



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:40 PM UTC

PDB ID : 6VQJ / pdb_00006vqj
EMDB ID : EMD-21352
Title : Mammalian V-ATPase from rat brain collar and peripheral stalks rotational state 2 (from focused refinement)
Authors : Abbas, Y.M.; Rubinstein, J.L.
Deposited on : 2020-02-05
Resolution : 5.70 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:

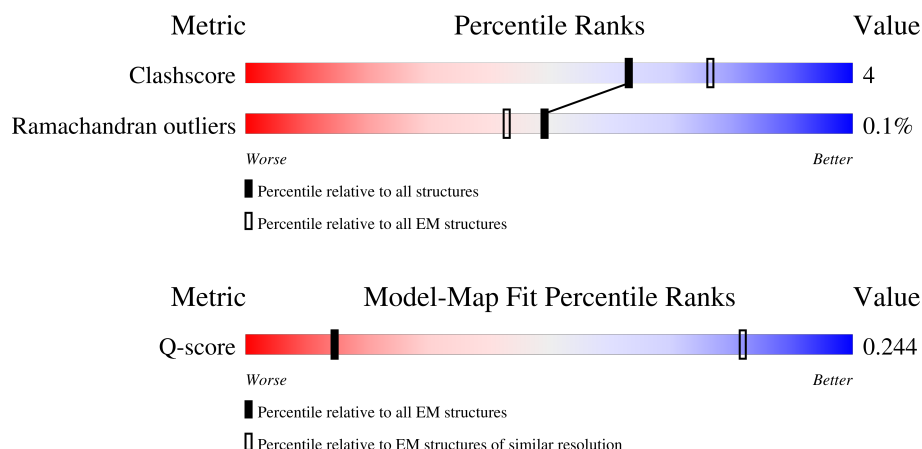
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 5.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	503 (5.20 - 6.20)

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	G	382	
2	I	226	
2	J	226	
2	K	226	
3	M	118	

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Mol	Chain	Length	Quality of chain
3	N	118	56% 43%
3	O	118	14% 53% 43%
4	a	838	35% 63%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5278 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 C 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	G	360	Total	C	N	O	0	0
			1790	1070	360	360		

- Molecule 2 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	I	64	Total	C	N	O	0	0
			319	191	64	64		
2	J	64	Total	C	N	O	0	0
			319	191	64	64		
2	K	64	Total	C	N	O	0	0
			319	191	64	64		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	M	67	Total	C	N	O	0	0
			332	198	67	67		
3	N	67	Total	C	N	O	0	0
			332	198	67	67		
3	O	67	Total	C	N	O	0	0
			332	198	67	67		

- Molecule 4 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	a	309	Total	C	N	O	0	0
			1535	917	309	309		

LEU PRO GLU ASP ILE ALA GLY GLY VAL GLU TYR ASN GLY ASP ARG LYS ILE LYS VAL SER ASN THR LEU GLU SER ARG ASP LEU ILE ALA GLN MET MET MET PRO GLU VAL ARG GLN ILE ALA LEU PHE GLY ALA ASN ALA ASN ARG LYS PHE LEU ASP

• Molecule 2: V-type proton ATPase subunit E 1

Chain K:  9% 27% 72%

MET A2 D5 A6 D7 V8 Q9 I12 K13 H16 A17 F18 I19 E20 A23 A27 D31 A32 E37 F38 K42 E58 E59 GLN LYS LYS LYS ILE GLN MET ASN LEU MET ASN GLN ALA ARG VAL LYS VAL ARG CYS ARG LYS SER ARG GLN MET ASP LEU PHE LEU ILE VAL GLN LYS ALA MET PRO GLU VAL ARG ILE

ASP LEU LEU ASN GLU LYS GLN ARG SER LYS VAL VAL LYS ASP THR THR ARG TYR GLN VAL PRO GLU ASP ILE ALA GLY LEU VAL GLN GLY ILE TYR ASN GLN ARG LEU ILE LYS PRO ARG VAL ILE SER ASN THR LEU CYS ARG LYS GLN MET ASP LEU PHE LEU ILE VAL GLN LYS ALA MET MET PRO GLU VAL ARG ILE

PRO MET TYR LYS ILE THR LYS VAL ASP LYS VAL GLN ILE ASP LEU THR ALA TYR LEU PRO GLU ASP ILE ALA GLY LEU VAL GLN GLY ILE TYR ASN GLN ARG LEU ILE LYS ILE LYS VAL ARG

GLY ALA LEU PHE GLY ALA ASN ALA ASN ARG LYS PHE LEU ASP

• Molecule 3: V-type proton ATPase subunit G

Chain M:  53% 43%

MET ALA S3 A14 A25 K29 L33 A36 A61 A62 S65 L69 SER ALA GLU VAL GLU GLN THR ARG GLN GLN MET GLN SER SER GLN GLN ARG ASN GLN ARG VAL LEU THR GLN LEU GLY MET VAL ARG ASP LEU THR GLN LEU MET VAL CYS ASP VAL ARG PRO GLN

VAL HIS PRO TYR ARG ILE THR VAL

• Molecule 3: V-type proton ATPase subunit G

Chain N:  56% 43%

MET ALA S3 A36 A61 A62 A63 L69 SER ALA GLU VAL GLU GLN THR ARG GLN GLN VAL GLN GLN MET MET GLN SER SER GLN GLN ARG ASN ARG VAL LEU THR GLN LEU GLY MET VAL CYS ASP VAL ARG PRO GLN GLN MET GLN SER SER GLN GLN THR ARG ASN TYR ARG ILE THR VAL

• Molecule 3: V-type proton ATPase subunit G

Chain O:  14% 53% 43%

MET ALA S3 Q4 S5 Q6 G7 I8 Q10 L11 L12 Q13 A14 K16 A19 E20 K21 V22 A23 D24 A25 A40 A61 A62 N68 L69 SER ALA GLU VAL GLN GLN THR ARG ARG GLN VAL GLN GLN MET GLN SER SER GLN GLN THR ARG ASN ARG GLU VAL THR

GLN LEU GLY MET VAL ASP VAL PRO GLN VAL HIS PRO ASN TYR ARG ILE THR VAL

• Molecule 4: V-type proton ATPase 116 kDa subunit a isoform 1

Chain a:  35% 63%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	74789	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.747	Depositor
Minimum map value	-1.100	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	360.4, 360.4, 360.4	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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	G	0.46	0/1788	1.12	6/2494 (0.2%)
2	I	0.41	0/318	1.01	0/443
2	J	0.54	0/318	1.15	0/443
2	K	0.41	0/318	1.01	0/443
3	M	0.41	0/331	1.06	1/460 (0.2%)
3	N	0.51	0/331	0.98	0/460
3	O	0.55	0/331	1.03	1/460 (0.2%)
4	a	0.51	0/1533	1.14	2/2137 (0.1%)
All	All	0.48	0/5268	1.10	10/7340 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	109	MET	N-CA-C	-6.24	104.77	112.38
1	G	314	VAL	CA-C-N	-6.20	112.28	120.95
1	G	314	VAL	C-N-CA	-6.20	112.28	120.95
4	a	188	TRP	N-CA-C	-5.78	104.89	111.07
3	M	65	SER	N-CA-C	5.55	118.25	111.82
1	G	119	LYS	N-CA-C	-5.46	105.23	111.07
1	G	78	ASP	CA-C-N	-5.45	112.68	120.42
1	G	78	ASP	C-N-CA	-5.45	112.68	120.42
3	O	40	ALA	N-CA-C	-5.09	105.73	111.28
4	a	47	PHE	N-CA-C	-5.04	105.68	111.07

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	G	1790	0	794	13	0
2	I	319	0	149	5	0
2	J	319	0	149	4	0
2	K	319	0	149	5	0
3	M	332	0	166	4	0
3	N	332	0	166	1	0
3	O	332	0	166	6	0
4	a	1535	0	661	7	0
All	All	5278	0	2400	32	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.

All (32) 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:G:3:GLU:HA	1:G:374:ILE:O	1.47	1.13
1:G:346:ALA:HB2	2:J:2:ALA:HB1	1.39	1.02
1:G:345:SER:CB	2:J:4:SER:CB	2.47	0.93
1:G:346:ALA:HB2	2:J:2:ALA:CB	2.06	0.86
1:G:6:LEU:O	1:G:371:TYR:HA	1.79	0.83
4:a:15:LEU:O	4:a:320:ILE:HA	1.80	0.80
2:K:27:ALA:HA	3:O:25:ALA:CB	2.14	0.78
2:K:27:ALA:HA	3:O:25:ALA:HB2	1.66	0.77
2:I:30:ILE:CB	3:M:25:ALA:HB1	2.17	0.75
1:G:181:TYR:O	1:G:231:LYS:N	2.27	0.67
2:K:19:ILE:CB	3:O:14:ALA:HB1	2.28	0.64
4:a:188:TRP:O	4:a:192:ARG:HA	2.00	0.62
2:K:27:ALA:CA	3:O:25:ALA:HB2	2.30	0.61
4:a:201:GLU:HA	4:a:217:LYS:O	2.02	0.59
4:a:208:ASP:O	4:a:212:GLY:N	2.36	0.58
2:I:30:ILE:CB	3:M:25:ALA:CB	2.82	0.57
2:J:42:LYS:CB	3:N:36:ALA:HB1	2.35	0.57
2:I:19:ILE:CB	3:M:14:ALA:HB1	2.36	0.56
1:G:205:ALA:HB2	1:G:237:PHE:N	2.21	0.55
1:G:101:TYR:O	1:G:105:PHE:N	2.41	0.54
1:G:7:ILE:HA	1:G:370:VAL:O	2.10	0.52
2:I:34:ALA:HB1	3:M:29:LYS:HA	1.92	0.51
1:G:307:VAL:O	1:G:311:GLY:N	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:27:ALA:CB	3:O:25:ALA:HB2	2.42	0.50
1:G:182:LEU:HA	1:G:229:LEU:O	2.12	0.48
4:a:14:GLN:HA	4:a:321:ALA:O	2.14	0.47
3:O:68:ASN:O	3:O:69:LEU:C	2.56	0.47
1:G:108:ASP:C	1:G:110:ALA:N	2.72	0.44
1:G:184:THR:HA	1:G:227:VAL:O	2.19	0.42
2:I:58:GLU:O	2:I:61:GLU:CB	2.68	0.42
4:a:18:GLN:O	4:a:22:ALA:N	2.49	0.41
4:a:187:LEU:O	4:a:188:TRP:C	2.62	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	G	356/382 (93%)	355 (100%)	1 (0%)	0	100	100
2	I	62/226 (27%)	62 (100%)	0	0	100	100
2	J	62/226 (27%)	61 (98%)	0	1 (2%)	7	37
2	K	62/226 (27%)	62 (100%)	0	0	100	100
3	M	65/118 (55%)	65 (100%)	0	0	100	100
3	N	65/118 (55%)	65 (100%)	0	0	100	100
3	O	65/118 (55%)	65 (100%)	0	0	100	100
4	a	305/838 (36%)	296 (97%)	9 (3%)	0	100	100
All	All	1042/2252 (46%)	1031 (99%)	10 (1%)	1 (0%)	49	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	64	ILE

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 oligosaccharides 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.

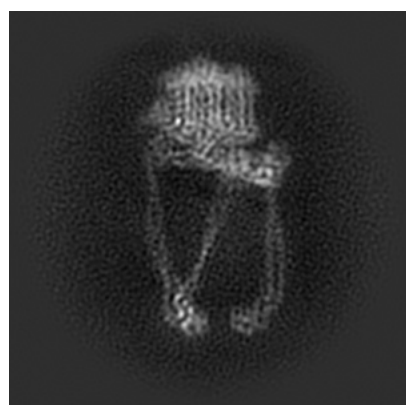
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21352. These allow visual inspection of the internal detail of the map and identification of artifacts.

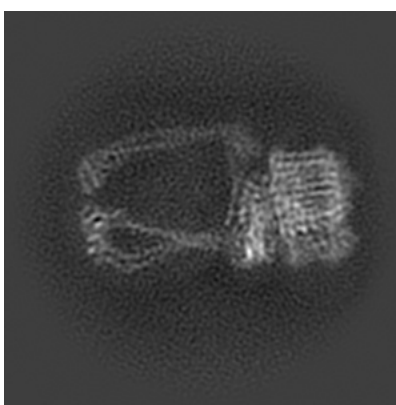
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

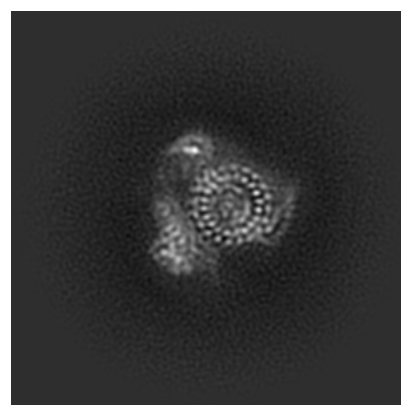
6.1.1 Primary map



X



Y

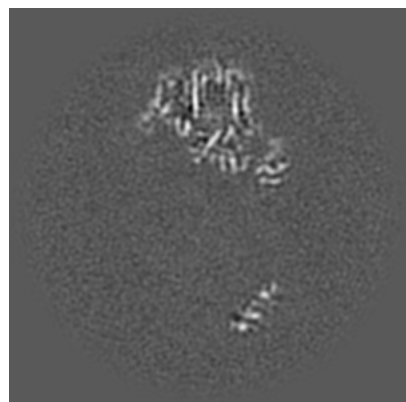


Z

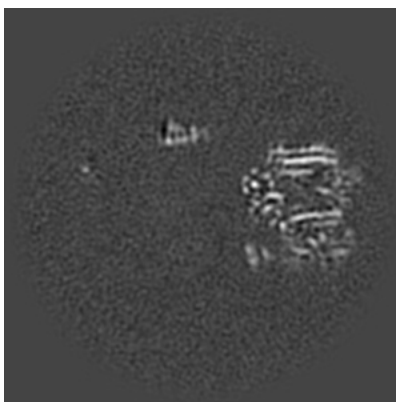
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

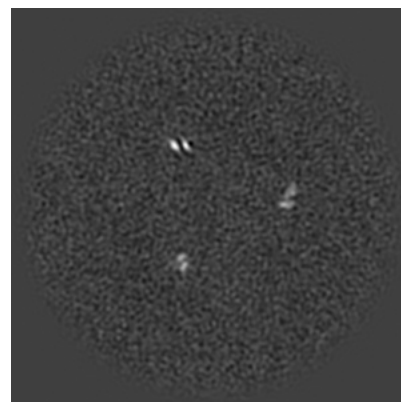
6.2.1 Primary map



X Index: 170



Y Index: 170

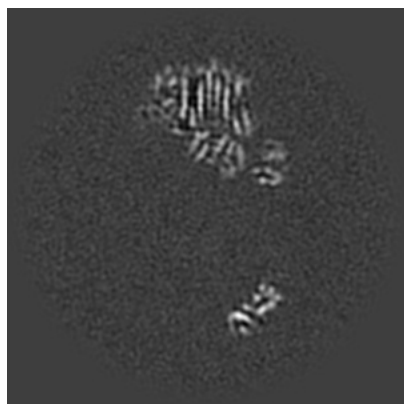


Z Index: 170

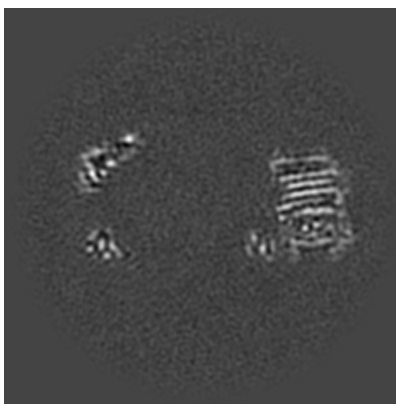
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

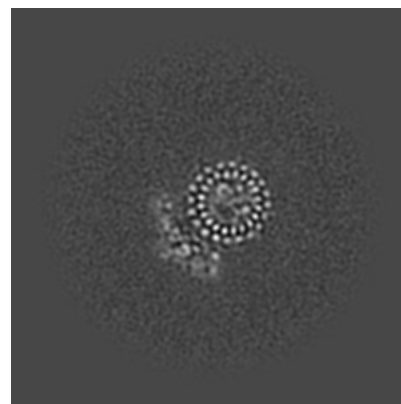
6.3.1 Primary map



X Index: 166



Y Index: 151

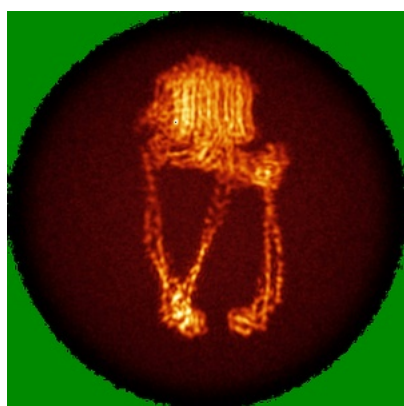


Z Index: 248

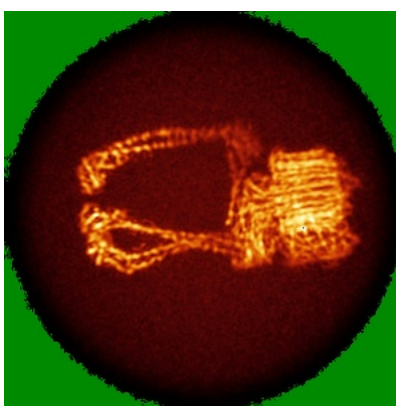
The images above show the largest variance slices of the map in three orthogonal directions.

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

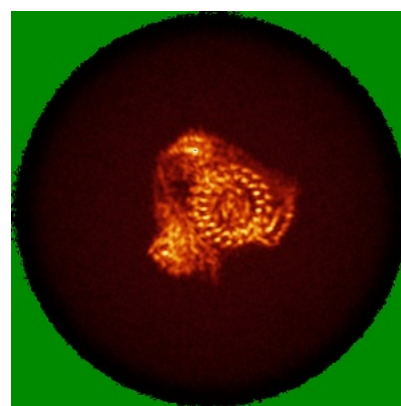
6.4.1 Primary map



X



Y

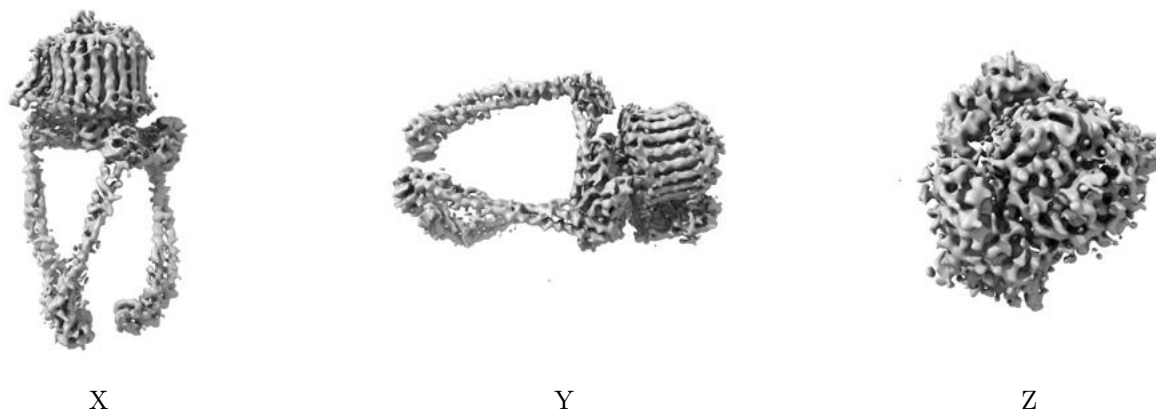


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

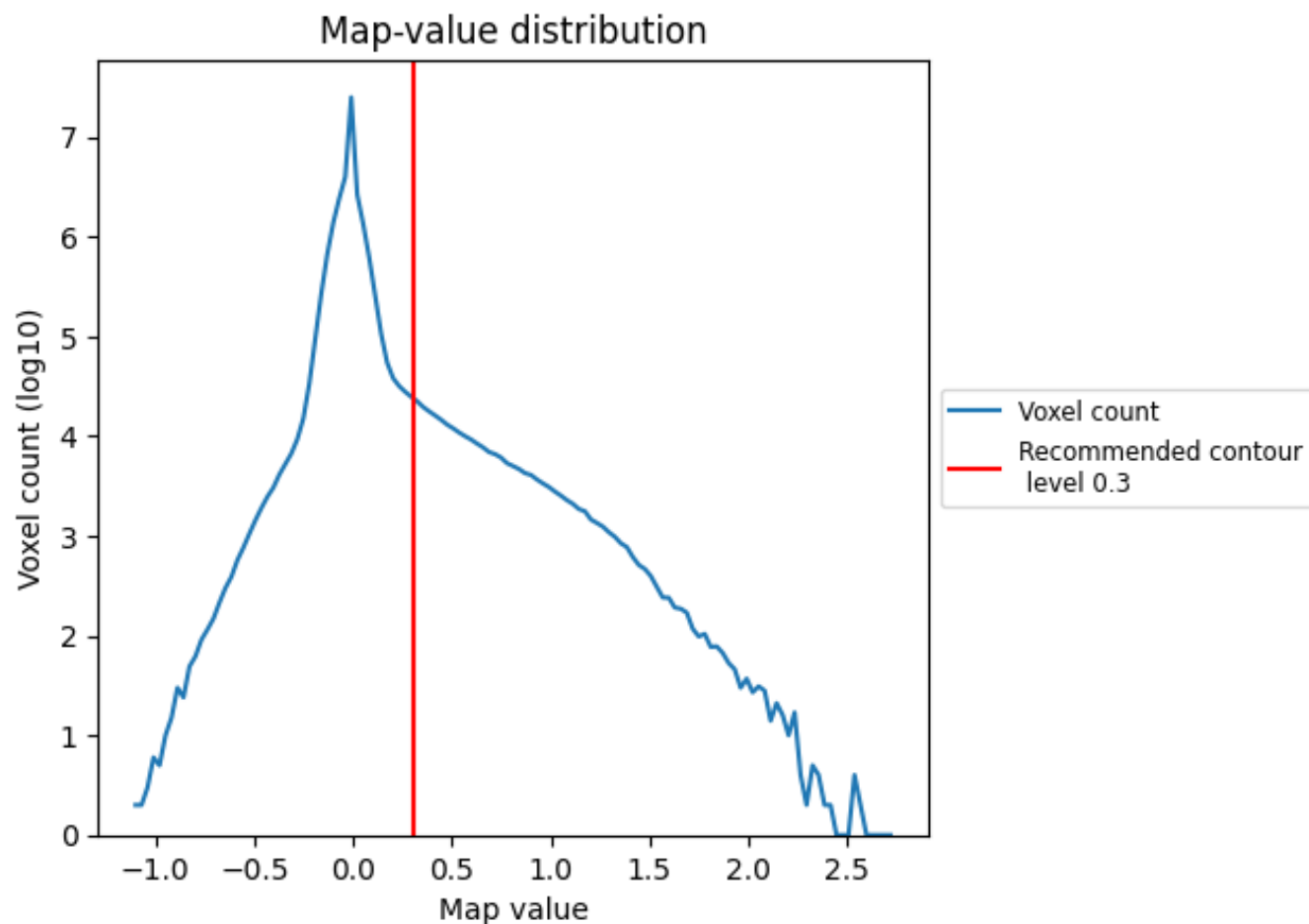
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

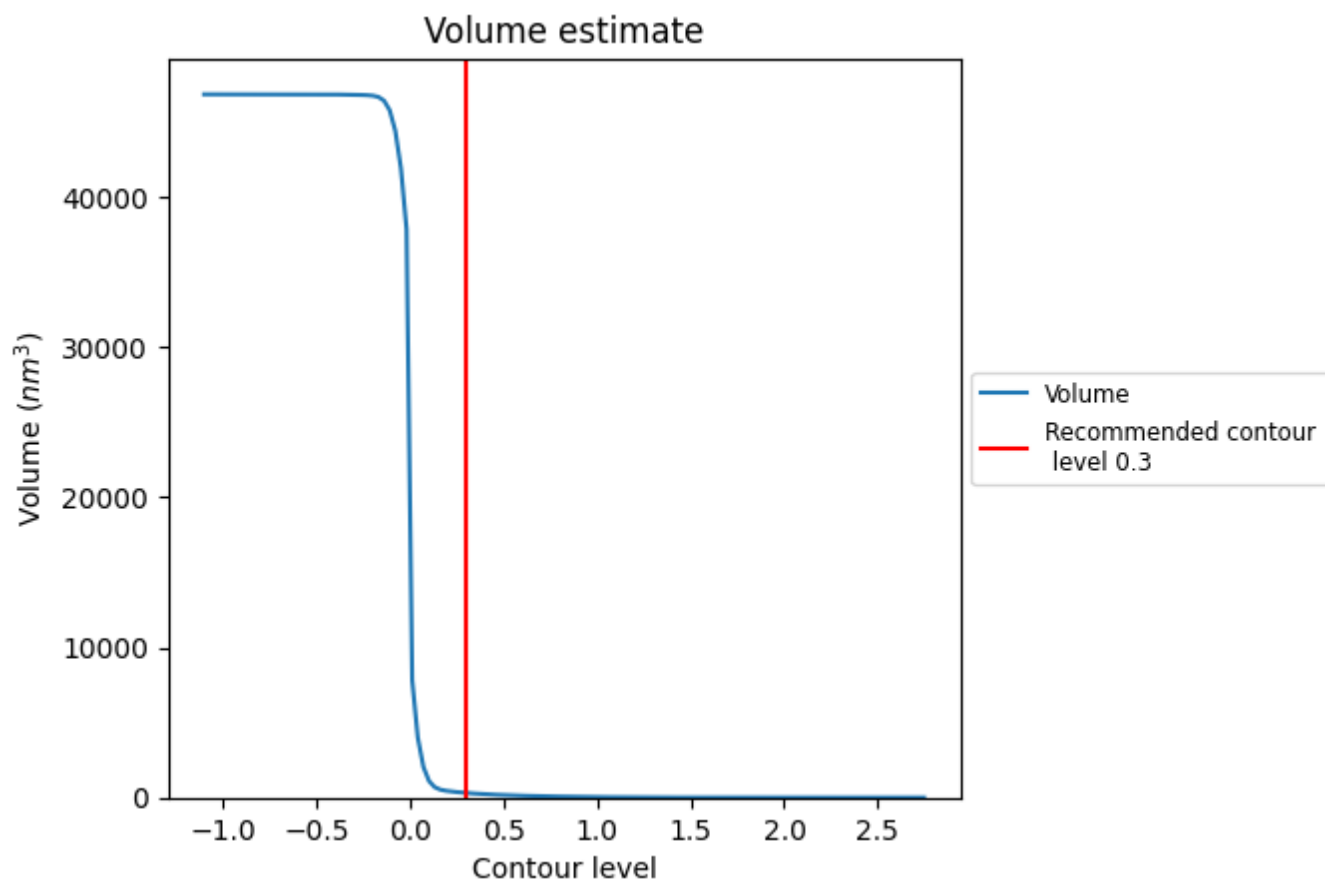
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

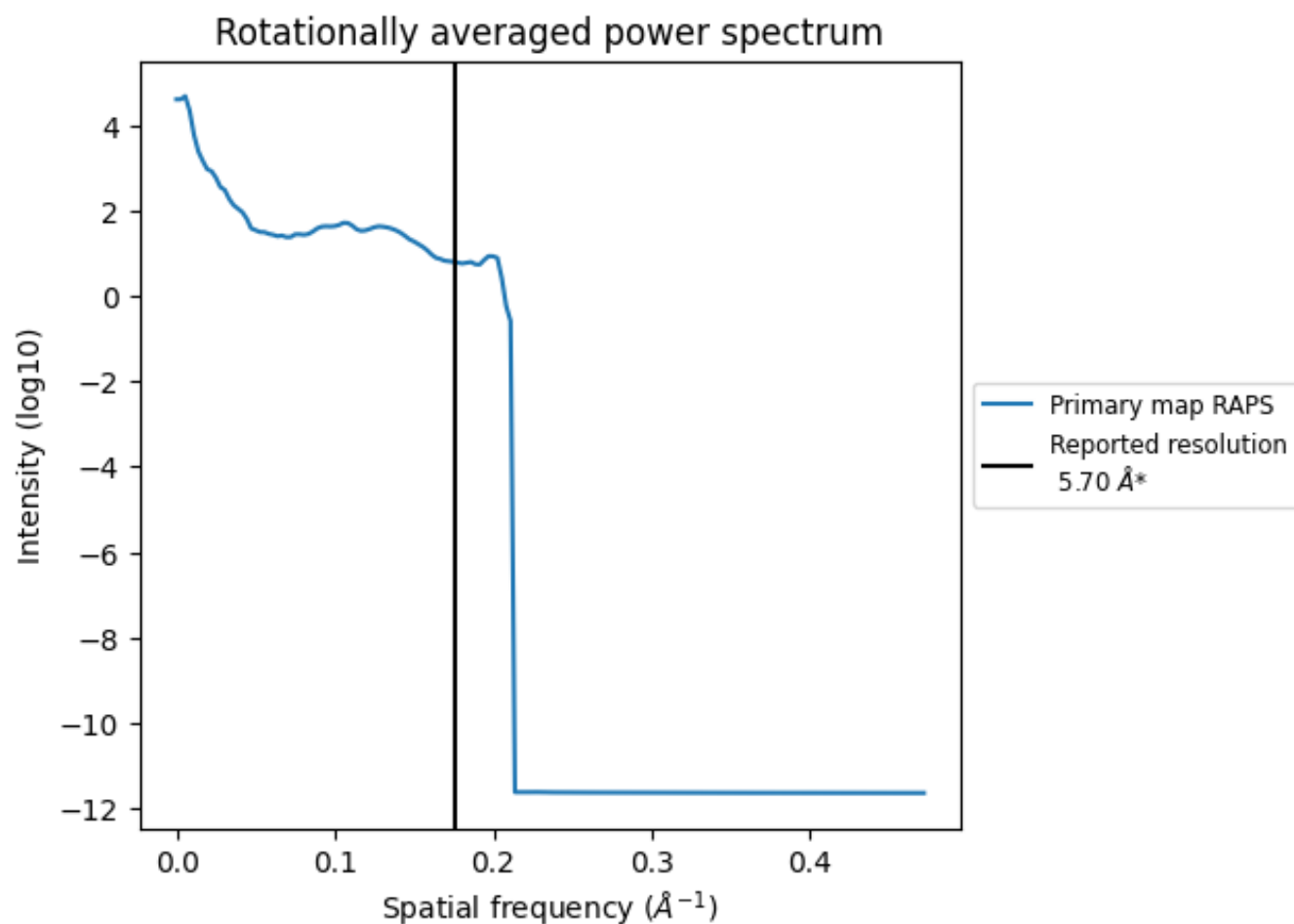
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 310 nm³; this corresponds to an approximate mass of 280 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.175 Å⁻¹

8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21352 and PDB model 6VQJ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

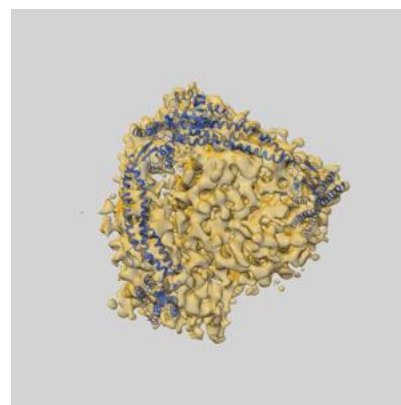
9.1 Map-model overlay [i](#)



X



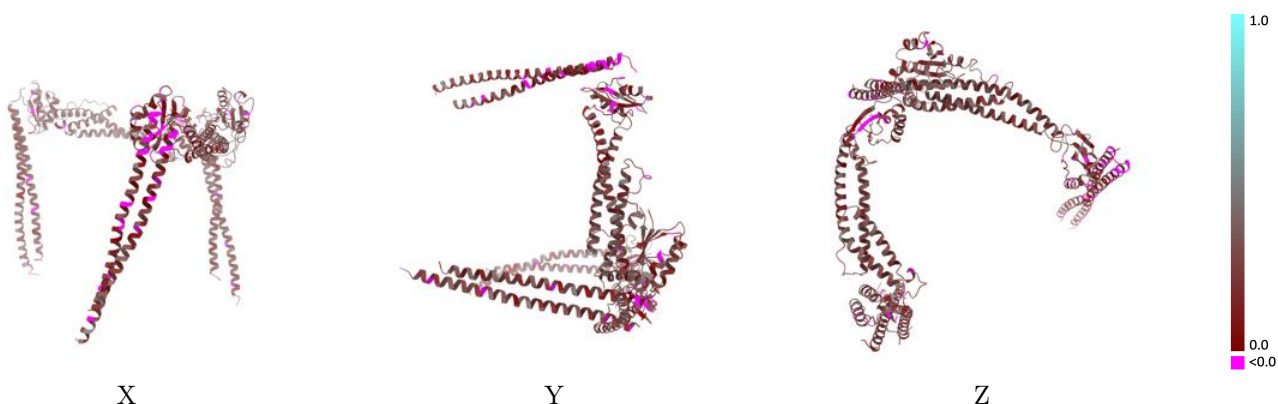
Y



Z

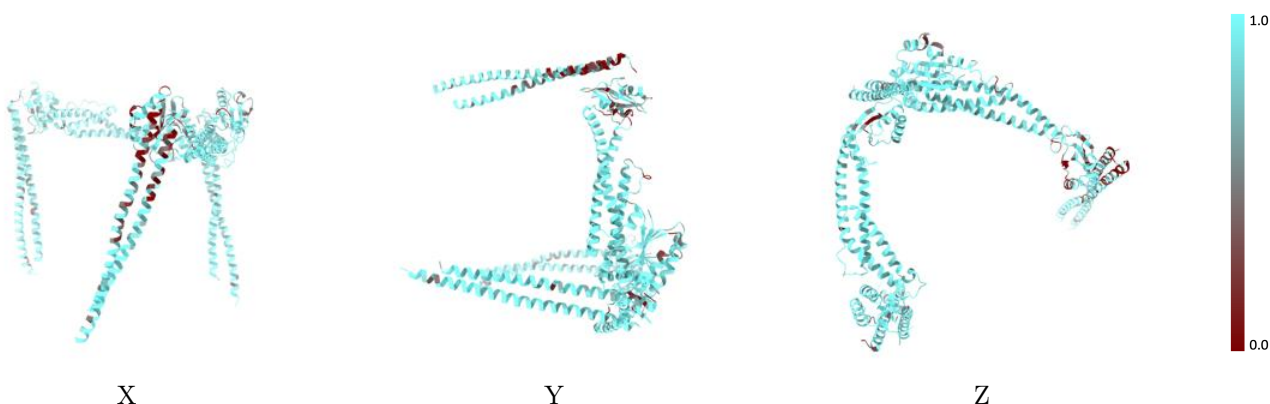
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



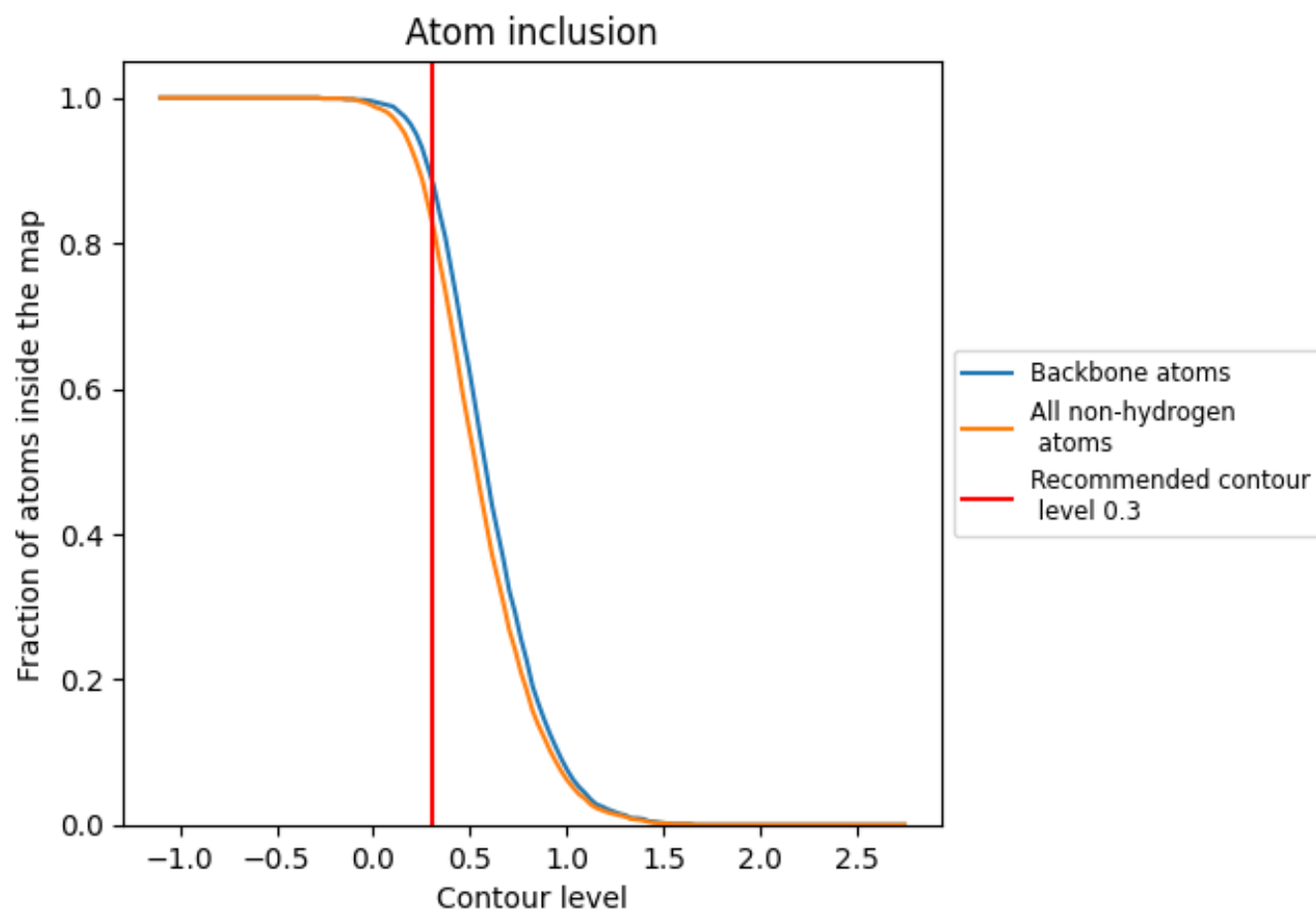
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8340	0.2440
G	0.8190	0.2570
I	0.8400	0.2350
J	0.8680	0.2290
K	0.6740	0.1390
M	0.8680	0.2420
N	0.9040	0.2430
O	0.7320	0.1810
a	0.8770	0.2690

1.0

0.0

<0.0