



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2022 – 12:07 AM EDT

PDB ID : 5TJ5
EMDB ID : EMD-8409
Title : Atomic model for the membrane-embedded motor of a eukaryotic V-ATPase
Authors : Mazhab-Jafari, M.T.; Rohou, A.; Schmidt, C.; Bueler, S.A.; Benlekbir, S.; Robinson, C.V.; Rubinstein, J.L.
Deposited on : 2016-10-03
Resolution : 3.90 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.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

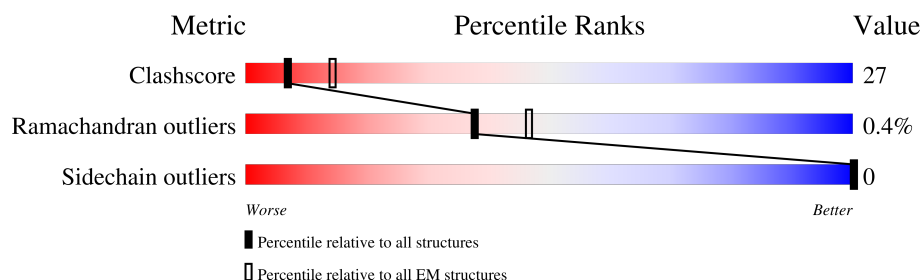
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.





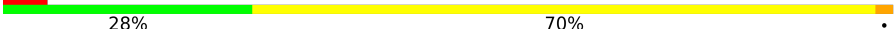
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	680	
2	B	213	
3	D	147	
4	E	150	
4	F	150	
4	G	150	
4	H	150	
4	I	150	

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Mol	Chain	Length	Quality of chain
4	J	150	 75% 25%
4	M	150	 63% 34% ..
4	N	150	 59% 38% ..
5	L	57	 5% 28% 70% .
6	O	54	 48% 52%
7	P	297	 69% 22% 9%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14976 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 a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	570	Total	C	N	O	S	0	0
			3391	2154	612	609	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	187	Total	C	N	O	S	0	0
			1266	834	201	227	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	147	Total	C	N	O	S	0	0
			914	596	156	157	5		

- Molecule 4 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	138	Total	C	N	O		0	0
			823	527	143	153			
4	F	150	Total	C	N	O	S	0	0
			885	569	154	161	1		
4	G	149	Total	C	N	O	S	0	0
			869	558	150	160	1		
4	H	150	Total	C	N	O	S	0	0
			895	579	151	164	1		
4	I	150	Total	C	N	O	S	0	0
			922	593	161	166	2		
4	J	150	Total	C	N	O	S	0	0
			866	549	152	164	1		
4	M	148	Total	C	N	O	S	0	0
			949	624	159	165	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	148	Total	C	N	O	S	0	0
			978	642	161	170	5		

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

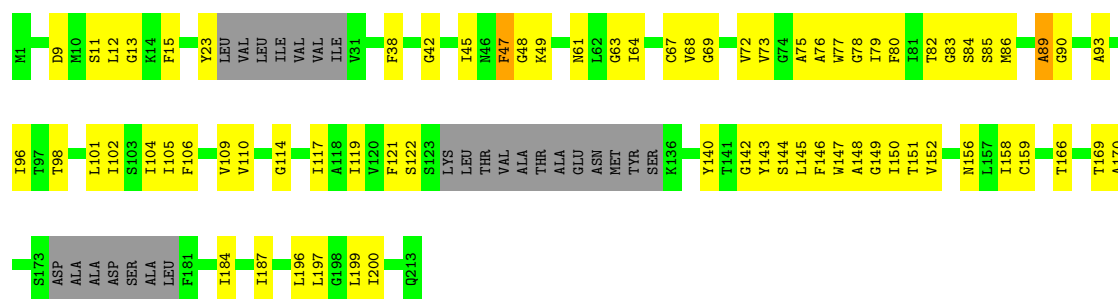
Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	57	Total	C	N	O	S	0	0
			411	274	66	67	4		

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

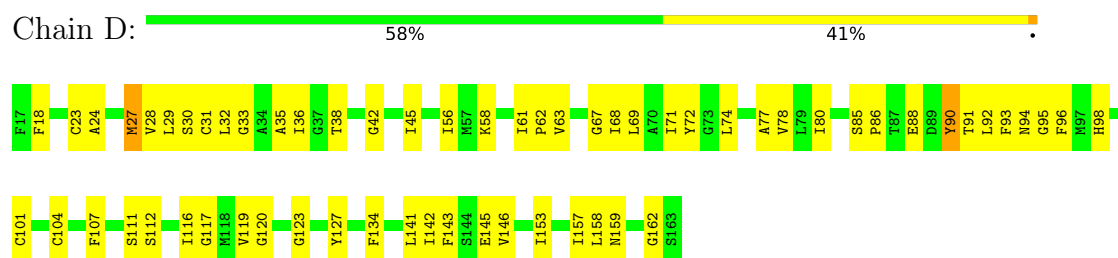
Mol	Chain	Residues	Atoms				AltConf	Trace
6	O	54	Total	C	N	O	0	0
			270	162	54	54		

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

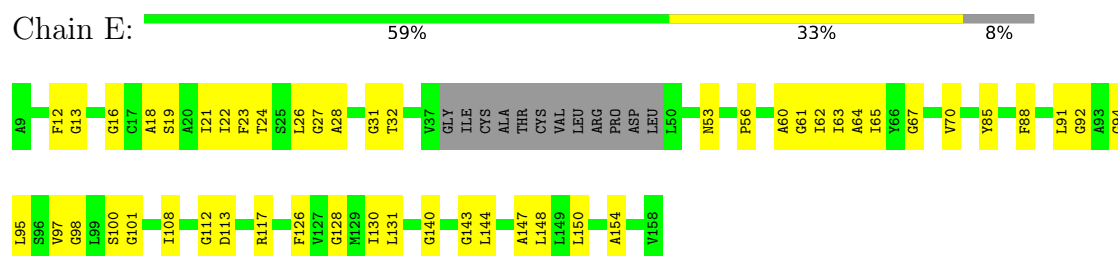
Mol	Chain	Residues	Atoms				AltConf	Trace
7	P	269	Total	C	N	O	0	0
			1537	964	280	293		



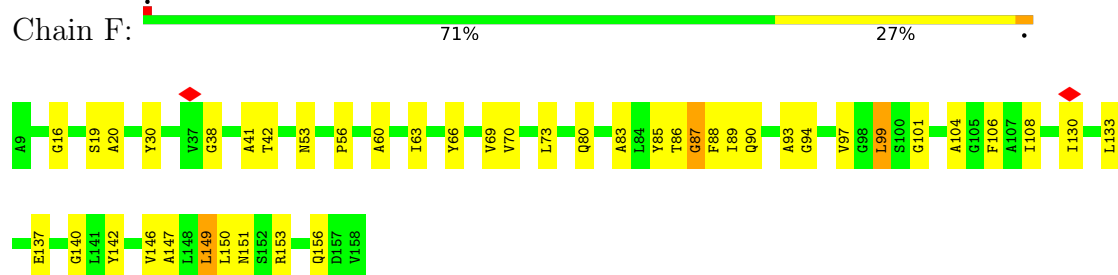
• Molecule 3: V-type proton ATPase subunit c'



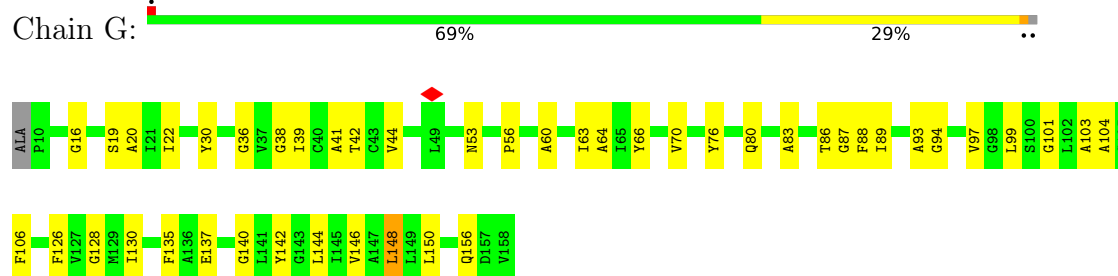
• Molecule 4: V-type proton ATPase subunit c



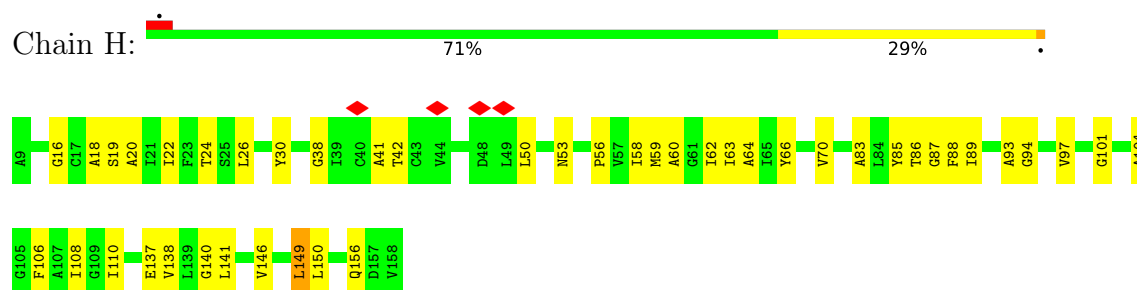
• Molecule 4: V-type proton ATPase subunit c



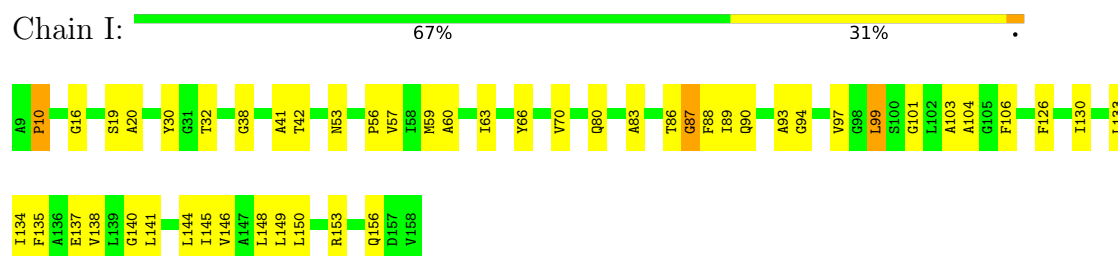
• Molecule 4: V-type proton ATPase subunit c



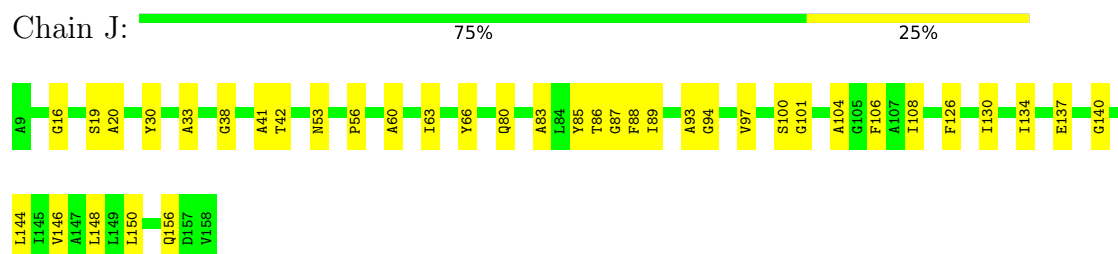
- Molecule 4: V-type proton ATPase subunit c



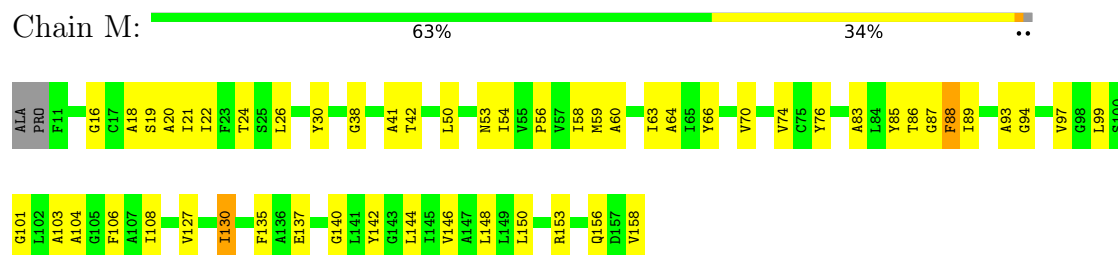
- Molecule 4: V-type proton ATPase subunit c



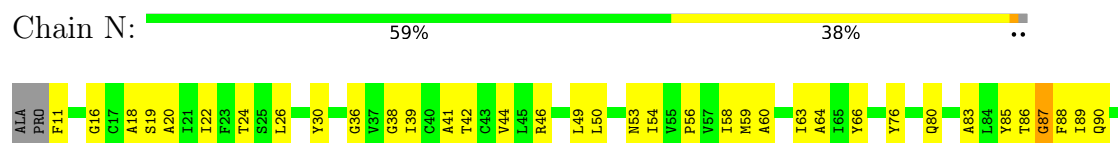
- Molecule 4: V-type proton ATPase subunit c



- Molecule 4: V-type proton ATPase subunit c

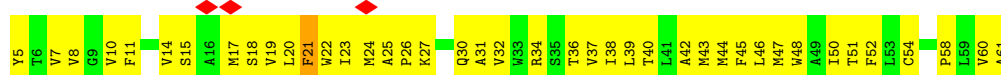


- Molecule 4: V-type proton ATPase subunit c





- Molecule 5: V-type proton ATPase subunit e



- Molecule 6: V-type proton ATPase subunit f



- Molecule 7: V-type proton ATPase subunit d



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	462842	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 ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	64350	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.270	Depositor
Minimum map value	-0.157	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0475	Depositor
Map size (\AA)	310.8, 310.8, 310.8	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.5539999, 1.5539999, 1.5539999	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	A	0.60	0/2196	0.70	3/3003 (0.1%)
2	B	0.62	0/1287	0.63	0/1752
3	D	0.49	0/925	0.64	1/1262 (0.1%)
4	E	0.53	0/831	0.58	0/1139
4	F	0.52	0/897	0.67	3/1233 (0.2%)
4	G	0.50	0/881	0.63	3/1210 (0.2%)
4	H	0.50	0/906	0.66	2/1245 (0.2%)
4	I	0.52	0/933	0.68	2/1278 (0.2%)
4	J	0.48	0/878	0.60	1/1204 (0.1%)
4	M	0.54	0/960	0.71	2/1312 (0.2%)
4	N	0.58	0/991	0.73	3/1352 (0.2%)
5	L	0.65	1/421 (0.2%)	0.77	0/579
7	P	0.47	0/1255	0.52	0/1735
All	All	0.54	1/13361 (0.0%)	0.66	20/18304 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	1
3	D	0	1
4	F	0	2
4	G	0	2
4	H	0	2
4	I	0	3
4	J	0	2
4	M	0	2
4	N	0	2
5	L	0	2
7	P	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	27

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	48	TRP	CB-CG	-5.85	1.39	1.50

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	570	GLY	N-CA-C	-8.96	90.71	113.10
4	M	130	ILE	CG1-CB-CG2	-7.41	95.11	111.40
4	F	88	PHE	N-CA-C	-6.71	92.89	111.00
4	G	88	PHE	N-CA-C	-6.70	92.91	111.00
4	N	88	PHE	N-CA-C	-6.70	92.91	111.00

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	UNK	Peptide
1	A	119	UNK	Peptide
1	A	229	UNK	Peptide
1	A	569	ILE	Peptide
1	A	606	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3391	0	1986	196	0
2	B	1266	0	1172	86	0
3	D	914	0	816	56	0
4	E	823	0	667	43	0
4	F	885	0	703	38	0
4	G	869	0	681	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	895	0	740	36	0
4	I	922	0	802	42	0
4	J	866	0	632	27	0
4	M	949	0	886	53	0
4	N	978	0	946	53	0
5	L	411	0	385	42	0
6	O	270	0	59	22	0
7	P	1537	0	796	43	0
All	All	14976	0	11271	710	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 27.

The worst 5 of 710 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:B:140:TYR:CD2	3:D:86:PRO:HA	1.81	1.14
1:A:604:PRO:HB2	1:A:605:ALA:HB2	1.44	1.00
7:P:97:TYR:HA	7:P:100:TYR:HD2	1.30	0.94
1:A:415:PHE:HB2	1:A:799:ARG:HG2	1.56	0.88
1:A:11:UNK:O	1:A:15:UNK:N	2.08	0.87

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	A	308/680 (45%)	244 (79%)	62 (20%)	2 (1%)	25	63
2	B	179/213 (84%)	158 (88%)	19 (11%)	2 (1%)	14	51
3	D	145/147 (99%)	132 (91%)	12 (8%)	1 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	134/150 (89%)	116 (87%)	18 (13%)	0	100	100
4	F	148/150 (99%)	128 (86%)	20 (14%)	0	100	100
4	G	147/150 (98%)	127 (86%)	20 (14%)	0	100	100
4	H	148/150 (99%)	127 (86%)	21 (14%)	0	100	100
4	I	148/150 (99%)	127 (86%)	20 (14%)	1 (1%)	22	60
4	J	148/150 (99%)	126 (85%)	22 (15%)	0	100	100
4	M	146/150 (97%)	126 (86%)	20 (14%)	0	100	100
4	N	146/150 (97%)	126 (86%)	20 (14%)	0	100	100
5	L	55/57 (96%)	34 (62%)	19 (34%)	2 (4%)	3	29
7	P	200/297 (67%)	177 (88%)	22 (11%)	1 (0%)	29	67
All	All	2052/2594 (79%)	1748 (85%)	295 (14%)	9 (0%)	38	71

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	622	ILE
3	D	56	ILE
7	P	338	ILE
1	A	571	ASN
2	B	47	PHE

5.3.2 Protein sidechains ⓘ

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	A	145/368 (39%)	145 (100%)	0	100	100
2	B	106/168 (63%)	106 (100%)	0	100	100
3	D	61/111 (55%)	61 (100%)	0	100	100
4	E	44/109 (40%)	44 (100%)	0	100	100
4	F	44/109 (40%)	44 (100%)	0	100	100
4	G	43/109 (39%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	50/109 (46%)	50 (100%)	0	100	100
4	I	58/109 (53%)	58 (100%)	0	100	100
4	J	37/109 (34%)	37 (100%)	0	100	100
4	M	68/109 (62%)	68 (100%)	0	100	100
4	N	80/109 (73%)	80 (100%)	0	100	100
5	L	37/50 (74%)	37 (100%)	0	100	100
7	P	45/217 (21%)	45 (100%)	0	100	100
All	All	818/1786 (46%)	818 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	HIS
1	A	559	HIS
1	A	725	ASN
1	A	743	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	10
7	P	5
6	O	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	295:UNK	C	307:UNK	N	67.70
1	A	365:UNK	C	400:ALA	N	58.47
1	A	224:UNK	C	225:UNK	N	30.05
1	A	210:UNK	C	211:UNK	N	26.91
1	A	248:UNK	C	268:UNK	N	24.15

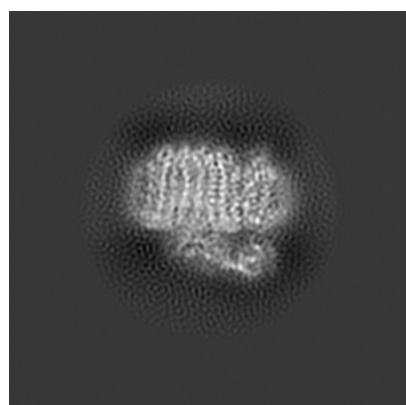
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8409. These allow visual inspection of the internal detail of the map and identification of artifacts.

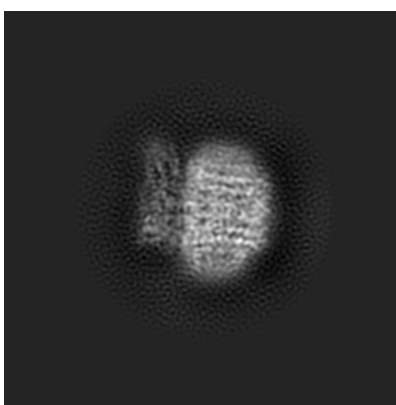
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

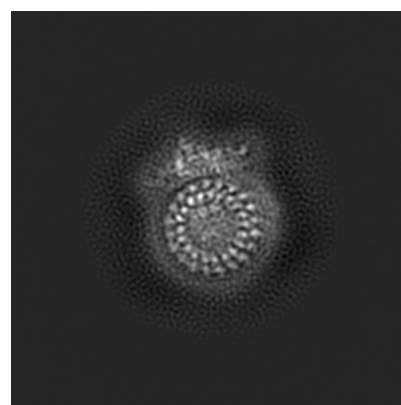
6.1.1 Primary map



X



Y

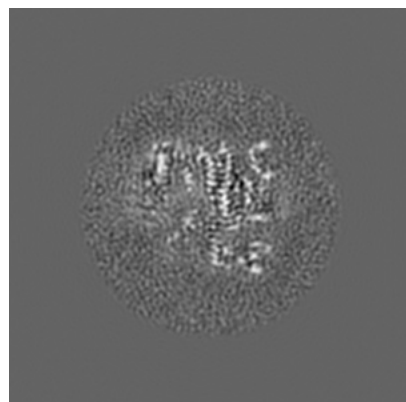


Z

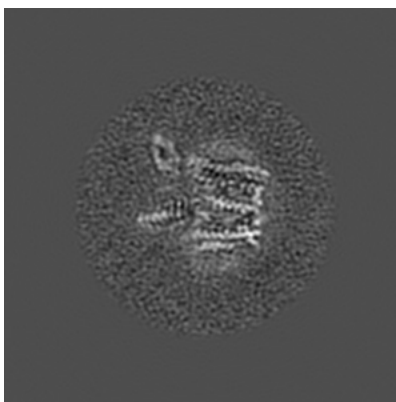
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

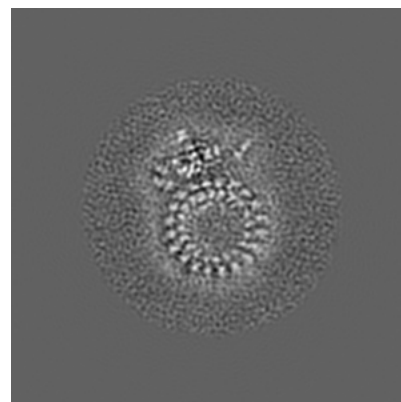
6.2.1 Primary map



X Index: 100



Y Index: 100

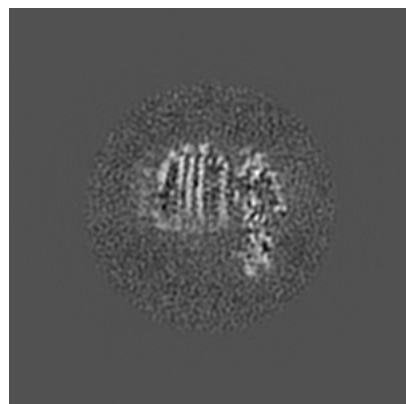


Z Index: 100

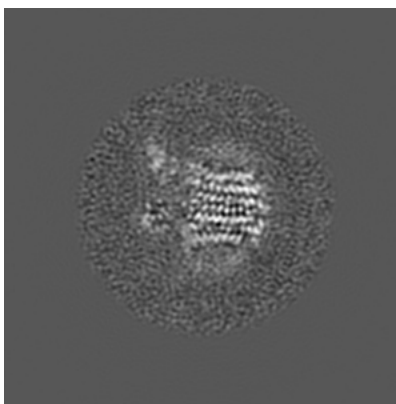
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

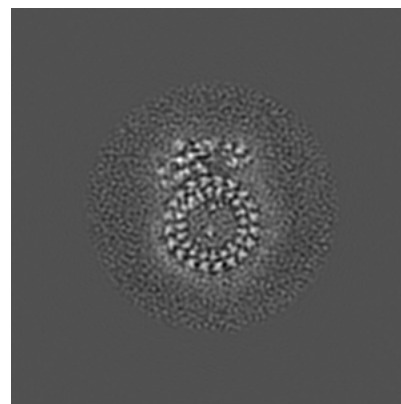
6.3.1 Primary map



X Index: 84



Y Index: 106



Z Index: 117

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

6.4 Orthogonal surface views [i](#)

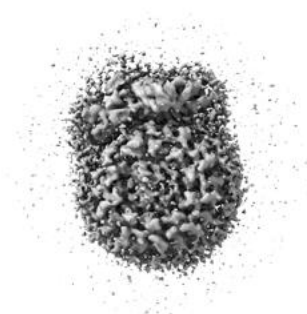
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0475. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

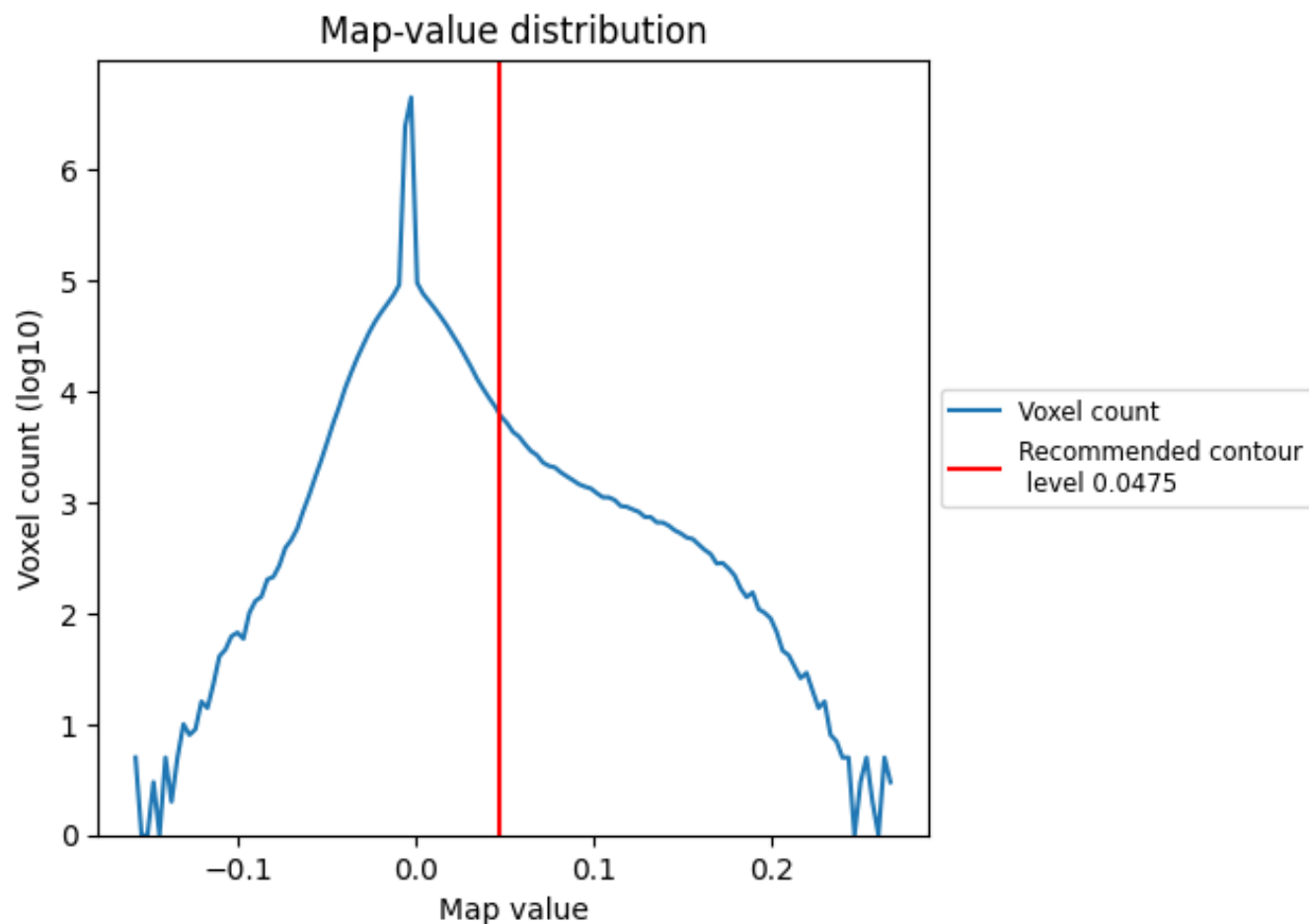
6.5 Mask visualisation

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

7 Map analysis [i](#)

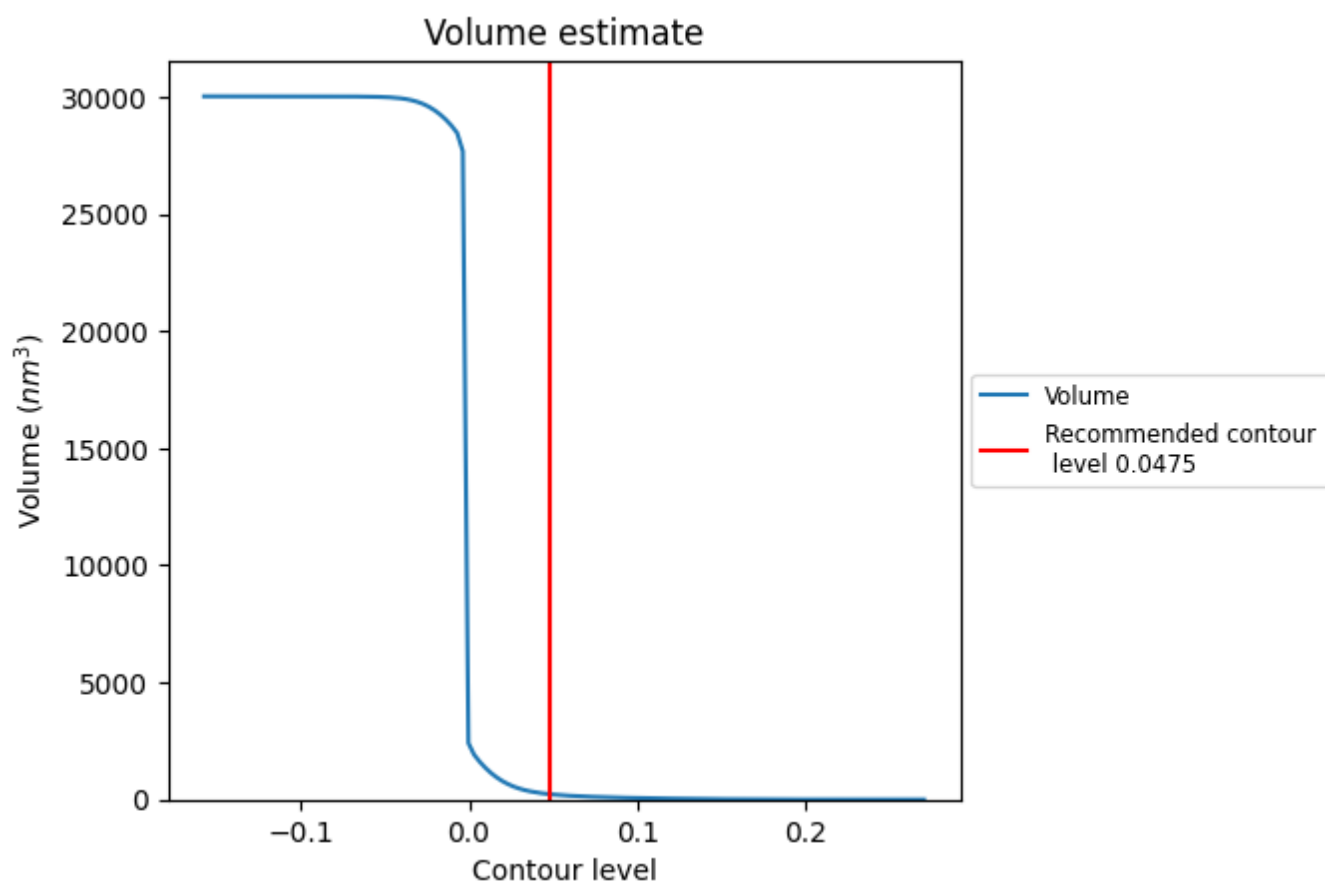
This section contains the results of statistical analysis of the map.

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.

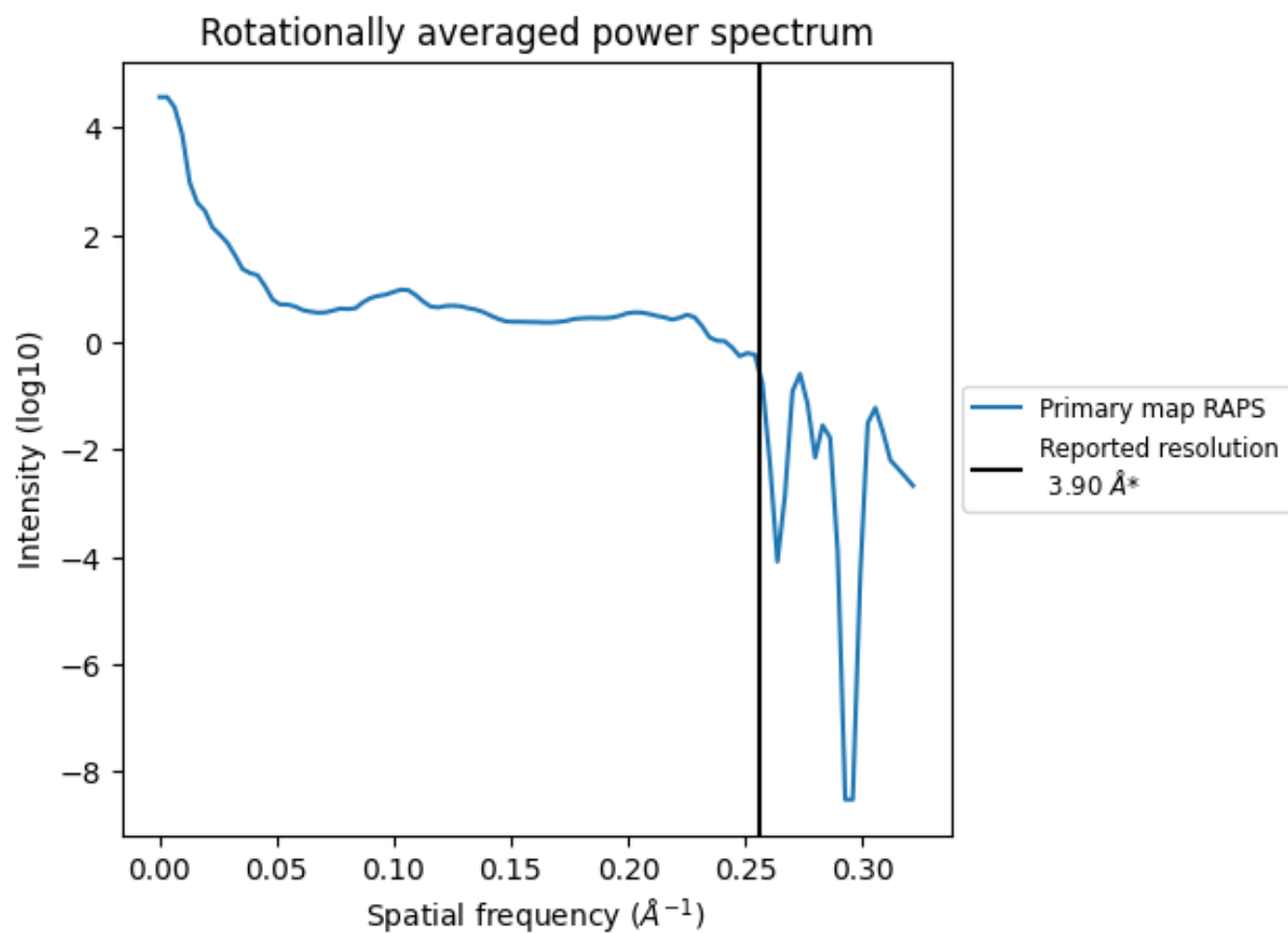
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 233 nm³; this corresponds to an approximate mass of 210 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 0.256 Å⁻¹

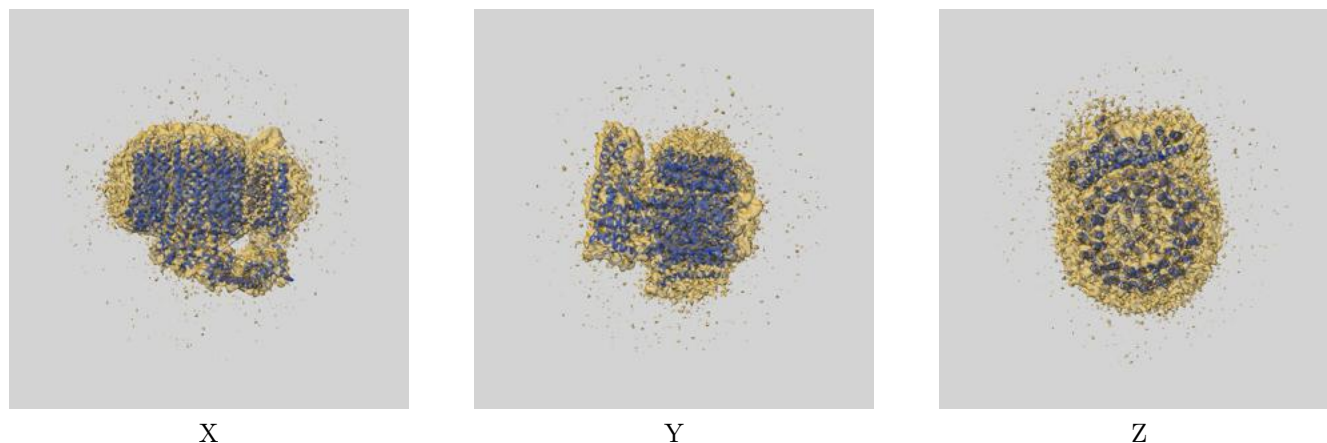
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

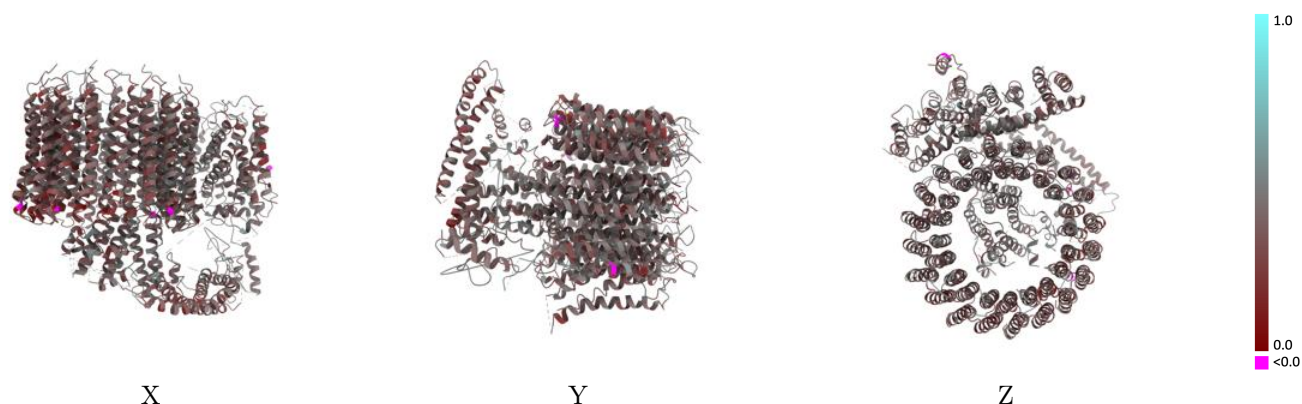
This section contains information regarding the fit between EMDB map EMD-8409 and PDB model 5TJ5. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



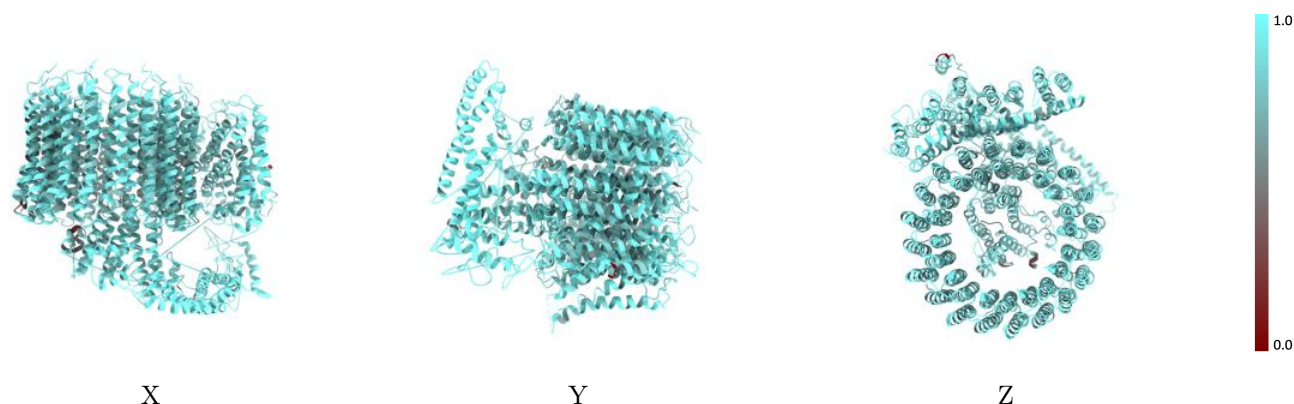
The images above show the 3D surface view of the map at the recommended contour level 0.0475 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



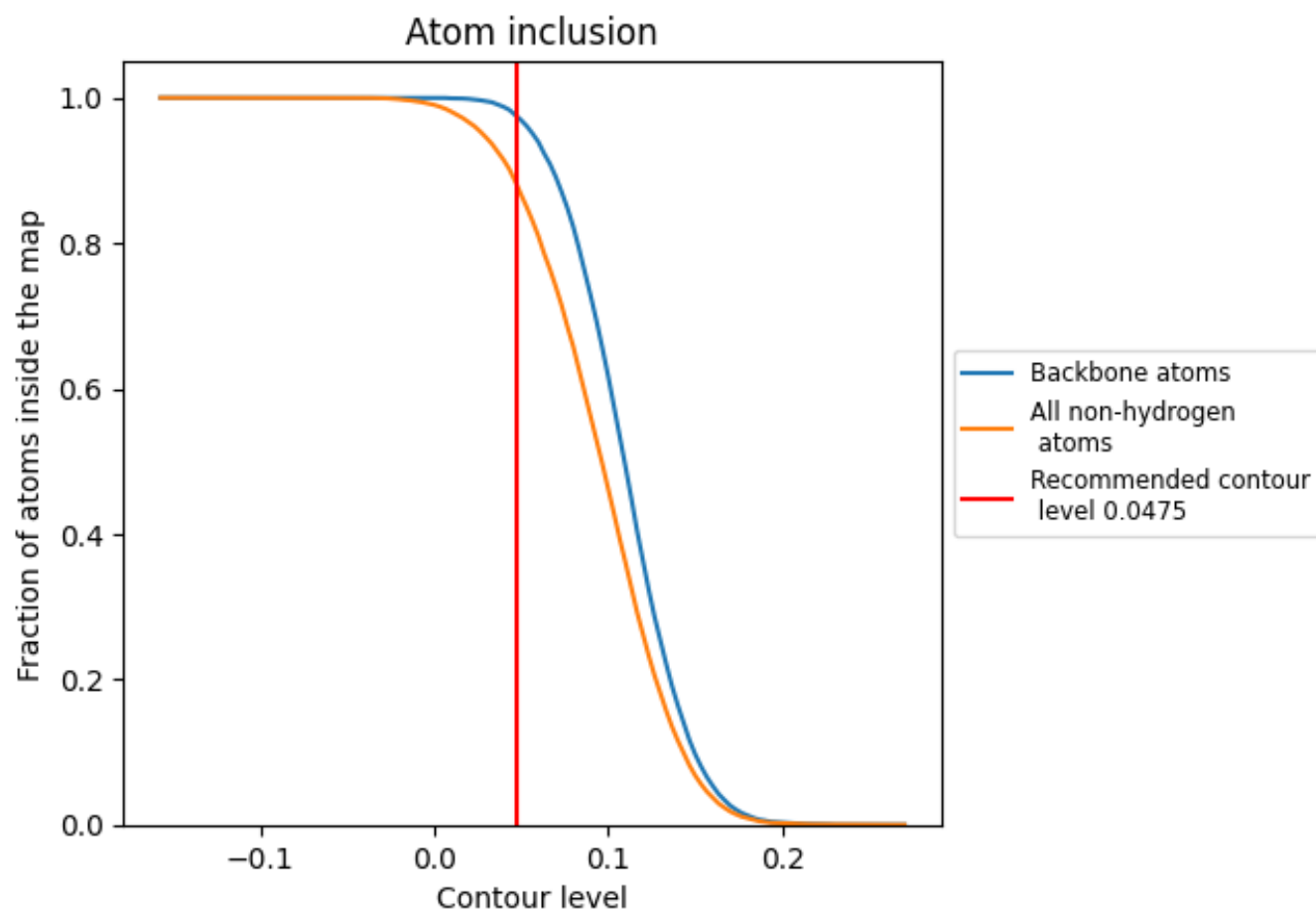
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0475).































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 88% 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 (0.0475) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8799	 0.3800
A	 0.9247	 0.4040
B	 0.8718	 0.4070
D	 0.8491	 0.3690
E	 0.8958	 0.3770
F	 0.8781	 0.3470
G	 0.8682	 0.3390
H	 0.8427	 0.3390
I	 0.8545	 0.3540
J	 0.8815	 0.3480
L	 0.8123	 0.3810
M	 0.8713	 0.3820
N	 0.8428	 0.3870
O	 0.9407	 0.3800
P	 0.8771	 0.4100

