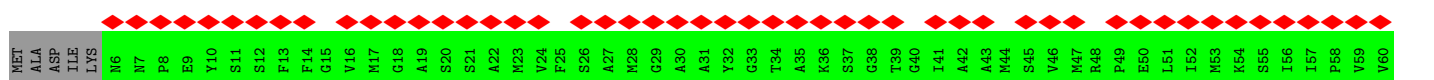
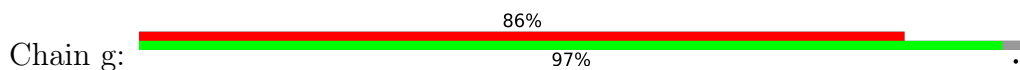
- Molecule 15: V-type proton ATPase subunit e 2



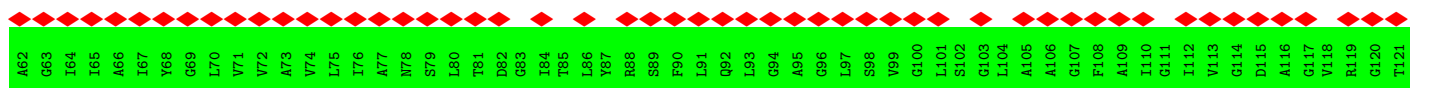
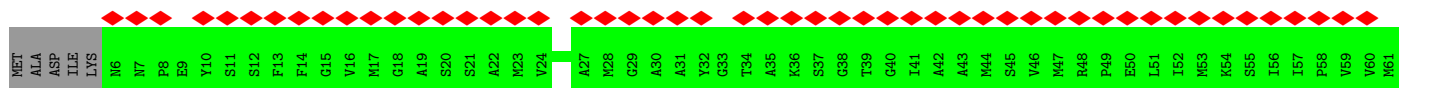
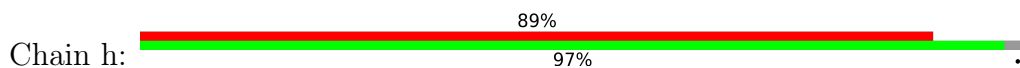
- Molecule 16: Rnasek protein

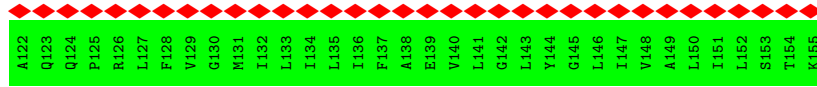


- Molecule 17: V-type proton ATPase 16 kDa proteolipid subunit c

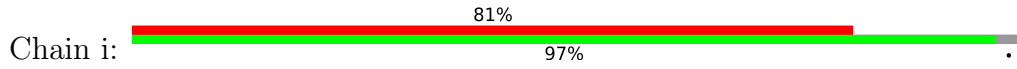


- Molecule 17: V-type proton ATPase 16 kDa proteolipid subunit c

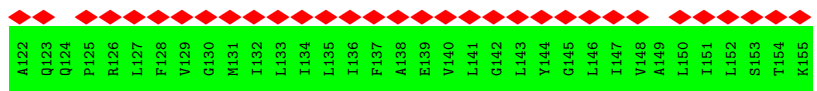




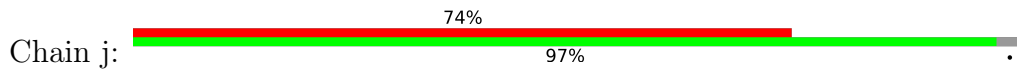
• Molecule 17: V-type proton ATPase 16 kDa proteolipid subunit c



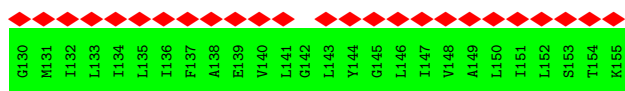
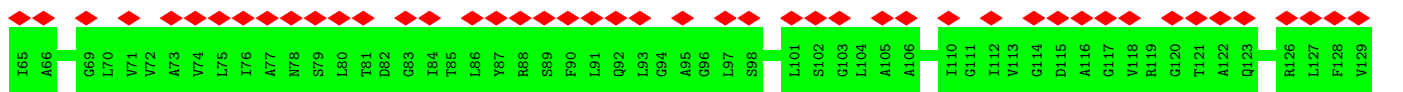
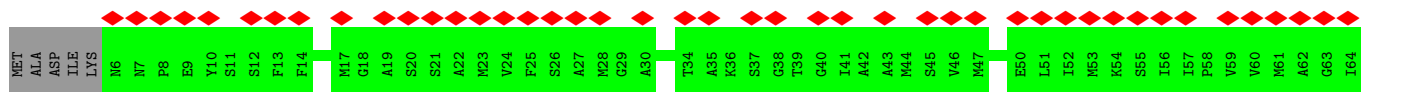
Chain i:



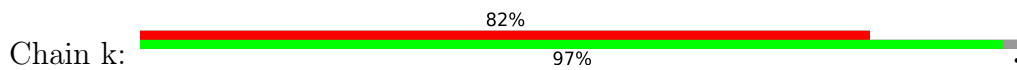
• Molecule 17: V-type proton ATPase 16 kDa proteolipid subunit c



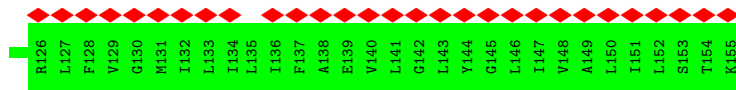
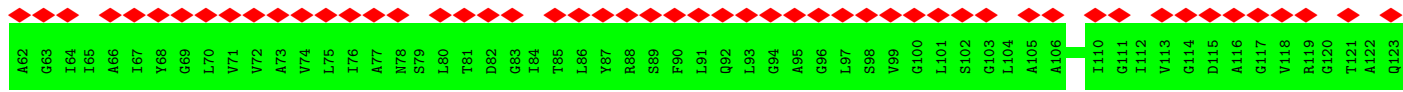
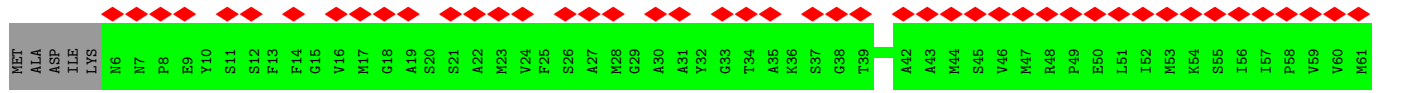
Chain j:



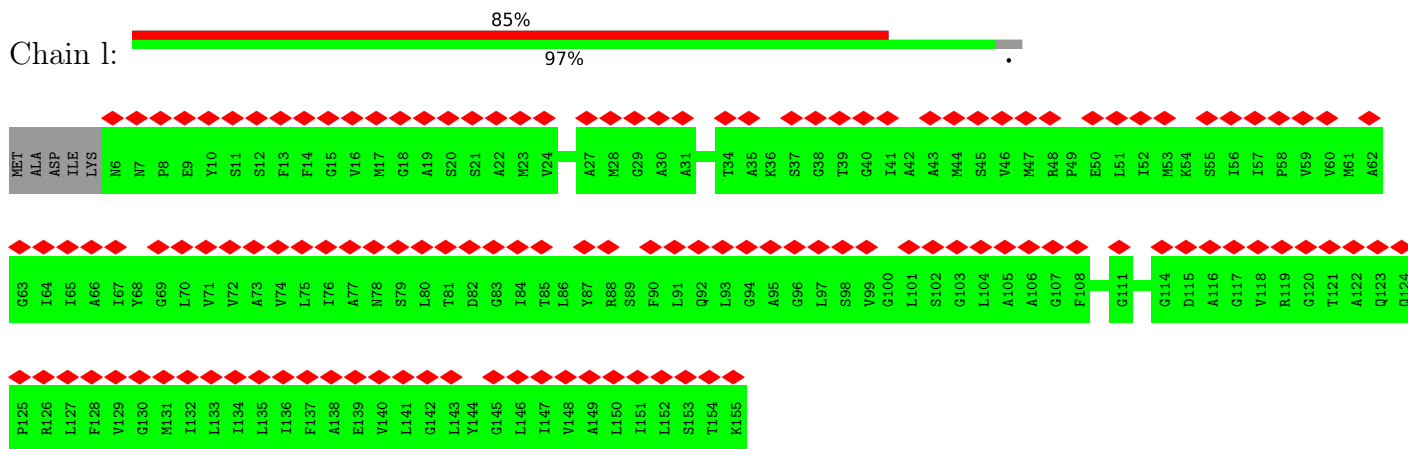
• Molecule 17: V-type proton ATPase 16 kDa proteolipid subunit c



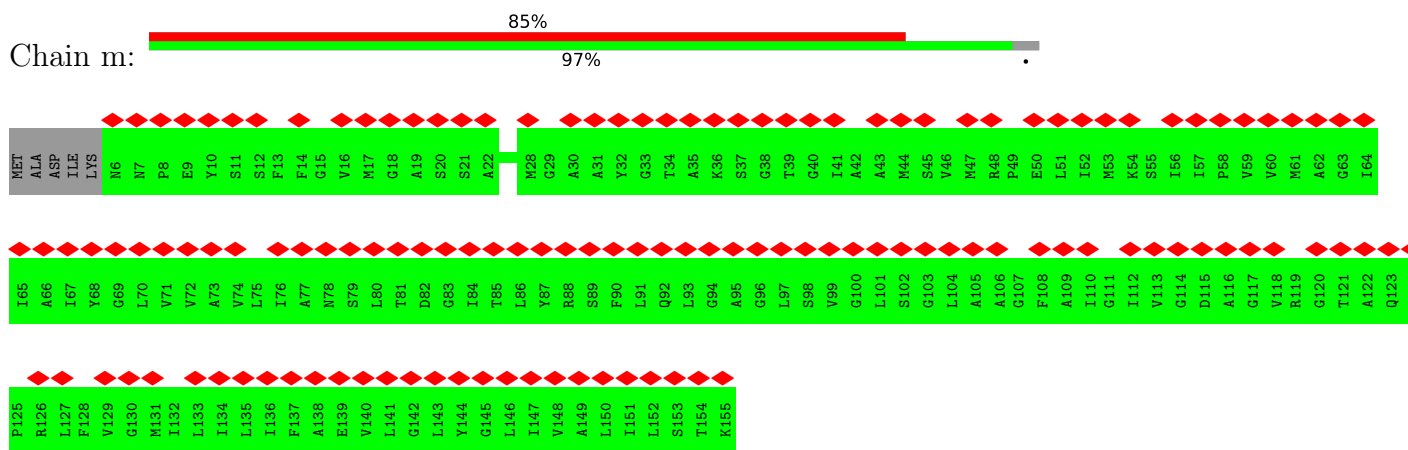
Chain k:



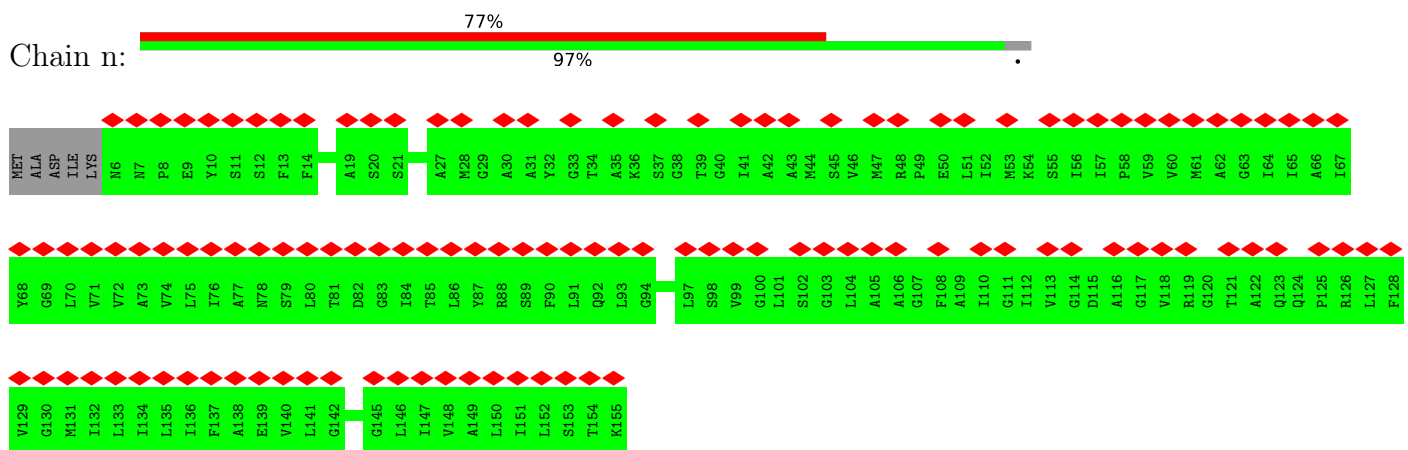
• Molecule 17: V-type proton ATPase 16 kDa proteolipid subunit c



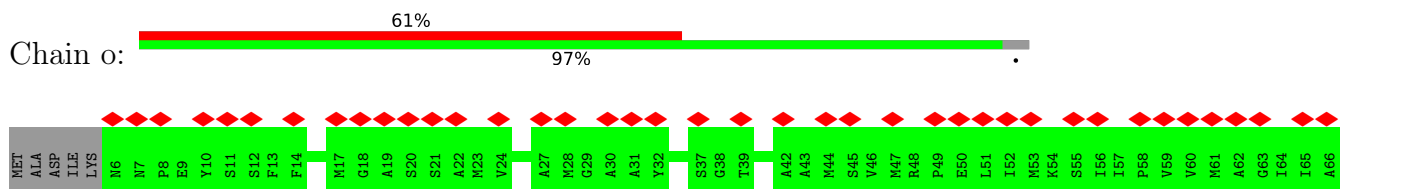
• Molecule 17: V-type proton ATPase 16 kDa proteolipid subunit c

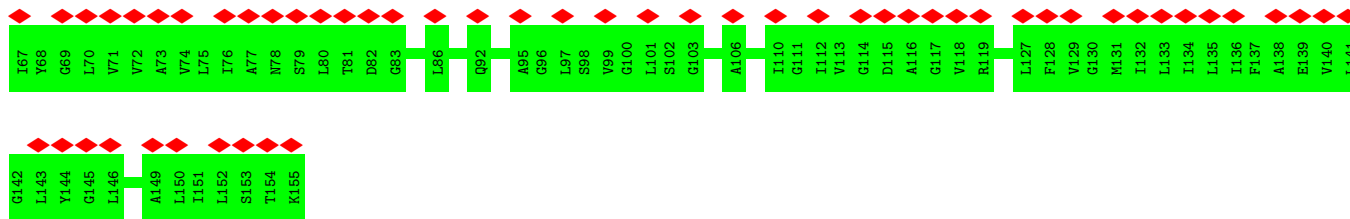


• Molecule 17: V-type proton ATPase 16 kDa proteolipid subunit c

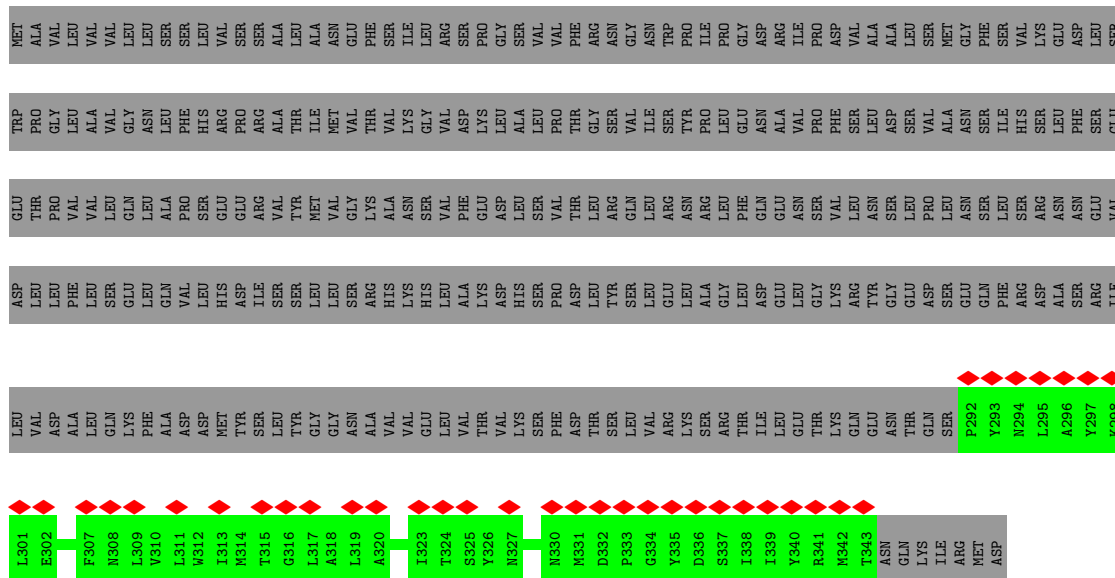


• Molecule 17: V-type proton ATPase 16 kDa proteolipid subunit c





• Molecule 18: Renin receptor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123220	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.295	Depositor
Minimum map value	-0.730	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	527.36, 527.36, 527.36	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3733333, 1.3733333, 1.3733333	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.28	0/2949	0.47	0/4097
1	B	0.27	0/2949	0.47	0/4097
1	C	0.29	0/2949	0.48	0/4097
2	D	0.29	0/2259	0.47	0/3139
2	E	0.29	0/2259	0.48	0/3139
2	F	0.29	0/2259	0.48	0/3139
3	G	0.24	0/1863	0.47	0/2600
4	H	0.25	0/1060	0.42	0/1477
5	I	0.25	0/1116	0.41	0/1556
5	J	0.25	0/1106	0.43	0/1542
5	K	0.25	0/1111	0.43	0/1549
6	L	0.24	0/541	0.48	0/751
7	M	0.25	0/564	0.40	0/785
7	N	0.26	0/559	0.42	0/778
7	O	0.25	0/559	0.40	0/778
8	P	0.28	0/1008	0.50	0/1403
9	Q	0.24	0/1324	0.43	0/1846
9	R	0.24	0/1305	0.41	0/1820
9	S	0.25	0/1309	0.42	0/1825
10	T	0.23	0/2134	0.42	0/2976
11	U	0.24	0/1054	0.45	0/1465
12	a	0.24	0/3814	0.45	0/5309
13	b	0.26	0/988	0.45	0/1366
14	d	0.25	0/1733	0.43	0/2415
15	e	0.26	0/393	0.44	0/545
16	f	0.24	0/421	0.42	0/583
17	g	0.28	0/728	0.47	0/1005
17	h	0.26	0/728	0.44	0/1005
17	i	0.27	0/728	0.45	0/1005
17	j	0.26	0/728	0.45	0/1005
17	k	0.26	0/728	0.46	0/1005
17	l	0.26	0/728	0.45	0/1005
17	m	0.27	0/728	0.46	0/1005
17	n	0.26	0/728	0.46	0/1005

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	o	0.26	0/728	0.45	0/1005
18	p	0.25	0/257	0.42	0/357
All	All	0.26	0/46395	0.45	0/64479

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2950	0	1348	3	0
1	B	2950	0	1348	0	0
1	C	2950	0	1348	0	0
2	D	2261	0	1019	0	0
2	E	2261	0	1019	3	0
2	F	2261	0	1019	4	0
3	G	1864	0	830	1	0
4	H	1061	0	493	0	0
5	I	1117	0	512	0	0
5	J	1107	0	505	0	0
5	K	1112	0	507	0	0
6	L	542	0	247	0	0
7	M	565	0	266	0	0
7	N	560	0	264	1	0
7	O	560	0	264	0	0
8	P	1009	0	443	1	0
9	Q	1325	0	573	0	0
9	R	1306	0	564	0	0
9	S	1310	0	567	0	0
10	T	2136	0	948	0	0
11	U	1055	0	489	2	0
12	a	3817	0	1672	0	0
13	b	989	0	489	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	d	1734	0	789	0	0
15	e	394	0	180	0	0
16	f	422	0	194	0	0
17	g	729	0	376	0	0
17	h	729	0	376	0	0
17	i	729	0	376	0	0
17	j	729	0	376	0	0
17	k	729	0	376	0	0
17	l	729	0	376	0	0
17	m	729	0	376	0	0
17	n	729	0	376	0	0
17	o	729	0	376	0	0
18	p	258	0	113	0	0
All	All	46437	0	21394	14	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 0.

All (14) 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)
11:U:31:ALA:HA	11:U:34:ALA:HB3	1.86	0.58
3:G:216:LEU:N	3:G:224:LEU:O	2.32	0.57
7:N:111:HIS:O	7:N:113:ASN:N	2.41	0.54
1:A:376:ALA:HB1	2:E:309:GLU:HA	1.92	0.52
2:F:206:ILE:O	2:F:210:ALA:HB2	2.13	0.49
1:A:40:TYR:N	1:A:54:ILE:O	2.43	0.47
2:F:129:GLY:N	2:F:257:VAL:O	2.42	0.47
2:F:122:PRO:CB	2:F:147:ALA:HB2	2.46	0.45
2:E:177:ILE:O	2:E:182:SER:N	2.50	0.45
8:P:326:TYR:O	8:P:329:SER:O	2.35	0.44
11:U:30:PHE:O	11:U:31:ALA:HB3	2.18	0.42
2:E:122:PRO:CB	2:E:147:ALA:HB2	2.50	0.42
1:A:248:ILE:O	1:A:409:ALA:HA	2.19	0.41
2:F:228:ALA:O	2:F:293:VAL:HA	2.20	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	598/647 (92%)	568 (95%)	30 (5%)	0	100	100
1	B	598/647 (92%)	571 (96%)	27 (4%)	0	100	100
1	C	598/647 (92%)	573 (96%)	25 (4%)	0	100	100
2	D	455/511 (89%)	432 (95%)	23 (5%)	0	100	100
2	E	455/511 (89%)	430 (94%)	25 (6%)	0	100	100
2	F	455/511 (89%)	438 (96%)	17 (4%)	0	100	100
3	G	373/382 (98%)	348 (93%)	24 (6%)	1 (0%)	41	75
4	H	212/247 (86%)	208 (98%)	4 (2%)	0	100	100
5	I	223/226 (99%)	223 (100%)	0	0	100	100
5	J	221/226 (98%)	217 (98%)	4 (2%)	0	100	100
5	K	222/226 (98%)	218 (98%)	4 (2%)	0	100	100
6	L	108/119 (91%)	103 (95%)	5 (5%)	0	100	100
7	M	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
7	N	111/118 (94%)	108 (97%)	3 (3%)	0	100	100
7	O	111/118 (94%)	109 (98%)	2 (2%)	0	100	100
8	P	202/463 (44%)	189 (94%)	13 (6%)	0	100	100
9	Q	265/573 (46%)	258 (97%)	7 (3%)	0	100	100
9	R	261/573 (46%)	259 (99%)	1 (0%)	1 (0%)	34	71
9	S	262/573 (46%)	258 (98%)	4 (2%)	0	100	100
10	T	426/463 (92%)	414 (97%)	12 (3%)	0	100	100
11	U	212/307 (69%)	209 (99%)	3 (1%)	0	100	100
12	a	766/838 (91%)	727 (95%)	38 (5%)	1 (0%)	51	83
13	b	201/205 (98%)	197 (98%)	4 (2%)	0	100	100
14	d	348/351 (99%)	339 (97%)	9 (3%)	0	100	100
15	e	78/81 (96%)	75 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	f	84/94 (89%)	81 (96%)	3 (4%)	0	100	100
17	g	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
17	h	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
17	i	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
17	j	148/155 (96%)	148 (100%)	0	0	100	100
17	k	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
17	l	148/155 (96%)	148 (100%)	0	0	100	100
17	m	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
17	n	148/155 (96%)	148 (100%)	0	0	100	100
17	o	148/155 (96%)	148 (100%)	0	0	100	100
18	p	50/350 (14%)	48 (96%)	2 (4%)	0	100	100
All	All	9339/11520 (81%)	9036 (97%)	300 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	189	VAL
9	R	99	SER
12	a	204	ASN

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

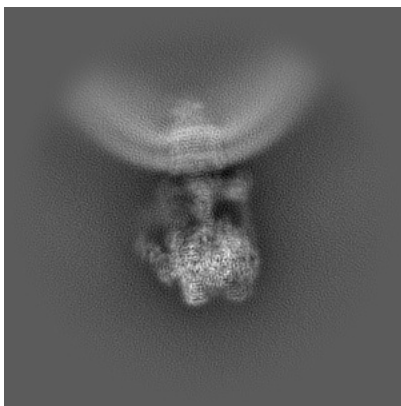
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44355. These allow visual inspection of the internal detail of the map and identification of artifacts.

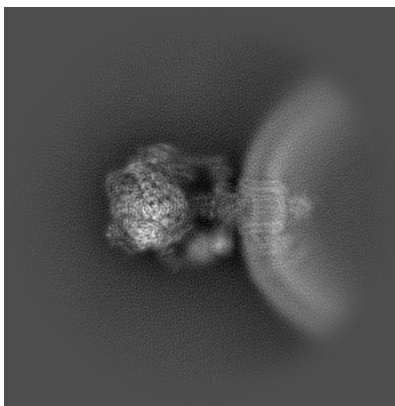
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

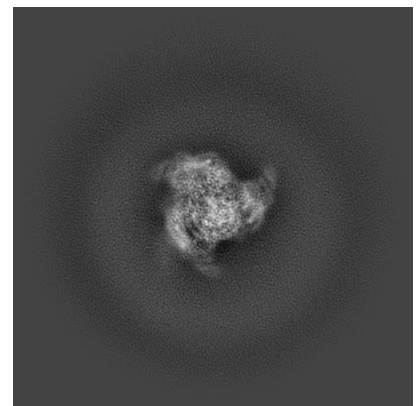
6.1.1 Primary map



X

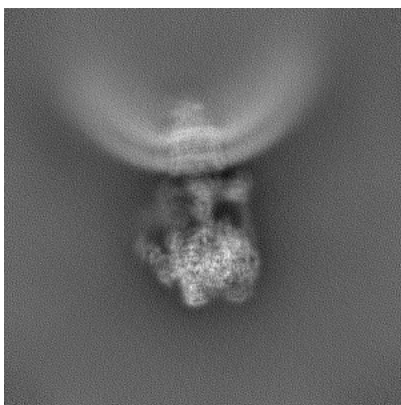


Y

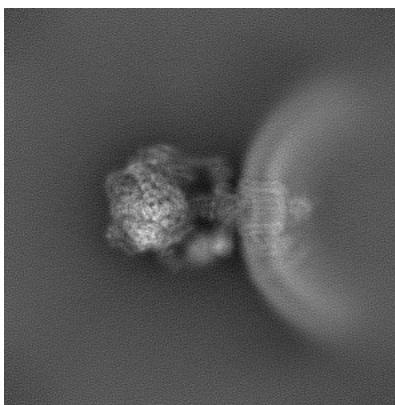


Z

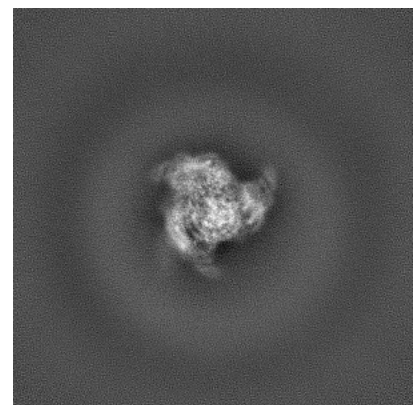
6.1.2 Raw map



X



Y



Z

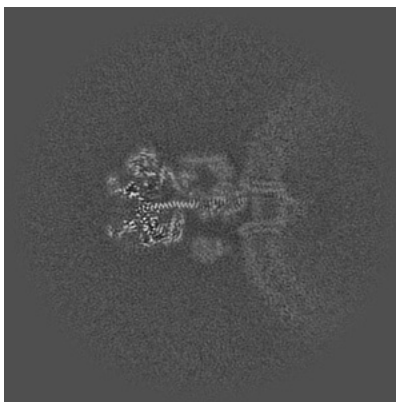
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

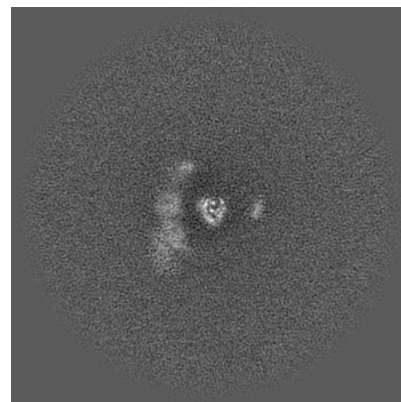
6.2.1 Primary map



X Index: 192

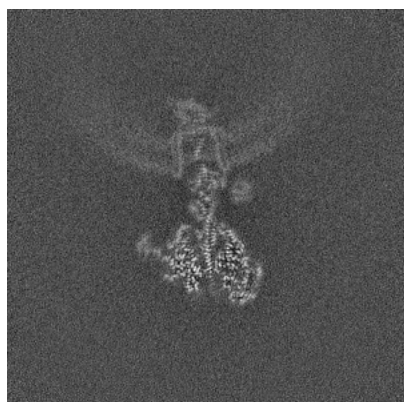


Y Index: 192

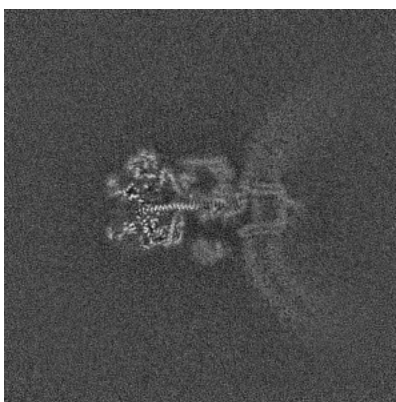


Z Index: 192

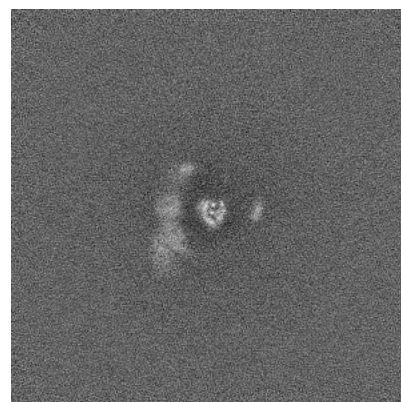
6.2.2 Raw map



X Index: 192



Y Index: 192

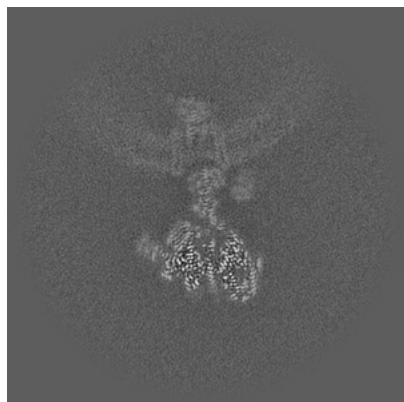


Z Index: 192

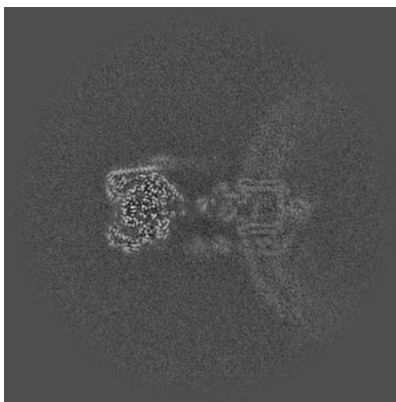
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

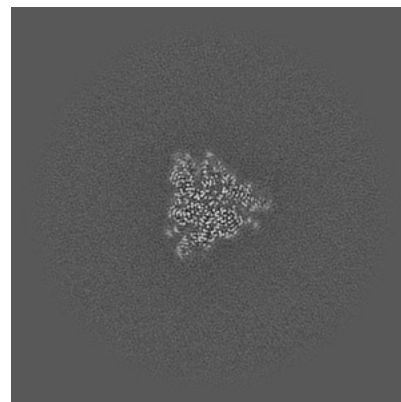
6.3.1 Primary map



X Index: 189

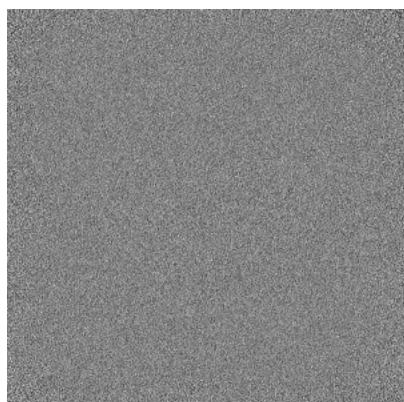


Y Index: 179

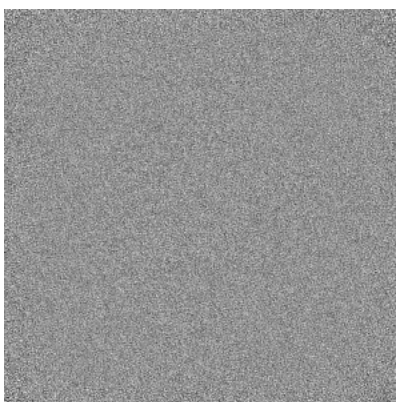


Z Index: 135

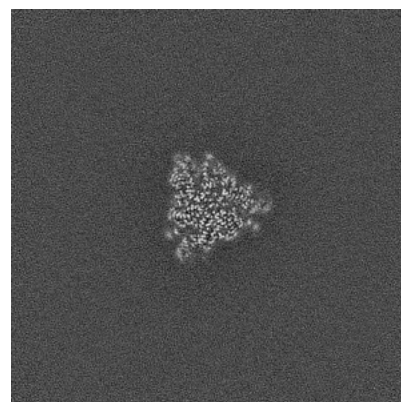
6.3.2 Raw map



X Index: 0



Y Index: 0

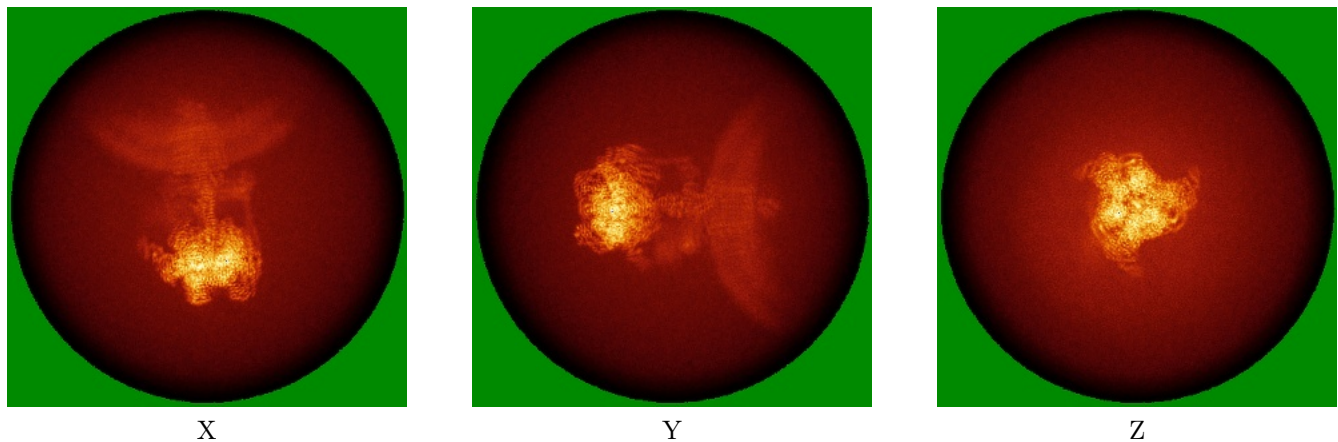


Z Index: 135

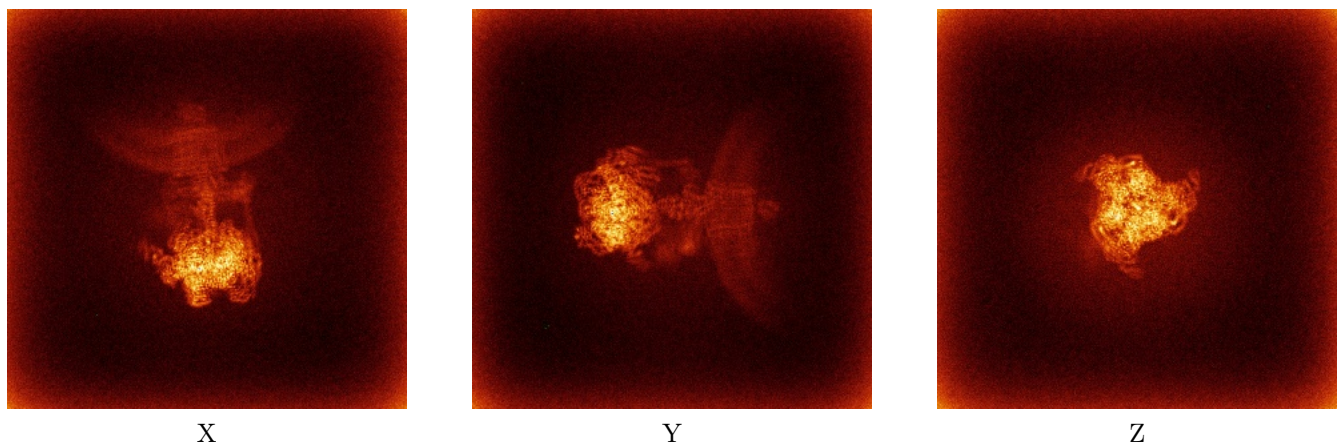
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



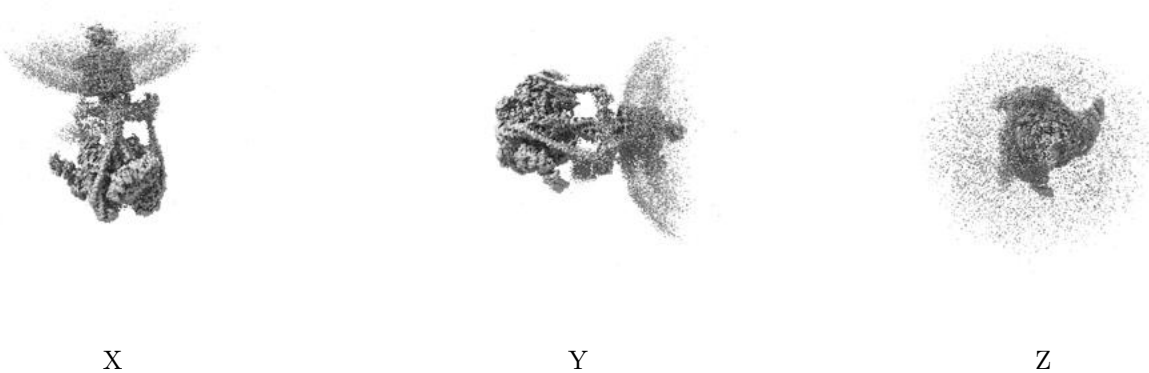
6.4.2 Raw map



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.

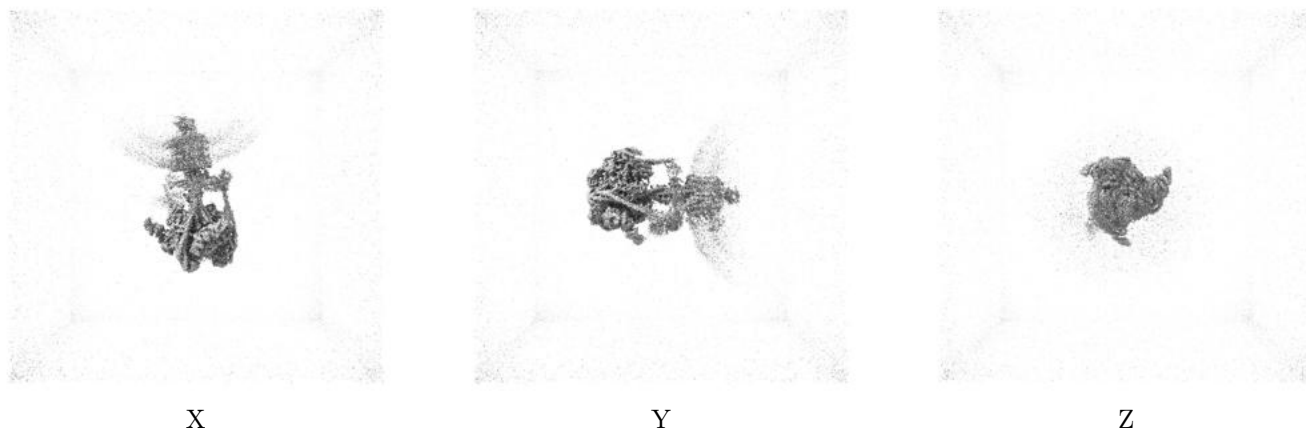
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. 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.

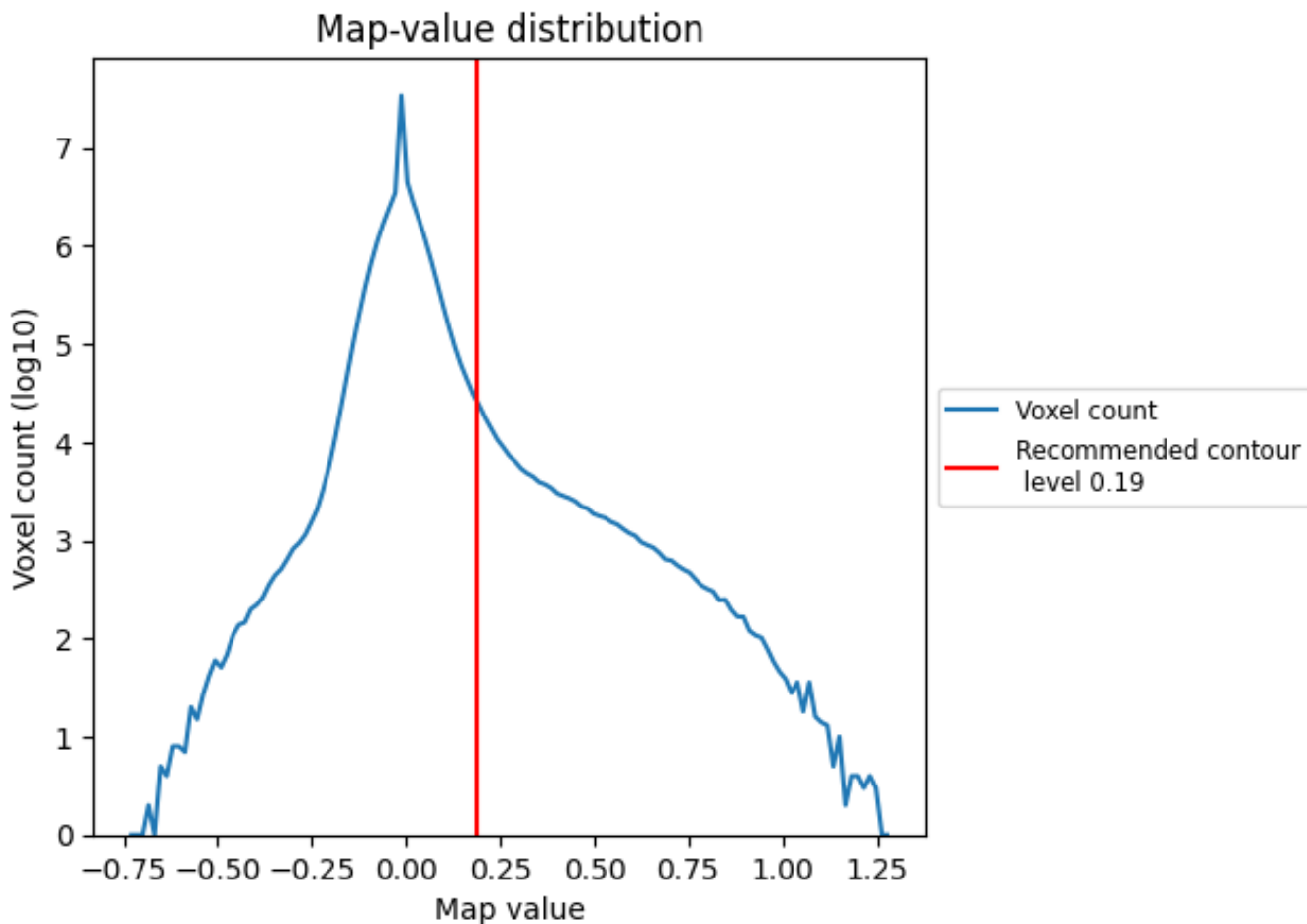
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

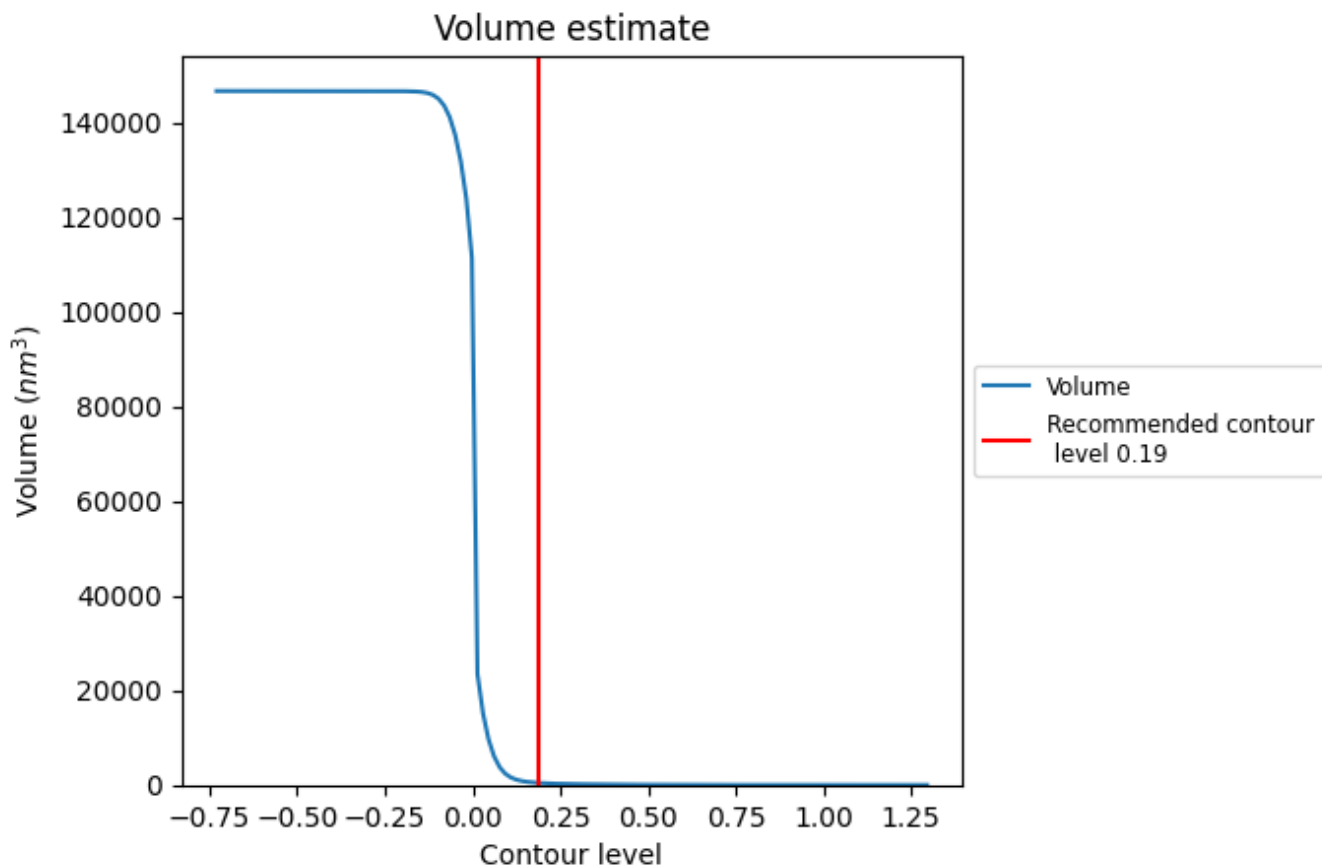
This section contains the results of statistical analysis of the map.

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.

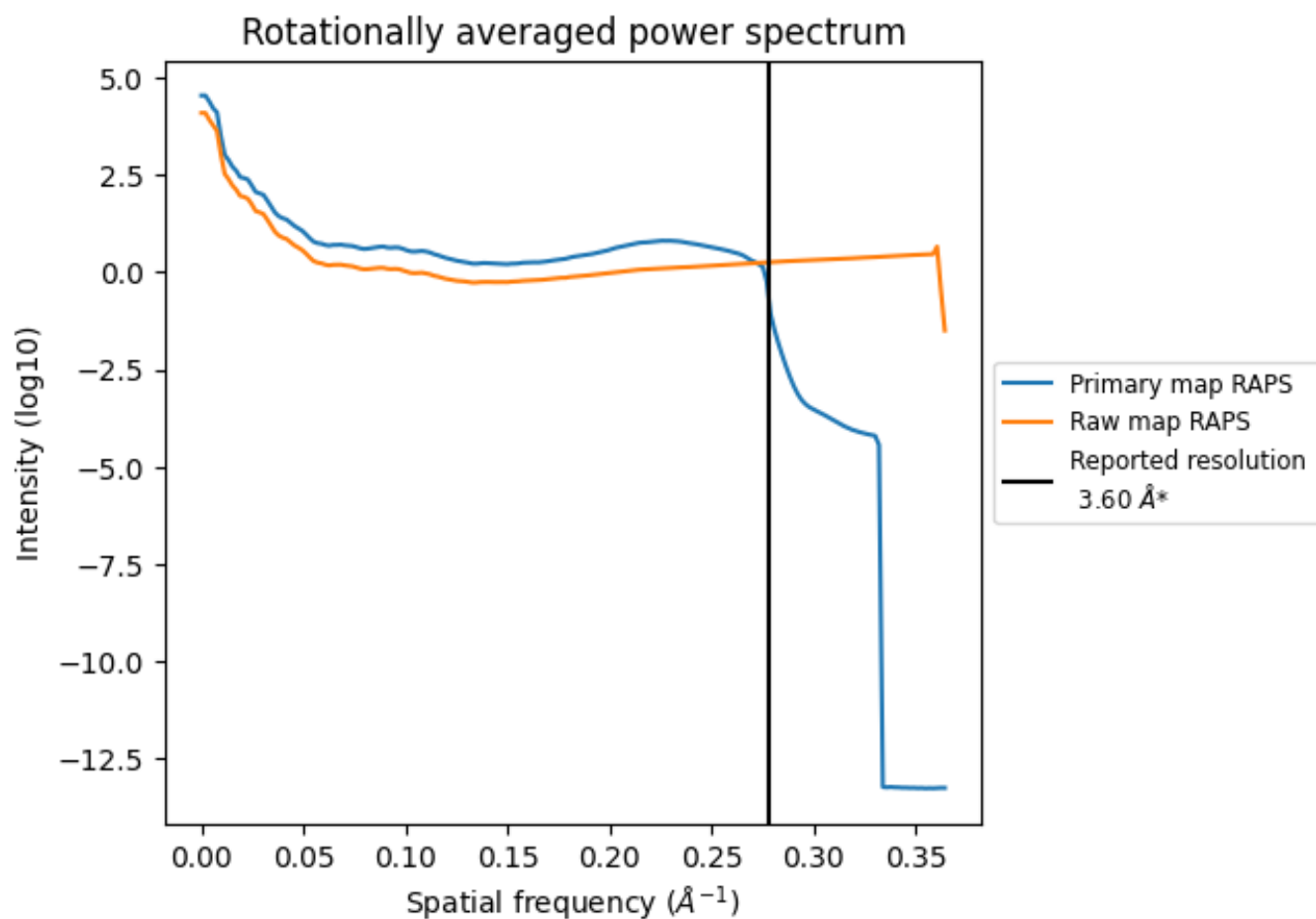
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 414 nm^3 ; this corresponds to an approximate mass of 374 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 i

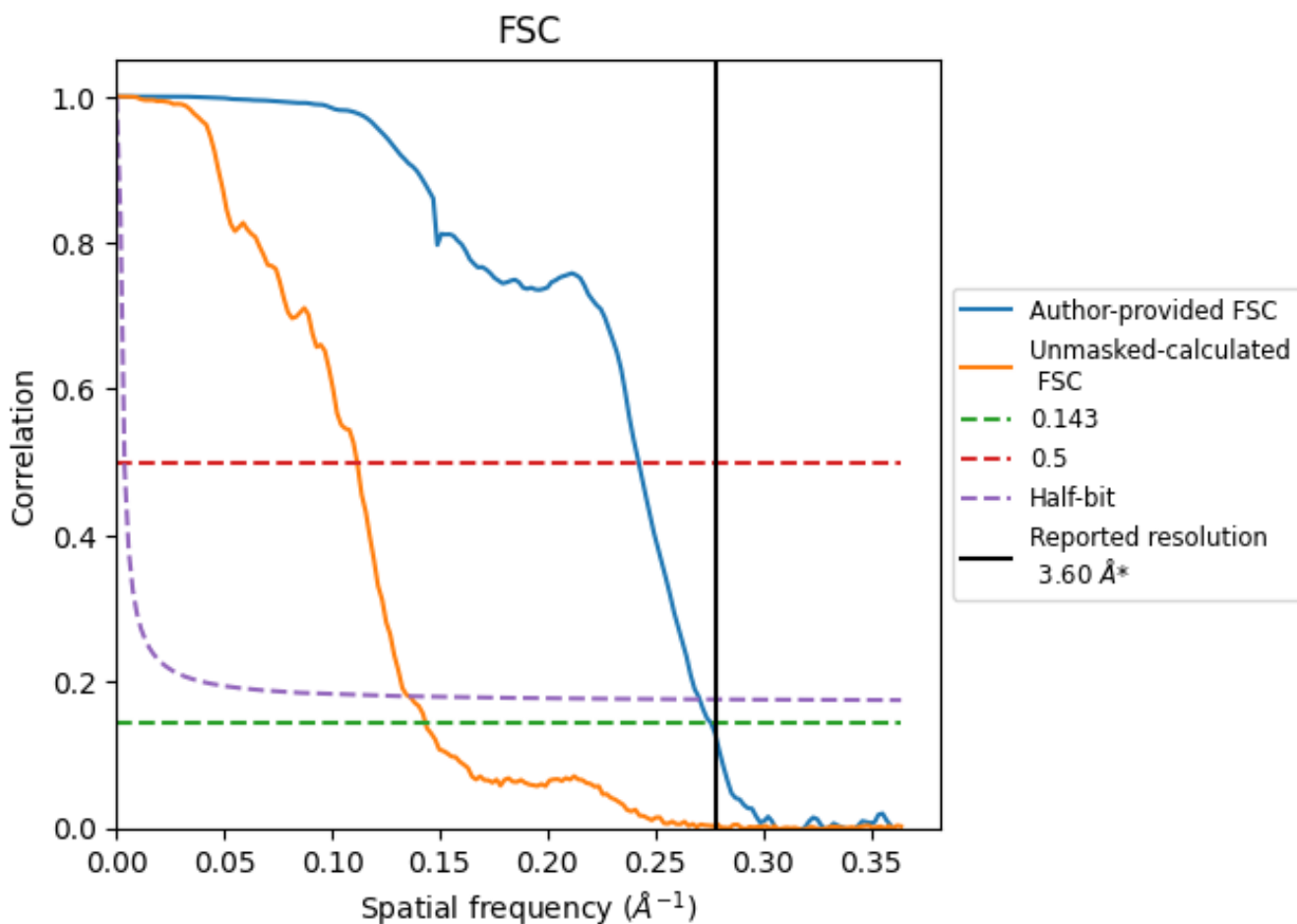


*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

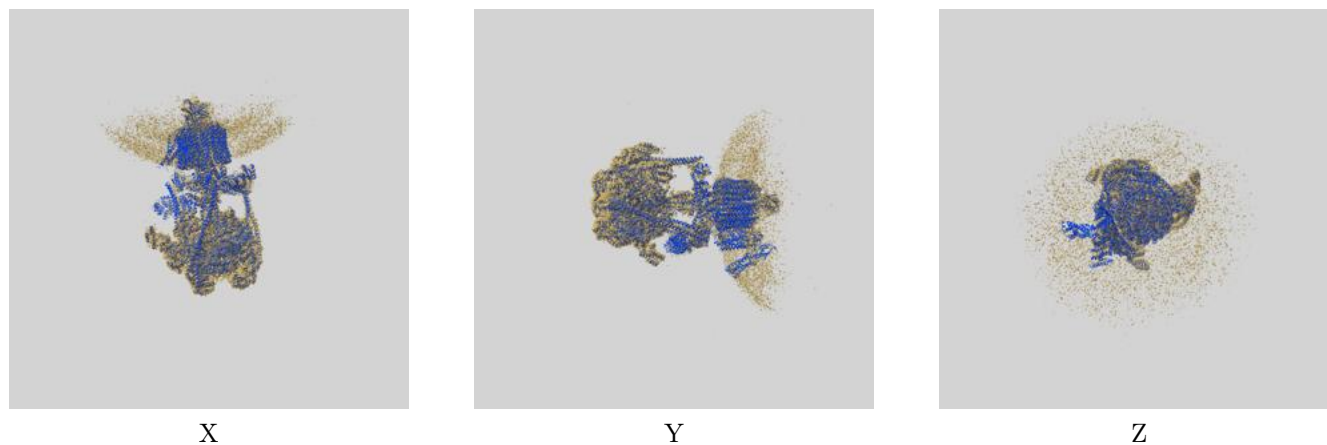
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.62	4.13	3.70
Unmasked-calculated*	6.97	8.95	7.36

*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 6.97 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

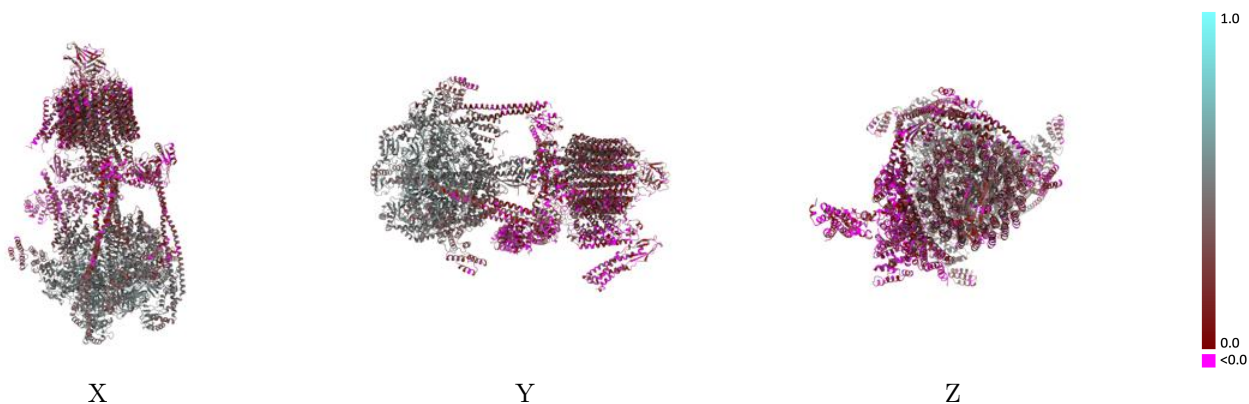
This section contains information regarding the fit between EMDB map EMD-44355 and PDB model 9BRB. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



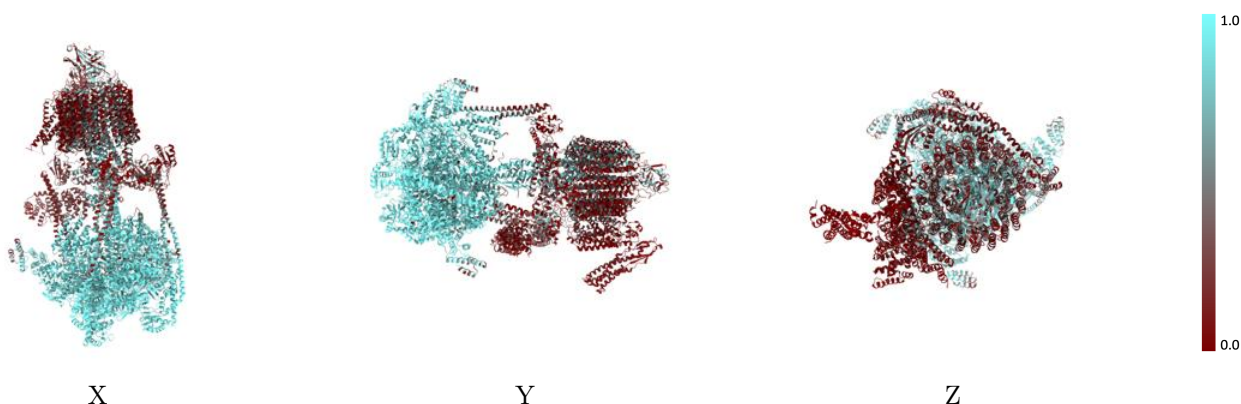
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



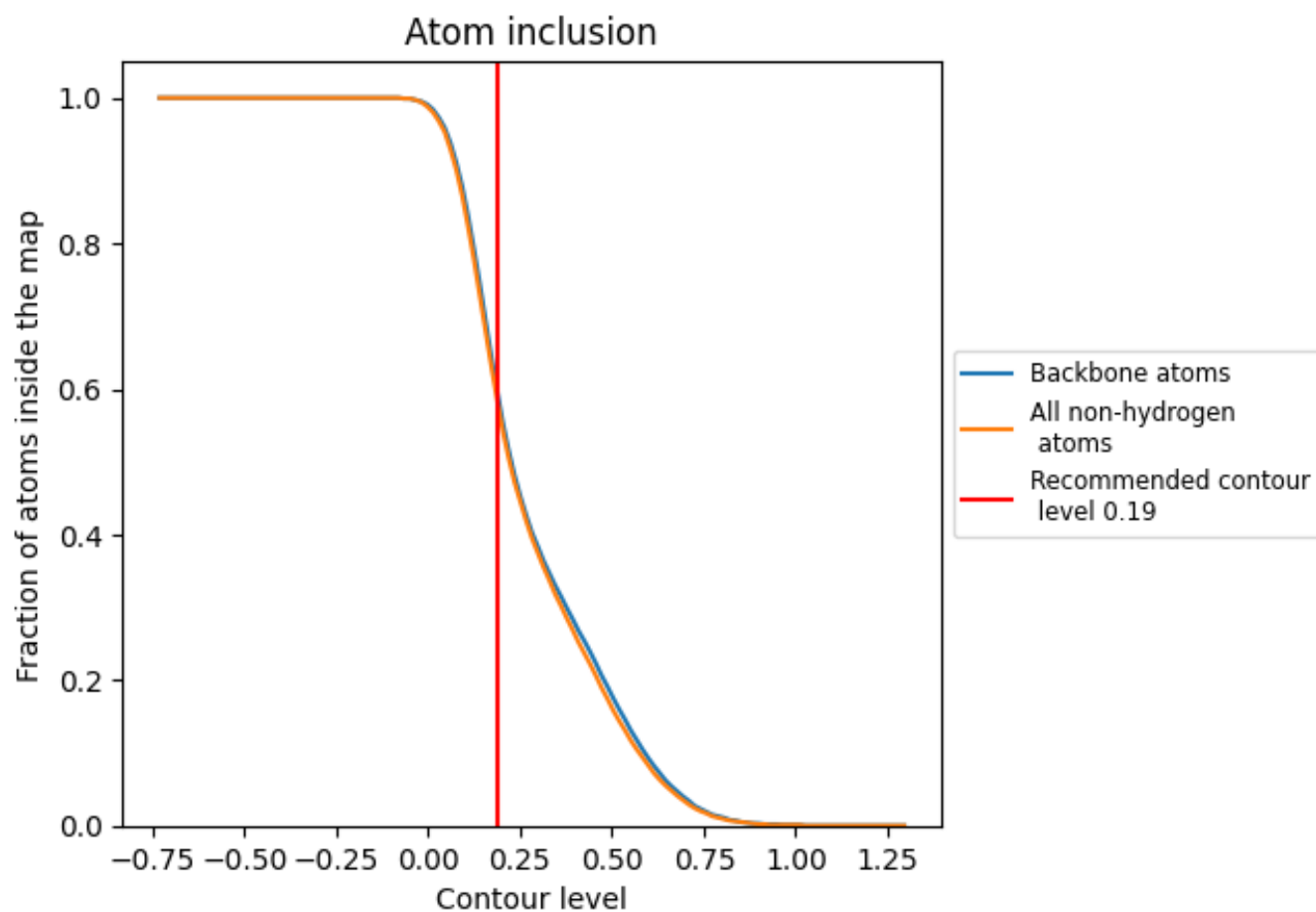
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 58% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5790	 0.3200
A	 0.9010	 0.4800
B	 0.8970	 0.4680
C	 0.9090	 0.4930
D	 0.9140	 0.5020
E	 0.9250	 0.5020
F	 0.9190	 0.5020
G	 0.1500	 0.0960
H	 0.8520	 0.4280
I	 0.7240	 0.3380
J	 0.8210	 0.3930
K	 0.8170	 0.3720
L	 0.7250	 0.3630
M	 0.5570	 0.3000
N	 0.6840	 0.2740
O	 0.6540	 0.2570
P	 0.3660	 0.2280
Q	 0.8340	 0.3480
R	 0.8800	 0.3620
S	 0.8460	 0.3720
T	 0.0590	 0.0630
U	 0.0090	 0.0390
a	 0.1660	 0.1160
b	 0.3580	 0.2620
d	 0.5250	 0.3150
e	 0.0510	 0.0760
f	 0.0430	 0.0470
g	 0.2000	 0.2200
h	 0.1620	 0.1960
i	 0.2350	 0.2350
j	 0.2950	 0.2250
k	 0.2030	 0.2240
l	 0.1740	 0.1960
m	 0.1890	 0.2120
n	 0.2540	 0.2270



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
o	 0.3730	 0.2740
p	 0.2790	 0.2920