



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 02:28 PM UTC

PDB ID : 6VQI / pdb_00006vqi
EMDB ID : EMD-21351
Title : Mammalian V-ATPase from rat brain collar and peripheral stalks rotational state 1 (from focused refinement)
Authors : Abbas, Y.M.; Rubinstein, J.L.
Deposited on : 2020-02-05
Resolution : 4.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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

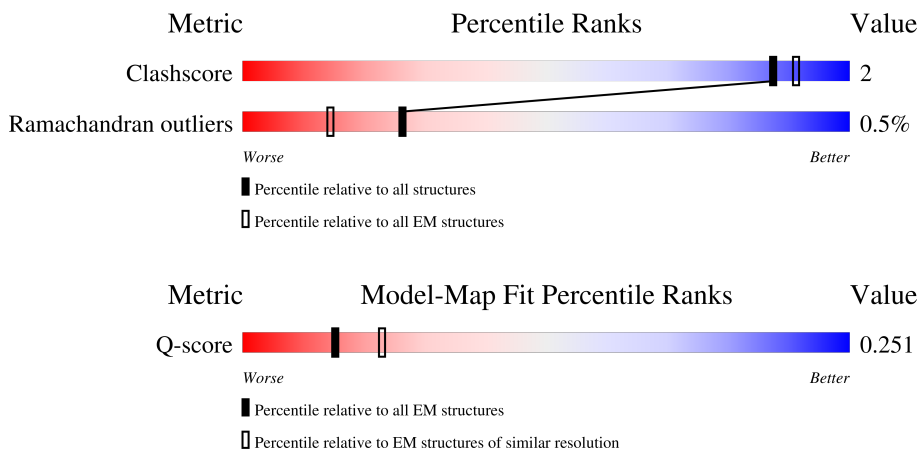
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	57% 43%
3	O	118	11% 56% 43%
4	a	838	36% 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		

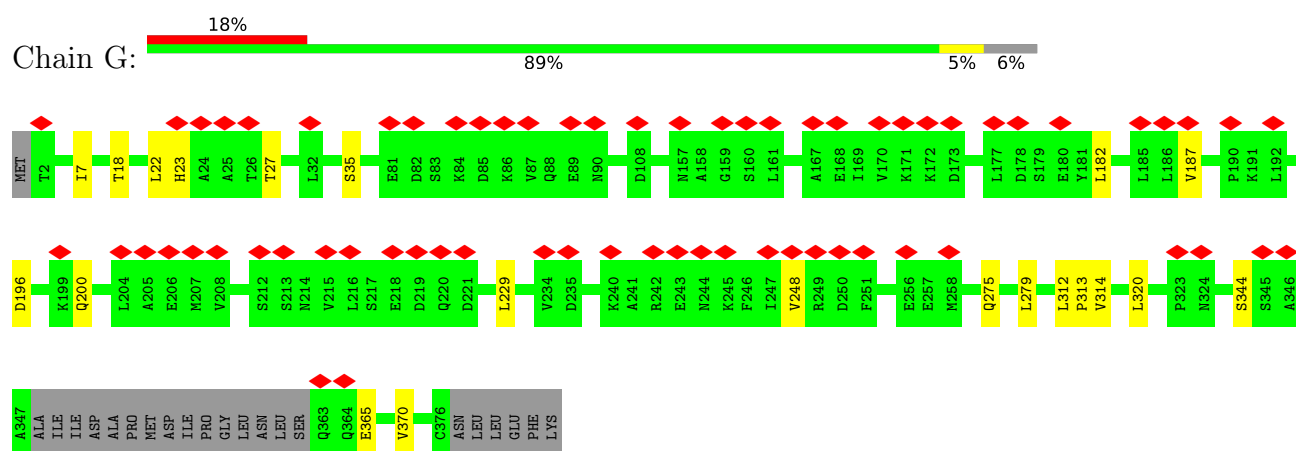
- Molecule 4 is a protein called V-type proton ATPase 116 kDa subunit a isoform 1.

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

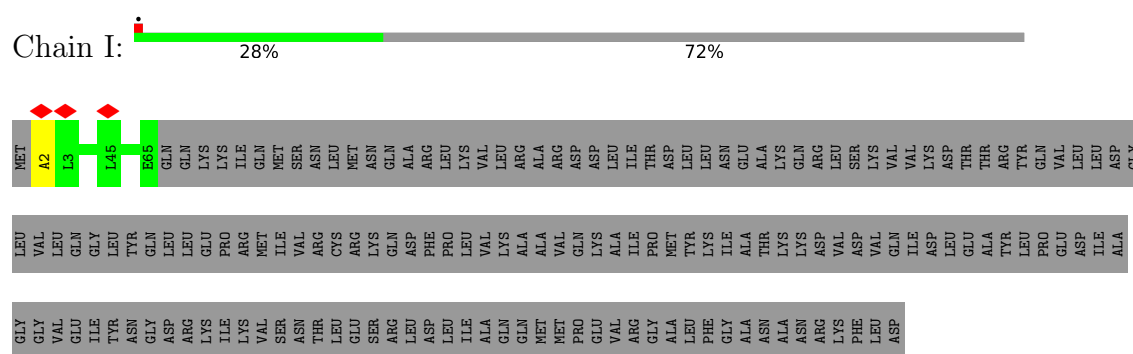
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

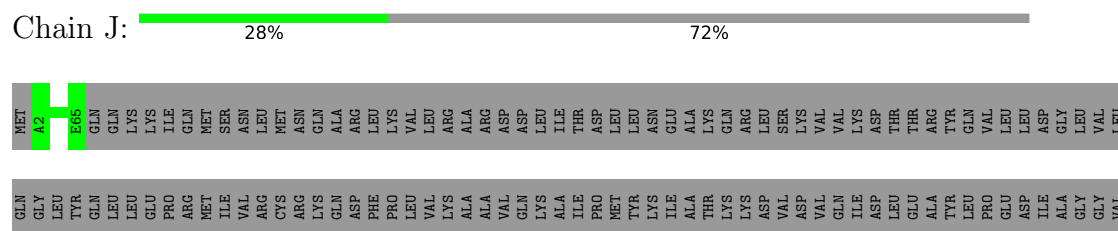
- Molecule 1: V-type proton ATPase subunit C 1



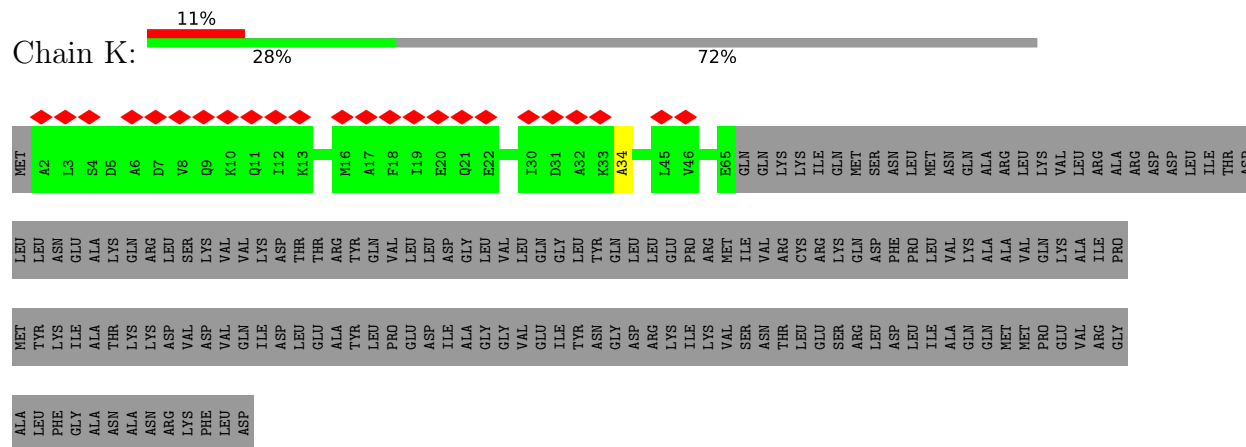
- Molecule 2: V-type proton ATPase subunit E 1



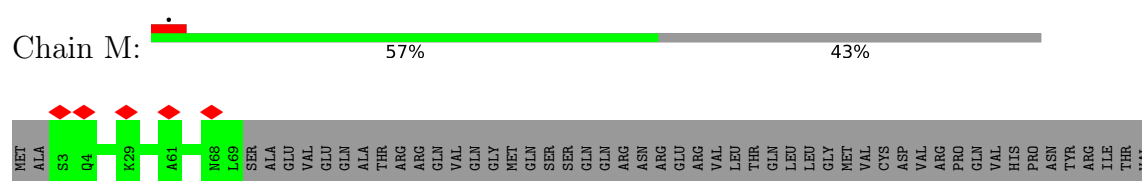
- Molecule 2: V-type proton ATPase subunit E 1



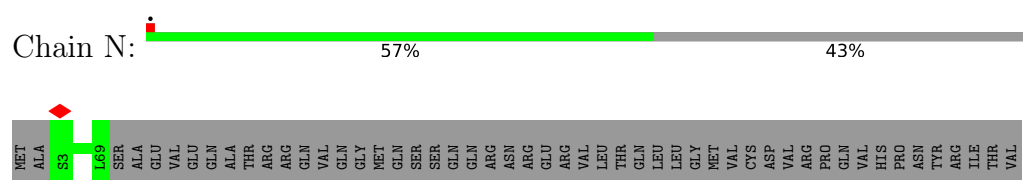
- Molecule 2: V-type proton ATPase subunit E 1



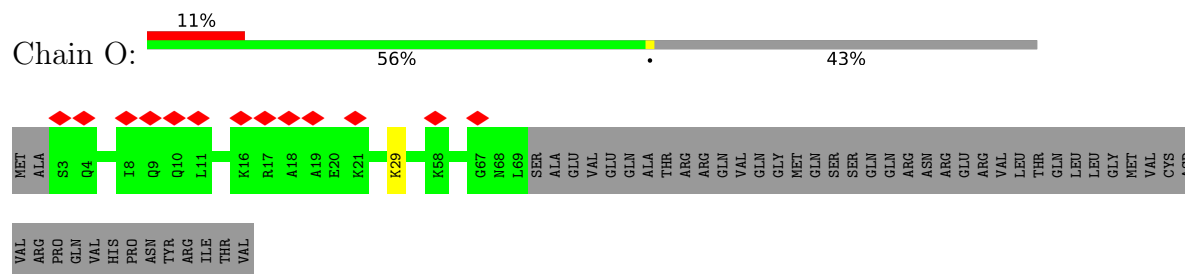
- Molecule 3: V-type proton ATPase subunit G



- Molecule 3: V-type proton ATPase subunit G



- Molecule 3: V-type proton ATPase subunit G



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



LEU	ARG	LEU	LEU	HIS	TRP	VAL	GLU	ALA	THR	SER	LYS	ASN	PHE	GLY	F170
LEU	LEU	SER	LEU	LEU	ASP	ALA	GLU	LEU	GLY	ASN	PRO	ALA	GLY	THR	I175
HIS	HIS	LEU	LEU	ALA	ALA	HIS	GLU	LEU	GLY	MET	ASN	PRO	TYR	ARG	R179
VAL	VAL	HIS	ALA	ALA	ILE	GLU	GLU	LEU	TYR	LEU	ILE	VAL	ILE	ILE	F183
GLU	PHE	GLN	LEU	GLN	ILE	ALA	ILE	GLY	SER	SER	PHE	PHE	ILE	ASN	E207
GLN	GLN	LEU	LEU	SER	HIS	SER	GLN	GLY	GLY	GLN	PHE	GLY	LEU	ALA	
ASN	ASN	SER	GLU	VAL	GLN	GLY	GLY	ILE	ILE	ASP	PRO	PRO	GLY	TYR	T211
LYS	PHE	VAL	VAL	VAL	GLN	GLY	ILE	GLU	PRO	TYR	TYR	TYR	LEU	THR	
TYR	TYR	TRP	LEU	LEU	LEU	ILE	ILE	GLU	PRO	PRO	PRO	PHE	PHE	VAL	Y214
THR	GLY	THR	THR	THR	SER	GLN	CYS	ILE	PHE	SER	ILE	ILE	THR	THR	S218
THR	THR	VAL	VAL	VAL	HIS	SER	PHE	ILE	ILE	ILE	TYR	PHE	PHE	THR	V219
GLY	GLY	MET	MET	MET	SER	VAL	LEU	SER	MET	ASP	THR	GLY	PHE	LEU	F220
PHE	PHE	ILE	ILE	ILE	ASP	HIS	ILE	VAL	SER	ILE	LEU	ILE	PHE	LEU	I221
LYS	LYS	HIS	HIS	ILE	ALA	ALA	VAL	VAL	LEU	TRP	TRP	ILE	PHE	ALA	I222
PHE	PHE	GLY	GLY	GLY	GLU	GLY	ALA	PHE	PHE	ASN	TYR	ASN	VAL	ALA	Y245
LEU	LEU	LEU	LEU	HIS	PRO	HIS	MET	GLY	ILE	ILE	ASN	VAL	VAL	MET	P246
PHE	PHE	HIS	VAL	VAL	THR	VAL	CYS	LEU	THR	THR	THR	CYS	PHE	PHE	S259
PHE	ARG	ARG	SER	SER	ASP	SER	PRO	VAL	ILE	LYS	LYS	ASN	PHE	ASP	
GLU	GLU	LEU	LEU	LEU	GLU	LEU	TRP	THR	LEU	LEU	THR	LEU	SER	PHE	T315
HIS	HIS	ALA	ALA	ALA	VAL	ALA	MET	VAL	ILE	THR	ALA	PHE	GLY	GLY	
ILE	ARG	GLY	GLY	GLY	PHE	GLY	LEU	PHE	PHE	THR	LYS	ASN	ILE	ILE	D331
GLU	GLU	GLY	GLY	GLY	ASP	LEU	PHE	LEU	LYS	TRP	SER	PHE	GLY	LEU	G345
LYS	LYS	GLY	GLY	GLY	GLY	GLY	LYS	THR	THR	ALA	PHE	PHE	GLY	MET	S346
LEU	PHE	LEU	PHE	PHE	ASP	LEU	PRO	LEU	ALA	TYR	LYS	LYS	SER	THR	T347
ASP	ASP	PHE	PHE	PHE	MET	PHE	ILE	ILE	ILE	ILE	TRP	TRP	PHE	PHE	T357
GLU	GLU	ILE	ILE	ILE	VAL	ILE	ILE	LEU	ASP	LYS	SER	SER	SER	ALA	ASN
		PHE	ALA	ALA	HIS	ALA	HIS	HIS	SER	SER	VAL	VAL	ARG	TRP	GLN
		ALA	ALA	ALA	ILE	ALA	THR	THR	SER	ILE	PRO	PRO	PRO	THR	THR
		ALA	ALA	ALA	ILE	ALA	THR	THR	ARG	ASN	GLY	GLY	PHE	VAL	PRO
		THR	THR	THR	ILE	THR	ARG	LYS	ILE	ILE	THR	THR	ARG	GLN	LYS
		LEU	LEU	LEU	THR	THR	GLY	PRO	PRO	ILE	GLY	GLY	ASN	ASN	THR
		VAL	VAL	VAL	THR	VAL	HIS	SER	SER	HIS	GLY	ASN	SER	LYS	ASN
		ALA	ALA	ALA	CYS	ALA	LEU	LEU	LEU	MET	ASN	THR	ARG	ILE	LYS
		ILE	ILE	ILE	GLY	ILE	GLY	LEU	ILE	LEU	THR	THR	THR	LEU	THR
		LEU	LEU	LEU	THR	ALA	ILE	THR	THR	LEU	TRP	TRP	THR	GLY	GLY
		LEU	LEU	LEU	ALA	LEU	ILE	PHE	PHE	GLY	ASN	ASN	GLY	GLY	ASN
		LEU	LEU	LEU	THR	ALA	ALA	THR	ALA	ILE	THR	THR	GLN	ASN	PHE
		SER	SER	SER	TYR	VAL	ARG	VAL	VAL	ARG	VAL	GLY	GLN	ASN	ASN
		PHE	PHE	PHE	LEU	VAL	VAL	VAL	PHE	SER	SER	MET	VAL	PHE	THR
		HIS	HIS	HIS	ARG	GLY	GLY	GLY	THR	ILE	THR	THR	GLN	ASN	THR
		ALA	ALA	ALA	THR	THR	ASN	THR	PRO	TYR	TYR	TYR	GLN	ASP	ALA
		THR	THR	THR	THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR
		THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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		THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		

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	1.733	Depositor
Minimum map value	-0.481	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.055	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 [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	G	0.32	0/1788	0.86	0/2494
2	I	0.31	0/318	0.81	0/443
2	J	0.53	0/318	1.01	0/443
2	K	0.45	0/318	0.99	0/443
3	M	0.31	0/331	0.75	0/460
3	N	0.49	0/331	0.90	0/460
3	O	0.30	0/331	0.83	0/460
4	a	0.40	0/1533	1.01	0/2137
All	All	0.38	0/5268	0.91	0/7340

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	G	1790	0	794	9	0
2	I	319	0	149	1	0
2	J	319	0	149	0	0
2	K	319	0	149	1	0
3	M	332	0	166	0	0
3	N	332	0	166	0	0
3	O	332	0	166	1	0
4	a	1535	0	661	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5278	0	2400	15	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.

The worst 5 of 15 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)
4:a:207:GLU:HA	4:a:214:TYR:HA	1.67	0.74
2:I:2:ALA:HB2	4:a:331:ASP:HA	1.76	0.66
4:a:179:ARG:O	4:a:183:PHE:N	2.33	0.61
1:G:196:ASP:O	1:G:200:GLN:N	2.34	0.56
1:G:275:GLN:O	1:G:279:LEU:N	2.39	0.56

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	G	356/382 (93%)	346 (97%)	7 (2%)	3 (1%)	16	52
2	I	62/226 (27%)	62 (100%)	0	0	100	100
2	J	62/226 (27%)	62 (100%)	0	0	100	100
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%)	7 (2%)	2 (1%)	18	55
All	All	1042/2252 (46%)	1023 (98%)	14 (1%)	5 (0%)	26	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	a	245	TYR
1	G	365	GLU
1	G	344	SER
1	G	314	VAL
4	a	79	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.

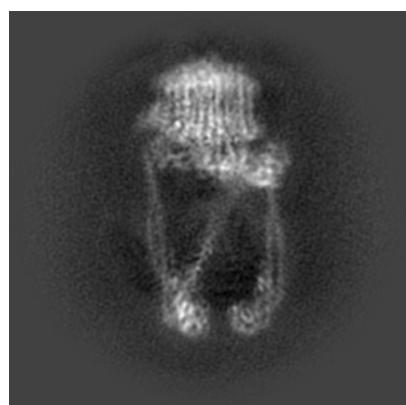
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21351. These allow visual inspection of the internal detail of the map and identification of artifacts.

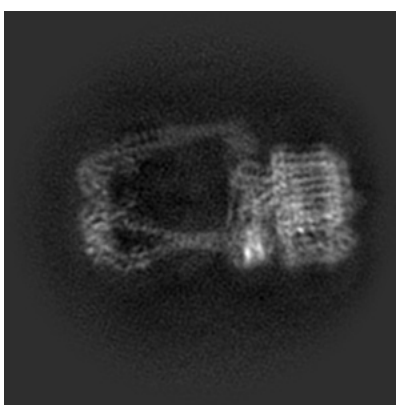
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

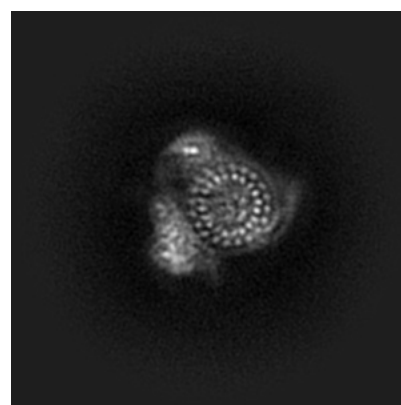
6.1.1 Primary map



X



Y

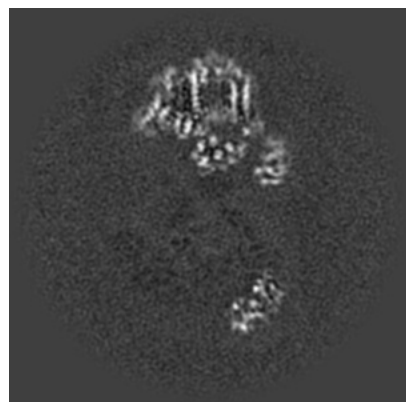


Z

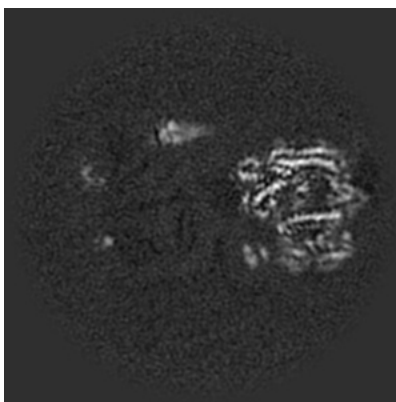
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

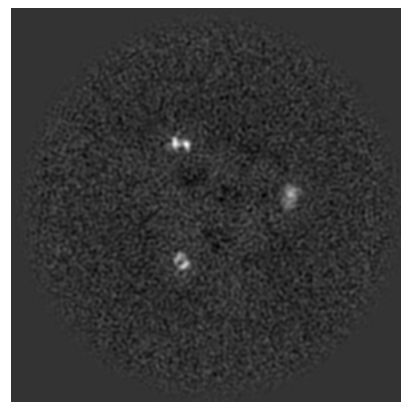
6.2.1 Primary map



X Index: 170



Y Index: 170

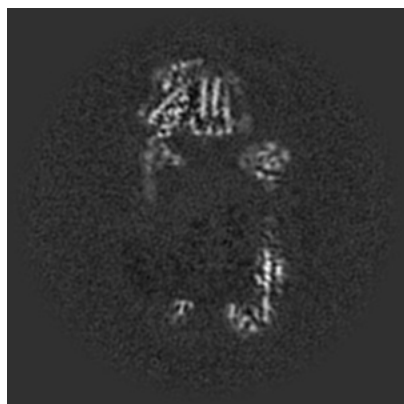


Z Index: 170

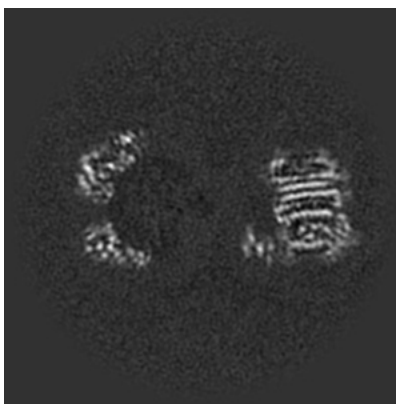
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

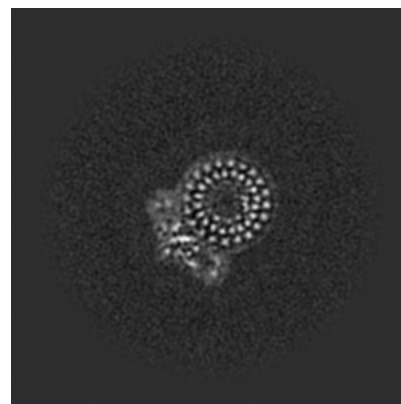
6.3.1 Primary map



X Index: 154



Y Index: 150

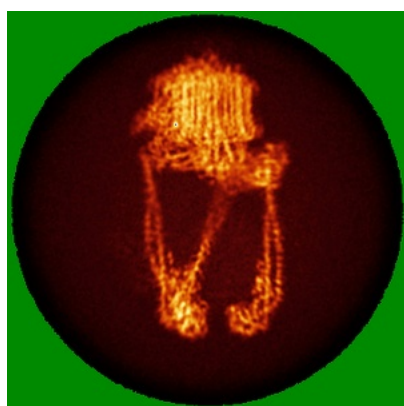


Z Index: 243

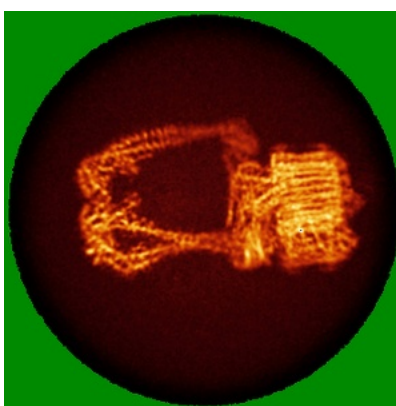
The images above show the largest variance slices of the map in three orthogonal directions.

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

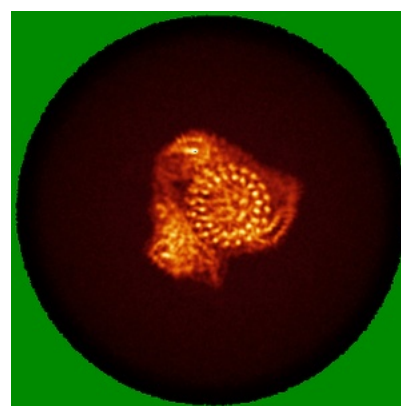
6.4.1 Primary map



X



Y

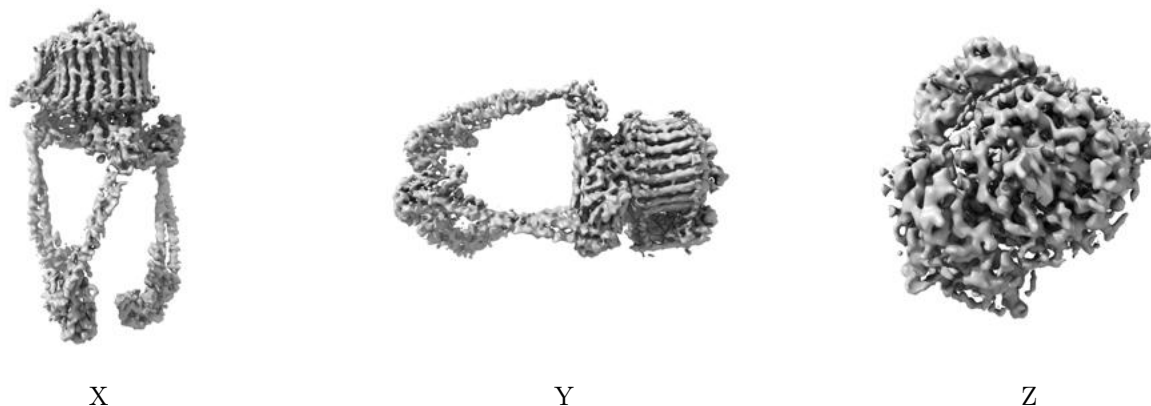


Z

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.

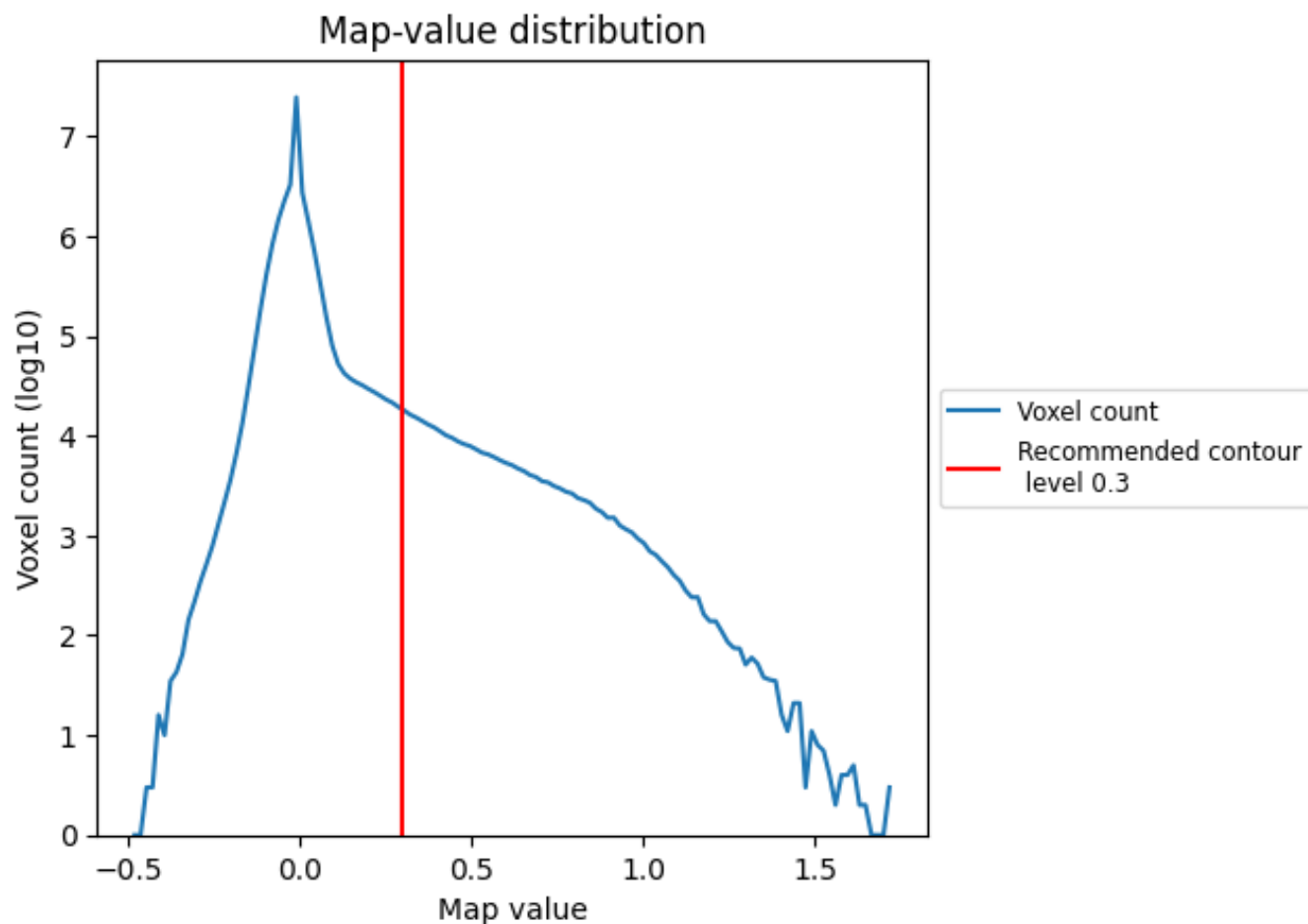
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

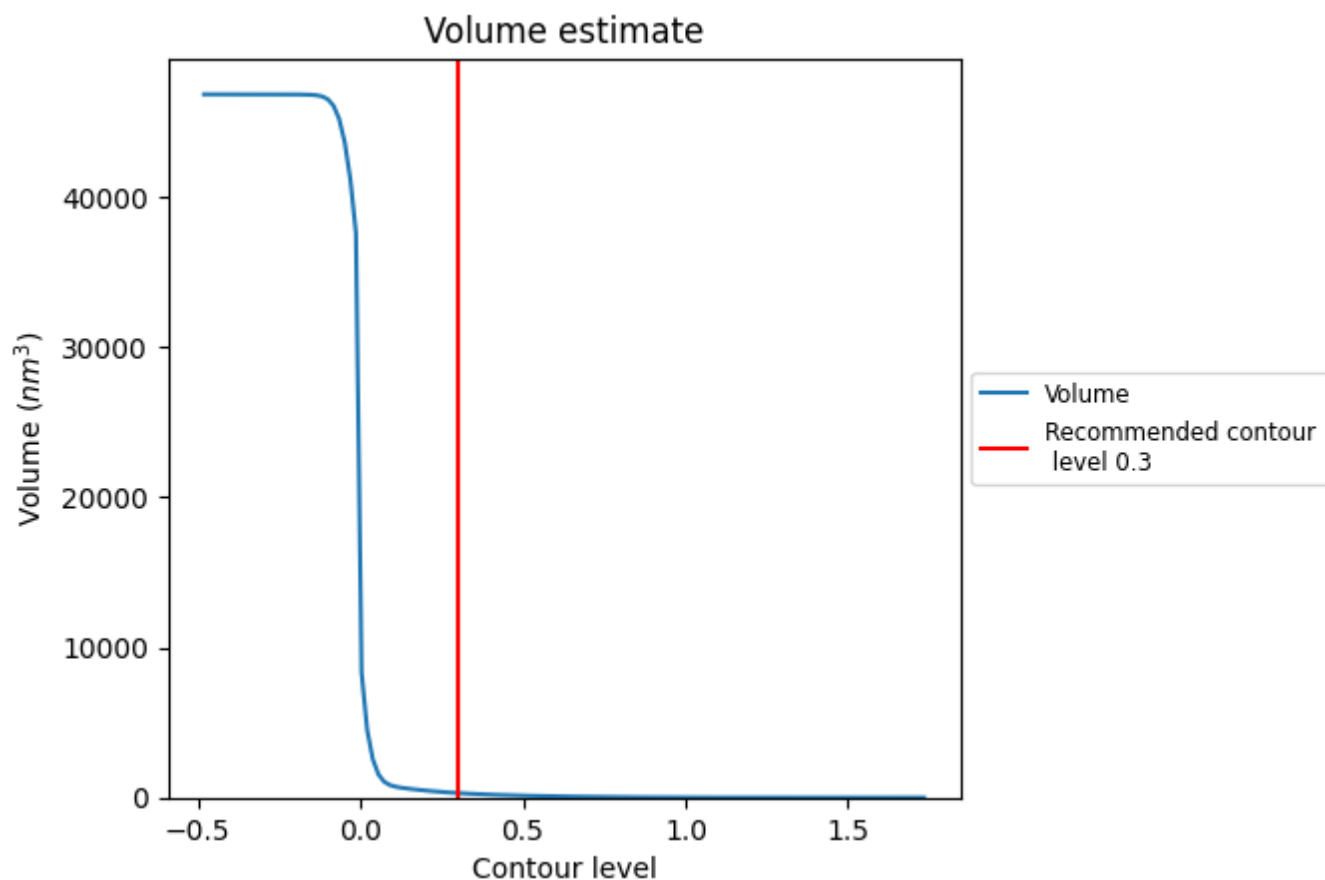
This section contains the results of statistical analysis of the map.

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.

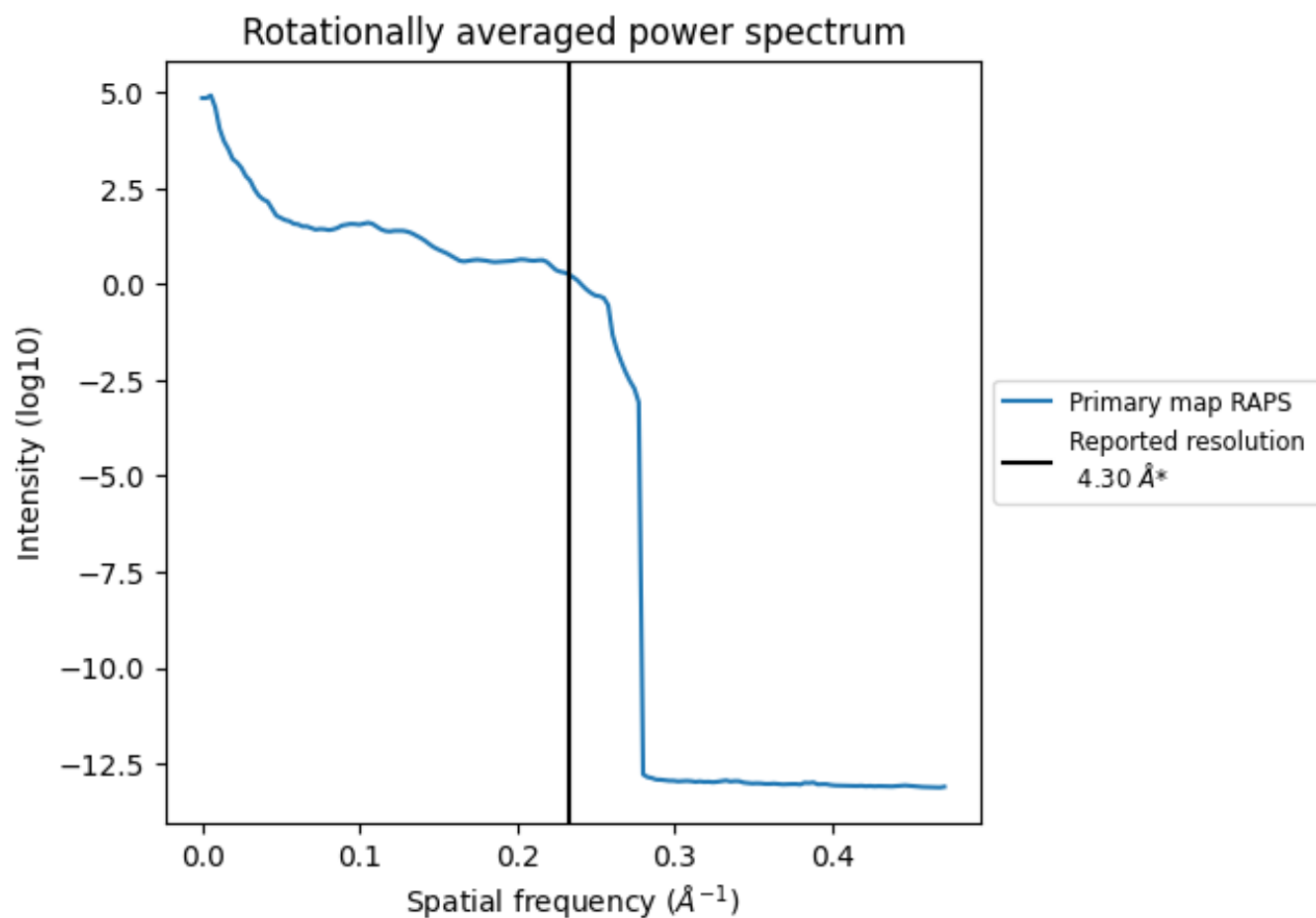
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 299 nm³; this corresponds to an approximate mass of 270 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 0.233 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-21351 and PDB model 6VQI. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

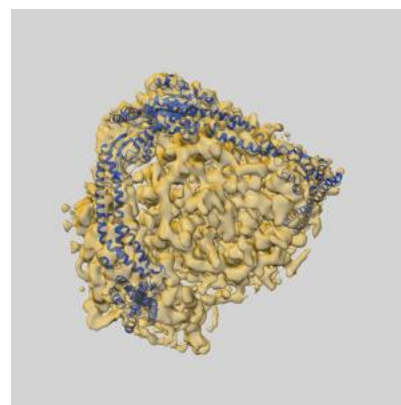
9.1 Map-model overlay [i](#)



X



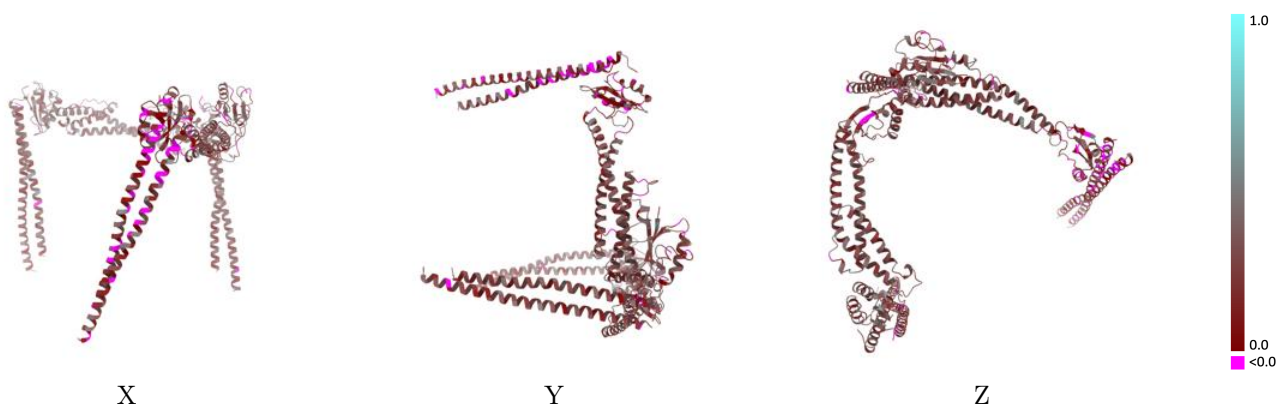
Y



Z

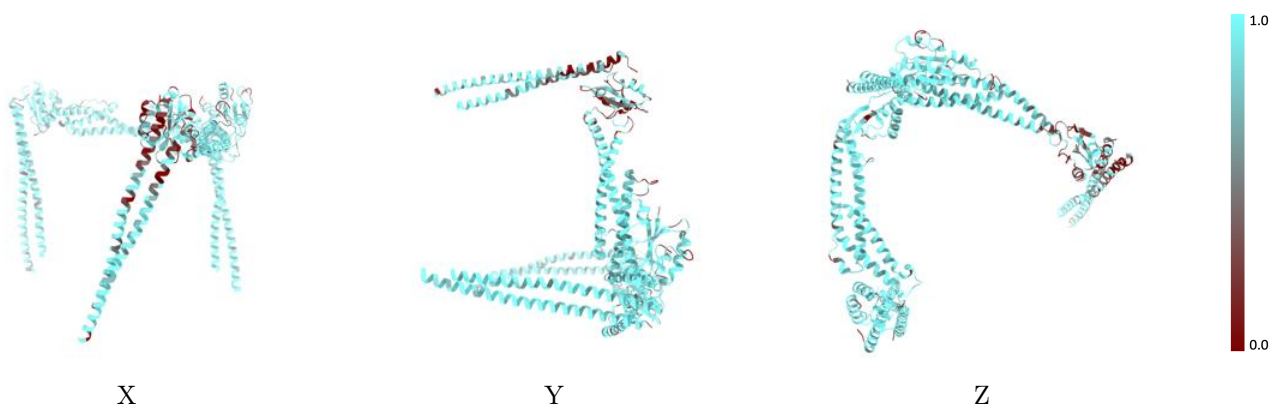
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



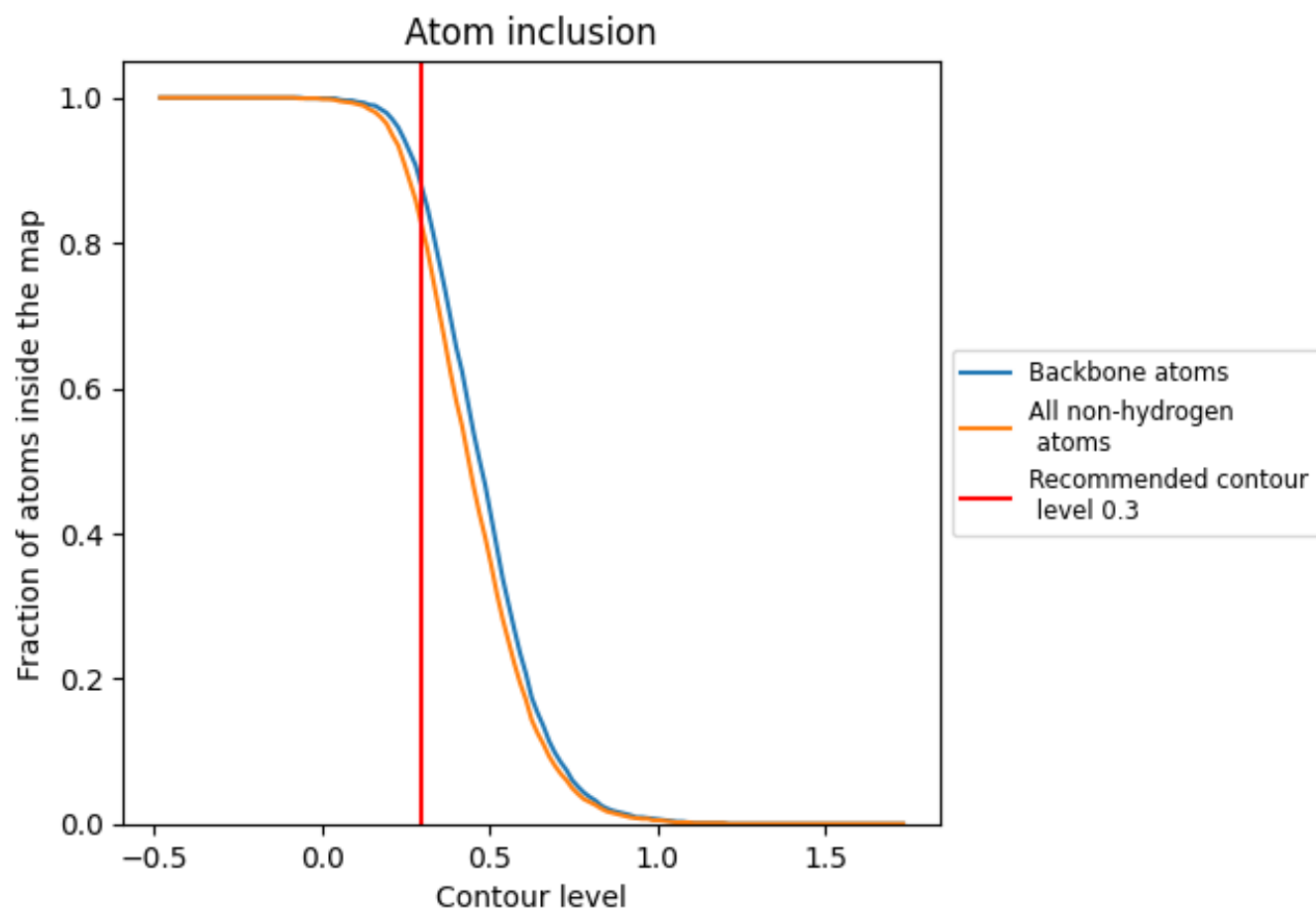
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 87% of all backbone atoms, 82% 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	0.8210	0.2510
G	0.7590	0.2510
I	0.8870	0.2540
J	0.9440	0.2670
K	0.6430	0.1560
M	0.8740	0.2250
N	0.9160	0.2460
O	0.7170	0.1590
a	0.8830	0.2920

1.0

0.0

<0.0