



Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 10:10 AM JST

PDB ID : 9K8L / pdb_00009k8l
EMDB ID : EMD-62177
Title : Cryo-EM structure of C3 symmetric interface of designed zinc-induced tetrahedron Cage-t32-Zn1-HEHE-36
Authors : Qu, Y.N.; Cao, L.X.
Deposited on : 2024-10-24
Resolution : 3.21 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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

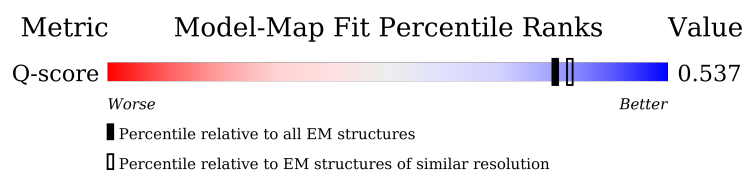
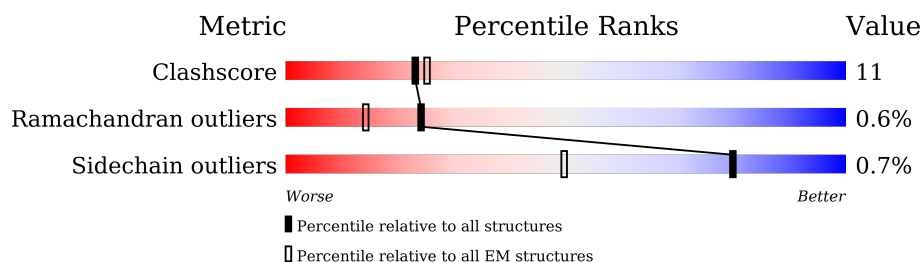
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.21 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14613 (2.71 - 3.71)

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	270	
1	B	270	
1	C	270	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1374 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 Cage-t32-Zn1-HEHE-36.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	55	Total	C	N	O	0	0
			457	279	87	91		
1	B	55	Total	C	N	O	0	0
			457	279	87	91		
1	C	55	Total	C	N	O	0	0
			457	279	87	91		

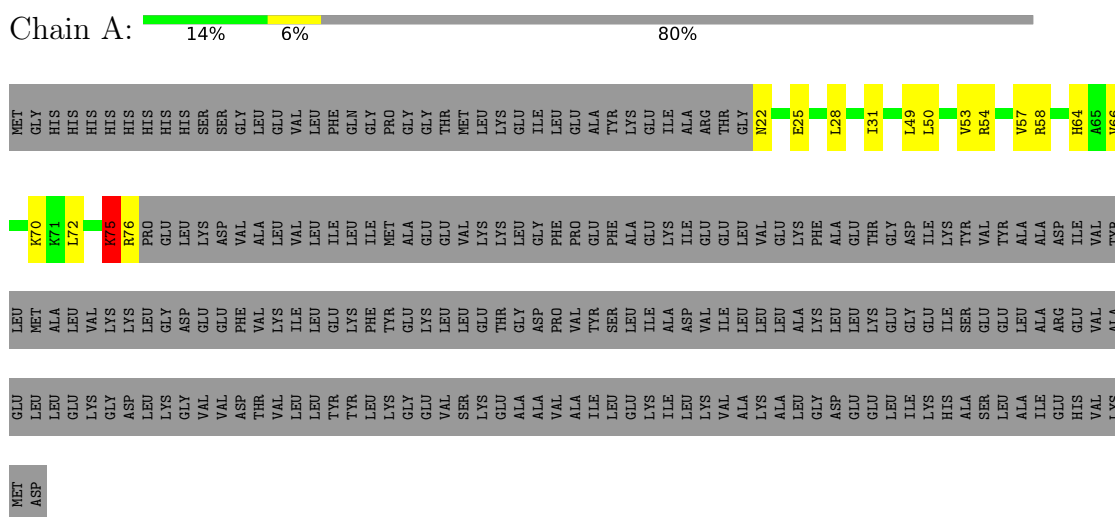
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	B	2	Total	Zn	0
			2	2	
2	C	1	Total	Zn	0
			1	1	

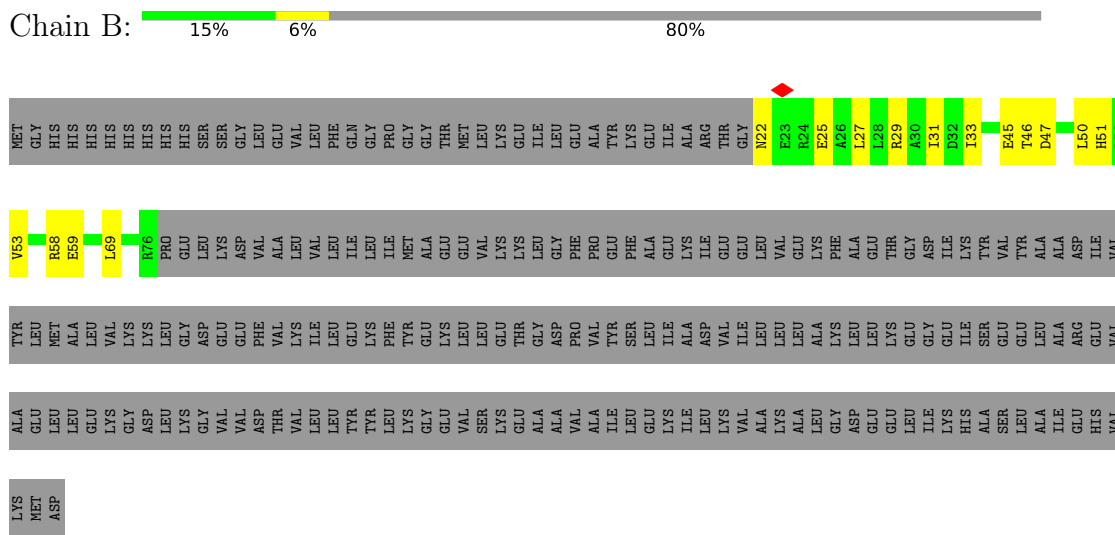
3 Residue-property plots

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: Cage-t32-Zn1-HEHE-36



- Molecule 1: Cage-t32-Zn1-HEHE-36



- Molecule 1: Cage-t32-Zn1-HEHE-36

HIS	ILE	LYS	R54	MET
ALA	SER	TYR	E57	GLY
SER	GLU	VAL	V57	HIS
LEU	GLU	TYR	R58	HIS
ALA	LEU	ALA	E59	HIS
ILE	ALA	ALA	L62	HIS
GLU	ARG	ASP	E63	HIS
HIS	GLU	ILE	E67	HIS
VAL	VAL	VAL	D68	HIS
LYS	ALA	TYR	L69	SER
MET	GLU	LEU	L72	GLY
ASP	LEU	MET	R75	SER
	LEU	ALA	K76	GLY
	GLU	LEU	P80	LEU
	GLY	GLY	GLU	PHE
	VAL	ASP	LEU	GLN
	VAL	GLU	LYS	GLY
	VAL	GLU	ASP	PRO
	ASP	PHE	VAL	GLY
	THR	VAL	ALA	THR
	VAL	LYS	LEU	MET
	LEU	ILE	VAL	LEU
	LEU	GLU	ILE	LYS
	TYR	LYS	LEU	GLU
	LEU	PHE	ILE	ILE
	LYS	TYR	MET	LEU
	GLY	GLU	ALA	GLU
	GLU	LYS	GLU	ALA
	VAL	LEU	VAL	TYR
	SER	LEU	VAL	LYS
	GLU	THR	LYS	GLU
	ALA	GLY	LEU	ILE
	ALA	ASP	LEU	ALA
	VAL	PRO	PHE	ARG
	VAL	VAL	GLY	THR
	ILE	TYR	PHO	GLY
	LEU	SER	PHE	N22
	GLU	LEU	ALA	E25
	ILE	ILE	GLU	I26
	ILE	ALA	LYS	L27
	LEU	ASP	ILE	A30
	LYS	VAL	GLU	I31
	VAL	ILE	GLU	D32
	ALA	LEU	LEU	I33
	LYS	LEU	VAL	V34
	ALA	LEU	GLU	R35
	GLY	LYS	LYS	D36
	ASP	LEU	PHE	E40
	GLU	LEU	ALA	E41
	GLU	LYS	THR	L49
	LEU	GLU	GLY	L50
	ILE	ILE	ASP	E53
	LYS	GLU	ILE	V53

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	341867	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.449	Depositor
Minimum map value	-5.274	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.158	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	258.552, 258.552, 258.552	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0773, 1.0773, 1.0773	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.45	1/459 (0.2%)	0.56	0/613
1	B	0.14	0/459	0.39	0/613
1	C	0.24	0/459	0.51	0/613
All	All	0.31	1/1377 (0.1%)	0.49	0/1839

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	LYS	CA-C	-5.29	1.45	1.52

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	A	457	0	463	10	0
1	B	457	0	463	7	0
1	C	457	0	463	14	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
All	All	1374	0	1389	30	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 11.

All (30) 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:A:28:LEU:HD21	1:A:58:ARG:HG3	1.74	0.69
1:B:53:VAL:HG21	1:B:69:LEU:HD13	1.78	0.65
1:B:58:ARG:NH2	1:B:59:GLU:OE2	2.38	0.56
1:B:22:ASN:OD1	1:B:25:GLU:N	2.35	0.54
1:A:54:ARG:HH11	1:A:58:ARG:HH21	1.56	0.53
1:A:64:HIS:ND1	1:C:36:ASP:OD1	2.35	0.52
1:B:46:THR:O	1:B:50:LEU:HD12	2.11	0.51
1:A:54:ARG:NH1	1:A:58:ARG:HH21	2.10	0.50
1:B:29:ARG:O	1:B:33:ILE:HG13	2.13	0.48
1:A:31:ILE:HG23	1:A:50:LEU:HD23	1.96	0.48
1:C:57:VAL:HG13	1:C:62:LEU:HD21	1.95	0.48
1:C:31:ILE:HG23	1:C:50:LEU:HD23	1.96	0.47
1:C:53:VAL:HG21	1:C:69:LEU:HD13	1.97	0.46
1:C:49:LEU:HD13	1:C:72:LEU:HD22	1.97	0.46
1:A:66:VAL:O	1:A:70:LYS:HB2	2.15	0.46
1:C:27:LEU:O	1:C:31:ILE:HD12	2.15	0.46
1:C:32:ASP:OD1	1:C:35:ARG:NH2	2.50	0.45
1:C:63:GLU:O	1:C:67:GLU:HG2	2.17	0.45
1:B:27:LEU:O	1:B:31:ILE:HG13	2.17	0.44
1:A:22:ASN:HB3	1:A:25:GLU:HG3	2.00	0.44
1:C:59:GLU:HA	1:C:59:GLU:OE1	2.17	0.44
1:C:75:LYS:HG2	1:C:76:ARG:HG3	1.99	0.44
1:B:47:ASP:O	1:B:51:HIS:HD2	2.02	0.43
1:A:53:VAL:O	1:A:57:VAL:HG23	2.19	0.42
1:C:22:ASN:OD1	1:C:25:GLU:HG2	2.19	0.42
1:A:49:LEU:HD13	1:A:72:LEU:HD22	2.02	0.42
1:C:35:ARG:HG3	1:C:50:LEU:HB2	2.02	0.42
1:C:54:ARG:HH11	1:C:58:ARG:HH21	1.68	0.41
1:C:30:ALA:O	1:C:34:VAL:HG12	2.21	0.41
1:A:75:LYS:HB2	1:A:76:ARG:H	1.77	0.40

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	A	53/270 (20%)	51 (96%)	1 (2%)	1 (2%)	6	32
1	B	53/270 (20%)	52 (98%)	1 (2%)	0	100	100
1	C	53/270 (20%)	53 (100%)	0	0	100	100
All	All	159/810 (20%)	156 (98%)	2 (1%)	1 (1%)	24	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	LYS

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	50/230 (22%)	50 (100%)	0	100	100
1	B	50/230 (22%)	49 (98%)	1 (2%)	50	73
1	C	50/230 (22%)	50 (100%)	0	100	100
All	All	150/690 (22%)	149 (99%)	1 (1%)	80	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	51	HIS
1	C	51	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

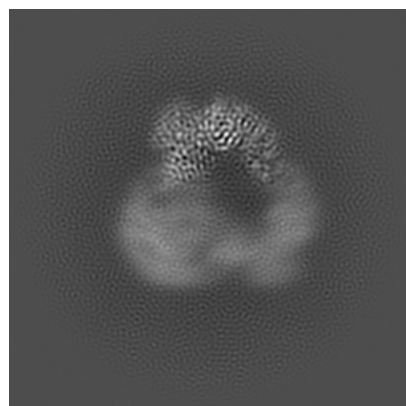
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62177. These allow visual inspection of the internal detail of the map and identification of artifacts.

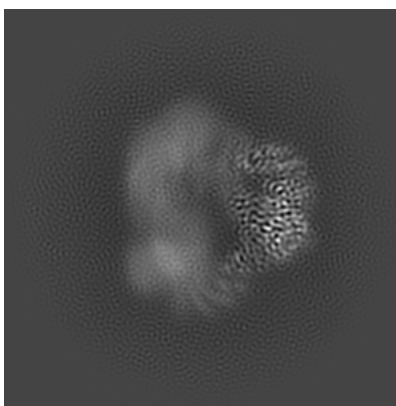
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

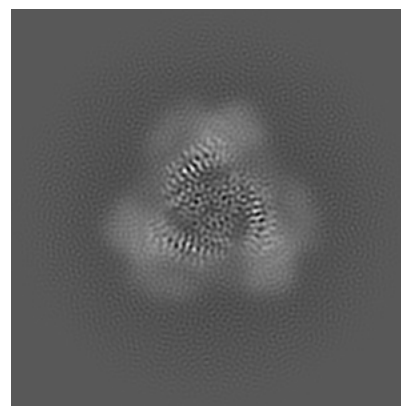
6.1.1 Primary map



X

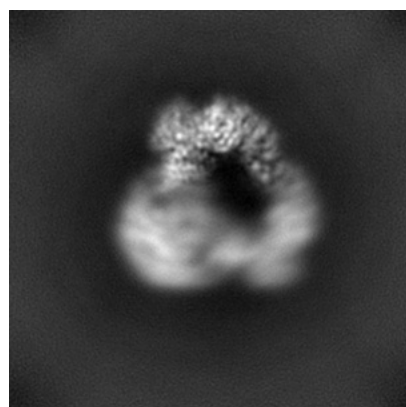


Y

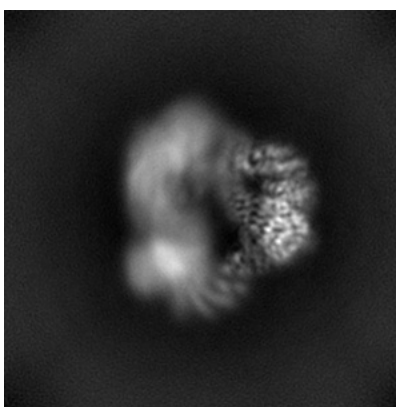


Z

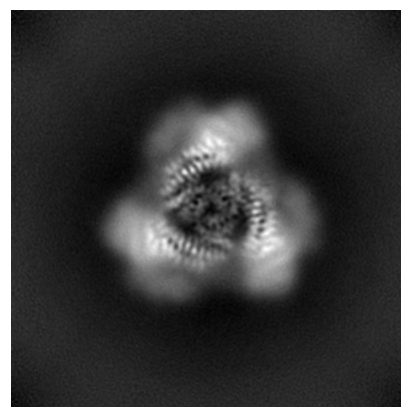
6.1.2 Raw map



X



Y

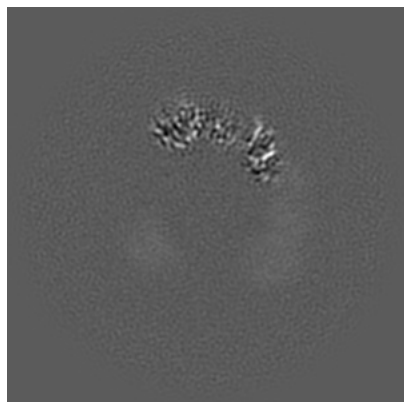


Z

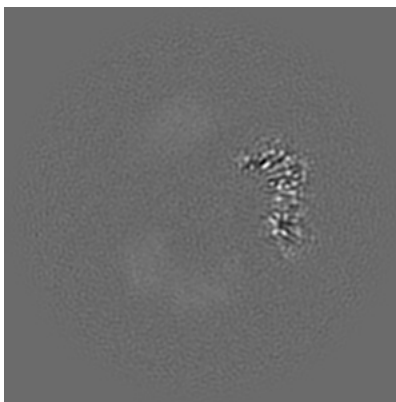
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

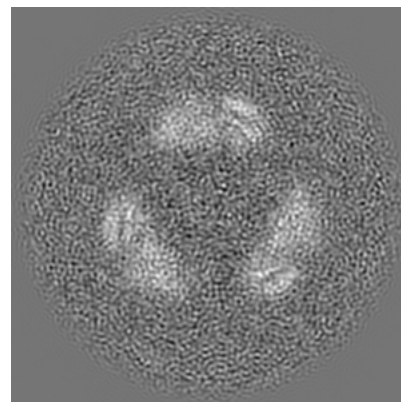
6.2.1 Primary map



X Index: 120

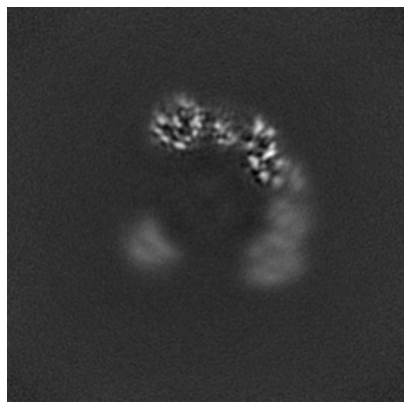


Y Index: 120

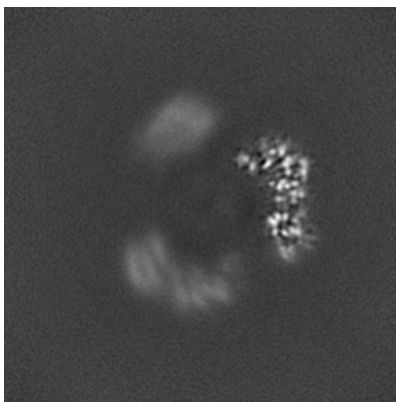


Z Index: 120

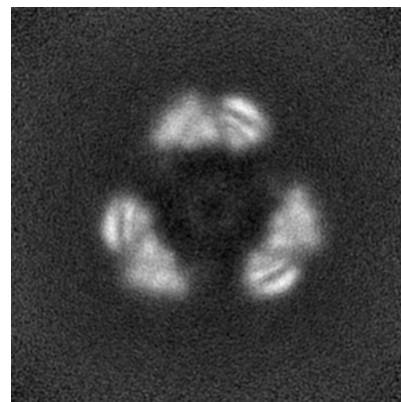
6.2.2 Raw map



X Index: 120



Y Index: 120

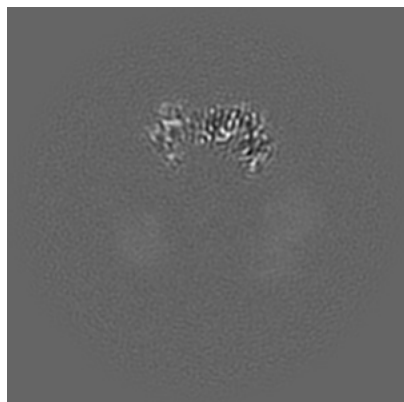


Z Index: 120

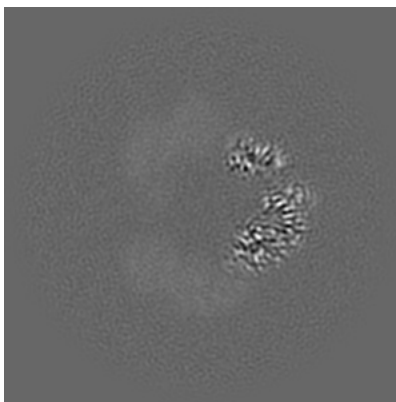
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

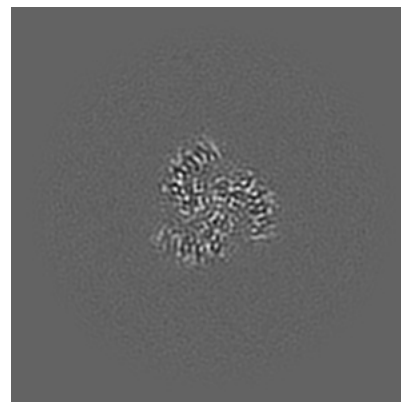
6.3.1 Primary map



X Index: 110

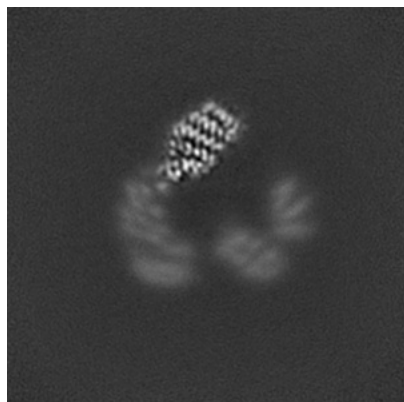


Y Index: 101

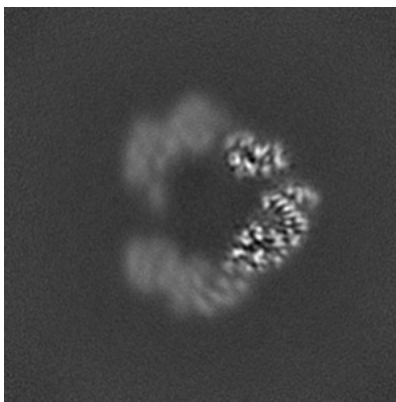


Z Index: 164

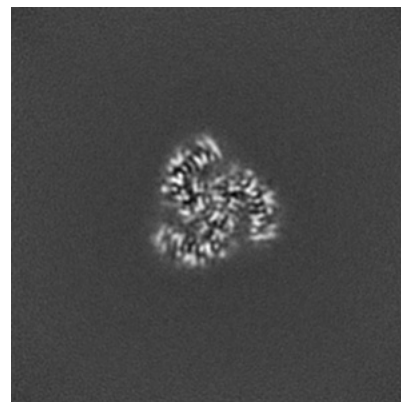
6.3.2 Raw map



X Index: 146



Y Index: 101

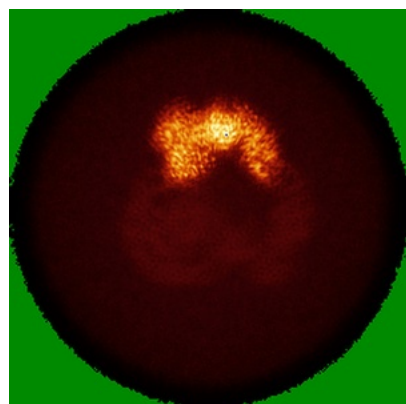


Z Index: 164

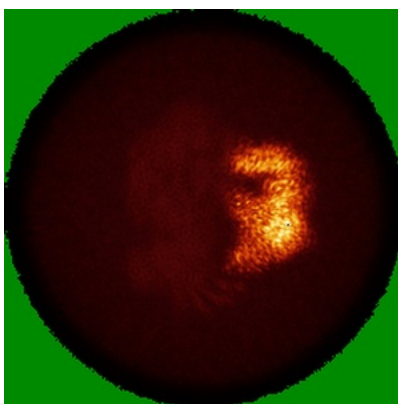
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

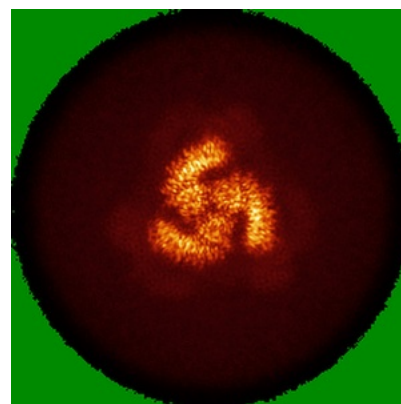
6.4.1 Primary map



X

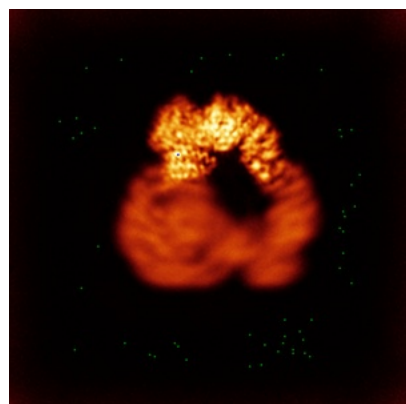


Y

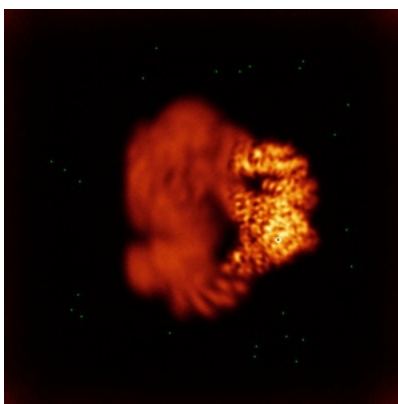


Z

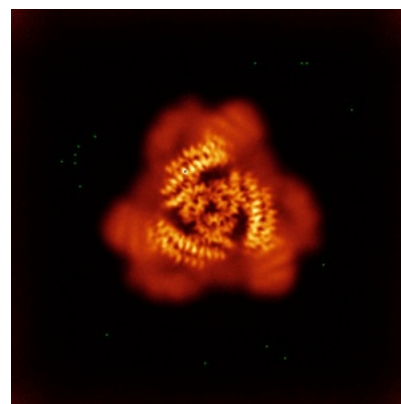
6.4.2 Raw map



X



Y

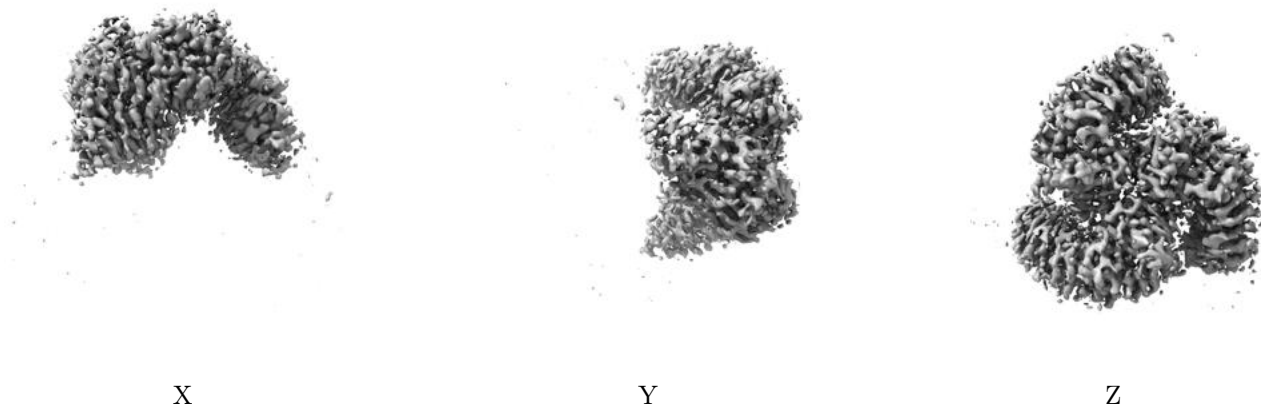


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

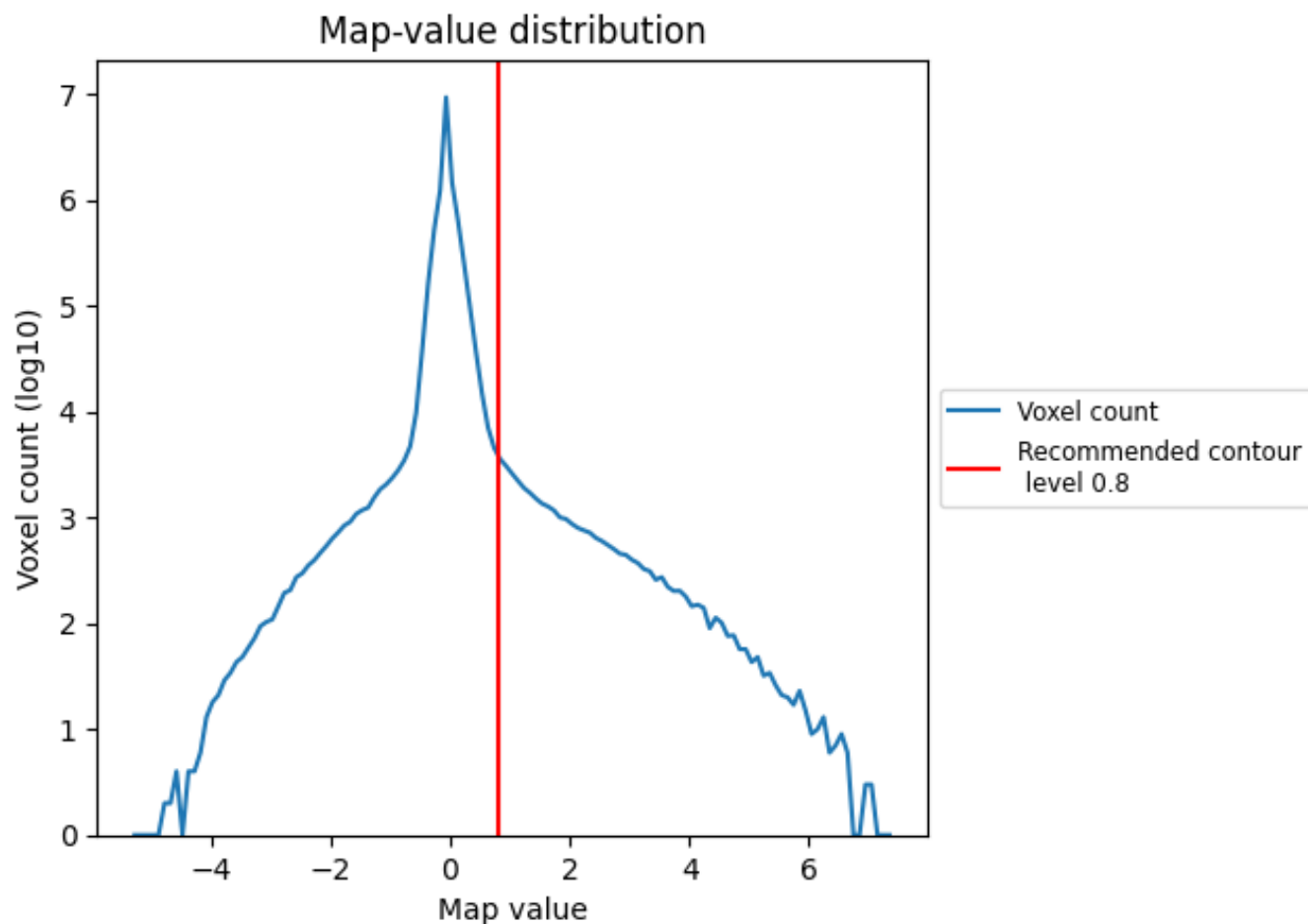
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

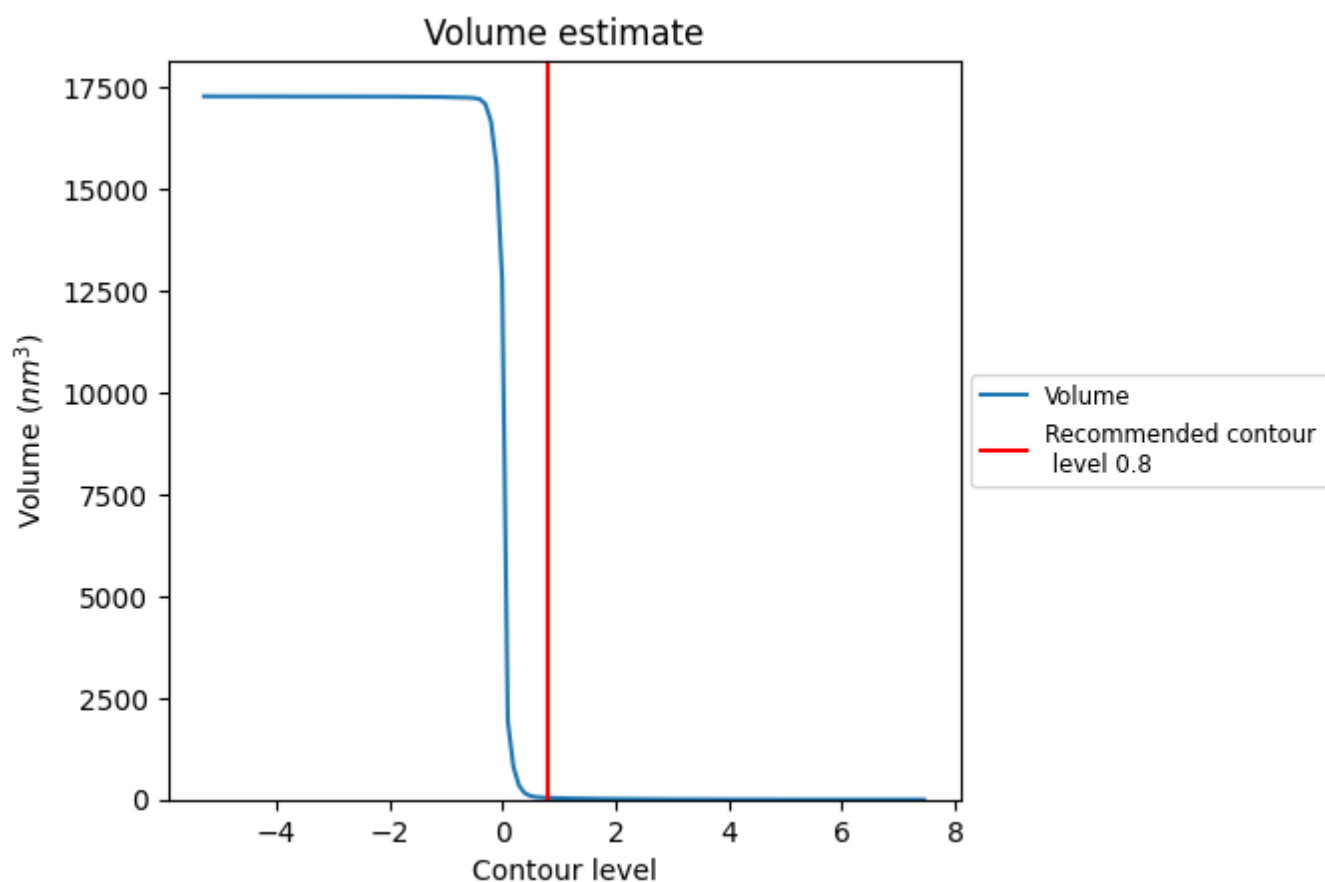
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

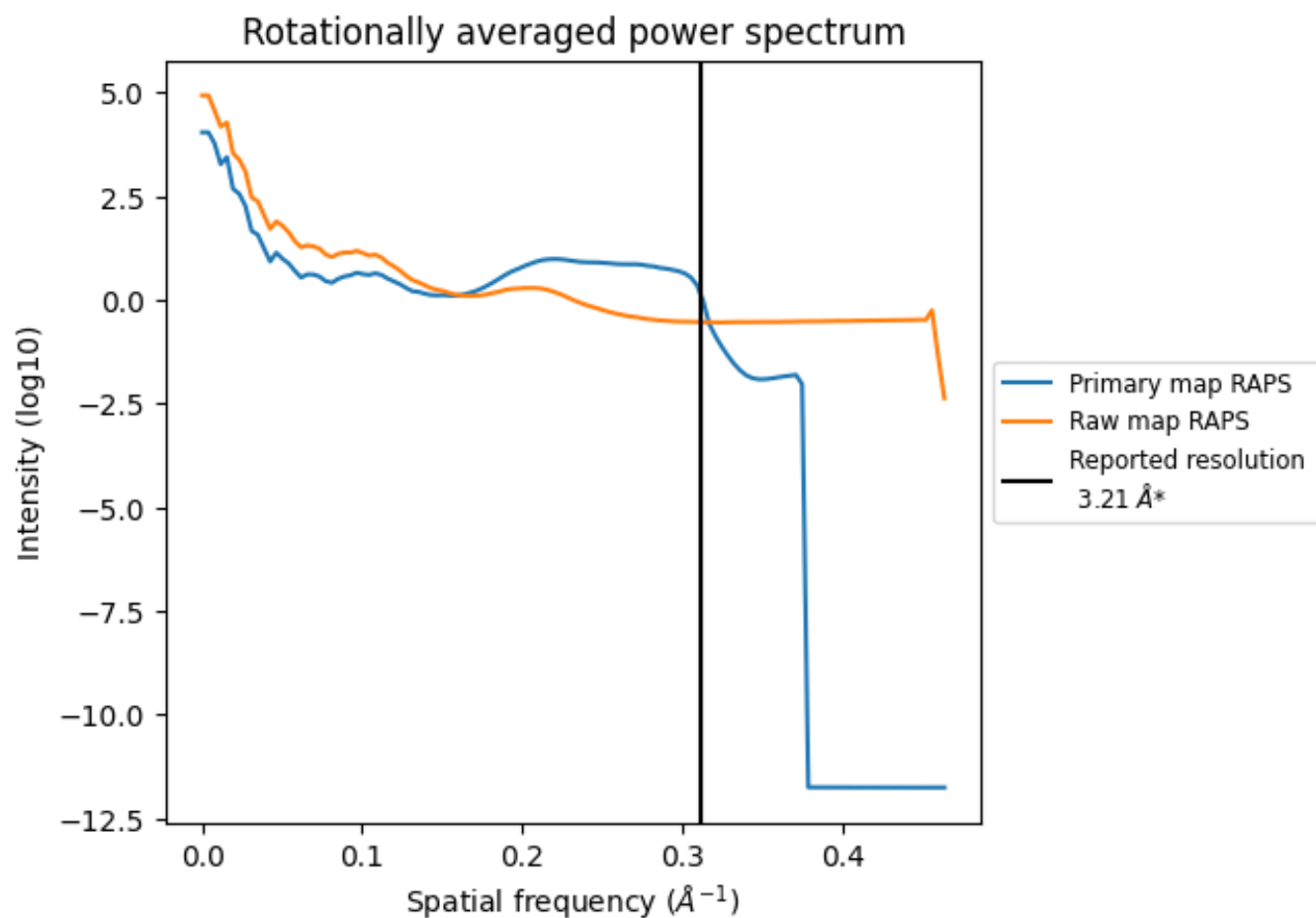
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 43 nm³; this corresponds to an approximate mass of 39 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 ⓘ

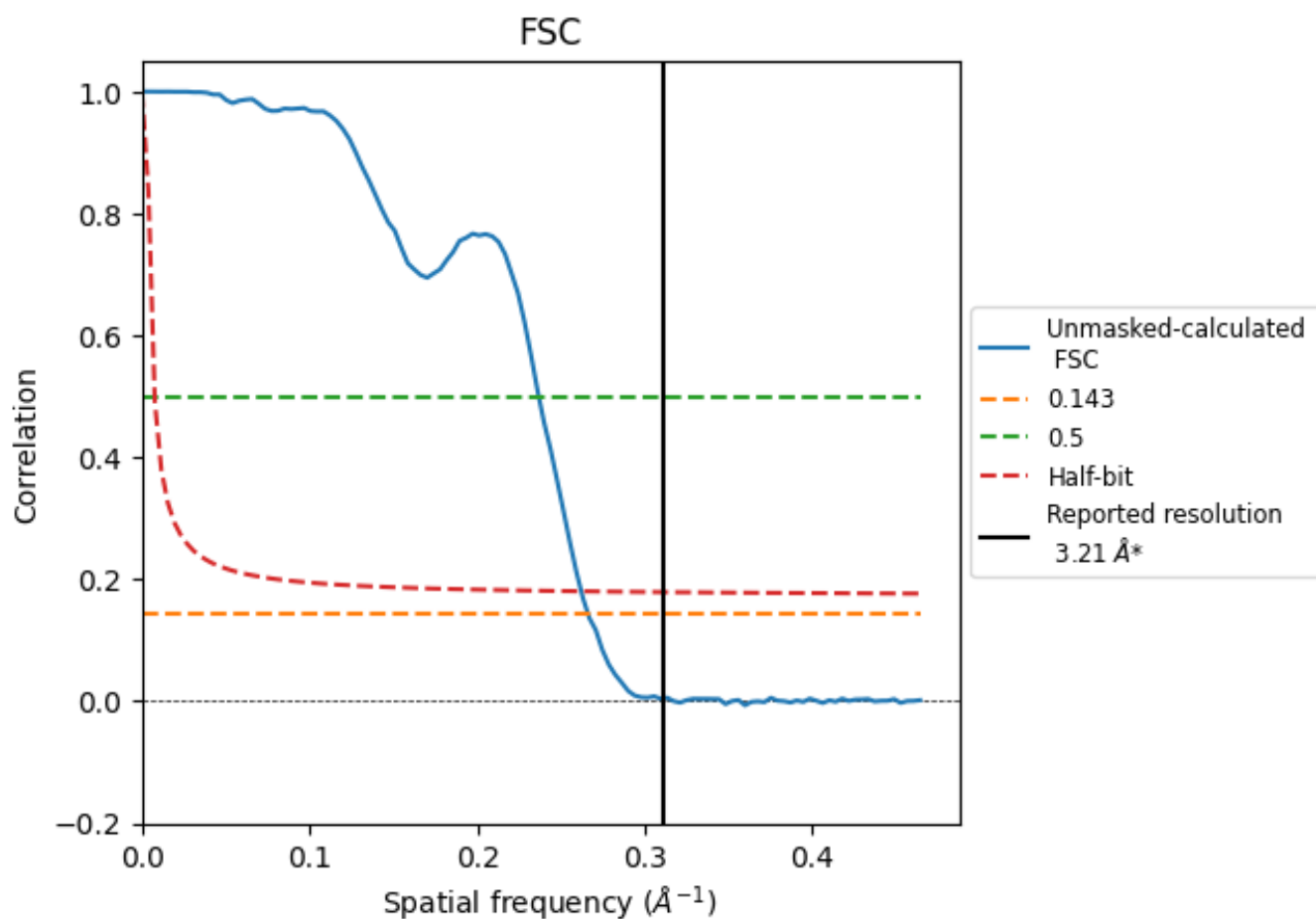


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

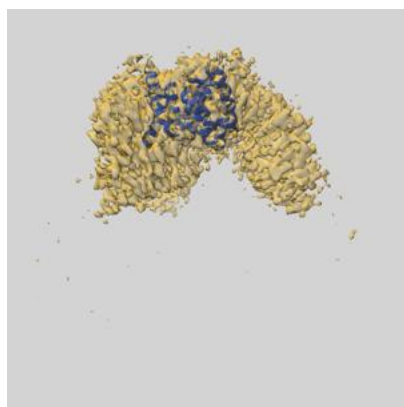
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.76	4.22	3.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 3.21 by more than 10 %

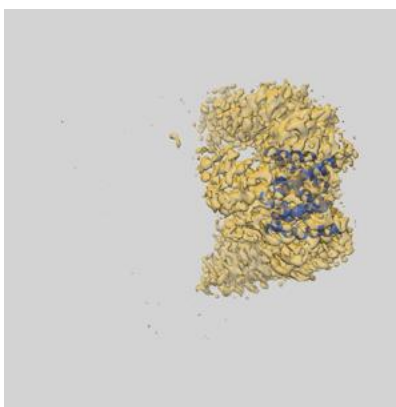
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62177 and PDB model 9K8L. Per-residue inclusion information can be found in section [3](#) on page [4](#).

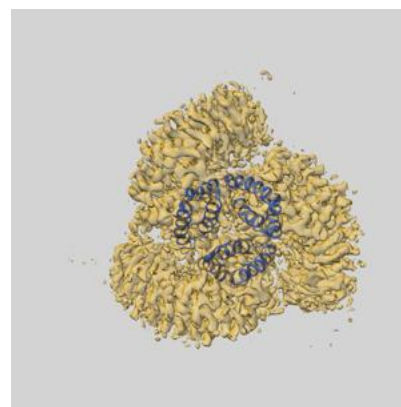
9.1 Map-model overlay [i](#)



X



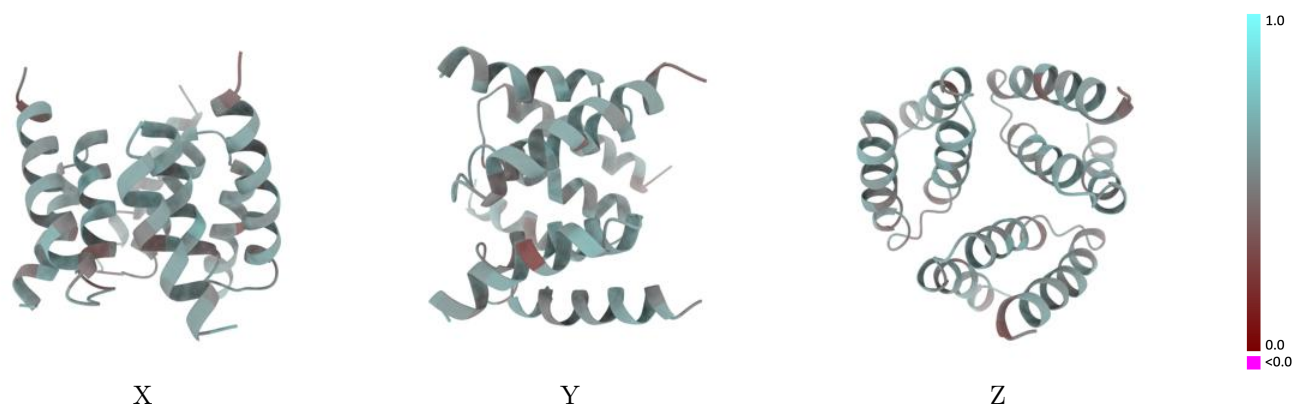
Y



Z

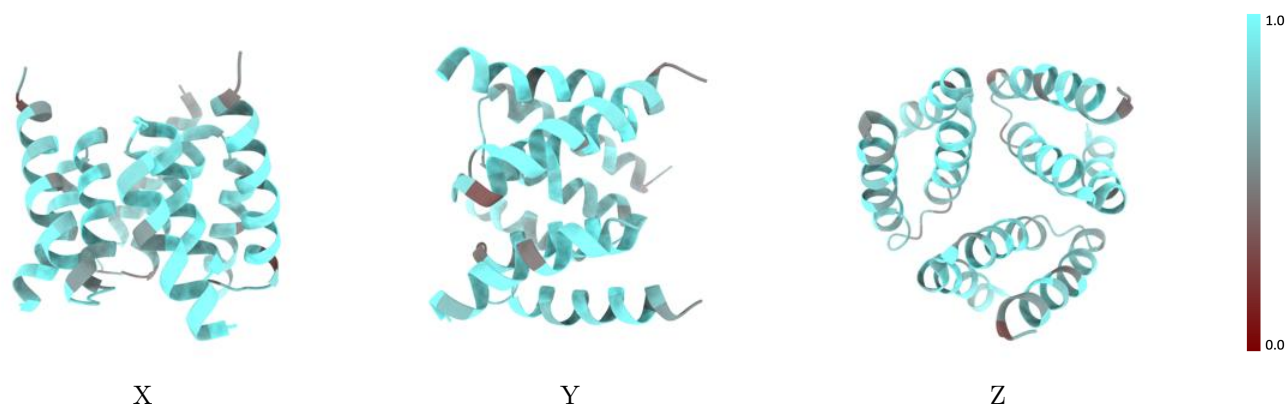
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



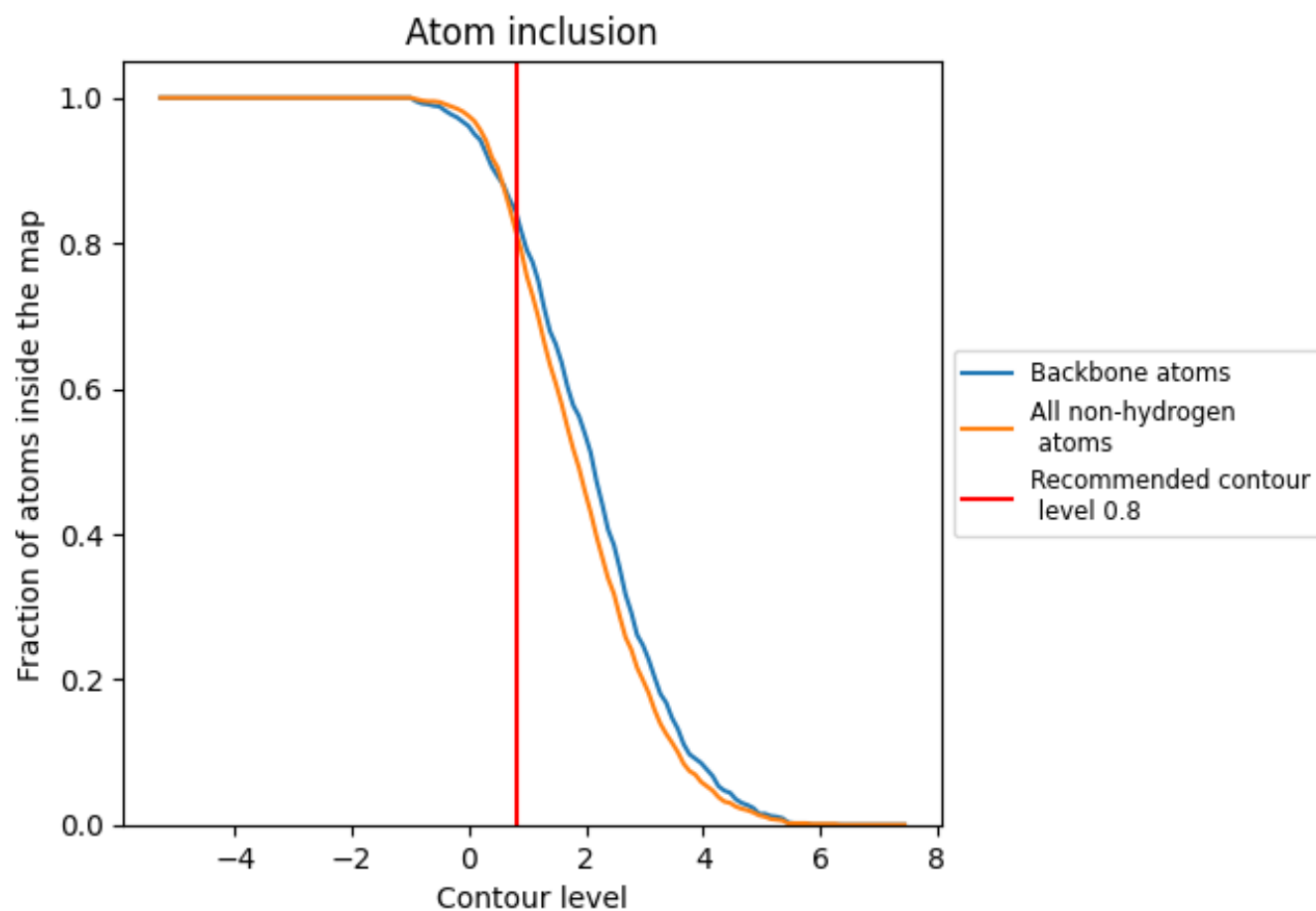
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8170	<div><div></div></div> 0.5370
A	<div><div></div></div> 0.8170	<div><div></div></div> 0.5360
B	<div><div></div></div> 0.8110	<div><div></div></div> 0.5310
C	<div><div></div></div> 0.8240	<div><div></div></div> 0.5430

