



wwPDB EM Validation Summary Report ⓘ

Jun 13, 2024 – 03:00 PM EDT

PDB ID : 9BRQ
EMDB ID : EMD-44840
Title : Intact V-ATPase State 3 and synaptophysin complex in mouse brain isolated synaptic vesicles
Authors : Wang, C.; Jiang, W.; Yang, K.; Wang, X.; Guo, Q.; Brunger, A.T.
Deposited on : 2024-05-11
Resolution : 4.30 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

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) : 2.36.2

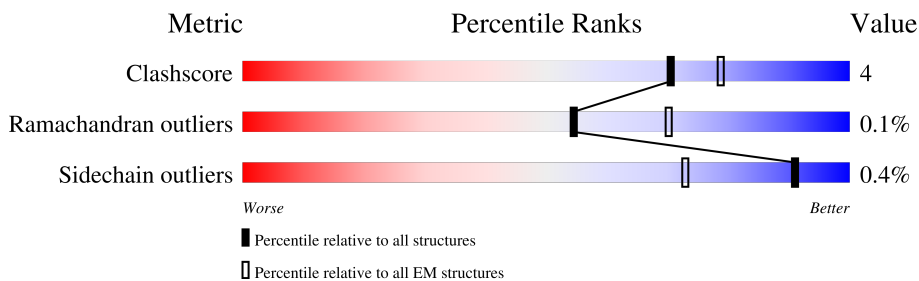
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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 ≥ 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	b	205	
2	g	155	
2	h	155	
2	i	155	
2	j	155	
2	k	155	
2	l	155	
2	m	155	

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Mol	Chain	Length	Quality of chain
2	n	155	13% 96%
2	o	155	95%
3	0	617	88% 6% 5%
3	1	617	92% 6%
3	2	617	91% 6%
4	3	511	86% 10%
4	4	511	87% 5% 8%
4	5	511	87% 8%
5	7	247	80% 6% 14%
6	8	226	96%
6	9	226	96%
6	Q	226	14% 95% 5%
7	R	118	94%
7	T	118	90% 7%
7	V	118	24% 92%
8	X	119	87% 6% 8%
9	6	382	37% 88% 6% 5%
10	U	483	10% 86% 12%
11	d	351	7% 100%
12	a	838	5% 89% 10%
13	c	463	43% 56%
14	p	350	14% 86%
15	f	98	13% 88% 12%
16	s	314	29% 67% 33%
17	e	81	5% 98%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 67167 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 V-type proton ATPase 21 kDa proteolipid subunit c^{''}.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	b	200	1484	983	234	256	11	0	0

- Molecule 2 is a protein called V-type proton ATPase 16 kDa proteolipid subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	g	150	1069	699	171	191	8	0	0
2	h	150	1069	699	171	191	8	0	0
2	i	150	1069	699	171	191	8	0	0
2	j	150	1069	699	171	191	8	0	0
2	k	150	1069	699	171	191	8	0	0
2	l	150	1069	699	171	191	8	0	0
2	m	150	1069	699	171	191	8	0	0
2	n	150	1069	699	171	191	8	0	0
2	o	150	1069	699	171	191	8	0	0

- Molecule 3 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1	600	4656	2953	787	889	27	0	0
3	2	600	4656	2953	787	889	27	0	0
3	0	585	4551	2891	768	866	26	0	0

- Molecule 4 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	461	Total	C	N	O	S	0	0
			3610	2290	615	685	20		
4	4	468	Total	C	N	O	S	0	0
			3667	2326	623	698	20		
4	5	468	Total	C	N	O	S	0	0
			3667	2326	623	698	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	213	Total	C	N	O	S	0	0
			1722	1096	310	311	5		

- Molecule 6 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		
6	9	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		
6	Q	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		

- Molecule 7 is a protein called V-type proton ATPase subunit G 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	114	Total	C	N	O	S	0	0
			925	552	192	176	5		
7	T	114	Total	C	N	O	S	0	0
			925	552	192	176	5		
7	V	114	Total	C	N	O	S	0	0
			925	552	192	176	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	110	Total	C	N	O	S	0	0
			875	553	157	163	2		

- Molecule 9 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	6	361	Total	C	N	O	S	0	0
			2931	1877	495	550	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	426	Total	C	N	O	S	0	0
			3501	2224	604	648	25		

- Molecule 11 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	351	Total	C	N	O	S	0	0
			2842	1834	461	532	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	752	Total	C	N	O	S	0	0
			6117	3991	1027	1058	41		

- Molecule 13 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	203	Total	C	N	O	S	0	0
			1642	1079	259	295	9		

- Molecule 14 is a protein called Renin receptor cytoplasmic fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	p	49	Total	C	N	O	S	0	0
			407	277	57	71	2		

- Molecule 15 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	86	Total	C	N	O	S	0	0
			666	440	103	116	7		

- Molecule 16 is a protein called Synaptophysin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	s	211	1671	1097	263	299	12	0	0

- Molecule 17 is a protein called V-type proton ATPase subunit e 2.

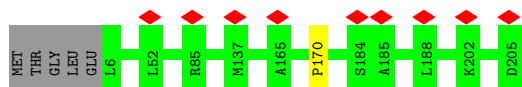
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	e	79	637	439	99	96	3	0	0

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.

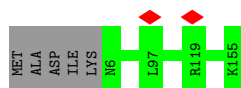
- Molecule 1: V-type proton ATPase 21 kDa proteolipid subunit c''

Chain b:  97%



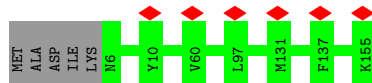
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c

Chain g:  97%



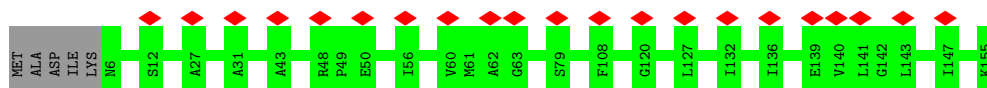
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c

Chain h:  97%



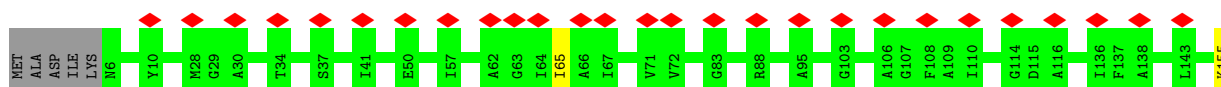
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c

Chain i:  14% 97%

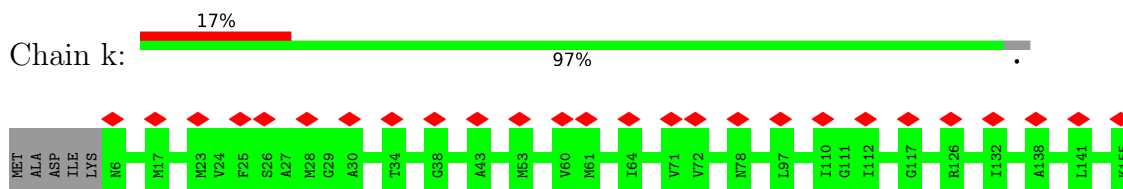


- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c

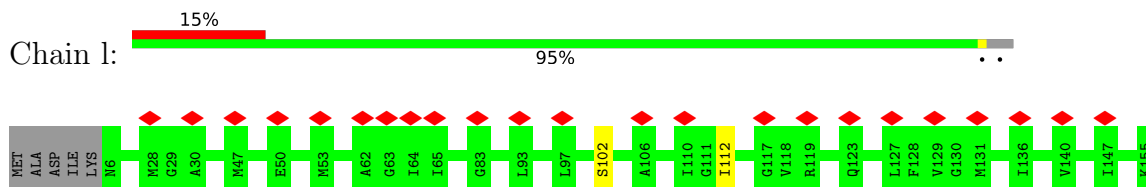
Chain j:  17% 95%



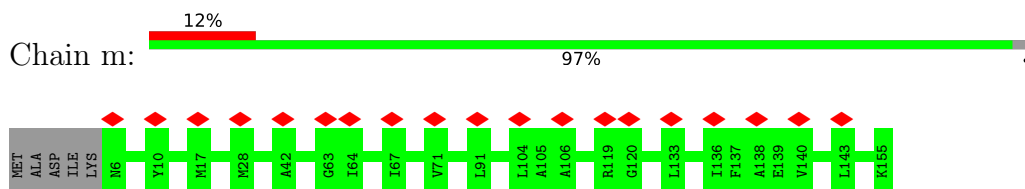
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c



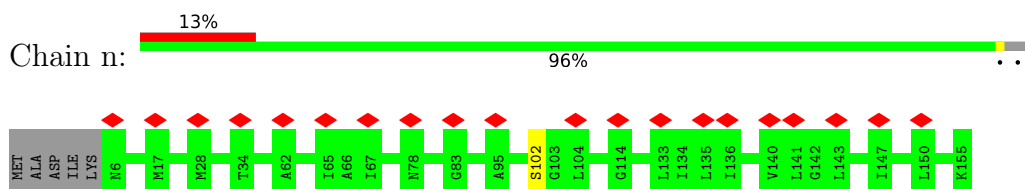
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c



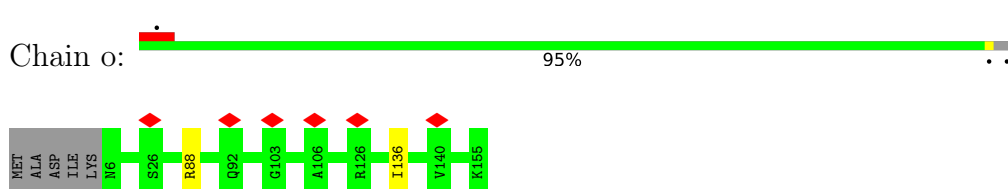
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c



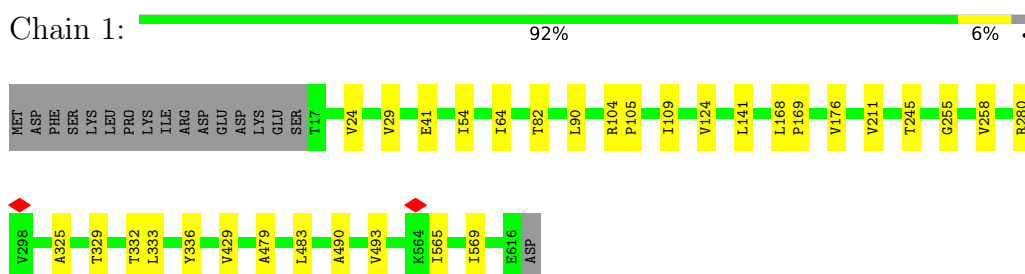
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c



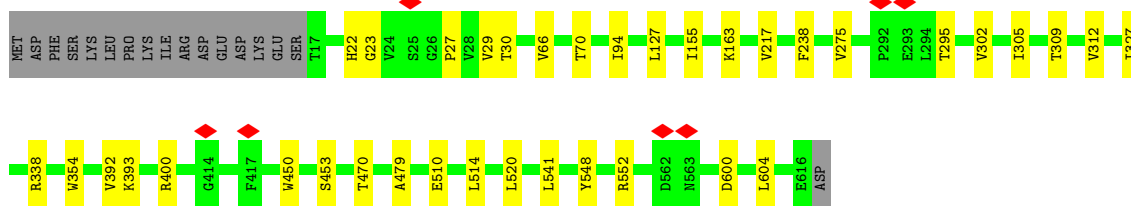
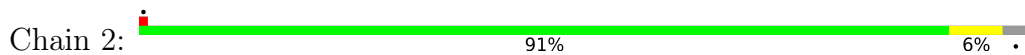
- Molecule 2: V-type proton ATPase 16 kDa proteolipid subunit c



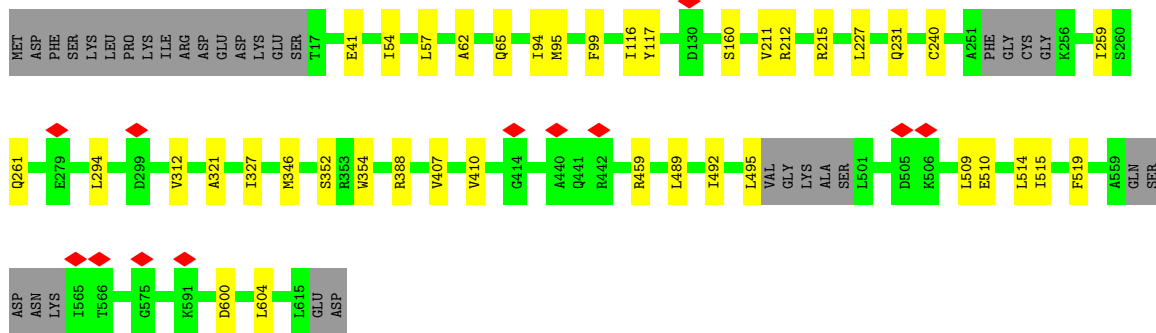
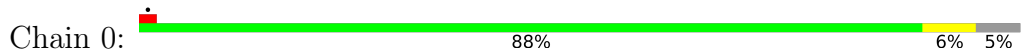
- Molecule 3: V-type proton ATPase catalytic subunit A



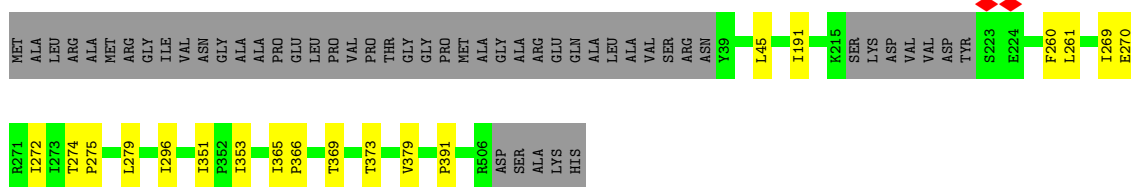
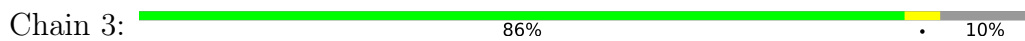
- Molecule 3: V-type proton ATPase catalytic subunit A



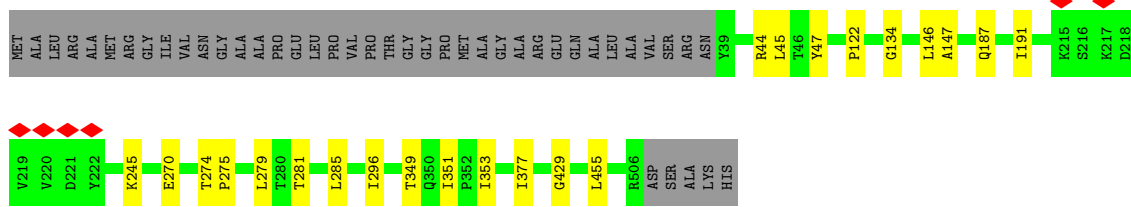
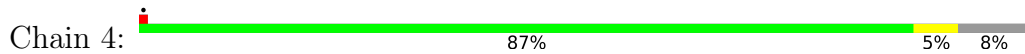
• Molecule 3: V-type proton ATPase catalytic subunit A



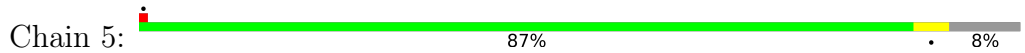
• Molecule 4: V-type proton ATPase subunit B, brain isoform

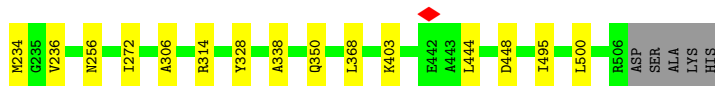
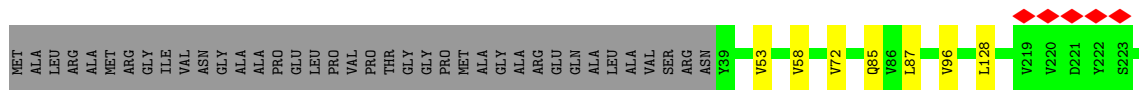


• Molecule 4: V-type proton ATPase subunit B, brain isoform

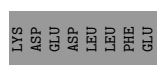
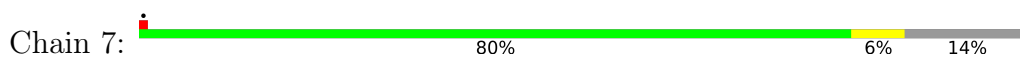


• Molecule 4: V-type proton ATPase subunit B, brain isoform

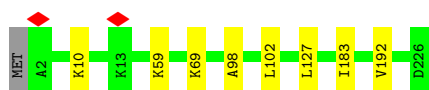




• Molecule 5: V-type proton ATPase subunit D



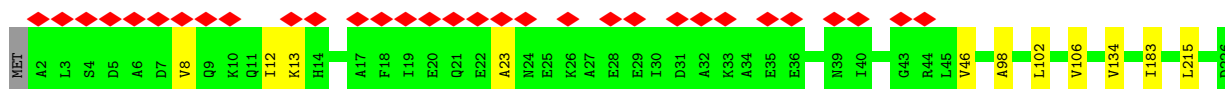
• Molecule 6: V-type proton ATPase subunit E 1



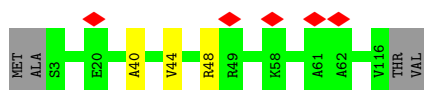
• Molecule 6: V-type proton ATPase subunit E 1



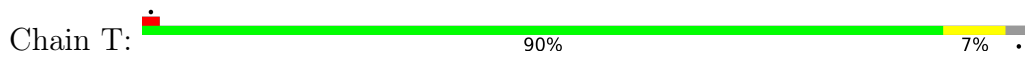
• Molecule 6: V-type proton ATPase subunit E 1



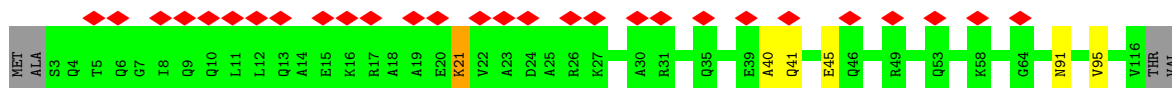
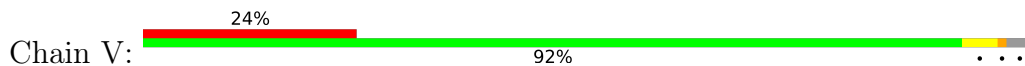
• Molecule 7: V-type proton ATPase subunit G 2



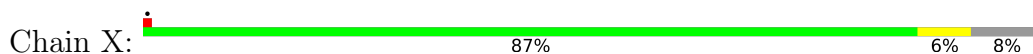
• Molecule 7: V-type proton ATPase subunit G 2



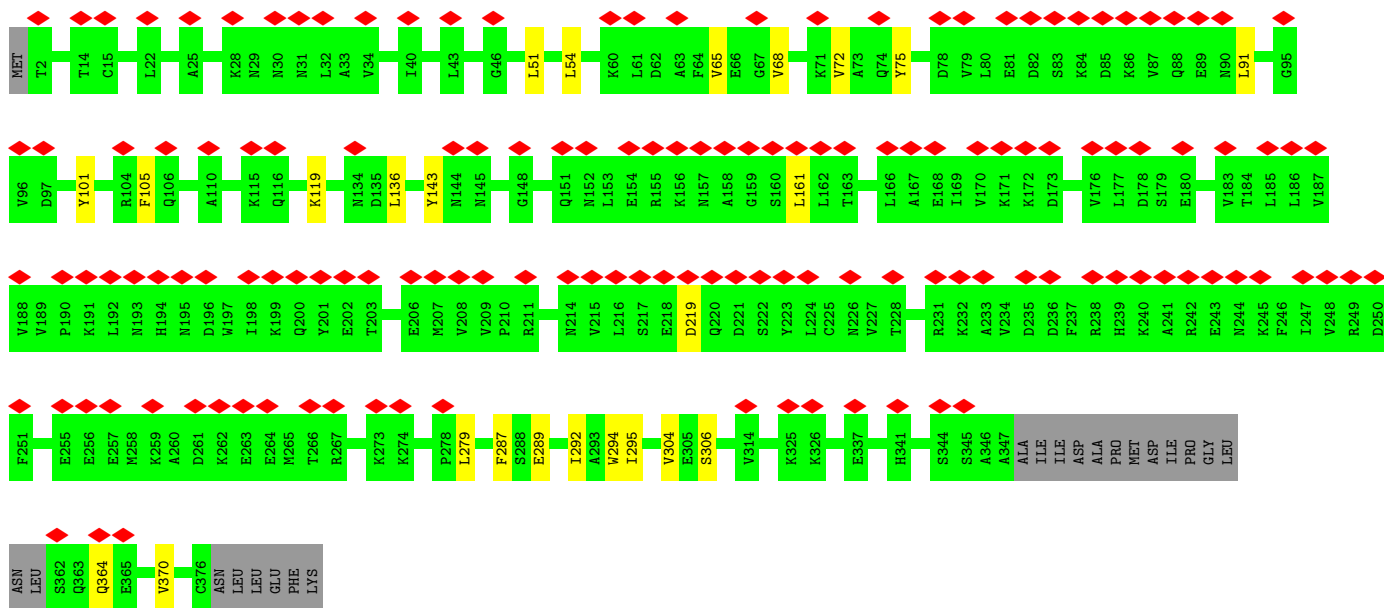
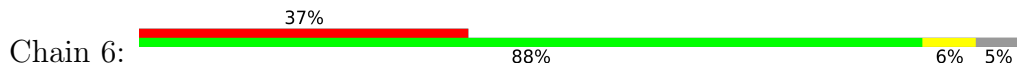
• Molecule 7: V-type proton ATPase subunit G 2



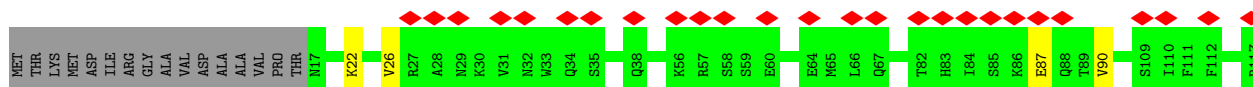
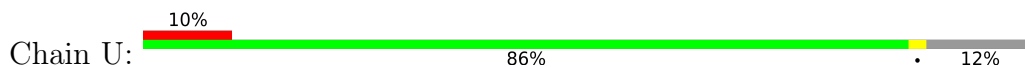
• Molecule 8: V-type proton ATPase subunit F



• Molecule 9: V-type proton ATPase subunit C 1



• Molecule 10: V-type proton ATPase subunit H



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34536	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.220	Depositor
Minimum map value	-0.510	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	497.8969, 497.8969, 497.8969	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.111377, 1.111377, 1.111377	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	b	0.36	0/1518	0.59	0/2061
2	g	0.32	0/1084	0.60	0/1466
2	h	0.32	0/1084	0.58	0/1466
2	i	0.28	0/1084	0.54	0/1466
2	j	0.49	0/1084	0.69	0/1466
2	k	0.32	0/1084	0.60	0/1466
2	l	0.37	0/1084	0.61	0/1466
2	m	0.30	0/1084	0.57	0/1466
2	n	0.39	0/1084	0.59	0/1466
2	o	0.41	0/1084	0.61	0/1466
3	0	0.28	0/4643	0.59	0/6284
3	1	0.29	0/4752	0.57	0/6433
3	2	0.27	0/4752	0.57	0/6433
4	3	0.27	0/3681	0.56	0/4987
4	4	0.28	0/3740	0.57	0/5069
4	5	0.28	0/3740	0.55	0/5069
5	7	0.30	0/1741	0.62	0/2328
6	8	0.31	0/1840	0.62	0/2462
6	9	0.29	0/1840	0.63	0/2462
6	Q	0.27	0/1840	0.55	0/2462
7	R	0.30	0/930	0.66	0/1237
7	T	0.32	0/930	0.73	0/1237
7	V	0.30	0/930	0.64	0/1237
8	X	0.28	0/889	0.59	0/1199
9	6	0.29	0/2985	0.55	0/4032
10	U	0.26	0/3568	0.55	0/4806
11	d	0.33	0/2908	0.56	0/3937
12	a	0.30	0/6274	0.59	0/8486
13	c	0.30	0/1697	0.58	0/2311
14	p	0.28	0/420	0.52	0/576
15	f	0.29	0/682	0.53	0/926
16	s	0.29	0/1716	0.54	0/2327
17	e	0.28	0/662	0.52	0/910
All	All	0.30	0/68434	0.58	0/92465

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	b	1484	0	1528	0	0
2	g	1069	0	1136	0	0
2	h	1069	0	1136	0	0
2	i	1069	0	1136	0	0
2	j	1069	0	1136	0	0
2	k	1069	0	1136	0	0
2	l	1069	0	1136	0	0
2	m	1069	0	1136	0	0
2	n	1069	0	1136	0	0
2	o	1069	0	1136	0	0
3	0	4551	0	4543	19	0
3	1	4656	0	4643	19	0
3	2	4656	0	4643	26	0
4	3	3610	0	3613	11	0
4	4	3667	0	3667	18	0
4	5	3667	0	3667	14	0
5	7	1722	0	1833	9	0
6	8	1823	0	1895	3	0
6	9	1823	0	1895	10	0
6	Q	1823	0	1895	8	0
7	R	925	0	935	2	0
7	T	925	0	935	7	0
7	V	925	0	935	6	0
8	X	875	0	883	4	0
9	6	2931	0	2969	15	0
10	U	3501	0	3481	6	0
11	d	2842	0	2782	0	0
12	a	6117	0	6154	0	0
13	c	1642	0	1568	0	0
14	p	407	0	403	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	f	666	0	663	0	0
16	s	1671	0	1649	0	0
17	e	637	0	652	0	0
All	All	67167	0	68055	162	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 4.

The worst 5 of 162 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)
9:6:72:VAL:HG22	9:6:136:LEU:HD22	1.70	0.74
3:1:141:LEU:HD21	3:1:176:VAL:HG11	1.69	0.72
3:2:450:TRP:CH2	3:2:520:LEU:HD13	2.27	0.70
3:2:548:TYR:CZ	3:2:552:ARG:HD2	2.28	0.68
3:2:548:TYR:CZ	3:2:552:ARG:CD	2.80	0.65

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	b	198/205 (97%)	193 (98%)	4 (2%)	1 (0%)	29	68
2	g	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
2	h	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
2	i	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
2	j	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
2	k	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
2	l	148/155 (96%)	143 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	m	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
2	n	148/155 (96%)	138 (93%)	10 (7%)	0	100	100
2	o	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
3	0	577/617 (94%)	518 (90%)	55 (10%)	4 (1%)	22	62
3	1	598/617 (97%)	556 (93%)	42 (7%)	0	100	100
3	2	598/617 (97%)	559 (94%)	39 (6%)	0	100	100
4	3	457/511 (89%)	435 (95%)	22 (5%)	0	100	100
4	4	466/511 (91%)	440 (94%)	26 (6%)	0	100	100
4	5	466/511 (91%)	445 (96%)	21 (4%)	0	100	100
5	7	211/247 (85%)	204 (97%)	7 (3%)	0	100	100
6	8	223/226 (99%)	213 (96%)	10 (4%)	0	100	100
6	9	223/226 (99%)	219 (98%)	4 (2%)	0	100	100
6	Q	223/226 (99%)	215 (96%)	8 (4%)	0	100	100
7	R	112/118 (95%)	110 (98%)	2 (2%)	0	100	100
7	T	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
7	V	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
8	X	108/119 (91%)	98 (91%)	10 (9%)	0	100	100
9	6	357/382 (94%)	334 (94%)	22 (6%)	1 (0%)	41	76
10	U	422/483 (87%)	396 (94%)	25 (6%)	1 (0%)	47	81
11	d	349/351 (99%)	334 (96%)	15 (4%)	0	100	100
12	a	746/838 (89%)	688 (92%)	58 (8%)	0	100	100
13	c	201/463 (43%)	170 (85%)	29 (14%)	2 (1%)	15	54
14	p	47/350 (13%)	45 (96%)	2 (4%)	0	100	100
15	f	84/98 (86%)	80 (95%)	4 (5%)	0	100	100
16	s	209/314 (67%)	201 (96%)	8 (4%)	0	100	100
17	e	77/81 (95%)	75 (97%)	2 (3%)	0	100	100
All	All	8508/9742 (87%)	8032 (94%)	467 (6%)	9 (0%)	54	85

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	U	134	ASP
3	0	160	SER

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Mol	Chain	Res	Type
9	6	364	GLN
13	c	374	LYS
3	0	388	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	b	154/158 (98%)	154 (100%)	0	100	100
2	g	109/113 (96%)	109 (100%)	0	100	100
2	h	109/113 (96%)	109 (100%)	0	100	100
2	i	109/113 (96%)	109 (100%)	0	100	100
2	j	109/113 (96%)	107 (98%)	2 (2%)	59	77
2	k	109/113 (96%)	109 (100%)	0	100	100
2	l	109/113 (96%)	107 (98%)	2 (2%)	59	77
2	m	109/113 (96%)	109 (100%)	0	100	100
2	n	109/113 (96%)	108 (99%)	1 (1%)	78	88
2	o	109/113 (96%)	107 (98%)	2 (2%)	59	77
3	0	496/524 (95%)	494 (100%)	2 (0%)	91	94
3	1	507/524 (97%)	505 (100%)	2 (0%)	91	94
3	2	507/524 (97%)	505 (100%)	2 (0%)	91	94
4	3	395/431 (92%)	395 (100%)	0	100	100
4	4	402/431 (93%)	401 (100%)	1 (0%)	93	96
4	5	402/431 (93%)	401 (100%)	1 (0%)	93	96
5	7	184/212 (87%)	183 (100%)	1 (0%)	88	93
6	8	197/198 (100%)	194 (98%)	3 (2%)	65	80
6	9	197/198 (100%)	197 (100%)	0	100	100
6	Q	197/198 (100%)	196 (100%)	1 (0%)	88	93
7	R	96/99 (97%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	96/99 (97%)	95 (99%)	1 (1%)	76	86
7	V	96/99 (97%)	95 (99%)	1 (1%)	76	86
8	X	94/100 (94%)	94 (100%)	0	100	100
9	6	326/344 (95%)	326 (100%)	0	100	100
10	U	384/429 (90%)	384 (100%)	0	100	100
11	d	306/306 (100%)	305 (100%)	1 (0%)	92	95
12	a	669/741 (90%)	665 (99%)	4 (1%)	86	92
13	c	180/395 (46%)	179 (99%)	1 (1%)	86	92
14	p	44/309 (14%)	44 (100%)	0	100	100
15	f	72/83 (87%)	72 (100%)	0	100	100
16	s	180/246 (73%)	180 (100%)	0	100	100
17	e	66/68 (97%)	66 (100%)	0	100	100
All	All	7228/8164 (88%)	7200 (100%)	28 (0%)	91	94

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	8	10	LYS
3	0	459	ARG
6	Q	13	LYS
12	a	815	LYS
6	8	69	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
9	6	214	ASN
10	U	405	GLN
3	0	430	GLN
12	a	442	HIS
12	a	619	HIS

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.

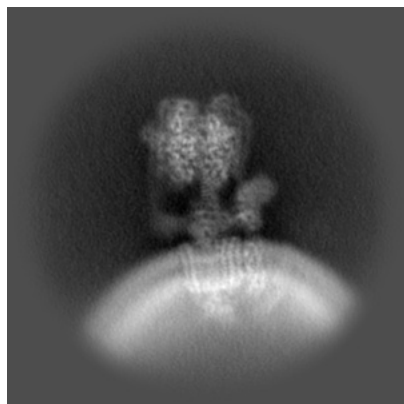
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44840. These allow visual inspection of the internal detail of the map and identification of artifacts.

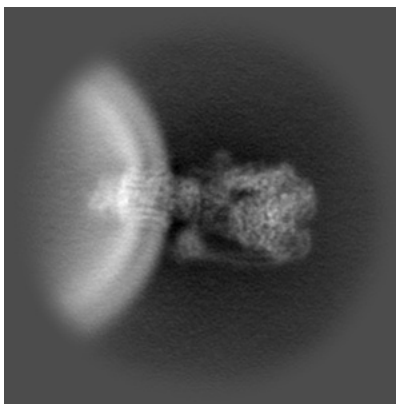
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

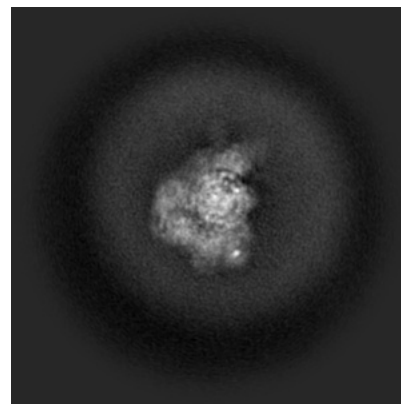
6.1.1 Primary map



X



Y

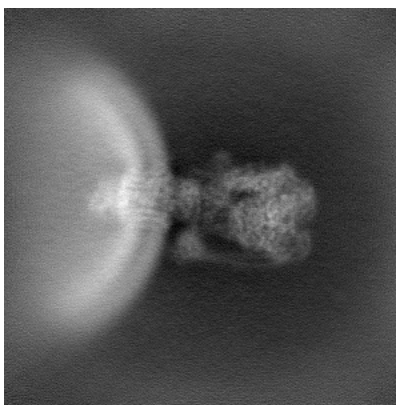


Z

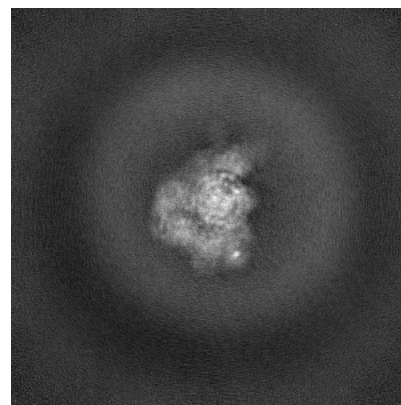
6.1.2 Raw map



X



Y

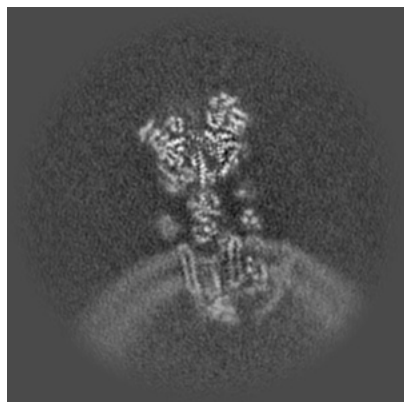


Z

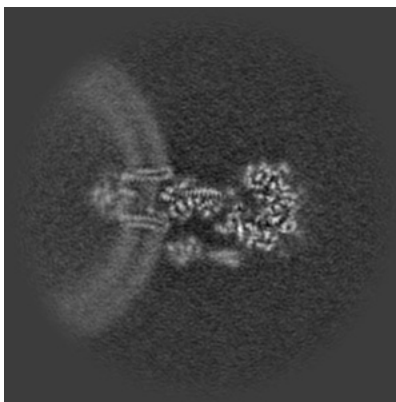
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

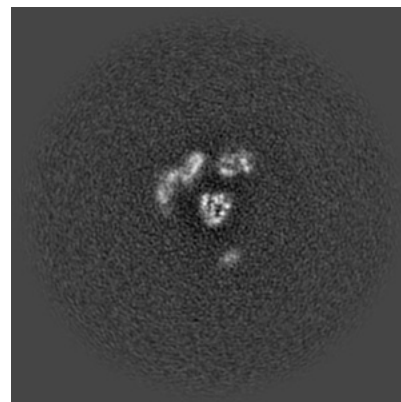
6.2.1 Primary map



X Index: 224

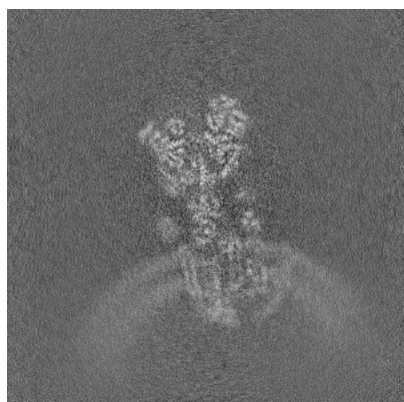


Y Index: 224

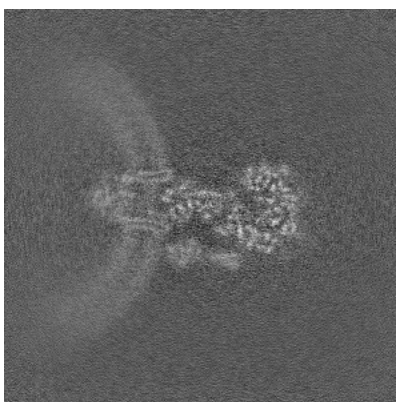


Z Index: 224

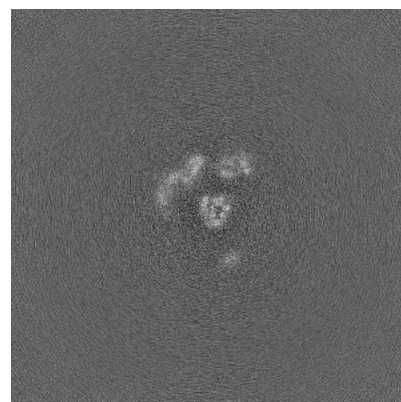
6.2.2 Raw map



X Index: 224



Y Index: 224

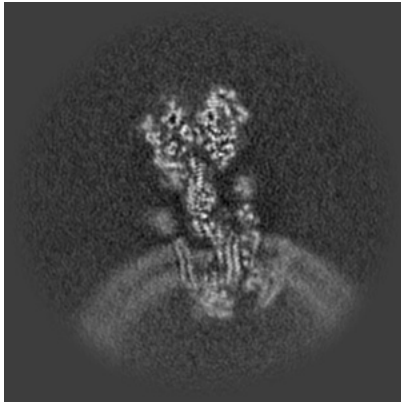


Z Index: 224

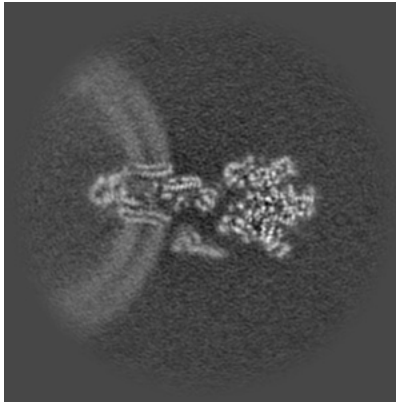
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

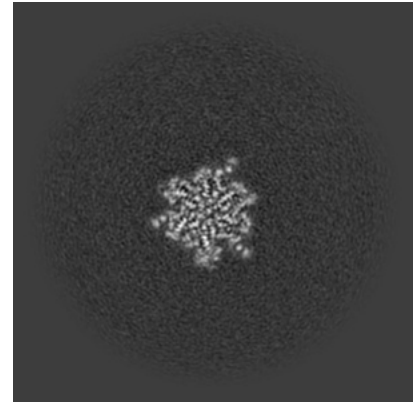
6.3.1 Primary map



X Index: 228

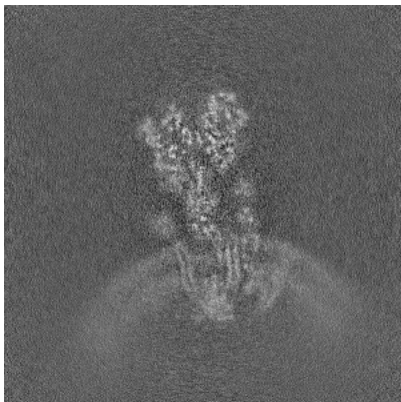


Y Index: 234

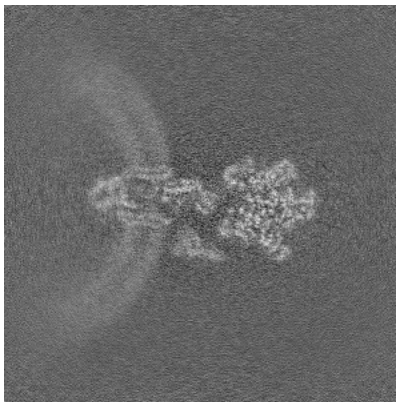


Z Index: 297

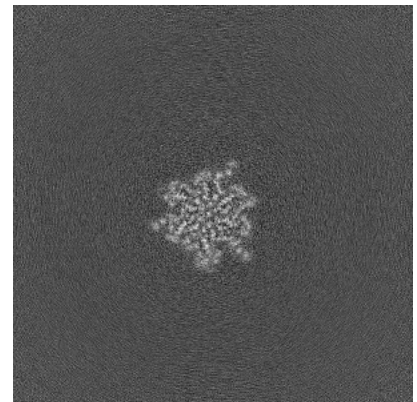
6.3.2 Raw map



X Index: 227



Y Index: 235

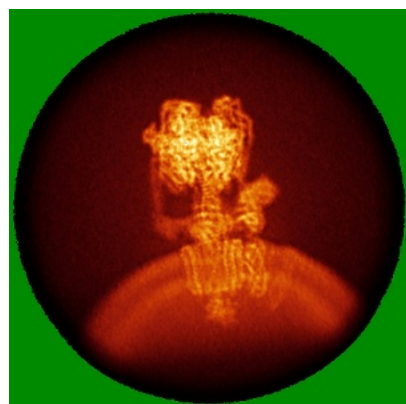


Z Index: 297

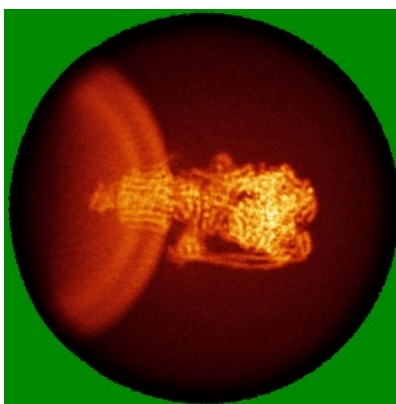
The images above show the largest variance slices of the map in three orthogonal directions.

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

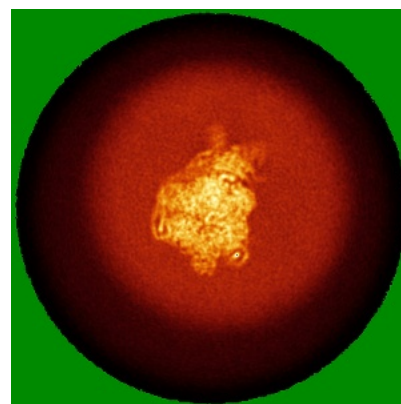
6.4.1 Primary map



X

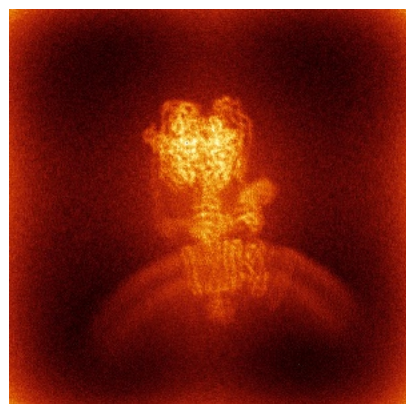


Y

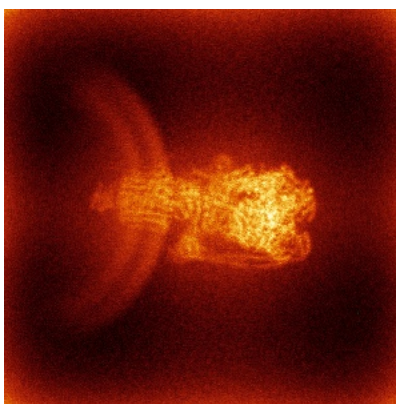


Z

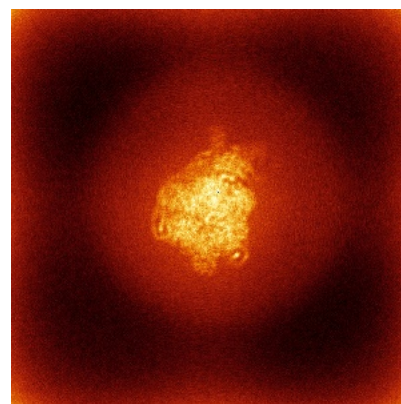
6.4.2 Raw map



X



Y

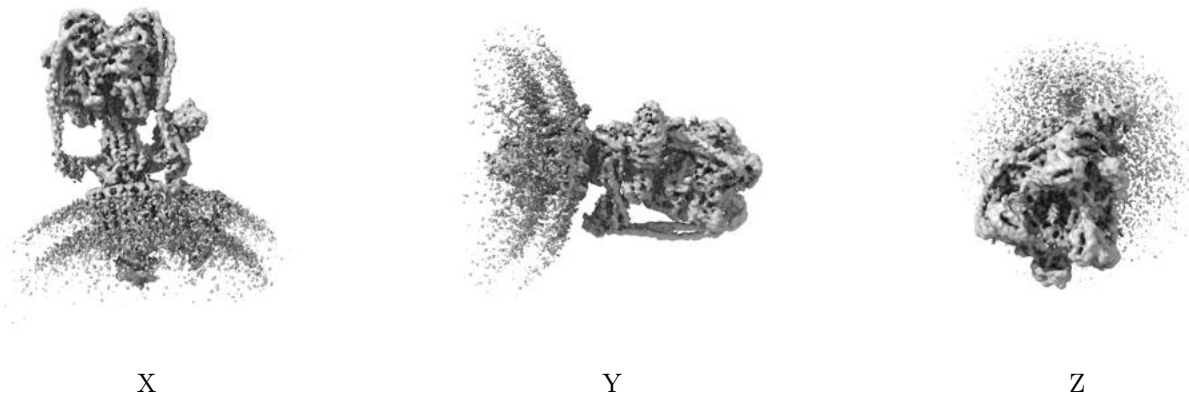


Z

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.

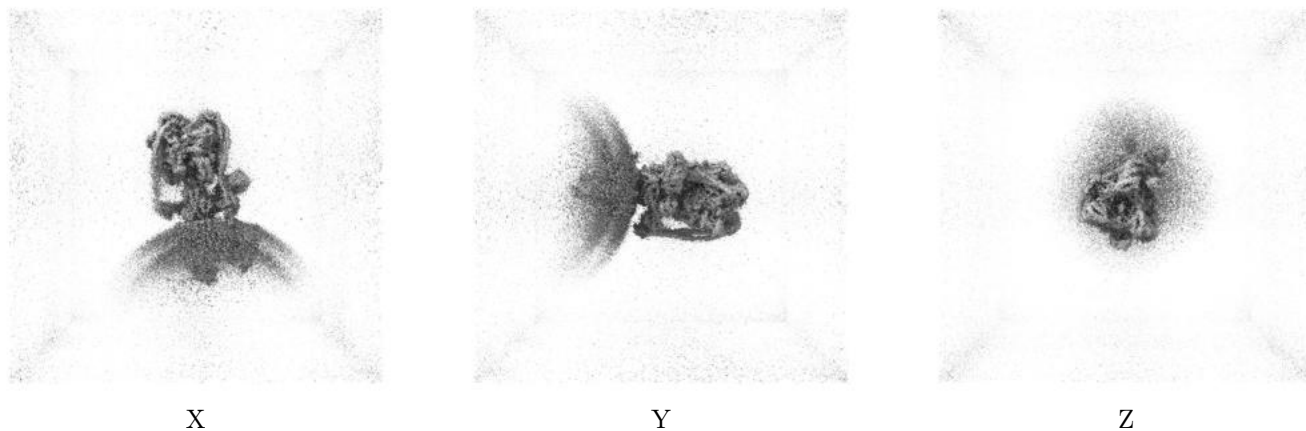
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.28. 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.

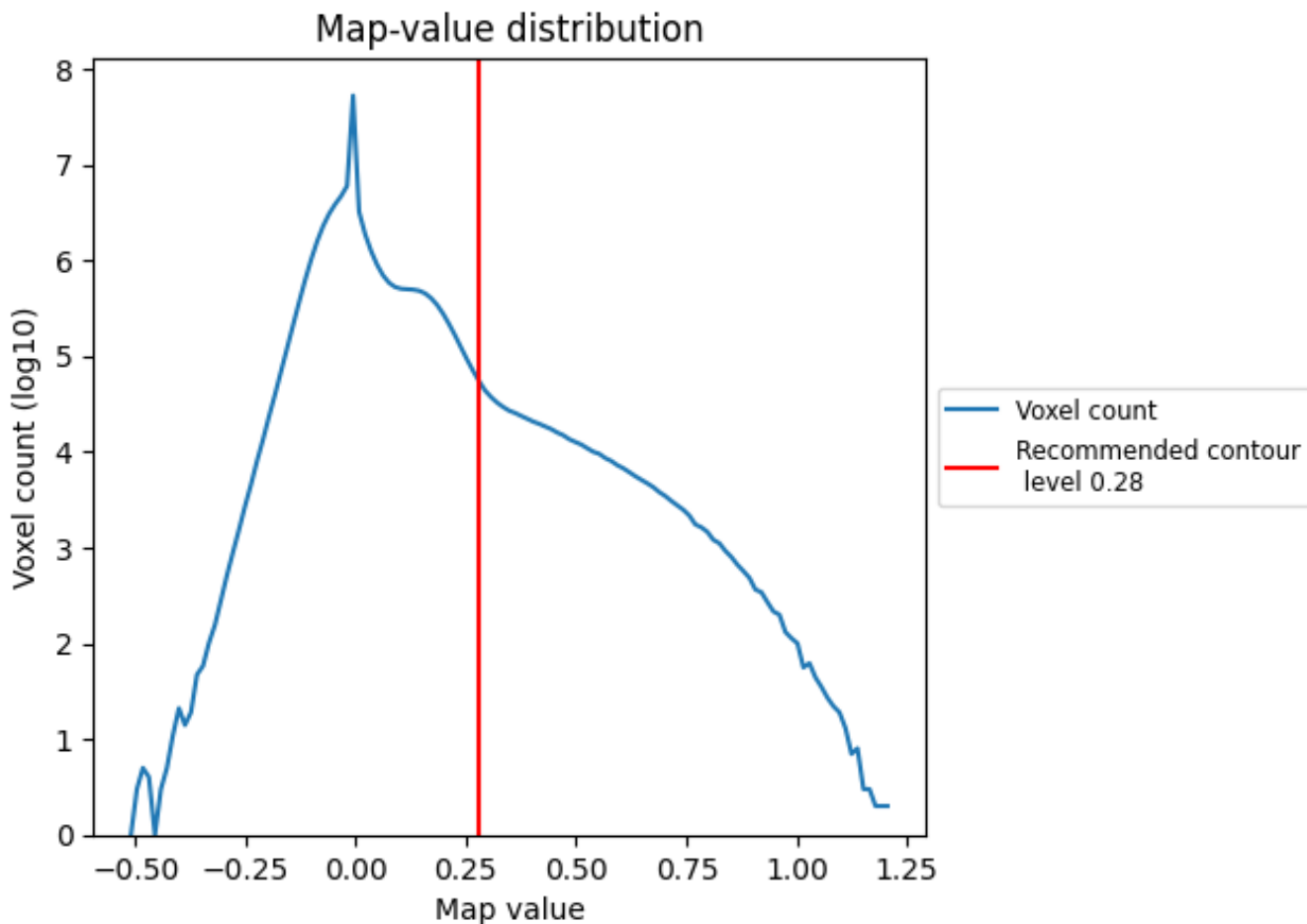
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

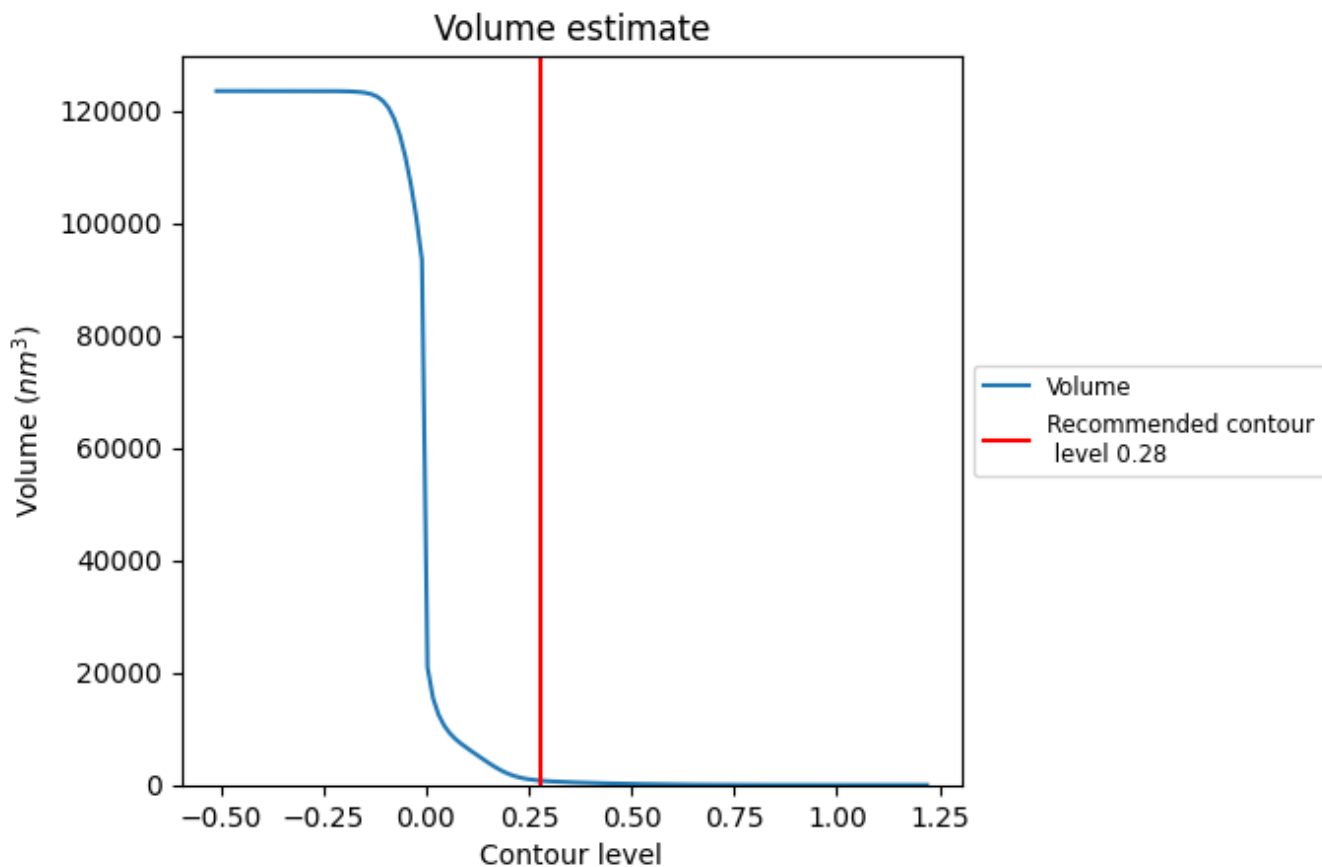
This section contains the results of statistical analysis of the map.

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.

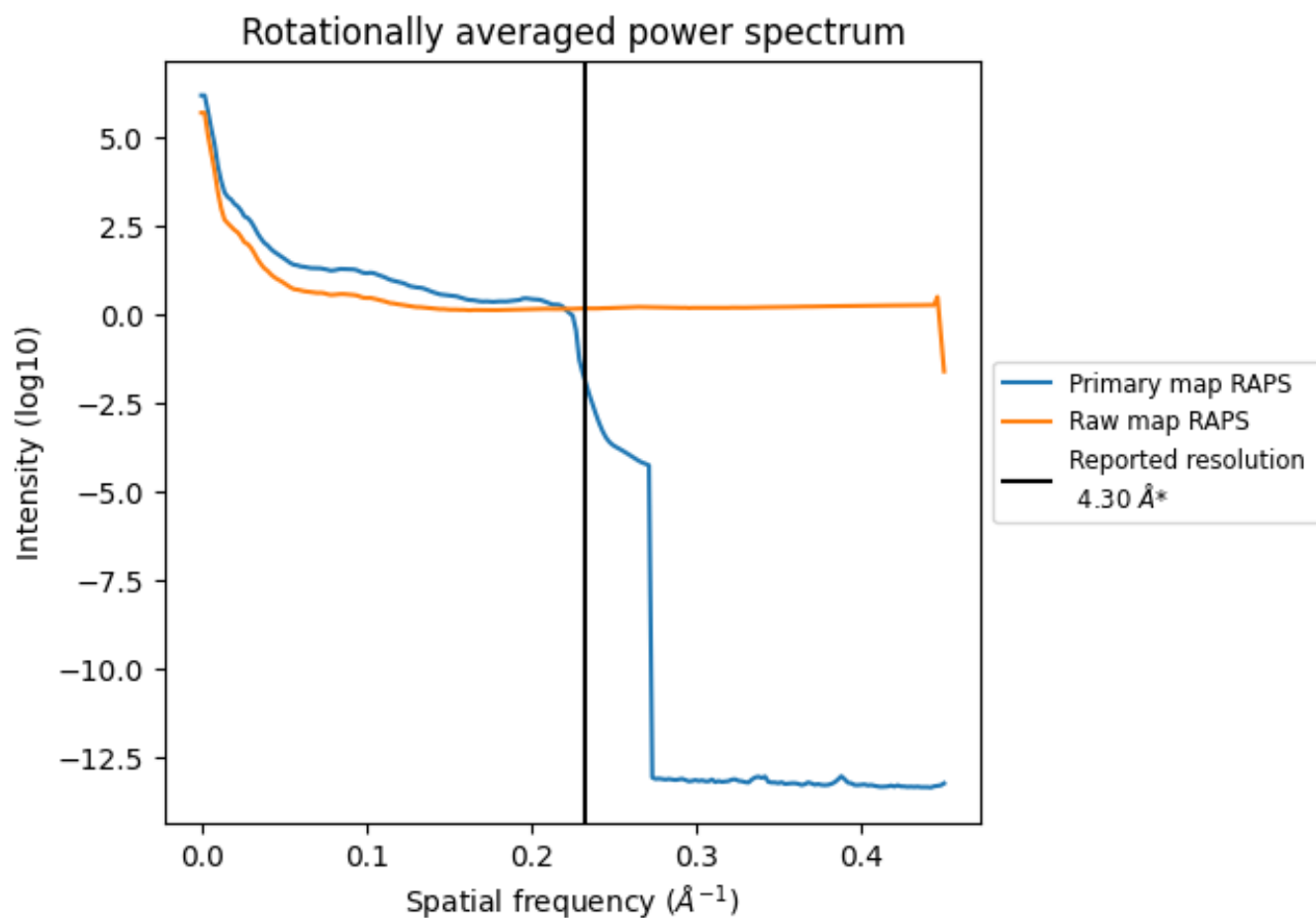
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 767 nm^3 ; this corresponds to an approximate mass of 693 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](#)

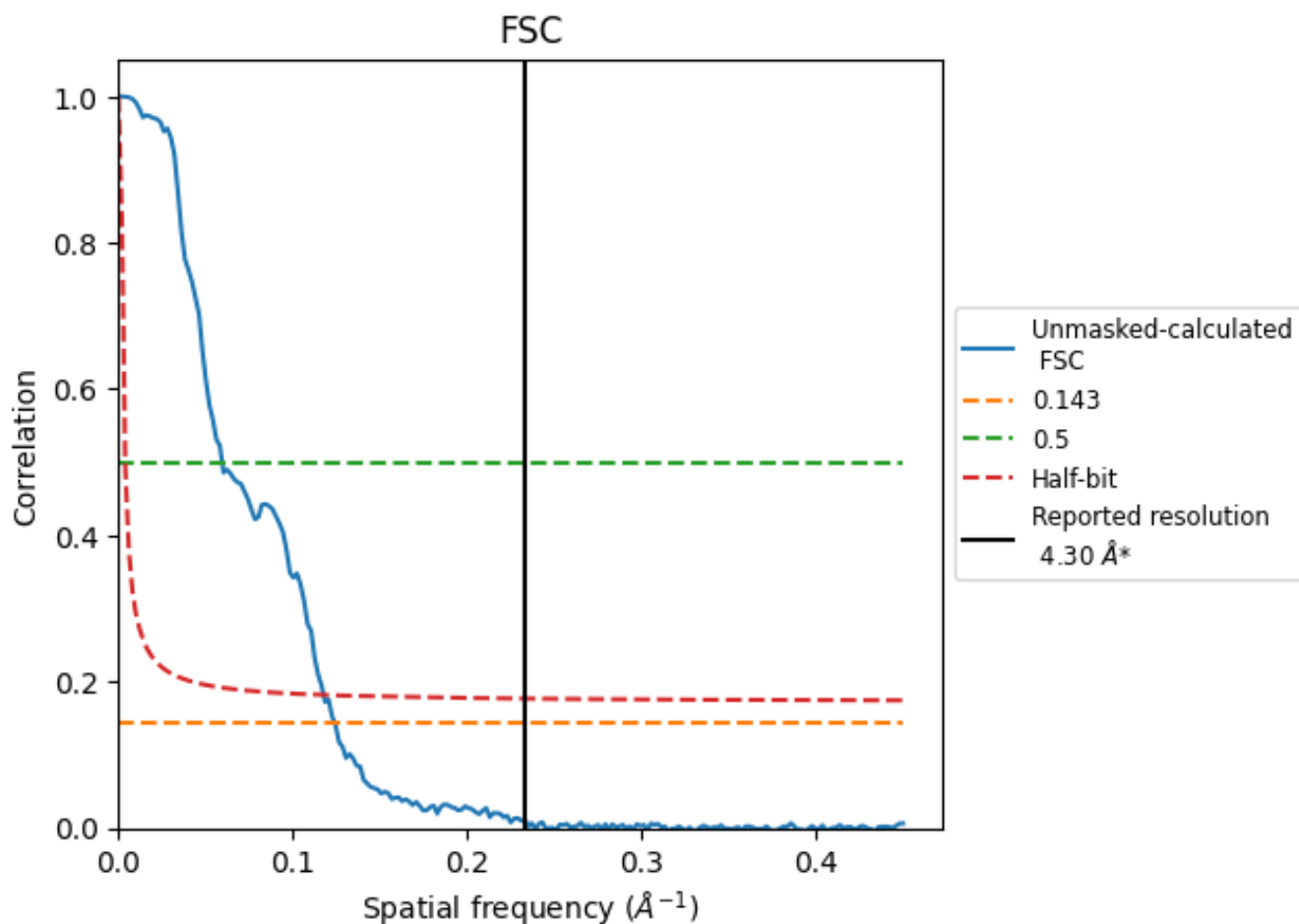


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

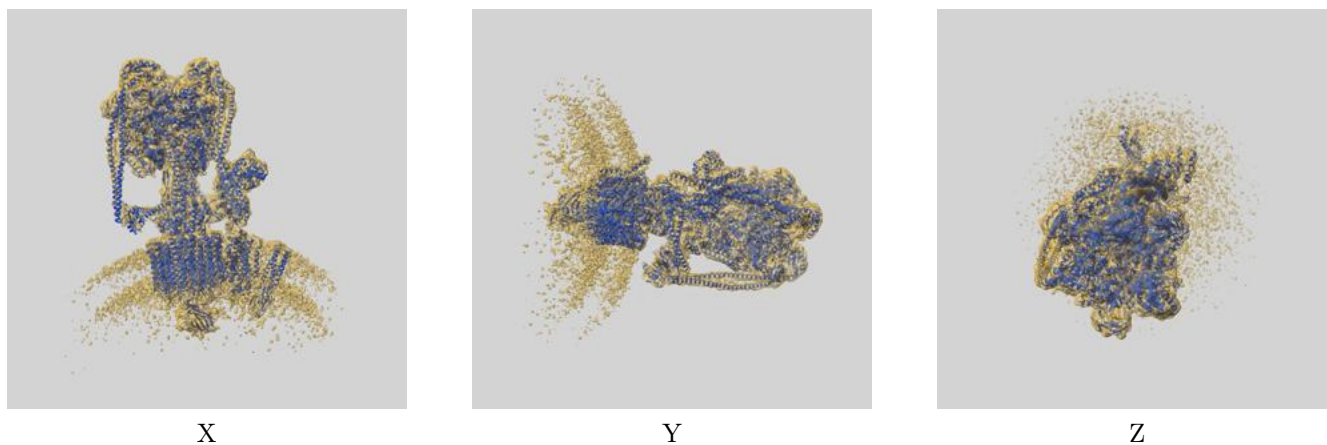
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.06	16.81	8.50

*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 8.06 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

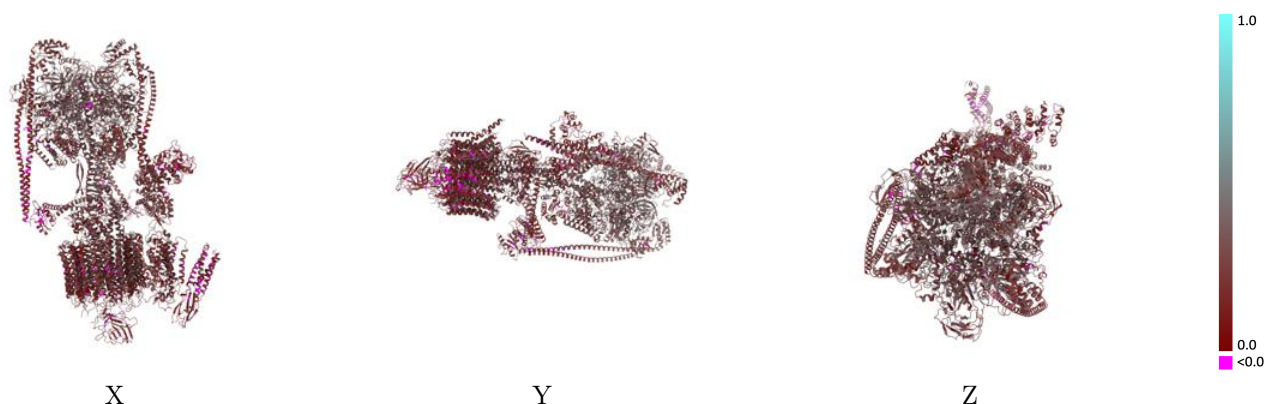
This section contains information regarding the fit between EMDB map EMD-44840 and PDB model 9BRQ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



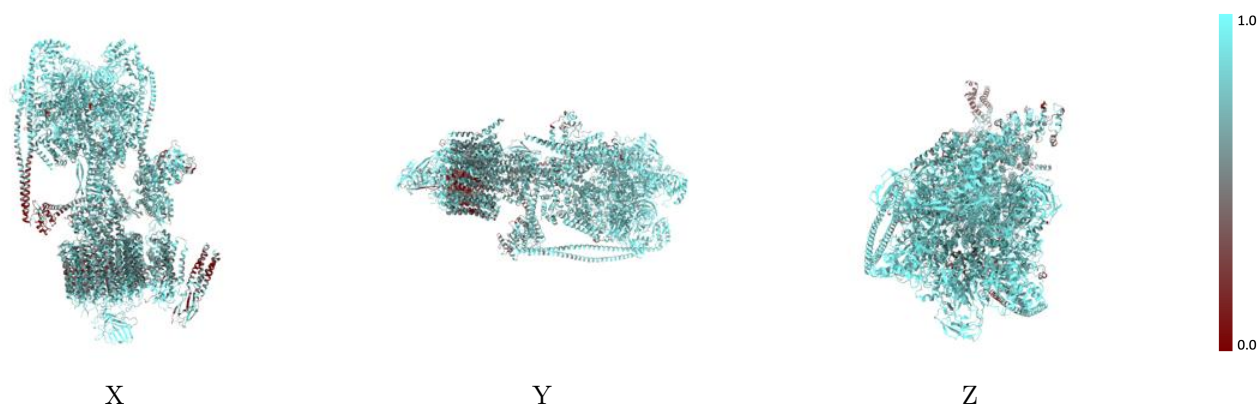
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



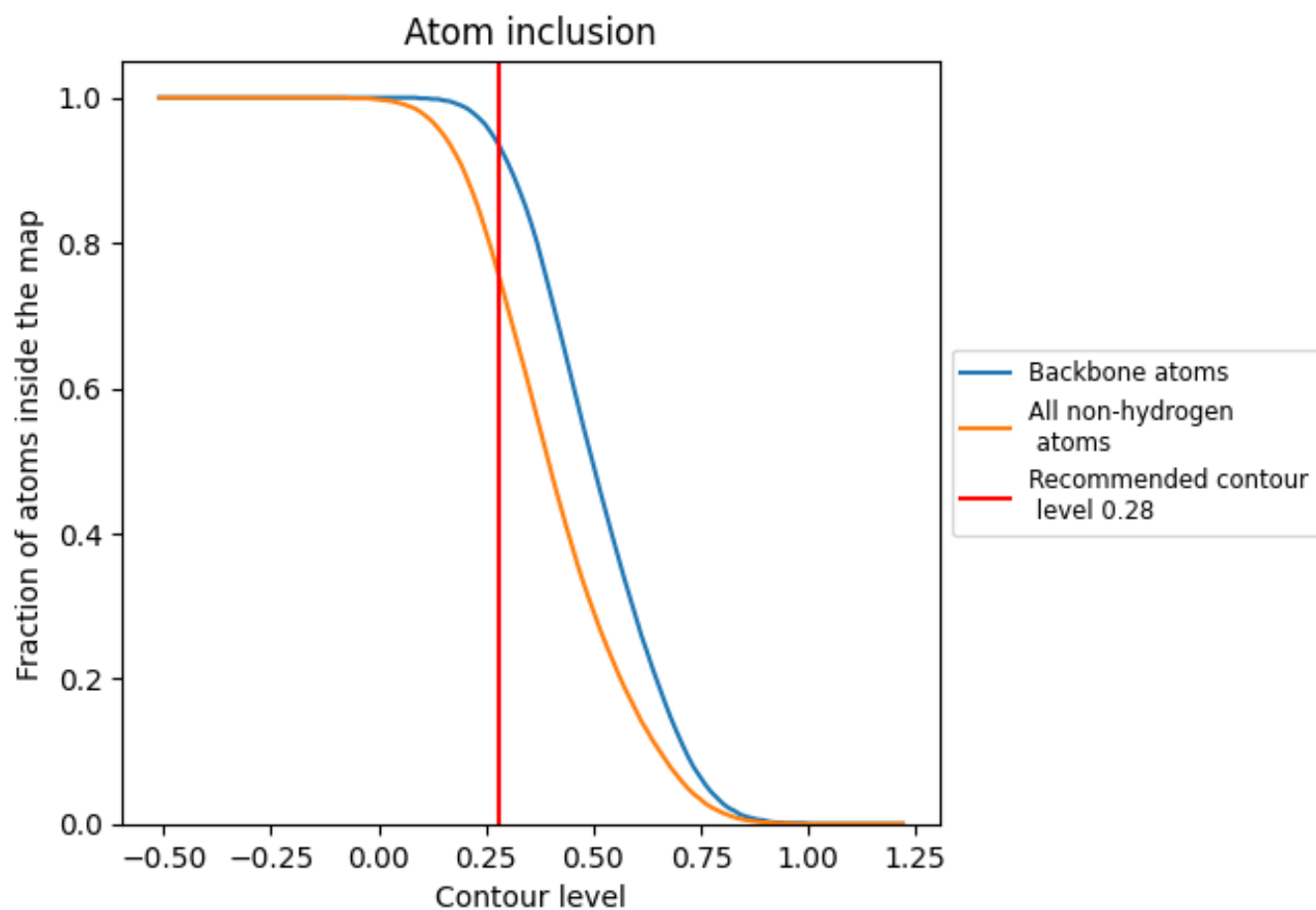
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.28).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 76% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7550	 0.2710
0	 0.8270	 0.2960
1	 0.8560	 0.3300
2	 0.8390	 0.3110
3	 0.8550	 0.3440
4	 0.8380	 0.3410
5	 0.8450	 0.3280
6	 0.5010	 0.1820
7	 0.8010	 0.3170
8	 0.8330	 0.2650
9	 0.8510	 0.2590
Q	 0.7250	 0.2370
R	 0.7800	 0.2480
T	 0.8250	 0.2370
U	 0.7110	 0.2120
V	 0.6540	 0.2190
X	 0.7930	 0.3350
a	 0.7140	 0.2460
b	 0.7270	 0.2590
c	 0.8440	 0.2420
d	 0.6970	 0.2870
e	 0.7320	 0.2470
f	 0.6480	 0.2110
g	 0.7180	 0.2640
h	 0.7000	 0.2460
i	 0.6610	 0.2340
j	 0.6440	 0.2420
k	 0.6580	 0.2110
l	 0.6740	 0.2220
m	 0.6910	 0.2190
n	 0.6630	 0.2400
o	 0.7000	 0.2580
p	 0.7290	 0.2700
s	 0.4700	 0.1450

