



wwPDB EM Validation Summary Report ⓘ

Feb 27, 2024 – 02:14 AM EST

PDB ID : 6VQC
EMDB ID : EMD-21348
Title : Mammalian V-ATPase from rat brain membrane-embedded Vo region rotational state 1 (from focused refinement)
Authors : Abbas, Y.M.; Rubinstein, J.L.
Deposited on : 2020-02-04
Resolution : 3.80 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.dev70
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

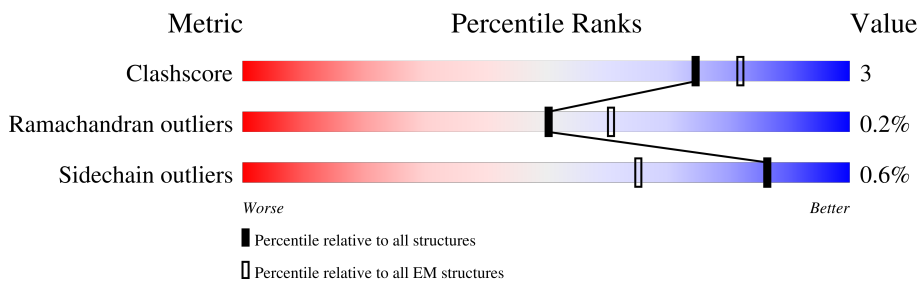
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	H	247	
2	L	119	
3	a	838	
4	b	205	
5	c	463	
6	d	351	
7	e	81	
8	f	98	

Continued on next page...

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Mol	Chain	Length	Quality of chain
9	g	155	 5% 96% ..
9	h	155	 5% 96% ..
9	i	155	 1% 97% .
9	j	155	 1% 97% .
9	k	155	 10% 97% .
9	l	155	 6% 97% .
9	m	155	 8% 96% ..
9	n	155	 7% 94% ..
9	o	155	 11% 95% ..
10	p	350	 15% 85%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 20991 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 ATPase H⁺-transporting V1 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	104	803	509	138	153	3	0	0

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

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

- Molecule 3 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	a	441	3495	2337	556	579	23	0	0

- Molecule 4 is a protein called ATPase, H⁺ transporting, V0 subunit B (Predicted), isoform CRA_a.

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

- Molecule 5 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	c	41	337	228	51	54	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	e	78	621	428	98	92	3	0	0

- Molecule 8 is a protein called Ribonuclease K.

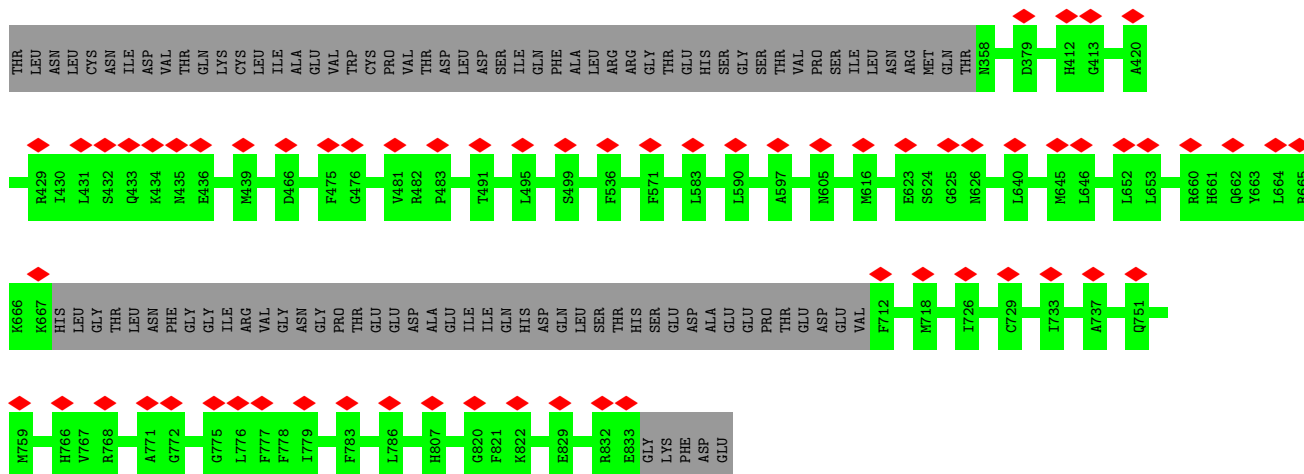
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	f	84	480	309	85	86	0	0

- Molecule 9 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

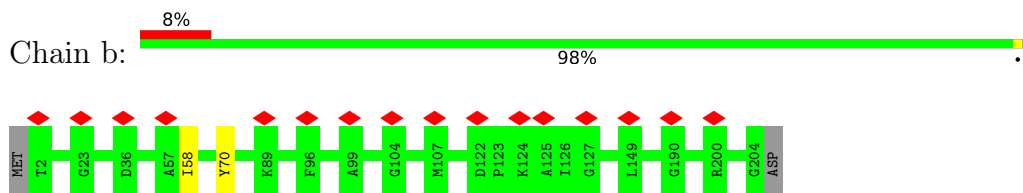
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	g	150	1068	699	171	190	8	0	0
9	h	150	1068	699	171	190	8	0	0
9	i	150	1068	699	171	190	8	0	0
9	j	150	1068	699	171	190	8	0	0
9	k	150	1068	699	171	190	8	0	0
9	l	150	1068	699	171	190	8	0	0
9	m	150	1068	699	171	190	8	0	0
9	n	150	1068	699	171	190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

- Molecule 10 is a protein called Renin receptor.

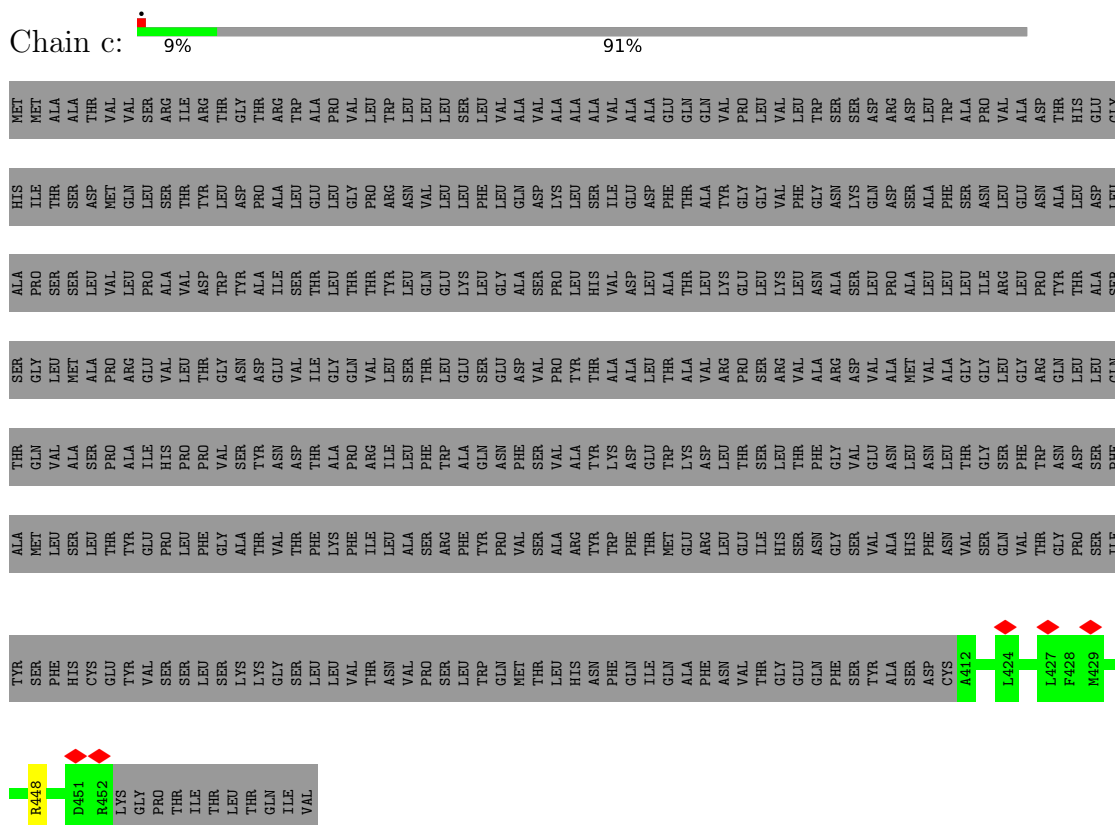
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	p	52	432	290	63	76	3	0	0



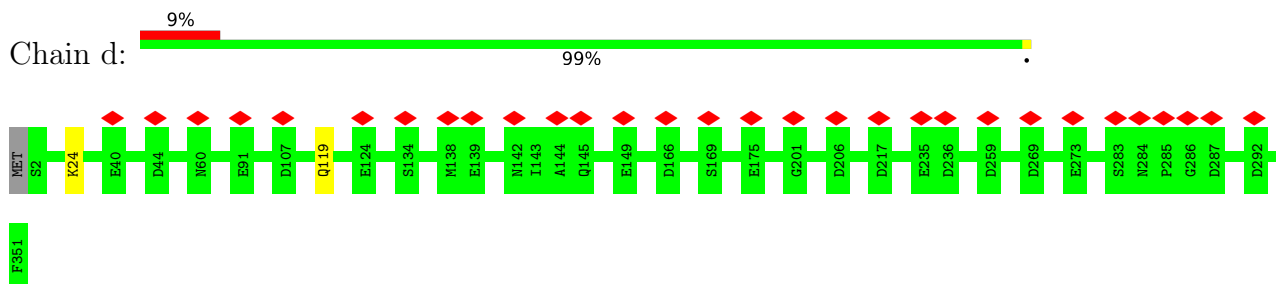
- Molecule 4: ATPase, H⁺ transporting, V₀ subunit B (Predicted), isoform CRA_a



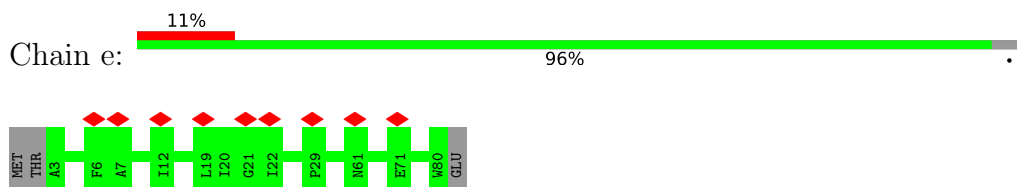
- Molecule 5: V-type proton ATPase subunit S1



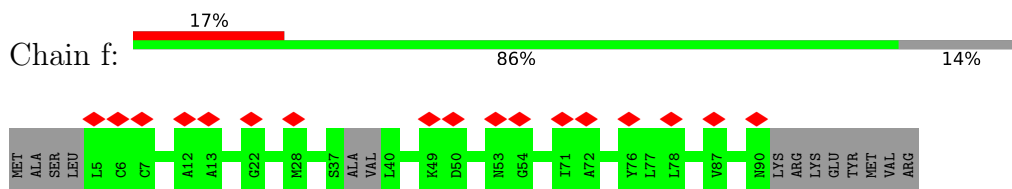
- Molecule 6: V-type proton ATPase subunit



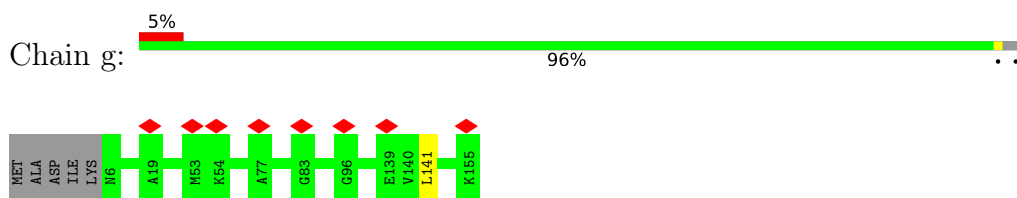
- Molecule 7: V-type proton ATPase subunit e 2



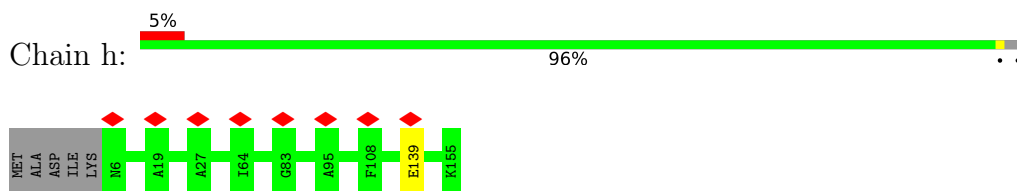
- Molecule 8: Ribonuclease K



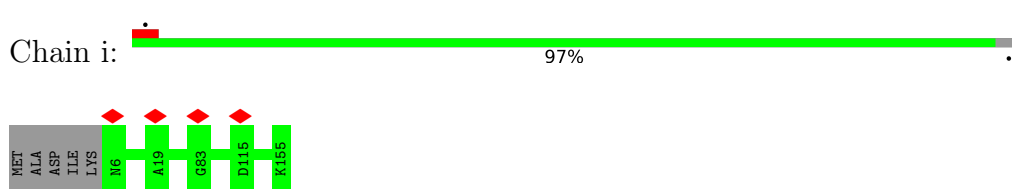
- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit



- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit

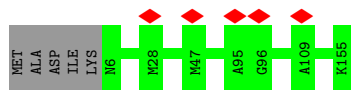


- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit

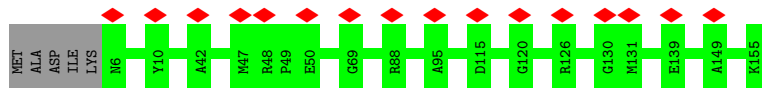


- Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit

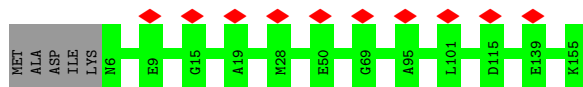




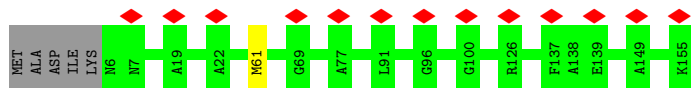
• Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit



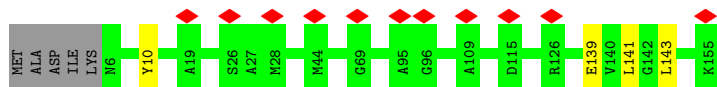
• Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit



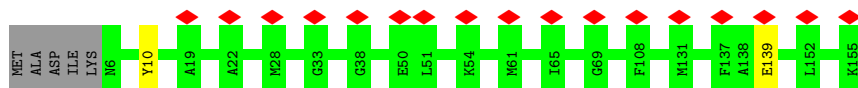
• Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit



• Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit



• Molecule 9: V-type proton ATPase 16 kDa proteolipid subunit



• Molecule 10: Renin receptor



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

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

LEU VAL
ASP ASP
ALA ALA
LEU LEU
GLN GLN
LYS LYS
PHE PHE
ALA ALA
ASP ASP
SER SER
MET MET
TYR TYR
SER SER
LEU LEU
TYR TYR
SER SER
GLY GLY
LEU LEU
VAL VAL
ASN ASN
ALA ALA
VAL VAL
VAL VAL
GLU GLU
LEU LEU
VAL VAL
THR THR
VAL VAL
LYS LYS
SER SER
PHE PHE
SER SER
THR THR
SER SER
LEU LEU
VAL VAL
ARG ARG
LYS LYS
SER SER
ARG ARG
THR THR
ILE ILE
LEU LEU
GLU GLU
THR THR
LYS LYS
GLN GLN
LEU LEU
TYR TYR
ASN ASN
SER SER
THR THR
GLN GLN
SER SER
P292
N300
G316
D322
P333
G334

Y335
D336
S337
I338
I339
Y340
R341
M342
T343
ASN
GLN
LYS
ILE
ARG
MET
ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	90648	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	2.773	Depositor
Minimum map value	-1.050	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.5	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 [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	H	0.84	0/812	0.64	0/1091
2	L	0.80	0/889	0.74	0/1199
3	a	0.52	0/3603	0.49	0/4888
4	b	0.51	0/1537	0.49	0/2088
5	c	0.48	0/347	0.54	0/466
6	d	0.73	0/2899	0.53	0/3927
7	e	0.47	0/645	0.44	0/887
8	f	0.40	0/490	0.50	0/676
9	g	0.50	0/1083	0.56	0/1466
9	h	0.47	0/1083	0.52	0/1466
9	i	0.49	0/1083	0.52	0/1466
9	j	0.47	0/1083	0.49	0/1466
9	k	0.49	0/1083	0.53	0/1466
9	l	0.48	0/1083	0.51	0/1466
9	m	0.49	0/1083	0.55	0/1466
9	n	0.47	0/1083	0.51	0/1466
9	o	0.49	0/1083	0.51	0/1466
10	p	0.49	0/445	0.60	0/609
All	All	0.56	0/21414	0.53	0/29025

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	H	803	0	828	4	0
2	L	875	0	883	12	0
3	a	3495	0	3434	0	0
4	b	1503	0	1551	0	0
5	c	337	0	338	0	0
6	d	2833	0	2770	0	0
7	e	621	0	639	0	0
8	f	480	0	288	0	0
9	g	1068	0	1136	0	0
9	h	1068	0	1136	0	0
9	i	1068	0	1136	0	0
9	j	1068	0	1136	0	0
9	k	1068	0	1136	0	0
9	l	1068	0	1136	0	0
9	m	1068	0	1136	0	0
9	n	1068	0	1136	0	0
9	o	1068	0	1136	0	0
10	p	432	0	428	0	0
All	All	20991	0	21383	13	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 3.

The worst 5 of 13 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)
2:L:58:ARG:HG2	2:L:60:ASP:H	1.65	0.61
2:L:85:ILE:N	2:L:86:PRO:CD	2.67	0.58
2:L:85:ILE:N	2:L:86:PRO:HD2	2.23	0.54
1:H:68:SER:OG	1:H:137:ASN:ND2	2.41	0.53
1:H:55:LYS:NZ	2:L:99:ASP:OD2	2.32	0.53

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	H	102/247 (41%)	97 (95%)	5 (5%)	0	100	100
2	L	108/119 (91%)	101 (94%)	5 (5%)	2 (2%)	8	42
3	a	435/838 (52%)	424 (98%)	11 (2%)	0	100	100
4	b	201/205 (98%)	197 (98%)	4 (2%)	0	100	100
5	c	39/463 (8%)	39 (100%)	0	0	100	100
6	d	348/351 (99%)	328 (94%)	19 (6%)	1 (0%)	41	74
7	e	76/81 (94%)	75 (99%)	1 (1%)	0	100	100
8	f	80/98 (82%)	77 (96%)	3 (4%)	0	100	100
9	g	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
9	h	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
9	i	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
9	j	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
9	k	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
9	l	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
9	m	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
9	n	148/155 (96%)	145 (98%)	2 (1%)	1 (1%)	22	60
9	o	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	22	60
10	p	50/350 (14%)	47 (94%)	2 (4%)	1 (2%)	7	41
All	All	2771/4147 (67%)	2692 (97%)	73 (3%)	6 (0%)	50	79

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	61	ILE
6	d	119	GLN
9	o	10	TYR
10	p	300	ASN
2	L	100	ALA

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	H	84/212 (40%)	84 (100%)	0	100	100
2	L	94/100 (94%)	93 (99%)	1 (1%)	73	85
3	a	362/743 (49%)	362 (100%)	0	100	100
4	b	156/158 (99%)	154 (99%)	2 (1%)	69	82
5	c	36/395 (9%)	35 (97%)	1 (3%)	43	68
6	d	305/306 (100%)	304 (100%)	1 (0%)	92	96
7	e	64/68 (94%)	64 (100%)	0	100	100
8	f	14/83 (17%)	14 (100%)	0	100	100
9	g	109/113 (96%)	108 (99%)	1 (1%)	78	88
9	h	109/113 (96%)	108 (99%)	1 (1%)	78	88
9	i	109/113 (96%)	109 (100%)	0	100	100
9	j	109/113 (96%)	109 (100%)	0	100	100
9	k	109/113 (96%)	109 (100%)	0	100	100
9	l	109/113 (96%)	109 (100%)	0	100	100
9	m	109/113 (96%)	108 (99%)	1 (1%)	78	88
9	n	109/113 (96%)	106 (97%)	3 (3%)	43	68
9	o	109/113 (96%)	108 (99%)	1 (1%)	78	88
10	p	47/313 (15%)	47 (100%)	0	100	100
All	All	2143/3395 (63%)	2131 (99%)	12 (1%)	86	92

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

Mol	Chain	Res	Type
9	m	61	MET
9	n	139	GLU
9	o	139	GLU
9	n	141	LEU
5	c	448	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	137	ASN

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Continued from previous page...

Mol	Chain	Res	Type
3	a	751	GLN
6	d	297	HIS
6	d	340	HIS
9	m	123	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

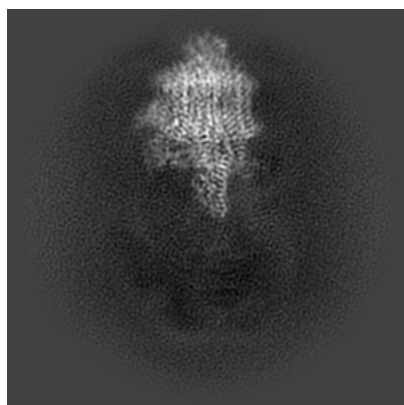
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21348. These allow visual inspection of the internal detail of the map and identification of artifacts.

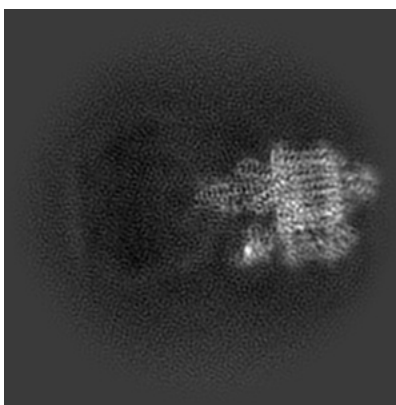
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

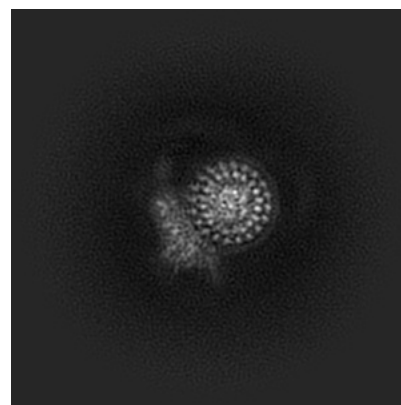
6.1.1 Primary map



X



Y



Z

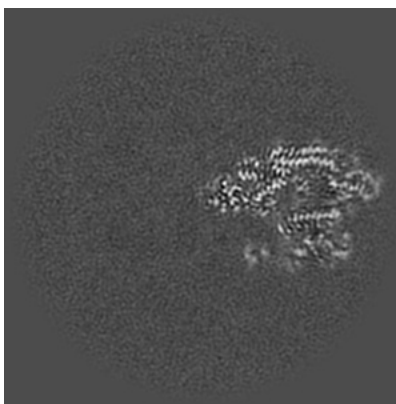
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

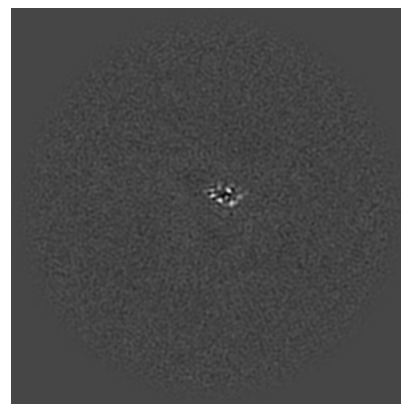
6.2.1 Primary map



X Index: 170



Y Index: 170

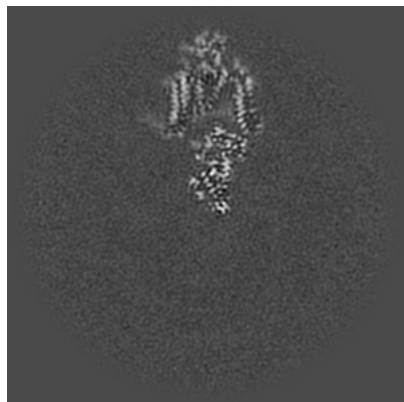


Z Index: 170

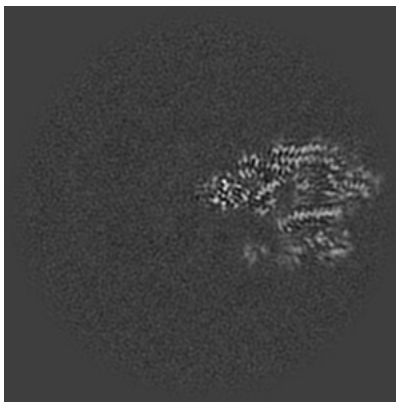
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

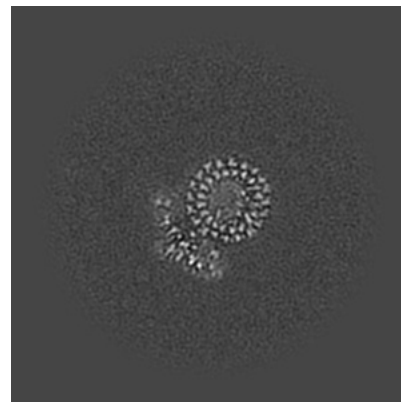
6.3.1 Primary map



X Index: 183



Y Index: 171

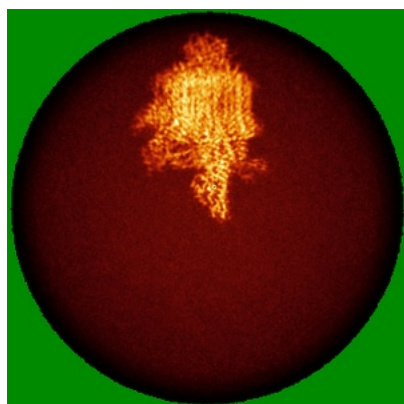


Z Index: 247

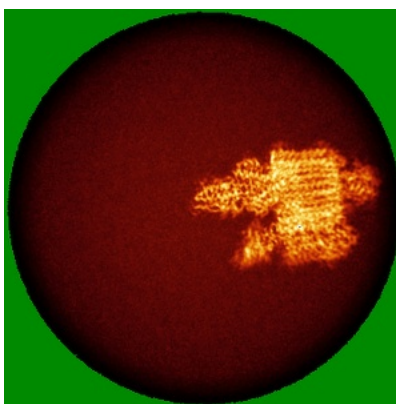
The images above show the largest variance slices of the map in three orthogonal directions.

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

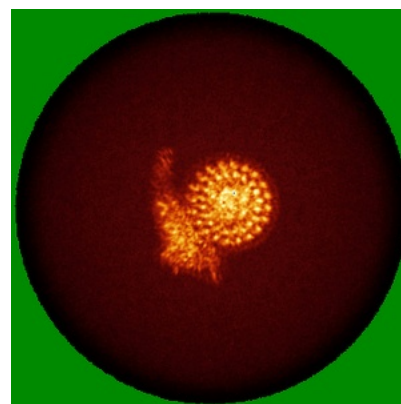
6.4.1 Primary map



X



Y

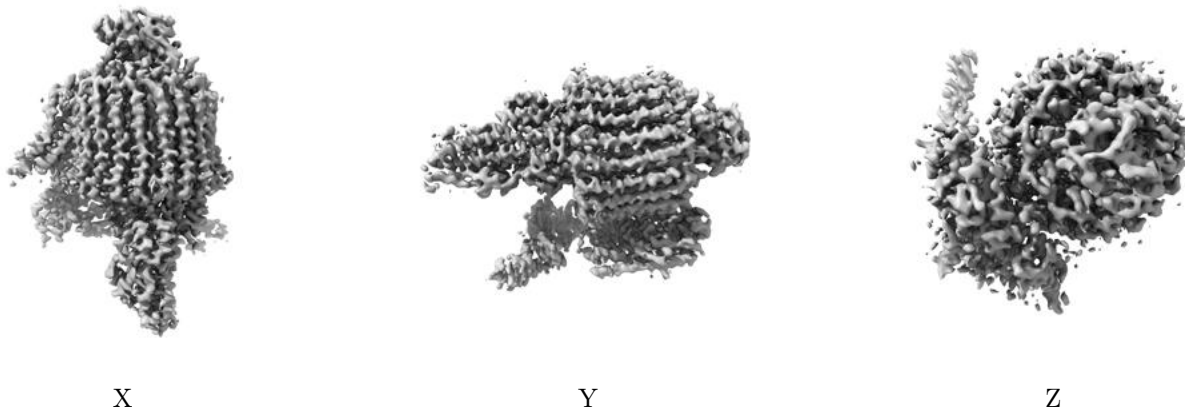


Z

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 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

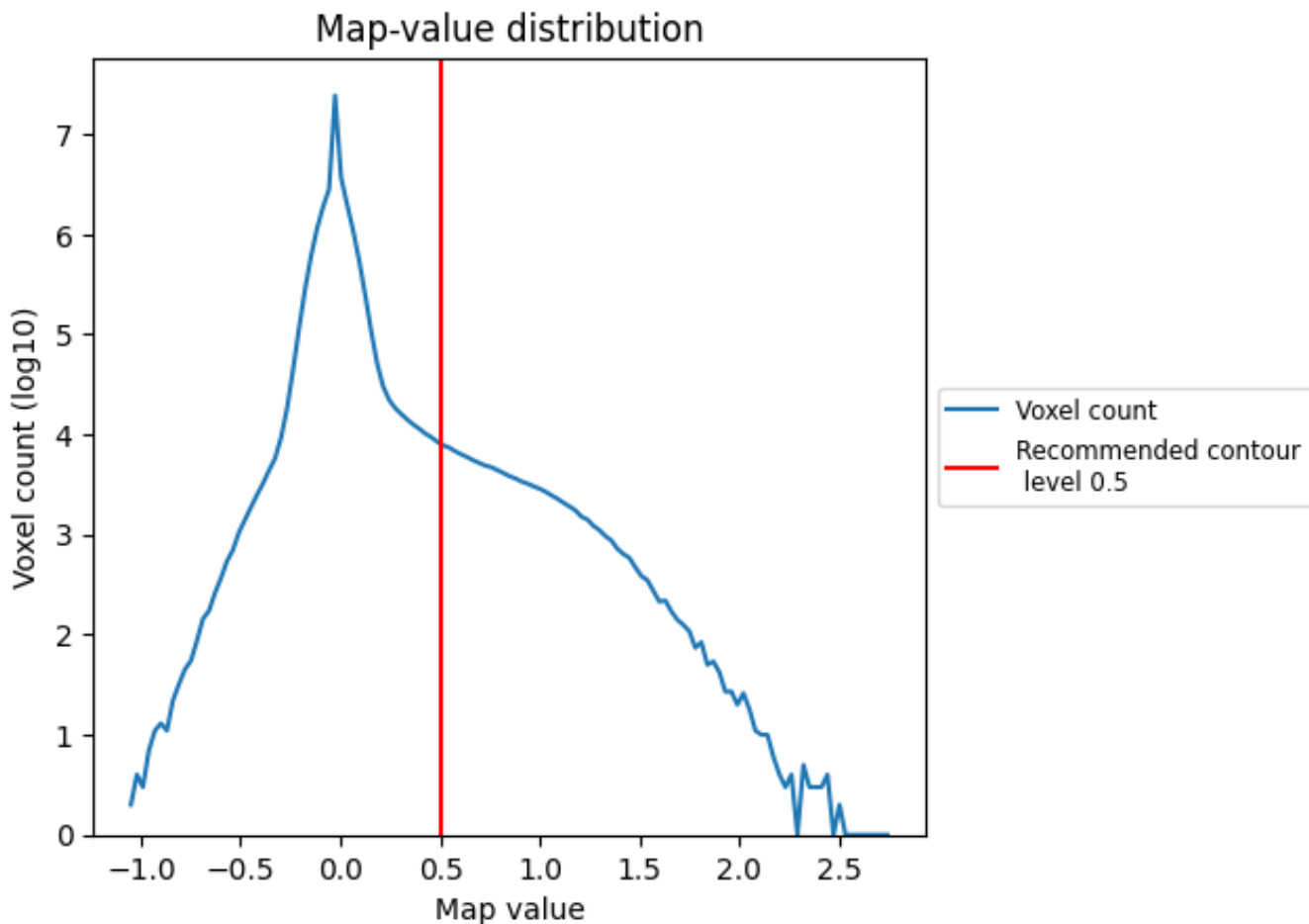
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

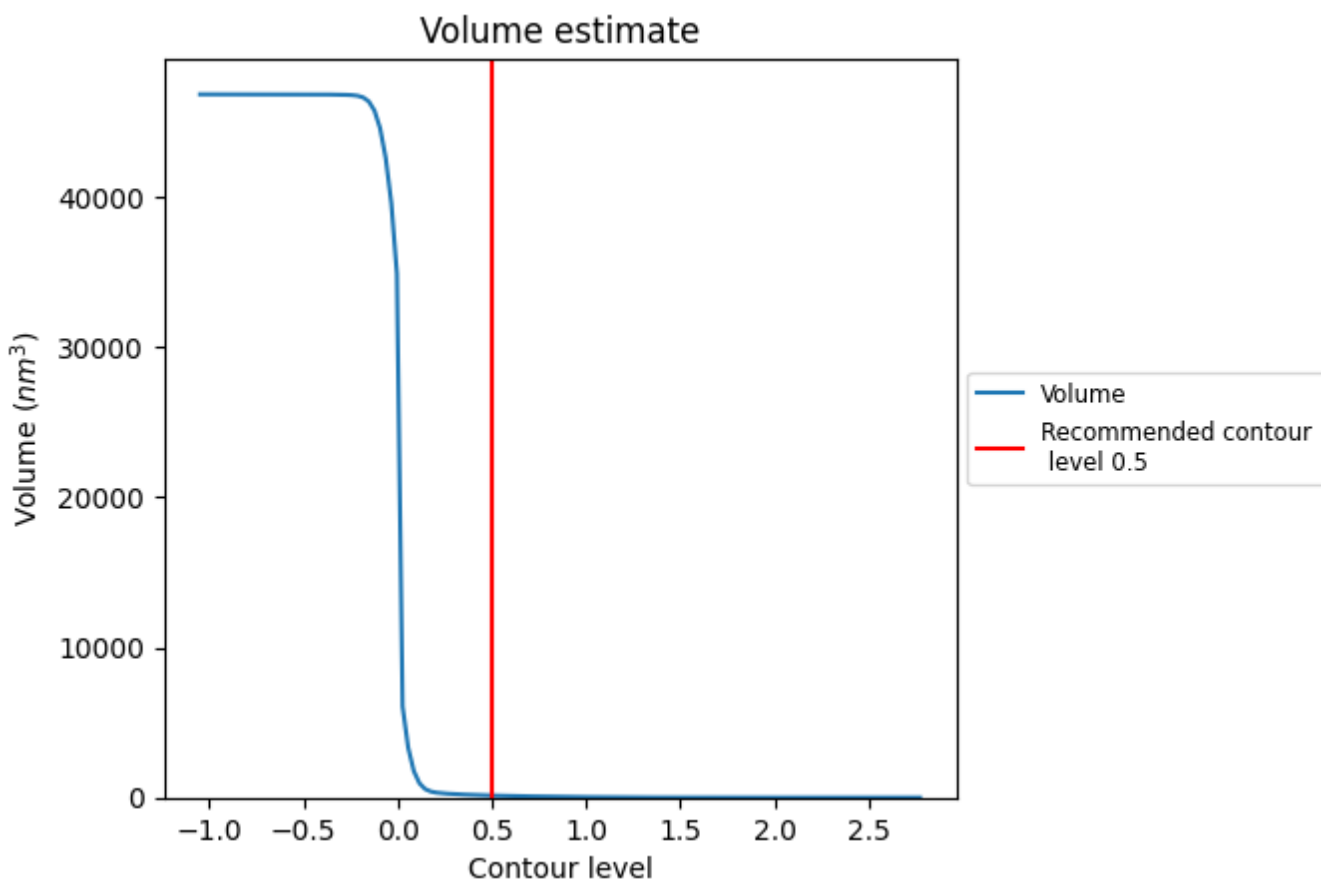
This section contains the results of statistical analysis of the map.

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.

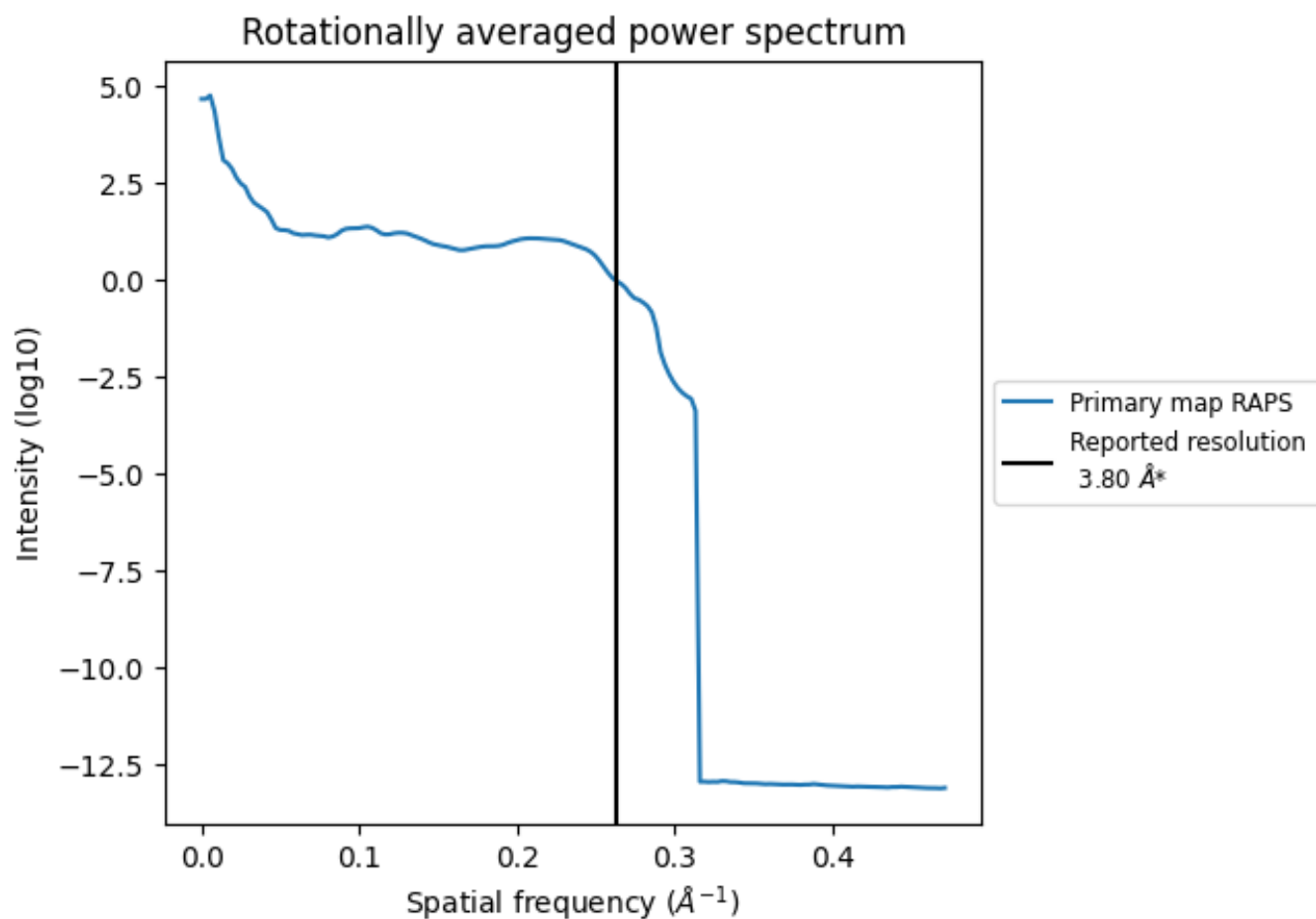
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 134 nm^3 ; this corresponds to an approximate mass of 121 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 0.263 Å⁻¹

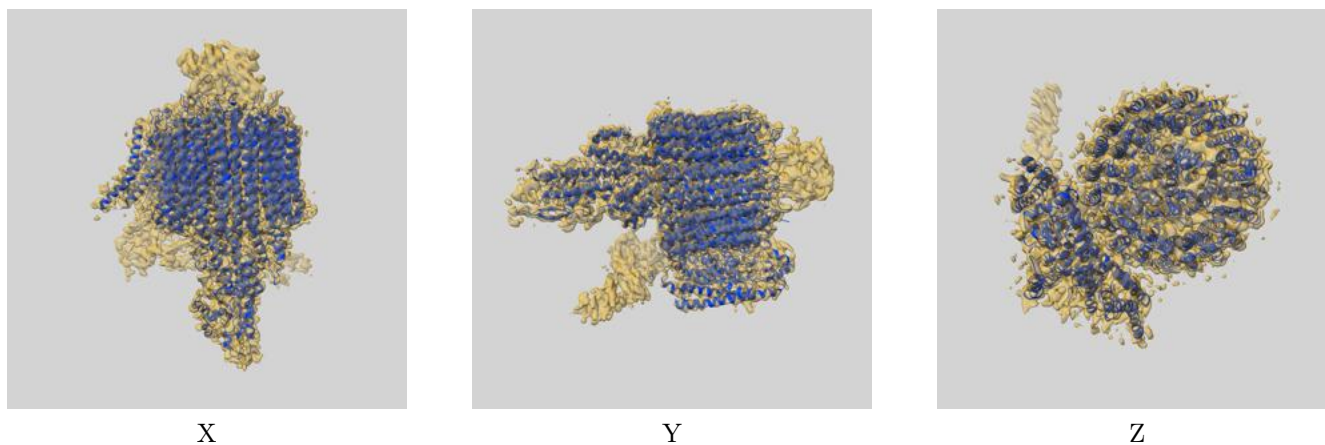
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

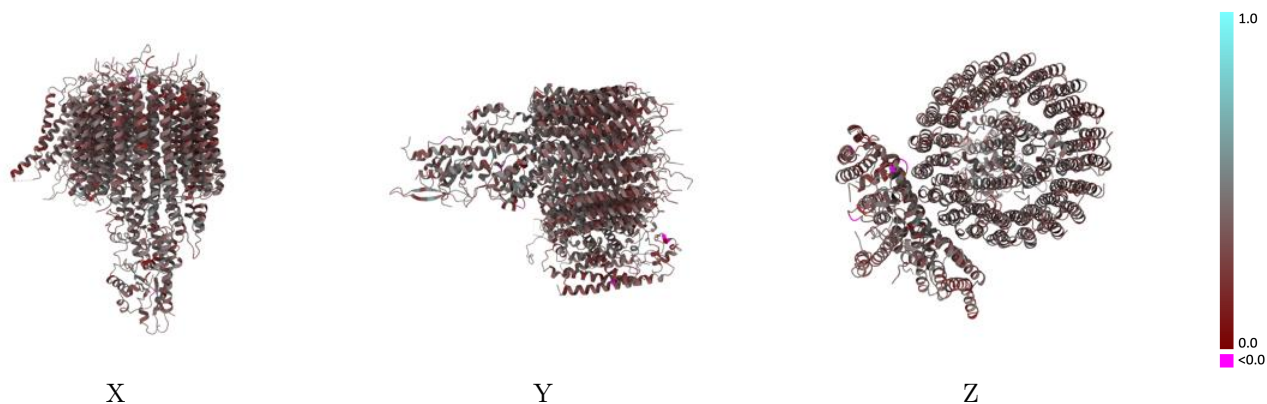
This section contains information regarding the fit between EMDB map EMD-21348 and PDB model 6VQC. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



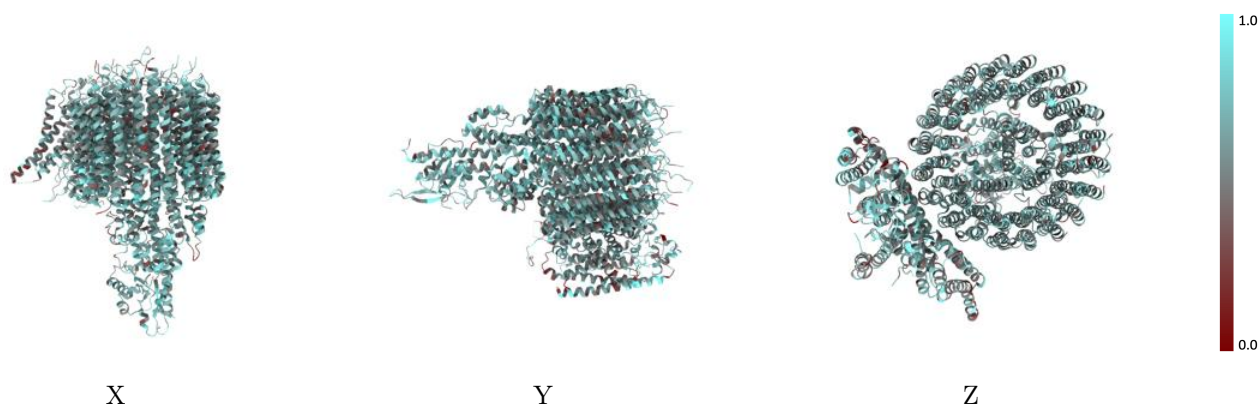
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



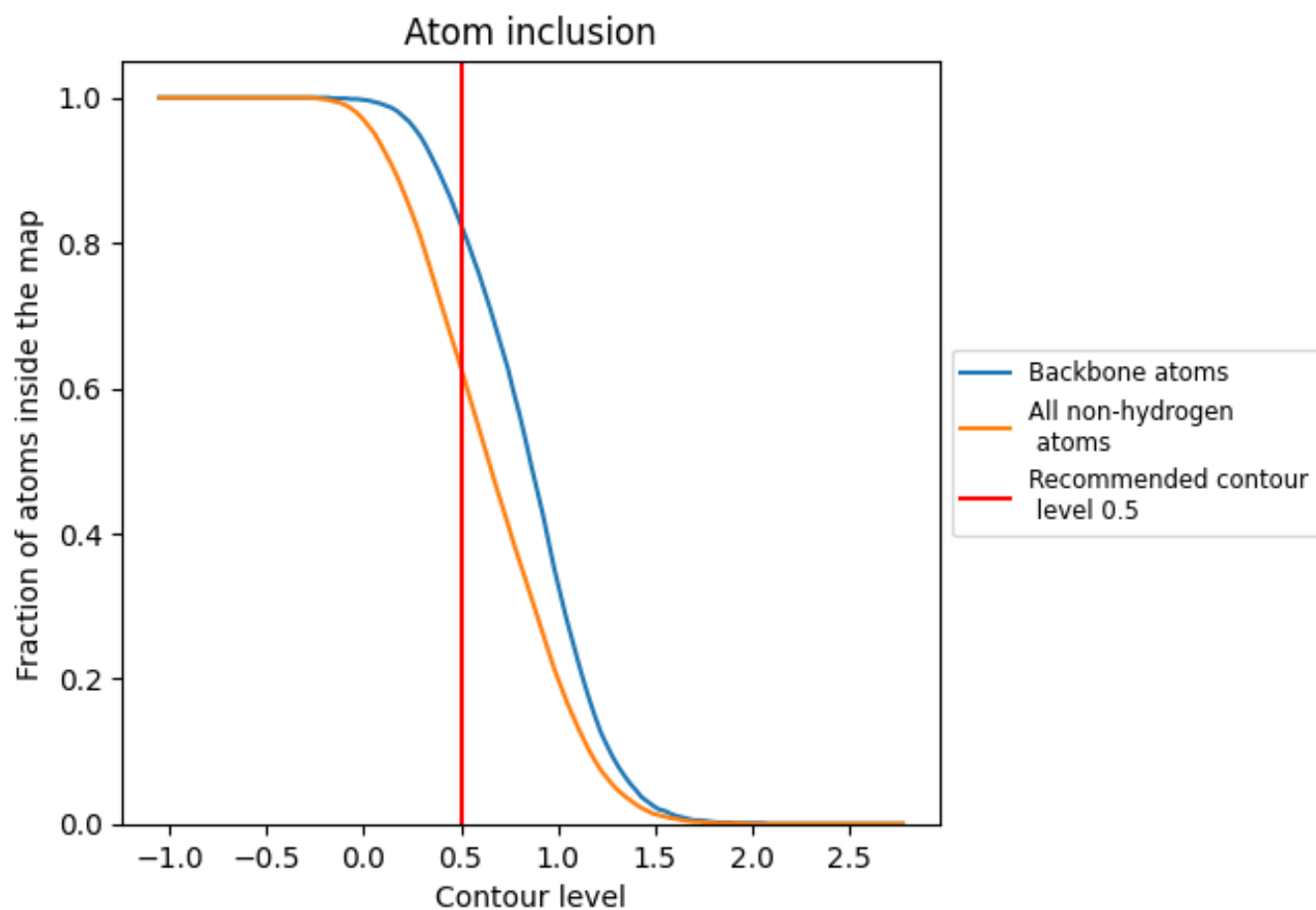
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6290	 0.3690
H	 0.6690	 0.3820
L	 0.6420	 0.3750
a	 0.6060	 0.3590
b	 0.6170	 0.3700
c	 0.5980	 0.3950
d	 0.6530	 0.3910
e	 0.6040	 0.3530
f	 0.6410	 0.3270
g	 0.6340	 0.3680
h	 0.6370	 0.3770
i	 0.6440	 0.3750
j	 0.6420	 0.3830
k	 0.6030	 0.3650
l	 0.6260	 0.3590
m	 0.6210	 0.3610
n	 0.6370	 0.3550
o	 0.6290	 0.3590
p	 0.6010	 0.3750

