



Full wwPDB EM Validation Report ⓘ

Jun 13, 2024 – 04:38 PM EDT

PDB ID : 9BRT
EMDB ID : EMD-44843
Title : Intact V-ATPase State 1 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 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) : 2.36.2

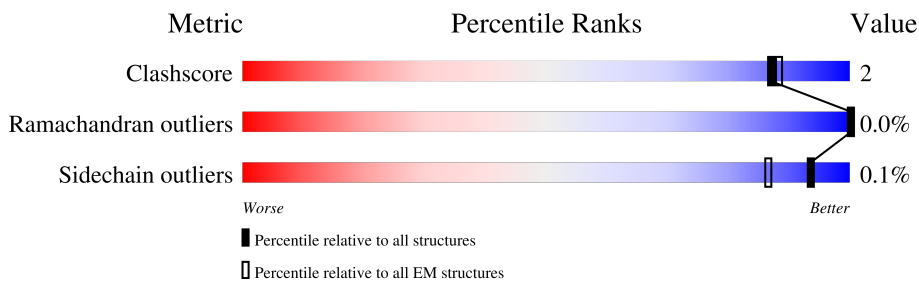
1 Overall quality at a glance

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	8	226	96%
1	9	226	98%
1	Q	226	9% 95% 5%
2	R	118	6% 92% 5%
2	T	118	90% 7%
2	V	118	93%
3	0	617	93% 5%
3	1	617	96%

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Mol	Chain	Length	Quality of chain
3	2	617	95%
4	3	511	87% 10%
4	4	511	88% 10%
4	5	511	88% 11%
5	6	382	23% 89% 5% 6%
6	7	247	19% 80% 16%
7	U	483	19% 83% 5% 12%
8	X	119	6% 86% 7% 8%
9	a	838	6% 89% 11%
10	b	205	16% 98%
11	d	351	9% 100%
12	g	155	22% 97%
12	h	155	23% 97%
12	i	155	16% 97%
12	j	155	18% 97%
12	k	155	27% 96%
12	l	155	27% 97%
12	m	155	21% 97%
12	n	155	18% 97%
12	o	155	17% 97%
13	p	350	15% 85%
14	c	463	43% 56%
15	f	98	21% 88% 12%
16	s	314	31% 67% 33%
17	e	81	17% 98%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 66930 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 subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	8	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		
1	9	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		
1	Q	225	Total	C	N	O	S	0	0
			1823	1146	322	345	10		

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

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

- 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	0	585	Total	C	N	O	S	0	0
			4551	2891	768	866	26		
3	1	596	Total	C	N	O	S	0	0
			4627	2937	782	881	27		
3	2	599	Total	C	N	O	S	0	0
			4647	2948	786	886	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	458	Total	C	N	O	S	0	0
			3584	2275	608	681	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	462	Total	C	N	O	S	0	0
			3617	2296	613	688	20		
4	5	457	Total	C	N	O	S	0	0
			3575	2270	607	678	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	360	Total	C	N	O	S	0	0
			2925	1874	494	548	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	208	Total	C	N	O	S	0	0
			1676	1064	303	304	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	427	Total	C	N	O	S	0	0
			3507	2227	605	650	25		

- 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 116 kDa subunit a 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	750	Total	C	N	O	S	0	0
			6105	3986	1021	1057	41		

- Molecule 10 is a protein called V-type proton ATPase 21 kDa proteolipid subunit c^{''}.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	203	Total	C	N	O	S	0	0
			1503	996	237	259	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	d	350	2833	1829	460	530	14	0	0

- Molecule 12 is a protein called V-type proton ATPase 16 kDa proteolipid subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	g	150	1068	699	171	190	8	0	0
12	h	150	1068	699	171	190	8	0	0
12	i	150	1068	699	171	190	8	0	0
12	j	150	1068	699	171	190	8	0	0
12	k	150	1068	699	171	190	8	0	0
12	l	150	1068	699	171	190	8	0	0
12	m	150	1068	699	171	190	8	0	0
12	n	150	1068	699	171	190	8	0	0
12	o	150	1068	699	171	190	8	0	0

- Molecule 13 is a protein called Renin receptor cytoplasmic fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	p	52	433	292	63	75	3	0	0

- Molecule 14 is a protein called V-type proton ATPase subunit S1.

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

- Molecule 15 is a protein called Ribonuclease kappa.

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

- 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

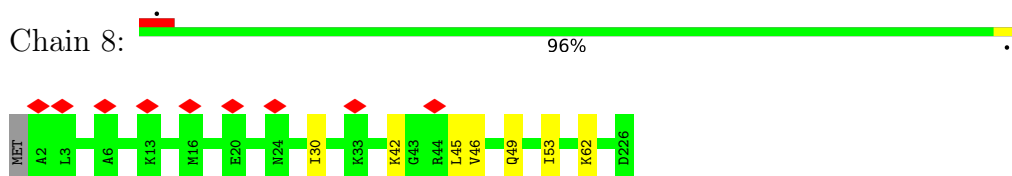
- Molecule 17 is a protein called V-type proton ATPase subunit e 2.

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

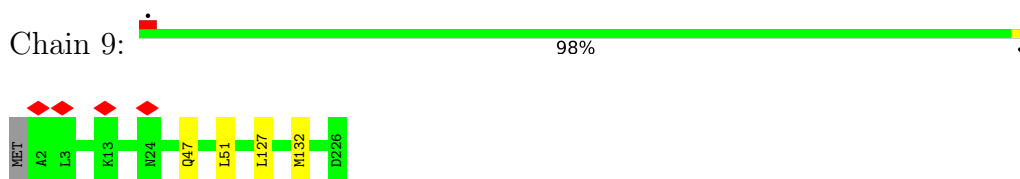
3 Residue-property plots [i](#)

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.

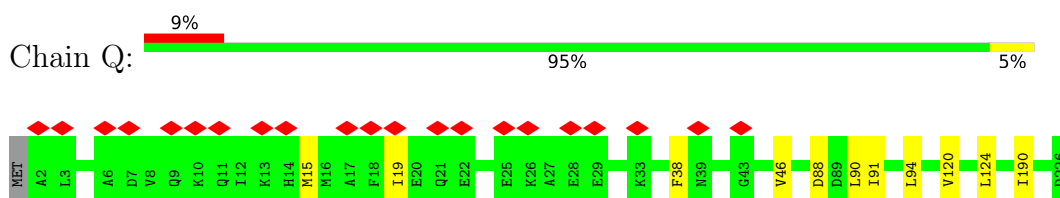
- Molecule 1: V-type proton ATPase subunit E 1



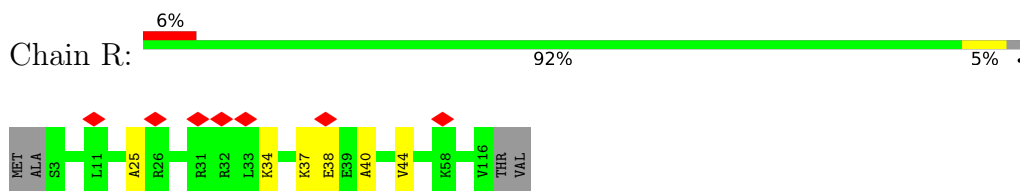
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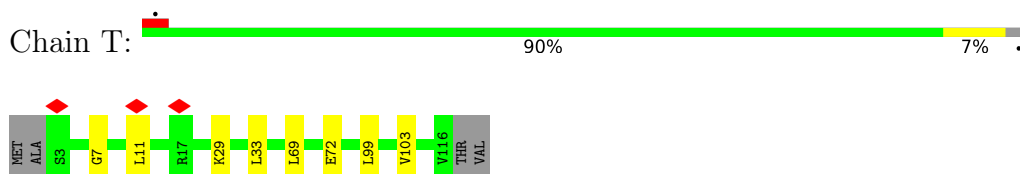
- Molecule 1: V-type proton ATPase subunit E 1



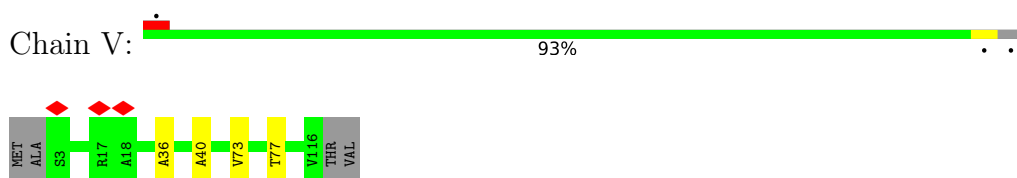
- Molecule 2: V-type proton ATPase subunit G 2



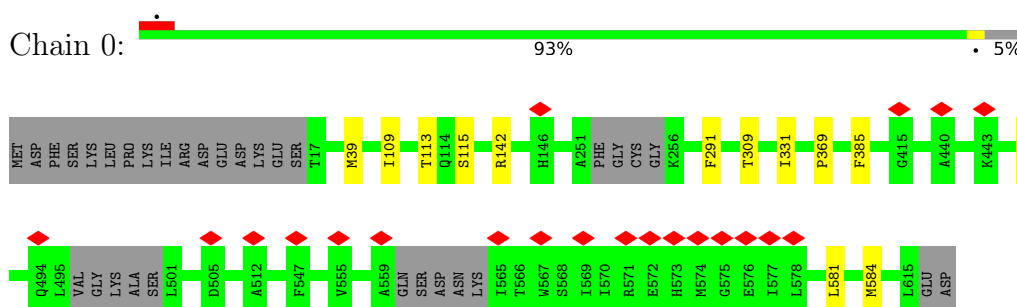
- Molecule 2: V-type proton ATPase subunit G 2



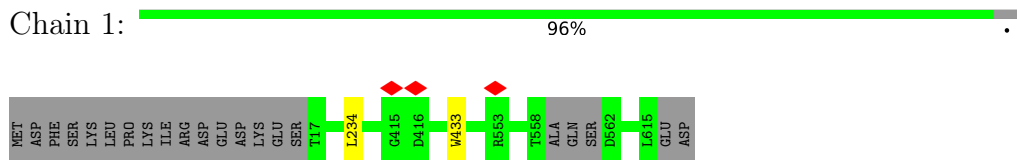
- Molecule 2: V-type proton ATPase subunit G 2



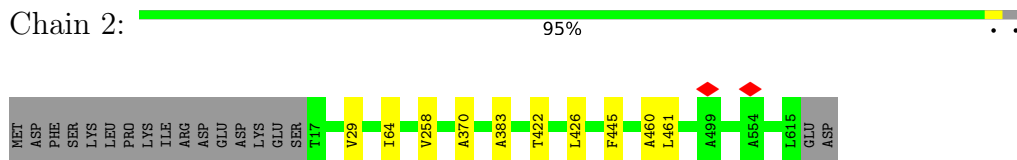
- Molecule 3: V-type proton ATPase catalytic subunit A



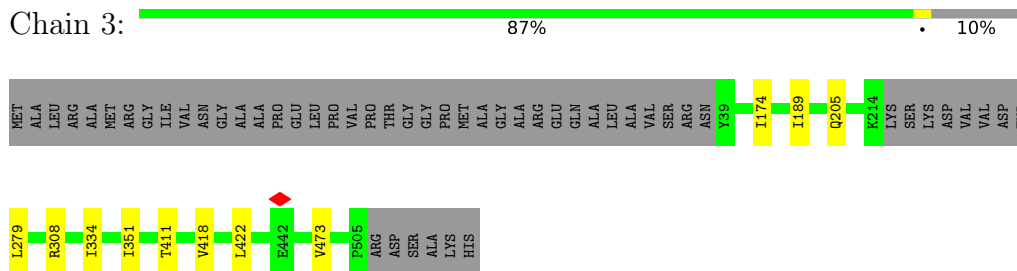
- Molecule 3: V-type proton ATPase catalytic subunit A



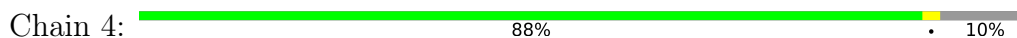
- Molecule 3: V-type proton ATPase catalytic subunit A

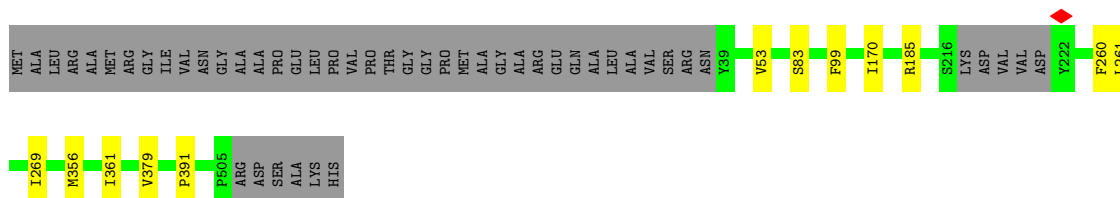


- Molecule 4: V-type proton ATPase subunit B, brain isoform

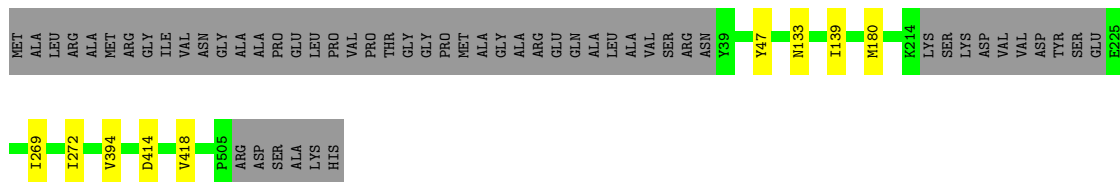
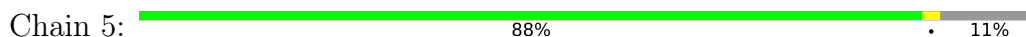


- Molecule 4: V-type proton ATPase subunit B, brain isoform

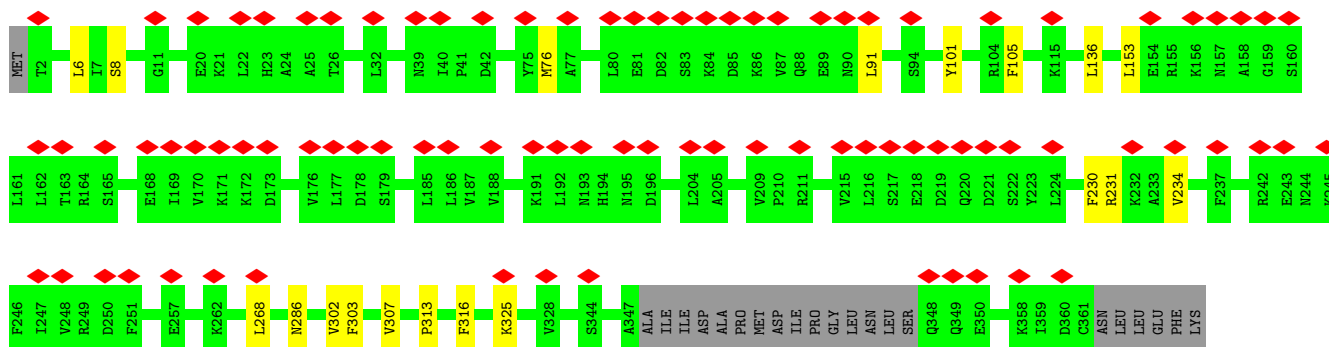
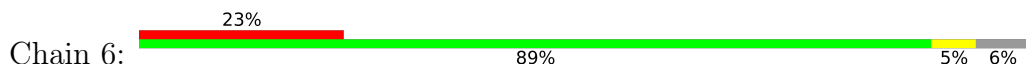




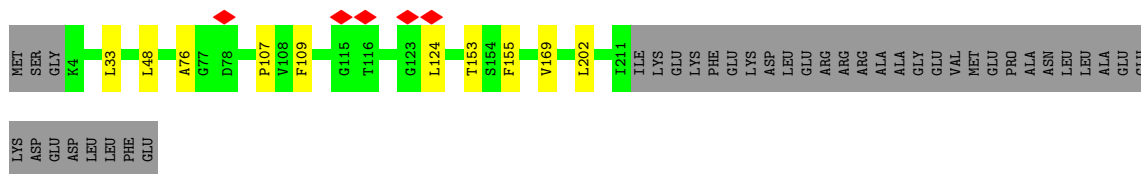
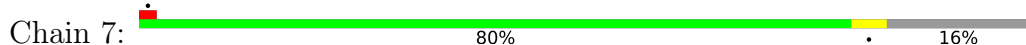
• Molecule 4: V-type proton ATPase subunit B, brain isoform



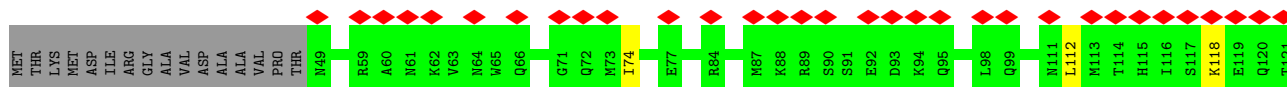
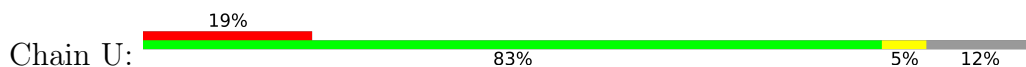
• Molecule 5: V-type proton ATPase subunit C 1

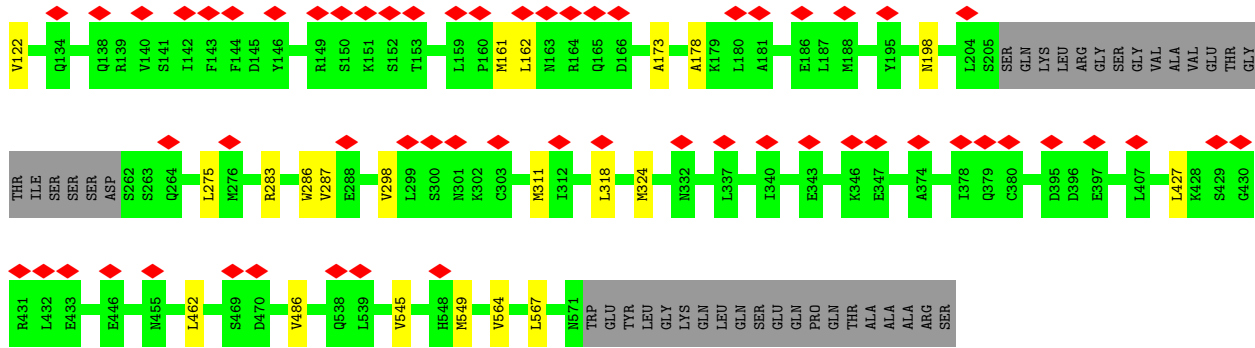


• Molecule 6: V-type proton ATPase subunit D

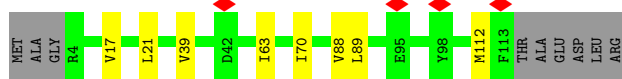
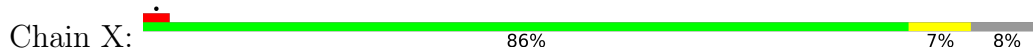


• Molecule 7: V-type proton ATPase subunit H

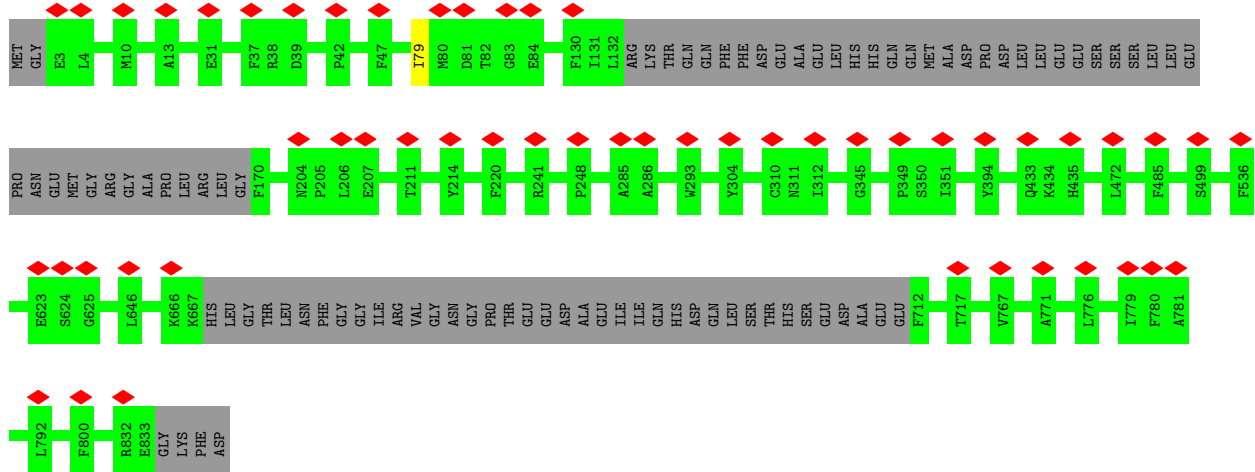
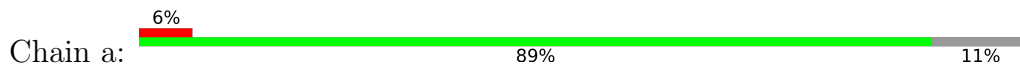




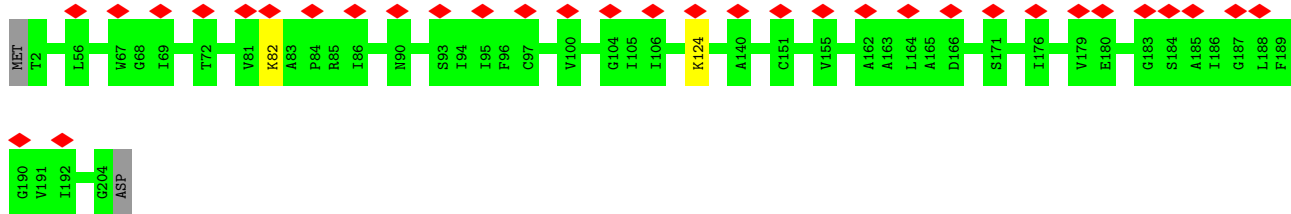
• Molecule 8: V-type proton ATPase subunit F



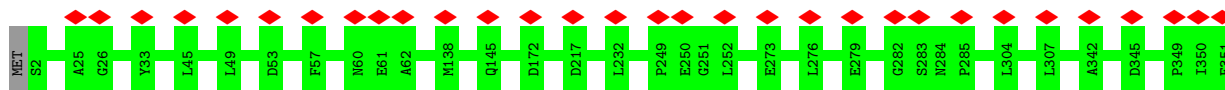
• Molecule 9: V-type proton ATPase 116 kDa subunit a 1



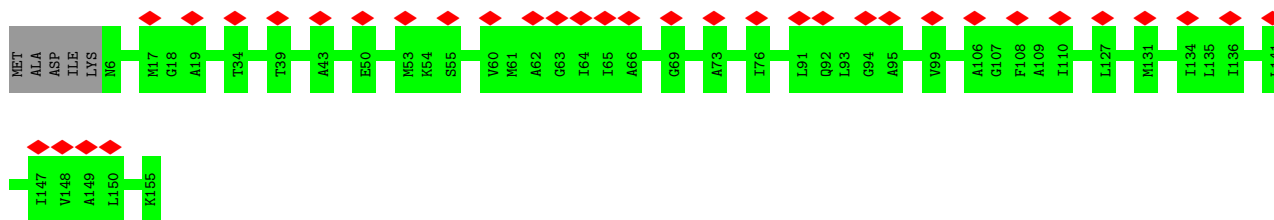
• Molecule 10: V-type proton ATPase 21 kDa proteolipid subunit c''



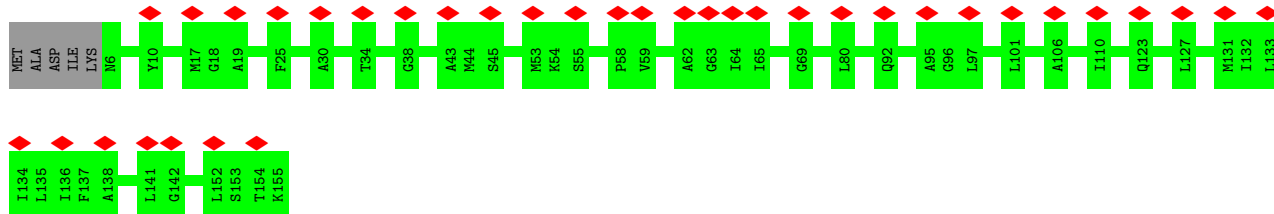
• Molecule 11: V-type proton ATPase subunit d 1



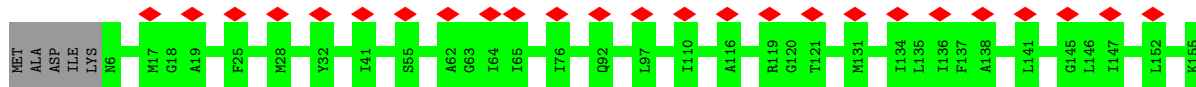
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c



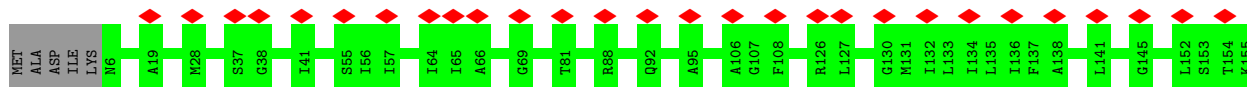
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c



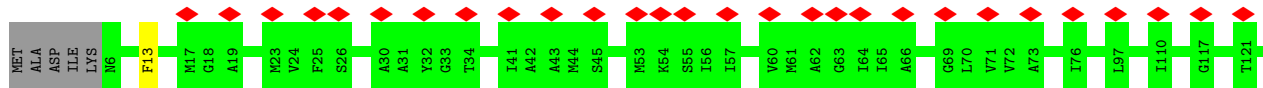
• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c

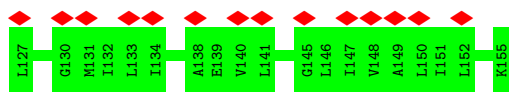


• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c

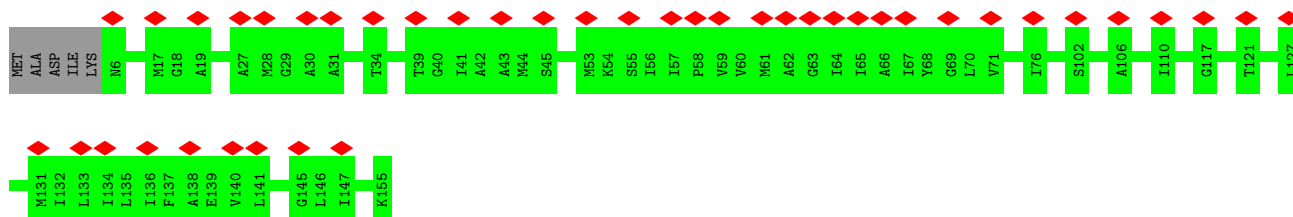


• Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c

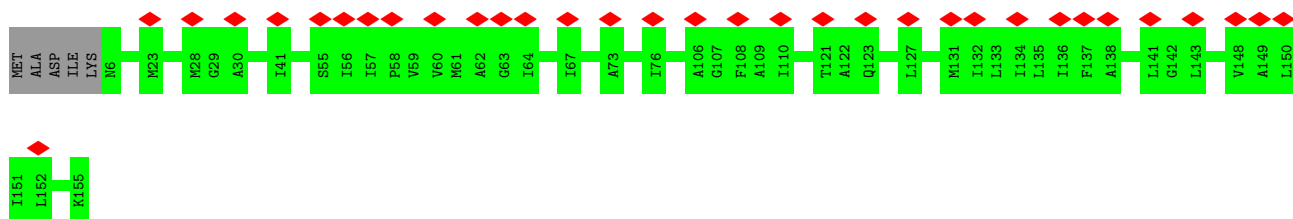




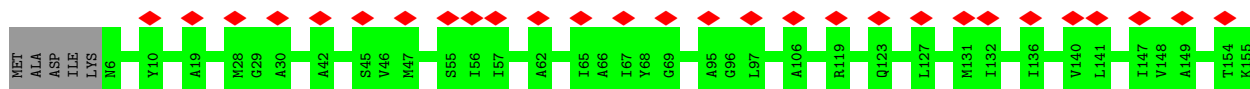
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c



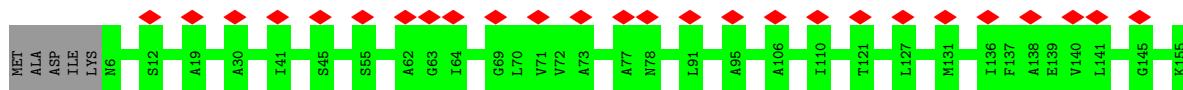
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c



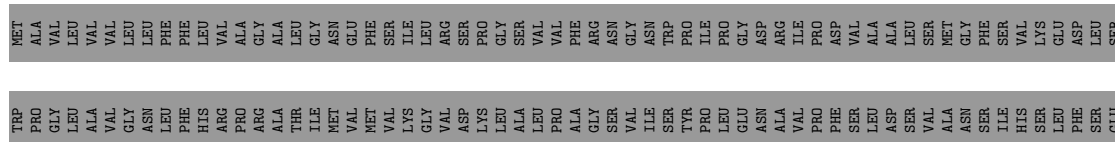
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c

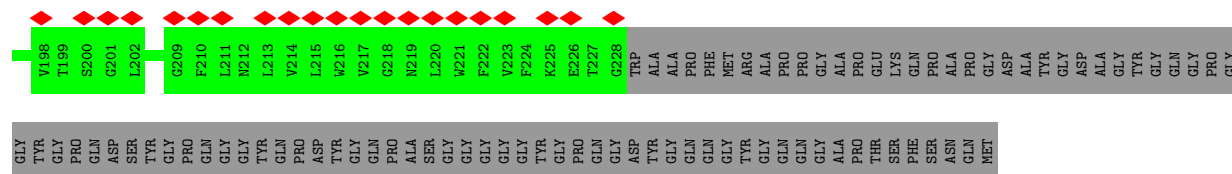


- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit c

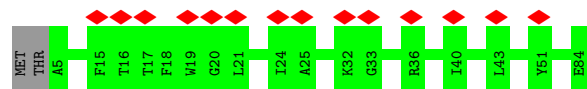


- Molecule 13: Renin receptor cytoplasmic fragment





• Molecule 17: V-type proton ATPase subunit e 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17889	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	1.434	Depositor
Minimum map value	-0.690	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.062	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	8	0.27	0/1840	0.54	0/2462
1	9	0.27	0/1840	0.52	0/2462
1	Q	0.27	0/1840	0.56	0/2462
2	R	0.29	0/930	0.60	0/1237
2	T	0.26	0/930	0.59	0/1237
2	V	0.27	0/930	0.57	0/1237
3	0	0.28	0/4643	0.54	0/6284
3	1	0.28	0/4722	0.54	0/6391
3	2	0.28	0/4743	0.54	0/6421
4	3	0.29	0/3655	0.55	0/4954
4	4	0.29	0/3689	0.55	0/4999
4	5	0.29	0/3646	0.55	0/4942
5	6	0.26	0/2979	0.50	0/4024
6	7	0.28	0/1694	0.57	0/2267
7	U	0.27	0/3574	0.53	0/4814
8	X	0.27	0/889	0.58	0/1199
9	a	0.28	0/6263	0.55	0/8473
10	b	0.32	0/1537	0.58	0/2088
11	d	0.29	0/2899	0.53	0/3927
12	g	0.31	0/1083	0.57	0/1466
12	h	0.28	0/1083	0.56	0/1466
12	i	0.31	0/1083	0.59	0/1466
12	j	0.31	0/1083	0.64	0/1466
12	k	0.32	0/1083	0.58	0/1466
12	l	0.32	0/1083	0.59	0/1466
12	m	0.30	0/1083	0.57	0/1466
12	n	0.31	0/1083	0.57	0/1466
12	o	0.34	0/1083	0.64	0/1466
13	p	0.27	0/446	0.51	0/610
14	c	0.27	0/1697	0.55	0/2311
15	f	0.28	0/682	0.50	0/926
16	s	0.27	0/1716	0.48	0/2327
17	e	0.30	0/662	0.57	0/910
All	All	0.29	0/68193	0.55	0/92158

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8	1823	0	1895	7	0
1	9	1823	0	1895	2	0
1	Q	1823	0	1895	7	0
2	R	925	0	935	8	0
2	T	925	0	935	4	0
2	V	925	0	935	3	0
3	0	4551	0	4543	11	0
3	1	4627	0	4618	1	0
3	2	4647	0	4637	6	0
4	3	3584	0	3582	8	0
4	4	3617	0	3614	9	0
4	5	3575	0	3576	5	0
5	6	2925	0	2964	10	0
6	7	1676	0	1781	8	0
7	U	3507	0	3486	18	0
8	X	875	0	883	6	0
9	a	6105	0	6131	0	0
10	b	1503	0	1551	0	0
11	d	2833	0	2770	0	0
12	g	1068	0	1136	0	0
12	h	1068	0	1136	0	0
12	i	1068	0	1136	0	0
12	j	1068	0	1136	0	0
12	k	1068	0	1136	0	0
12	l	1068	0	1136	0	0
12	m	1068	0	1136	0	0
12	n	1068	0	1136	0	0
12	o	1068	0	1136	0	0
13	p	433	0	432	0	0
14	c	1642	0	1568	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	66930	0	67814	95	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 2.

All (95) 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)
1:Q:46:VAL:HG21	2:V:40:ALA:HB1	1.69	0.72
7:U:162:LEU:HD22	7:U:198:ASN:HB2	1.71	0.71
1:8:45:LEU:HD22	2:R:37:LYS:HE2	1.73	0.70
6:7:109:PHE:CD2	8:X:63:ILE:HD11	2.31	0.66
4:3:174:ILE:HD11	4:3:205:GLN:HG2	1.79	0.65
6:7:48:LEU:HD22	8:X:112:MET:HE1	1.79	0.65
1:8:45:LEU:HD22	2:R:37:LYS:CE	2.30	0.61
7:U:162:LEU:HD22	7:U:198:ASN:CB	2.30	0.61
7:U:178:ALA:HB1	7:U:275:LEU:HD23	1.83	0.60
1:8:49:GLN:HB3	2:R:44:VAL:HG21	1.84	0.60
7:U:298:VAL:HG13	7:U:311:MET:CE	2.33	0.58
2:V:73:VAL:O	2:V:77:THR:HG23	2.04	0.57
2:R:40:ALA:O	2:R:44:VAL:HG23	2.04	0.57
4:3:189:ILE:O	4:3:351:ILE:HD12	2.05	0.56
6:7:48:LEU:HD21	6:7:155:PHE:CE1	2.40	0.56
3:0:39:MET:CE	4:4:53:VAL:HG11	2.37	0.55
5:6:231:ARG:O	5:6:234:VAL:HG22	2.07	0.54
1:Q:120:VAL:O	1:Q:124:LEU:HD23	2.07	0.54
5:6:153:LEU:HD12	5:6:268:LEU:HD12	1.89	0.53
5:6:307:VAL:HG22	5:6:313:PRO:HG3	1.91	0.53
7:U:298:VAL:HG13	7:U:311:MET:HE1	1.91	0.53
7:U:427:LEU:HD21	7:U:462:LEU:HD21	1.91	0.53
3:0:581:LEU:HD23	3:0:584:MET:HE3	1.91	0.52
1:9:127:LEU:HD23	1:9:132:MET:HG3	1.91	0.52
3:0:109:ILE:O	3:0:113:THR:HG22	2.10	0.52
1:9:47:GLN:O	1:9:51:LEU:HD23	2.10	0.51
7:U:283:ARG:HG3	7:U:318:LEU:HD23	1.92	0.51
7:U:564:VAL:HA	7:U:567:LEU:HD12	1.91	0.51
1:Q:15:MET:SD	1:Q:19:ILE:HD12	2.51	0.50
5:6:136:LEU:HD13	5:6:286:ASN:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:581:LEU:HD23	3:0:584:MET:CE	2.43	0.49
4:3:418:VAL:O	4:3:422:LEU:HD23	2.12	0.49
7:U:545:VAL:HG12	7:U:564:VAL:HG23	1.94	0.49
6:7:33:LEU:HD23	6:7:169:VAL:HG22	1.94	0.49
5:6:6:LEU:HG	5:6:302:VAL:HG21	1.94	0.49
7:U:545:VAL:CG1	7:U:564:VAL:HG23	2.43	0.49
4:5:47:TYR:CD2	1:Q:190:ILE:HD13	2.47	0.48
1:Q:90:LEU:O	1:Q:94:LEU:HD23	2.13	0.48
5:6:230:PHE:O	5:6:234:VAL:HG13	2.13	0.48
1:Q:38:PHE:CD1	2:V:36:ALA:HB2	2.49	0.48
3:2:370:ALA:HB1	4:3:308:ARG:HH21	1.79	0.48
4:3:279:LEU:HD12	4:3:334:ILE:HD12	1.96	0.48
5:6:303:PHE:O	5:6:307:VAL:HG23	2.14	0.47
1:8:42:LYS:O	1:8:46:VAL:HG23	2.14	0.47
3:0:113:THR:HG23	3:0:115:SER:H	1.80	0.47
1:8:53:ILE:HD11	2:R:44:VAL:HG22	1.97	0.47
8:X:39:VAL:HG11	8:X:70:ILE:HD11	1.97	0.47
6:7:48:LEU:HD22	8:X:112:MET:CE	2.46	0.46
4:4:170:ILE:HD11	4:4:185:ARG:HG2	1.97	0.46
4:3:351:ILE:HG23	4:3:351:ILE:O	2.15	0.46
7:U:486:VAL:HG21	7:U:567:LEU:HD21	1.98	0.45
8:X:17:VAL:O	8:X:21:LEU:HD23	2.17	0.45
4:5:269:ILE:O	4:5:272:ILE:HG22	2.17	0.45
6:7:107:PRO:HG2	6:7:153:THR:HG22	1.99	0.44
3:0:39:MET:HE3	4:4:53:VAL:HG11	1.98	0.44
4:5:133:ASN:HB3	4:5:139:ILE:HG21	1.99	0.44
7:U:161:MET:HB3	7:U:173:ALA:HB2	2.00	0.44
1:8:53:ILE:HD11	2:R:44:VAL:HG13	1.99	0.44
4:3:411:THR:HG22	4:3:473:VAL:HG21	1.99	0.44
5:6:101:TYR:HH	5:6:105:PHE:HE1	1.66	0.44
6:7:76:ALA:HB1	6:7:124:LEU:HB3	2.00	0.44
4:4:99:PHE:CE1	4:4:269:ILE:HG21	2.53	0.43
5:6:76:MET:HG2	5:6:91:LEU:HD11	2.00	0.43
2:T:69:LEU:HD23	2:T:72:GLU:OE1	2.18	0.43
8:X:88:VAL:C	8:X:89:LEU:HD22	2.38	0.43
4:4:356:MET:HE1	4:4:361:ILE:HD12	2.00	0.43
7:U:287:VAL:HG11	7:U:324:MET:HE1	2.00	0.43
2:R:34:LYS:O	2:R:38:GLU:OE1	2.37	0.43
2:T:7:GLY:O	2:T:11:LEU:HD23	2.17	0.43
7:U:74:ILE:HA	7:U:112:LEU:HD11	2.01	0.43
3:2:460:ALA:C	3:2:461:LEU:HD22	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:234:LEU:HD13	3:1:433:TRP:CZ3	2.55	0.42
4:4:83:SER:HG	4:4:99:PHE:HD2	1.65	0.42
7:U:486:VAL:HG21	7:U:567:LEU:CD2	2.48	0.42
4:4:379:VAL:HG13	4:4:391:PRO:HG2	2.01	0.42
3:2:29:VAL:O	3:2:64:ILE:HD12	2.20	0.42
5:6:8:SER:HG	5:6:316:PHE:HD2	1.67	0.42
3:2:422:THR:O	3:2:426:LEU:HD23	2.19	0.41
4:5:414:ASP:O	4:5:418:VAL:HG23	2.19	0.41
7:U:118:LYS:O	7:U:122:VAL:HG12	2.20	0.41
3:2:258:VAL:HG11	3:2:445:PHE:CZ	2.55	0.41
7:U:549:MET:CE	7:U:564:VAL:HG11	2.50	0.41
1:Q:88:ASP:HA	1:Q:91:ILE:HG22	2.03	0.41
3:0:39:MET:HE1	4:4:53:VAL:HG11	2.01	0.41
3:2:383:ALA:HB1	4:3:264:ALA:HB1	2.03	0.41
4:5:180:MET:HG3	4:5:394:VAL:HG21	2.03	0.41
3:0:331:ILE:HD11	3:0:385:PHE:CE1	2.55	0.41
7:U:286:TRP:CZ3	7:U:318:LEU:HD11	2.56	0.41
1:8:30:ILE:HG22	2:R:25:ALA:HB2	2.02	0.41
4:4:260:PHE:O	4:4:261:LEU:HD22	2.21	0.40
3:0:461:LEU:HD12	3:0:464:TYR:HB3	2.02	0.40
3:0:291:PHE:CE2	3:0:309:THR:HG21	2.56	0.40
2:T:29:LYS:O	2:T:33:LEU:HD23	2.21	0.40
3:0:369:PRO:HD2	6:7:202:LEU:HD11	2.02	0.40
2:T:99:LEU:O	2:T:103:VAL:HG23	2.21	0.40

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	8	223/226 (99%)	218 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9	223/226 (99%)	219 (98%)	4 (2%)	0	100	100
1	Q	223/226 (99%)	216 (97%)	7 (3%)	0	100	100
2	R	112/118 (95%)	107 (96%)	5 (4%)	0	100	100
2	T	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
2	V	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
3	0	577/617 (94%)	536 (93%)	41 (7%)	0	100	100
3	1	592/617 (96%)	558 (94%)	34 (6%)	0	100	100
3	2	597/617 (97%)	567 (95%)	30 (5%)	0	100	100
4	3	454/511 (89%)	426 (94%)	28 (6%)	0	100	100
4	4	458/511 (90%)	441 (96%)	17 (4%)	0	100	100
4	5	453/511 (89%)	428 (94%)	25 (6%)	0	100	100
5	6	356/382 (93%)	334 (94%)	22 (6%)	0	100	100
6	7	206/247 (83%)	195 (95%)	11 (5%)	0	100	100
7	U	423/483 (88%)	400 (95%)	23 (5%)	0	100	100
8	X	108/119 (91%)	97 (90%)	11 (10%)	0	100	100
9	a	744/838 (89%)	696 (94%)	47 (6%)	1 (0%)	51	85
10	b	201/205 (98%)	199 (99%)	2 (1%)	0	100	100
11	d	348/351 (99%)	330 (95%)	18 (5%)	0	100	100
12	g	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
12	h	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
12	i	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
12	j	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
12	k	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
12	l	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
12	m	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
12	n	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
12	o	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
13	p	50/350 (14%)	47 (94%)	3 (6%)	0	100	100
14	c	201/463 (43%)	175 (87%)	25 (12%)	1 (0%)	29	68
15	f	84/98 (86%)	80 (95%)	4 (5%)	0	100	100
16	s	209/314 (67%)	203 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	e	77/81 (95%)	71 (92%)	6 (8%)	0	100	100
All	All	8475/9742 (87%)	8058 (95%)	415 (5%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	c	366	GLU
9	a	79	ILE

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	8	197/198 (100%)	196 (100%)	1 (0%)	88	93
1	9	197/198 (100%)	197 (100%)	0	100	100
1	Q	197/198 (100%)	197 (100%)	0	100	100
2	R	96/99 (97%)	96 (100%)	0	100	100
2	T	96/99 (97%)	96 (100%)	0	100	100
2	V	96/99 (97%)	96 (100%)	0	100	100
3	0	496/524 (95%)	495 (100%)	1 (0%)	93	96
3	1	504/524 (96%)	504 (100%)	0	100	100
3	2	506/524 (97%)	506 (100%)	0	100	100
4	3	392/431 (91%)	392 (100%)	0	100	100
4	4	396/431 (92%)	396 (100%)	0	100	100
4	5	391/431 (91%)	391 (100%)	0	100	100
5	6	325/344 (94%)	324 (100%)	1 (0%)	92	95
6	7	179/212 (84%)	179 (100%)	0	100	100
7	U	385/429 (90%)	385 (100%)	0	100	100
8	X	94/100 (94%)	94 (100%)	0	100	100
9	a	668/741 (90%)	668 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	b	156/158 (99%)	154 (99%)	2 (1%)	69	82
11	d	305/306 (100%)	305 (100%)	0	100	100
12	g	109/113 (96%)	109 (100%)	0	100	100
12	h	109/113 (96%)	109 (100%)	0	100	100
12	i	109/113 (96%)	109 (100%)	0	100	100
12	j	109/113 (96%)	109 (100%)	0	100	100
12	k	109/113 (96%)	108 (99%)	1 (1%)	78	88
12	l	109/113 (96%)	109 (100%)	0	100	100
12	m	109/113 (96%)	109 (100%)	0	100	100
12	n	109/113 (96%)	109 (100%)	0	100	100
12	o	109/113 (96%)	109 (100%)	0	100	100
13	p	47/309 (15%)	47 (100%)	0	100	100
14	c	180/395 (46%)	179 (99%)	1 (1%)	86	92
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	7202/8164 (88%)	7195 (100%)	7 (0%)	93	97

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

Mol	Chain	Res	Type
1	8	62	LYS
3	0	142	ARG
5	6	325	LYS
10	b	82	LYS
10	b	124	LYS
12	k	13	PHE
14	c	444	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	0	573	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.

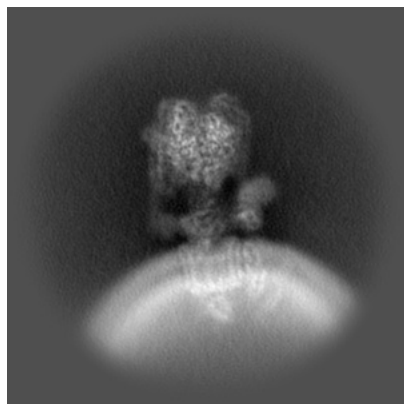
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44843. These allow visual inspection of the internal detail of the map and identification of artifacts.

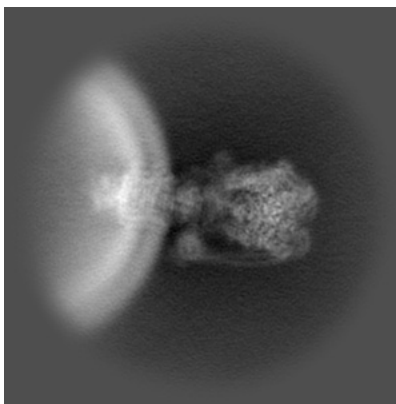
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

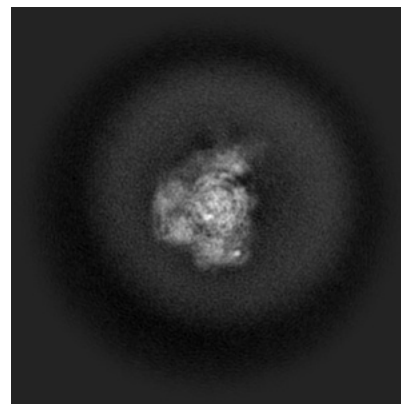
6.1.1 Primary map



X

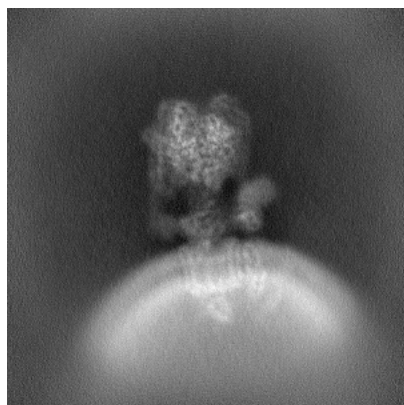


Y

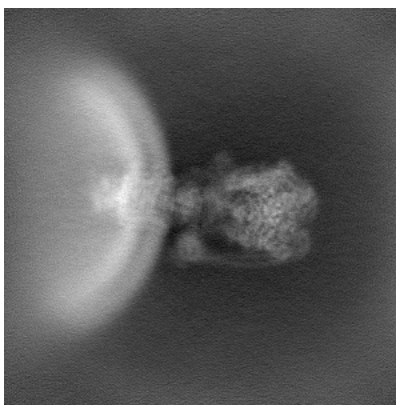


Z

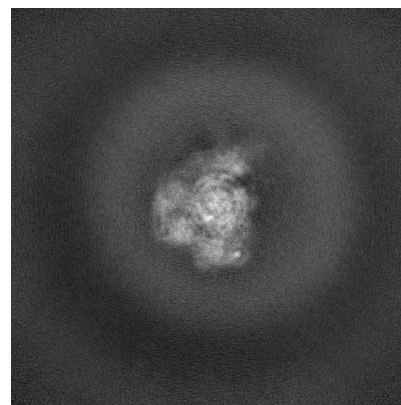
6.1.2 Raw map



X



Y

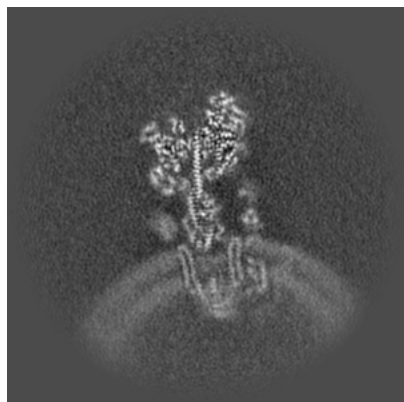


Z

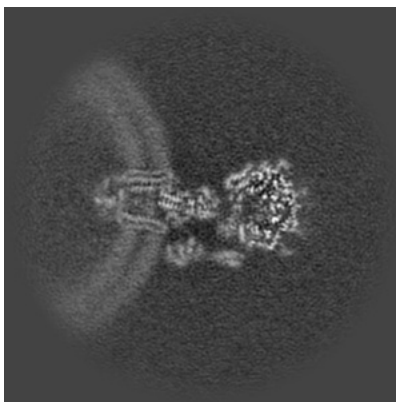
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

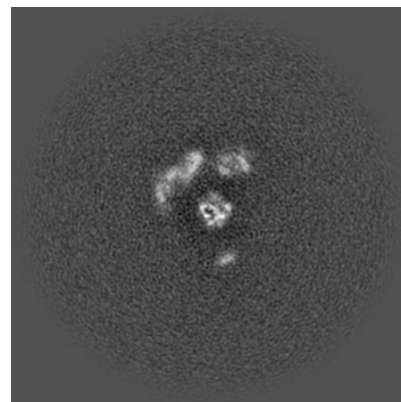
6.2.1 Primary map



X Index: 224

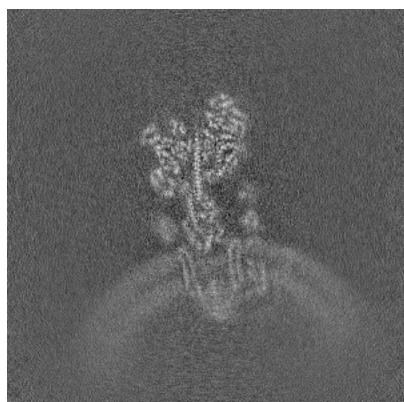


Y Index: 224

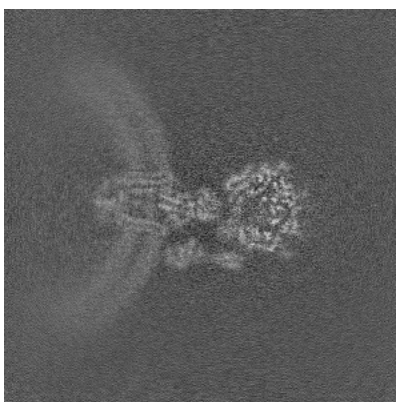


Z Index: 224

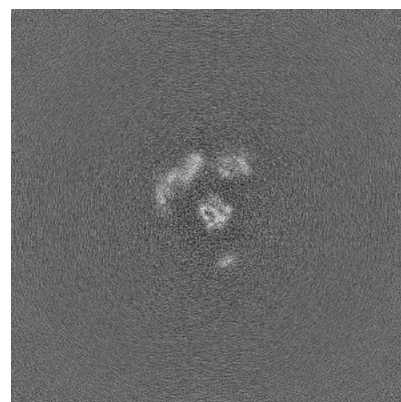
6.2.2 Raw map



X Index: 224



Y Index: 224

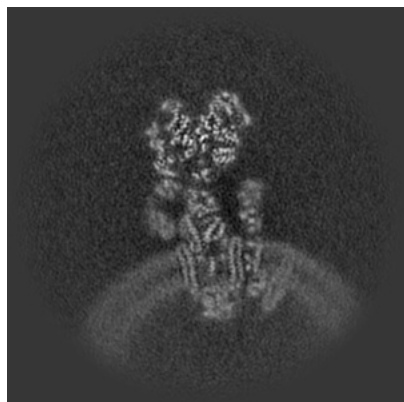


Z Index: 224

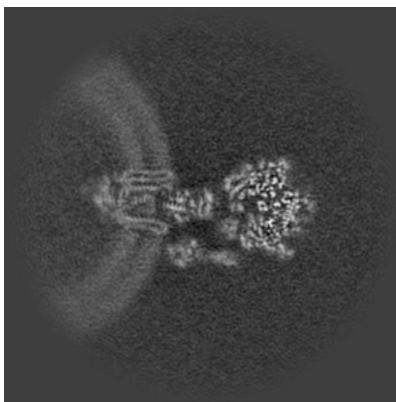
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

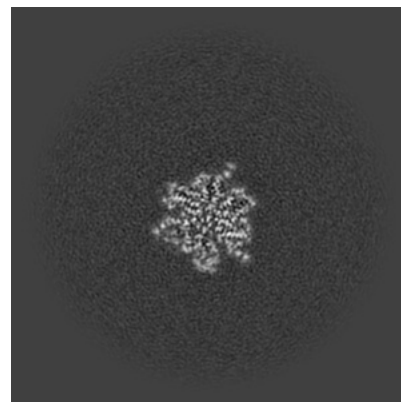
6.3.1 Primary map



X Index: 232

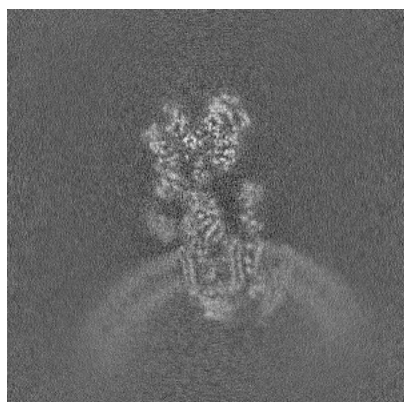


Y Index: 227

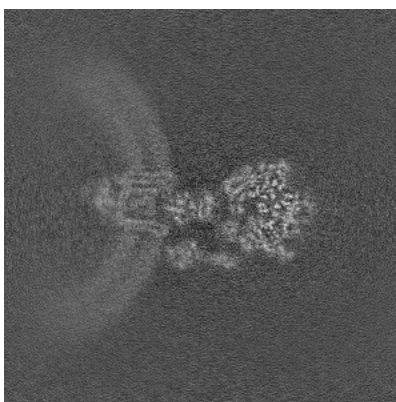


Z Index: 299

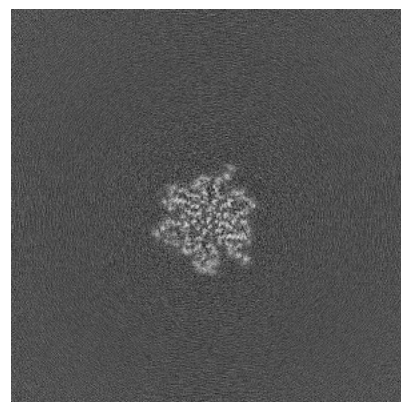
6.3.2 Raw map



X Index: 230



Y Index: 227

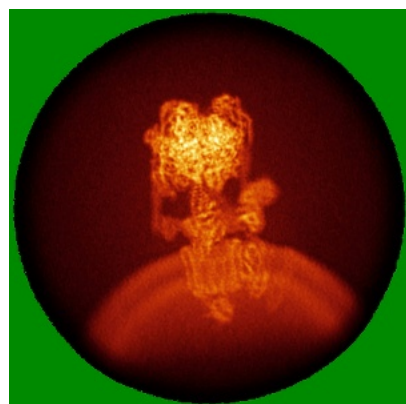


Z Index: 299

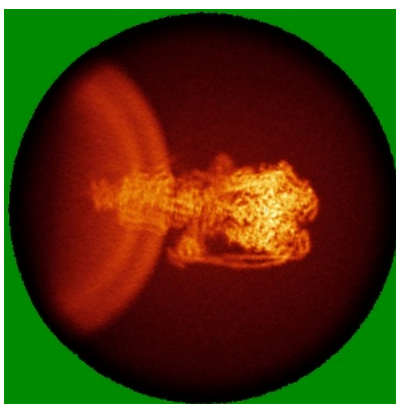
The images above show the largest variance slices of the map in three orthogonal directions.

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

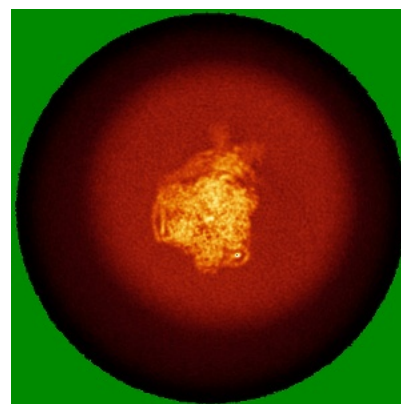
6.4.1 Primary map



X

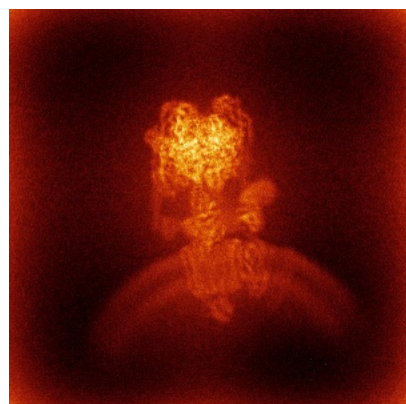


Y

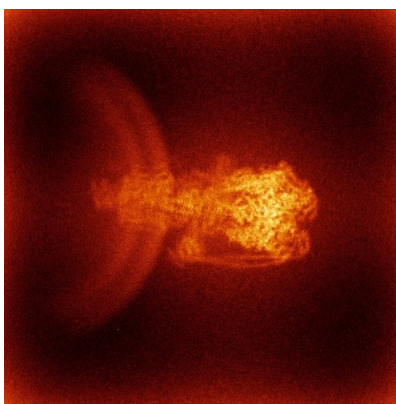


Z

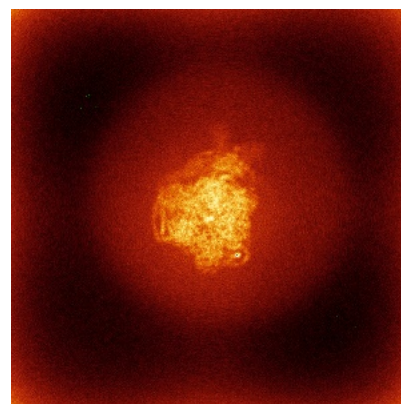
6.4.2 Raw map



X



Y

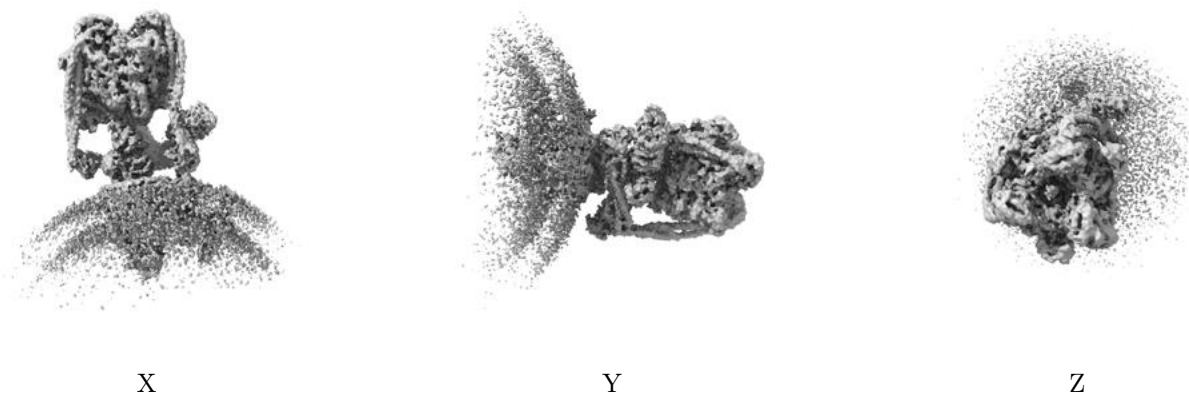


Z

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.

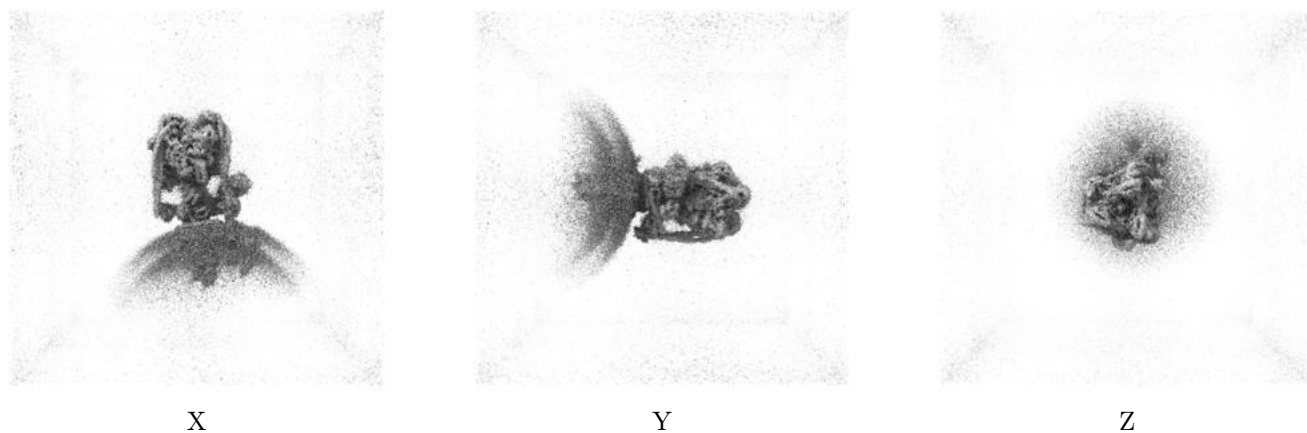
6.5 Orthogonal surface views [i](#)

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.

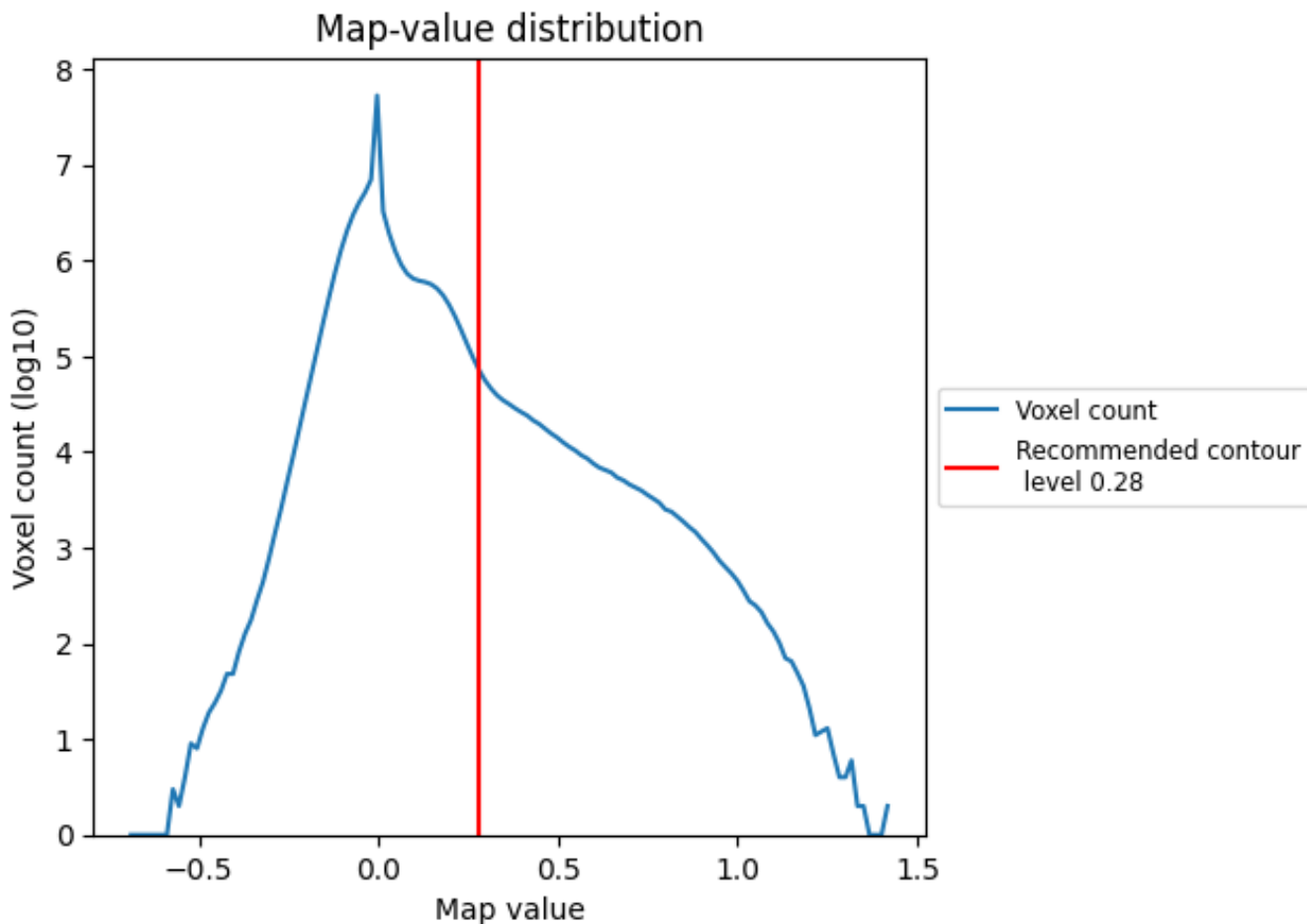
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

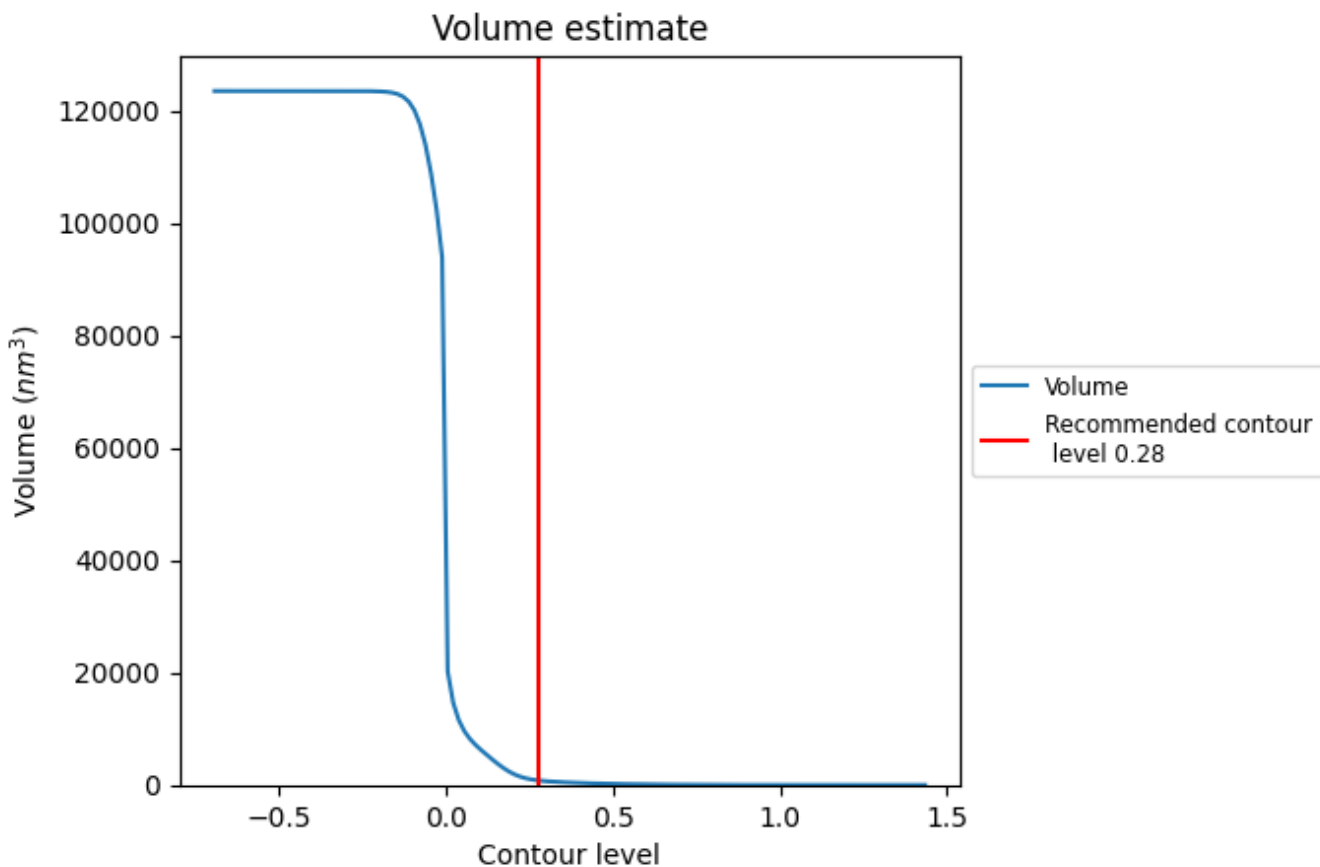
This section contains the results of statistical analysis of the map.

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.

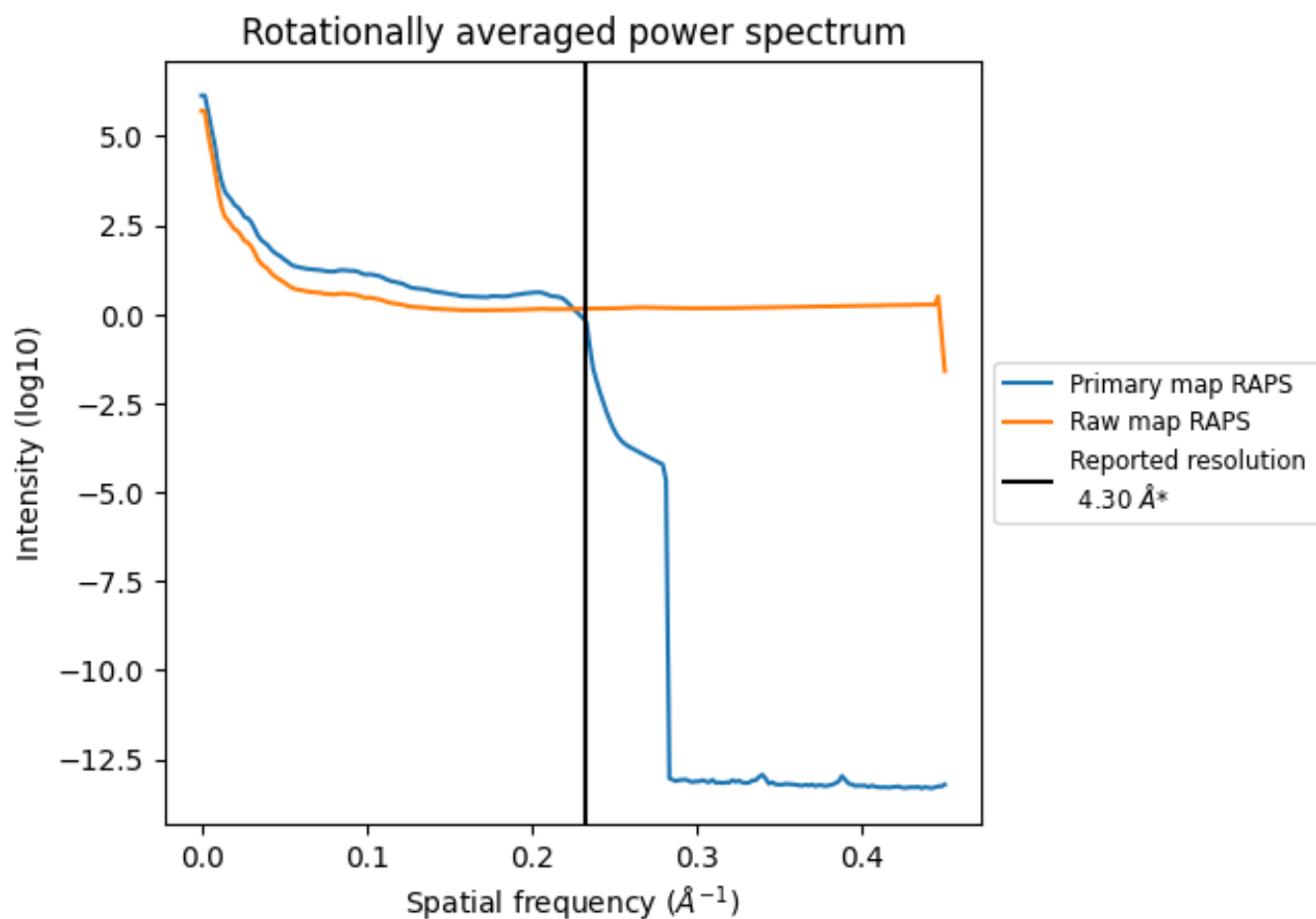
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 793 nm^3 ; this corresponds to an approximate mass of 716 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](#)

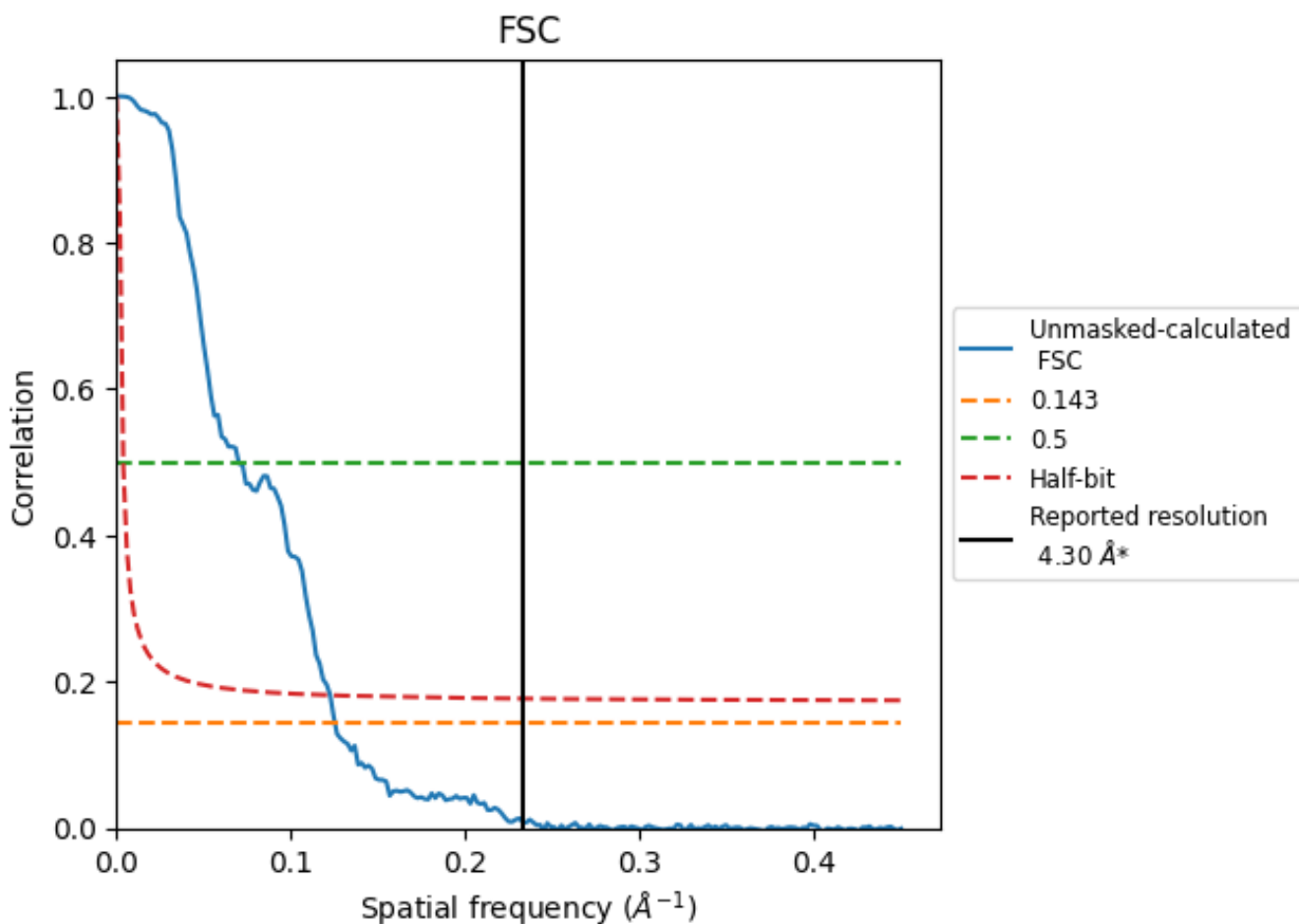


*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

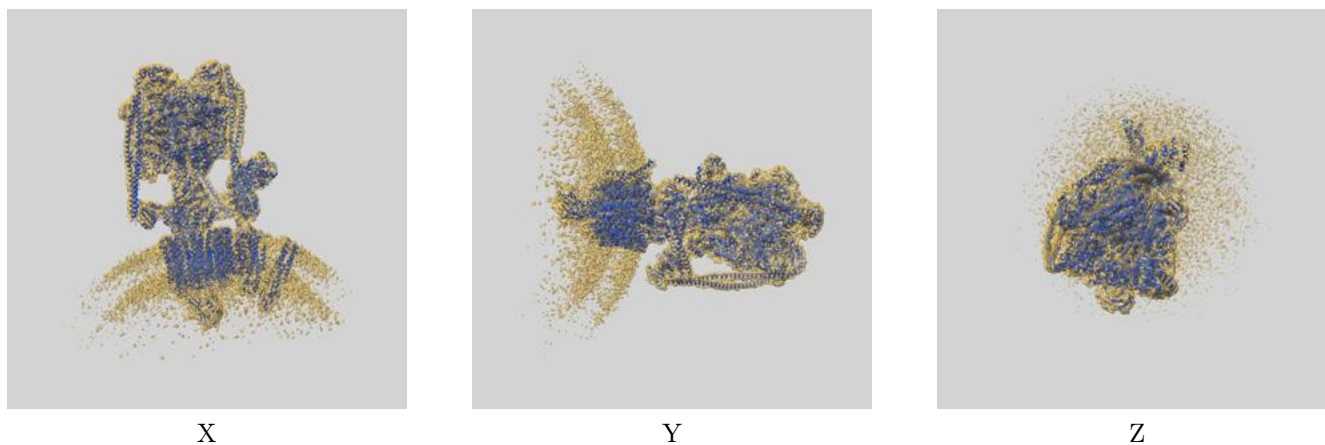
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.98	14.27	8.16

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

9 Map-model fit [i](#)

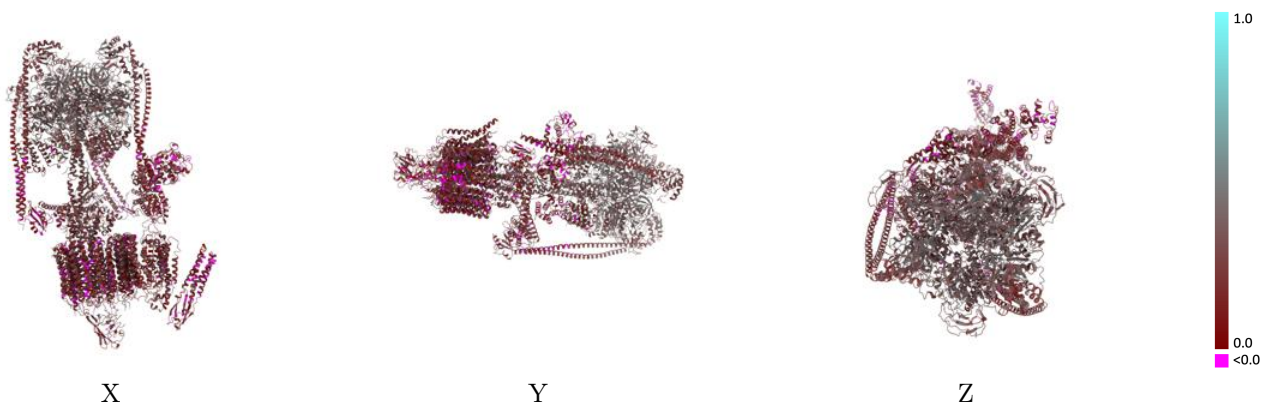
This section contains information regarding the fit between EMDB map EMD-44843 and PDB model 9BRT. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



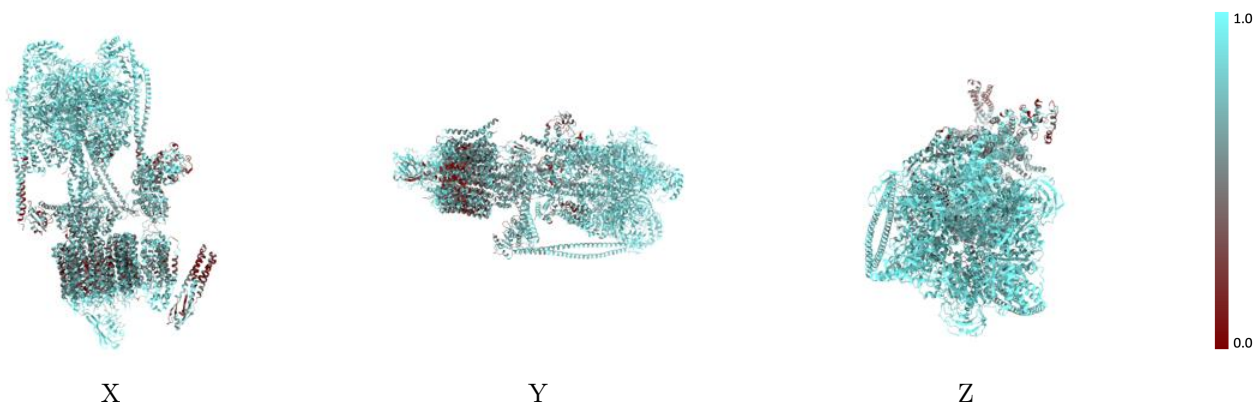
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



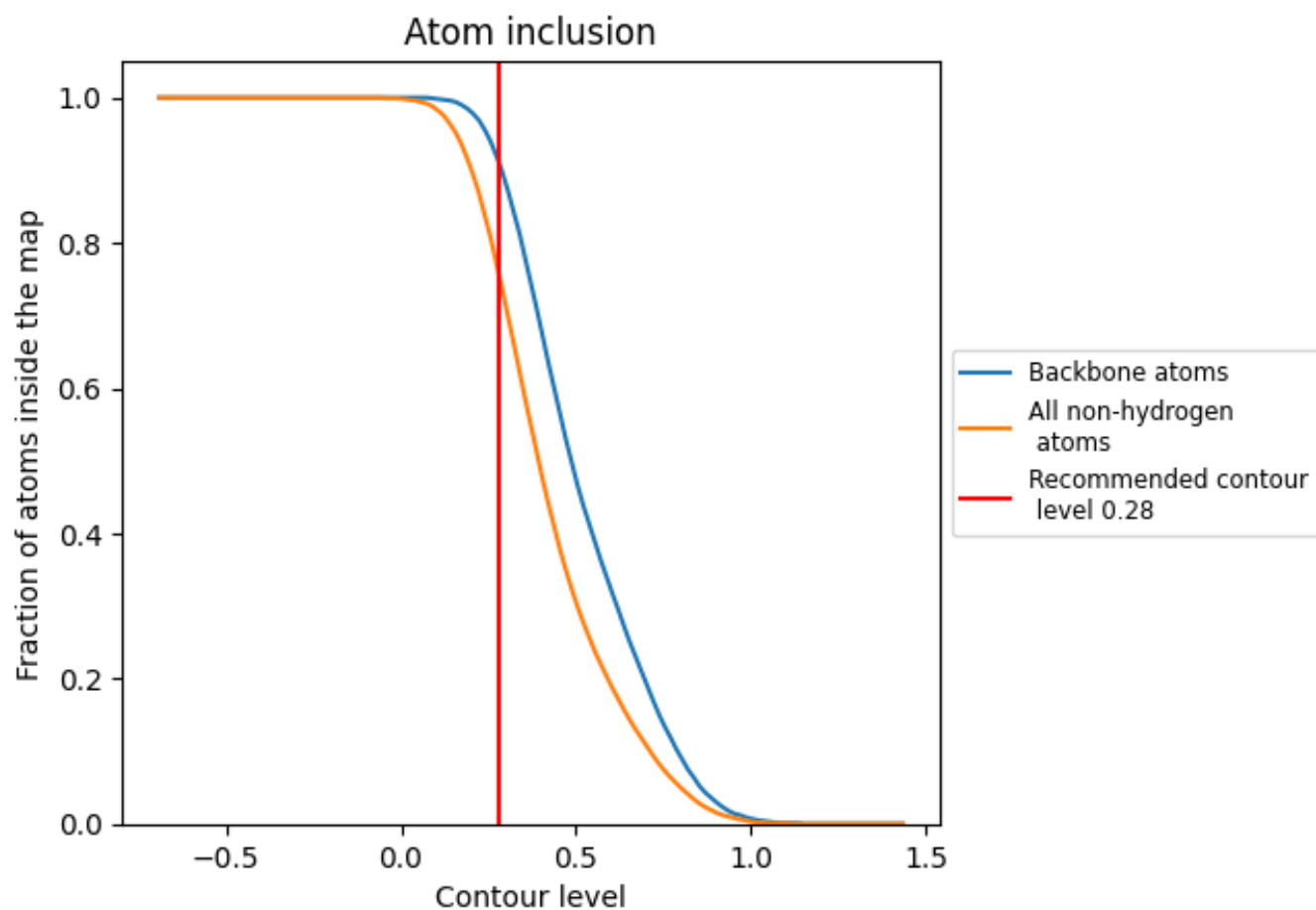
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 91% 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	 0.7570	 0.2710
0	 0.8300	 0.3270
1	 0.8730	 0.3480
2	 0.8830	 0.3670
3	 0.8860	 0.3820
4	 0.8810	 0.3840
5	 0.8850	 0.3760
6	 0.5880	 0.1740
7	 0.8060	 0.3290
8	 0.8230	 0.2710
9	 0.8290	 0.2560
Q	 0.7750	 0.2520
R	 0.7600	 0.2250
T	 0.8290	 0.2330
U	 0.6130	 0.1610
V	 0.7920	 0.2230
X	 0.7890	 0.3110
a	 0.6920	 0.2150
b	 0.6920	 0.2330
c	 0.8600	 0.2520
d	 0.6910	 0.2720
e	 0.6720	 0.2310
f	 0.6420	 0.1940
g	 0.6390	 0.1870
h	 0.6210	 0.1970
i	 0.6770	 0.2320
j	 0.6690	 0.1950
k	 0.6060	 0.1540
l	 0.6100	 0.1730
m	 0.6290	 0.1820
n	 0.6770	 0.2030
o	 0.6990	 0.2160
p	 0.7010	 0.2850
s	 0.4180	 0.1250

