



wwPDB EM Validation Summary Report ⓘ

Dec 7, 2024 – 06:29 am GMT

PDB ID : 9G40
EMDB ID : EMD-51020
Title : Structure of the Position 7 CMG-decorated gamma-Tubulin Ring Complex from Pig Brain
Authors : Munoz-Hernandez, H.; Krutyholowa, R.; Wieczorek, M.
Deposited on : 2024-07-12
Resolution : 4.30 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

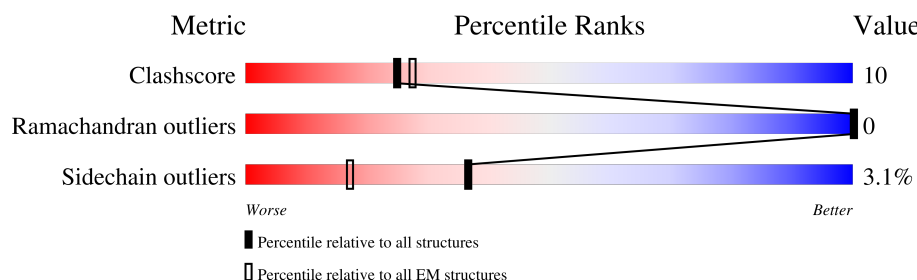
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	F	910	<div> <div>11%</div> <div>52%</div> <div>15%</div> <div>32%</div> </div>
2	G	905	<div> <div>7%</div> <div>63%</div> <div>24%</div> <div>12%</div> </div>
3	X	155	<div> <div>21%</div> <div>7%</div> <div>71%</div> </div>
4	u	1893	<div> <div>98%</div> </div>
4	v	1893	<div> <div>98%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24900 atoms, of which 12457 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 Gamma-tubulin complex component 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	F	617	Total	C	H	N	O	S	0	0
			10098	3221	5034	905	913	25		

- Molecule 2 is a protein called Gamma-tubulin complex component.

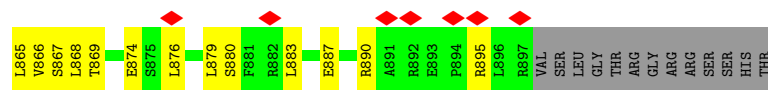
Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	797	Total	C	H	N	O	S	0	0
			12901	4108	6467	1096	1196	34		

- Molecule 3 is a protein called Mitotic-spindle organizing protein 2A isoform X4.

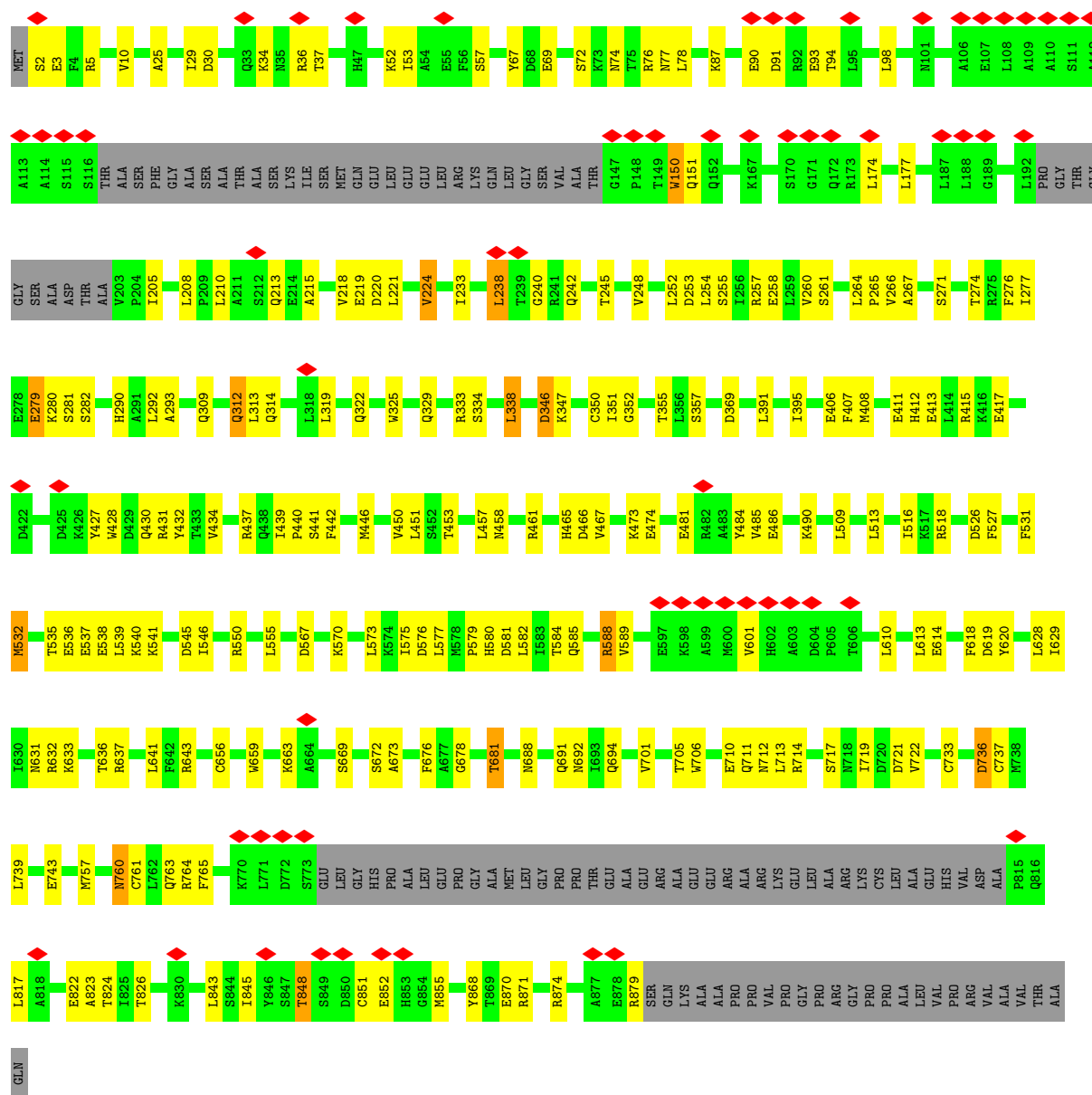
Mol	Chain	Residues	Atoms						AltConf	Trace
3	X	45	Total	C	H	N	O	S	0	0
			679	217	346	51	62	3		

- Molecule 4 is a protein called CDK5 regulatory subunit-associated protein 2.

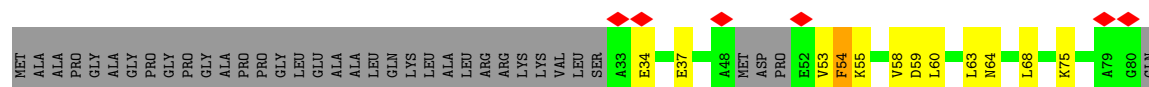
Mol	Chain	Residues	Atoms						AltConf	Trace
4	u	34	Total	C	H	N	O	S	0	0
			611	193	305	54	57	2		
4	v	34	Total	C	H	N	O	S	0	0
			611	193	305	54	57	2		



• Molecule 2: Gamma-tubulin complex component



• Molecule 3: Mitotic-spindle organizing protein 2A isoform X4



[illegible]

- Molecule 4: CDK5 regulatory subunit-associated protein 2

Chain u:

MET	MET	ASP	LEU	VAL	LEU	GLU	GLU	ASP	VAL	THR	VAL	PRO	GLY	THR	LEU	SER	GLY	CYS	SER	GLY	VAL	PRO	SER	VAL	PRO	ASP	ASP	LEU	ASP	GLY	ILE	ASN	PRO	ASN	ALA	GLY	LEU	GLY	ASN	VAL	SER	PRO	THR	ARG	R58	R59
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GLU	ASP	ALA	ALA	ARG	LYS	LYS	VAL	GLN	GLN	VAL	GLU	ASP	LEU	LEU	THR	LYS	ARG	ILE	LEU	LEU	LEU	GLU	LYS	ASP	VAL	THR	ALA	ALA	GLN	GLU	GLU	GLU	LYS	GLU	THR	GLY	GLY	THR	GLU	THR	GLU	GLU	GLU	LYS	ALA	ALA	LEU	LEU	ARG	ARG	LEU	LEU	SER	GLU	MET	LYS	LYS	LYS	LYS	MET	HIS
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GLU GLY ASP ASP LEU LEU ALA ALA MET MET ALA ALA LEU LEU VAL VAL LEU LEU LEU LEU ASP ASP GLU GLU LYS LYS ARG ARG ASP ASP LEU LEU ILE ILE LEU LEU GLU GLU GLU GLU LYS LYS SER SER LYS LYS GLU GLU ALA ALA LEU LEU ILE ILE GLN GLN CYS CYS LEU LEU LEU LEU LYS LYS GLU GLU GLU GLU LYS LYS SER SER SER SER MET MET ALA ALA CYS CYS PRO PRO ASP ASP GLU GLU ASN ASN VAL VAL SER SER SER SER GLY GLY GLU GLU LEU LEU ARG ARG GLY GLY LEU LEU CYS CYS CYS CYS ALA ALA ALA ALA PRO PRO

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

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

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

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

[illegible]

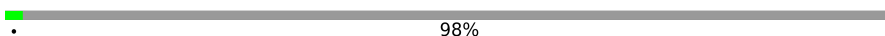
GLY TYR LEU LEU ARG HIS THR GLU LYS ILE SER ASP CYS ASP GLY ALA ALA PRO GLY CYS LEU LEU GLU GLY GLY ALA ALA PHE ASN ASN ASN THR LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU VAL VAL ARG GLU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU

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

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

- Molecule 4: CDK5 regulatory subunit-associated protein 2

Chain v: [illegible]





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93207	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.034	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0075	Depositor
Map size (\AA)	452.2656, 452.2656, 452.2656	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.41333, 1.41333, 1.41333	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	F	0.24	0/5174	0.48	0/6990
2	G	0.25	0/6562	0.46	0/8869
3	X	0.24	0/335	0.36	0/449
4	u	0.24	0/309	0.47	0/408
4	v	0.25	0/309	0.50	0/408
All	All	0.25	0/12689	0.47	0/17124

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	F	5064	5034	5034	87	0
2	G	6434	6467	6467	155	0
3	X	333	346	346	11	0
4	u	306	305	305	0	0
4	v	306	305	305	0	0
All	All	12443	12457	12457	245	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 10.

The worst 5 of 245 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:F:409:THR:O	1:F:415:ARG:NH1	2.10	0.85
1:F:500:CYS:O	1:F:555:LYS:NZ	2.15	0.80
1:F:866:VAL:O	1:F:869:THR:OG1	1.98	0.80
2:G:461:ARG:NH2	2:G:466:ASP:OD2	2.14	0.80
2:G:442:PHE:O	2:G:484:TYR:OH	1.98	0.79

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	F	611/910 (67%)	587 (96%)	24 (4%)	0	100	100
2	G	789/905 (87%)	742 (94%)	47 (6%)	0	100	100
3	X	41/155 (26%)	40 (98%)	1 (2%)	0	100	100
4	u	32/1893 (2%)	31 (97%)	1 (3%)	0	100	100
4	v	32/1893 (2%)	32 (100%)	0	0	100	100
All	All	1505/5756 (26%)	1432 (95%)	73 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	F	548/783 (70%)	534 (97%)	14 (3%)	41	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	712/790 (90%)	690 (97%)	22 (3%)	35	56
3	X	34/115 (30%)	32 (94%)	2 (6%)	16	39
4	u	34/1704 (2%)	31 (91%)	3 (9%)	8	26
4	v	34/1704 (2%)	33 (97%)	1 (3%)	37	58
All	All	1362/5096 (27%)	1320 (97%)	42 (3%)	37	56

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	656	CYS
2	G	879	ARG
2	G	681	THR
2	G	848	THR
3	X	54	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	694	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 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.

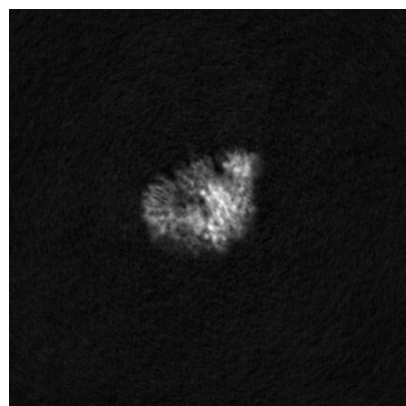
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51020. These allow visual inspection of the internal detail of the map and identification of artifacts.

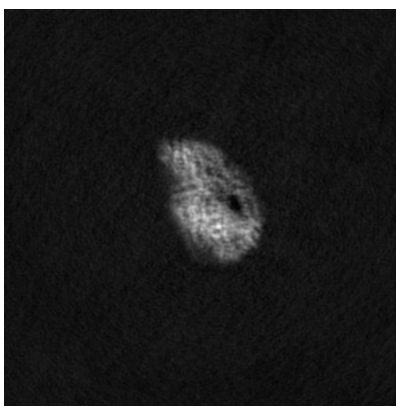
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

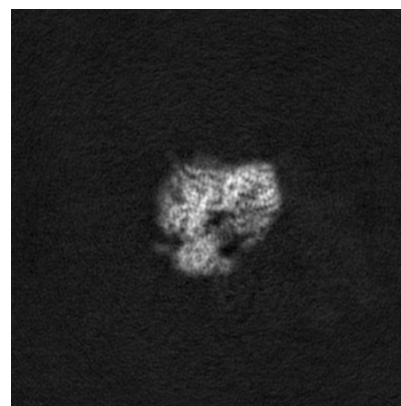
6.1.1 Primary map



X

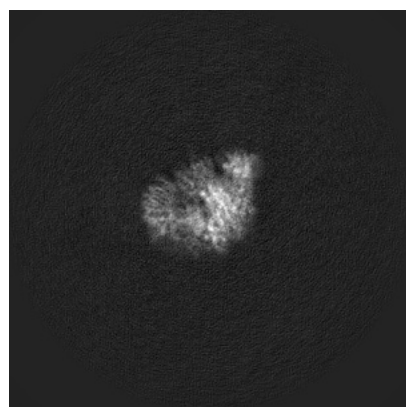


Y

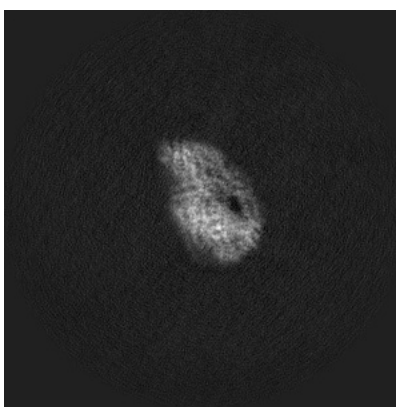


Z

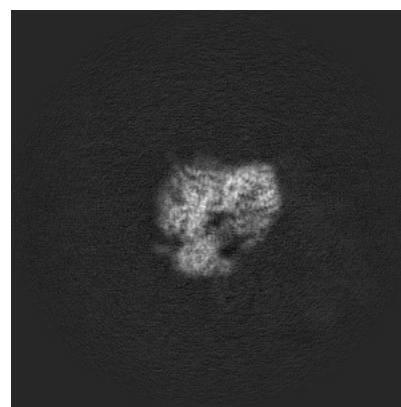
6.1.2 Raw map



X



Y

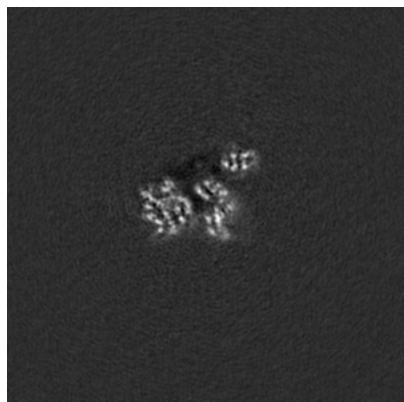


Z

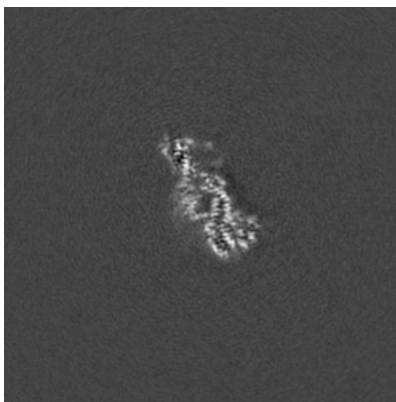
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

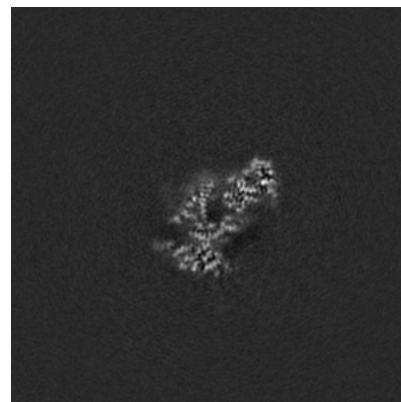
6.2.1 Primary map



X Index: 160

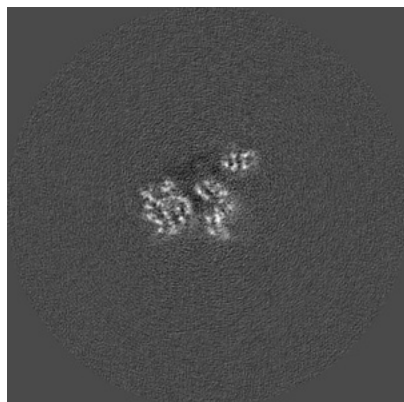


Y Index: 160

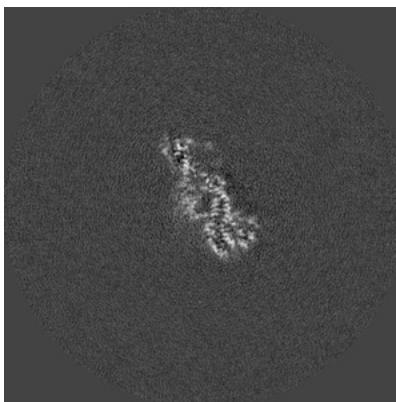


Z Index: 160

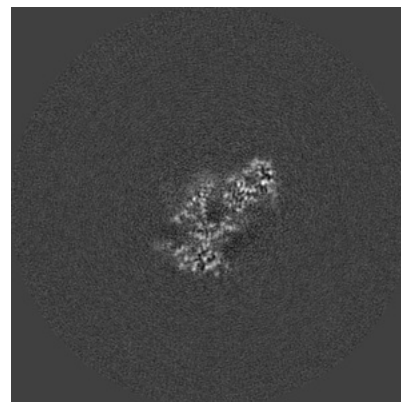
6.2.2 Raw map



X Index: 160



Y Index: 160

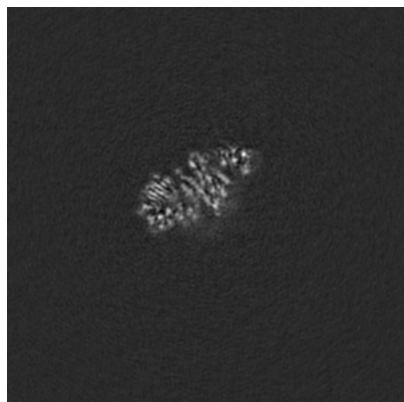


Z Index: 160

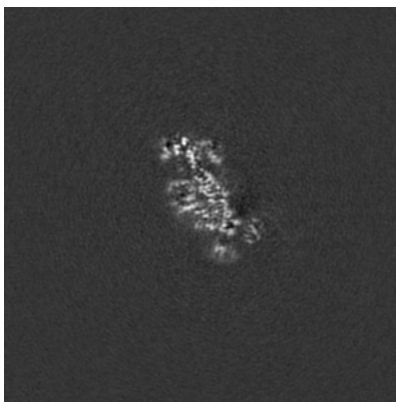
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

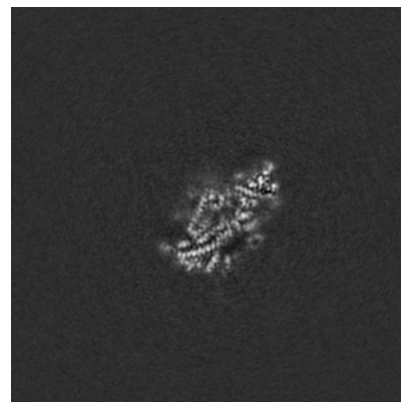
6.3.1 Primary map



X Index: 146

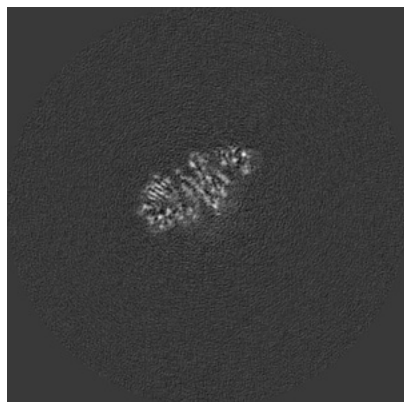


Y Index: 169

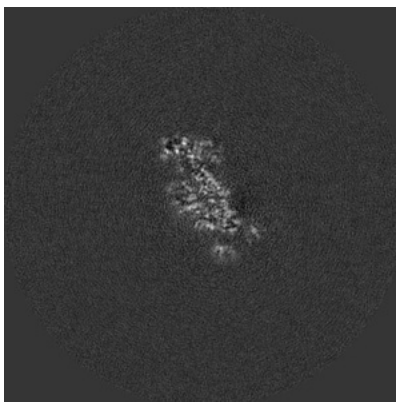


Z Index: 152

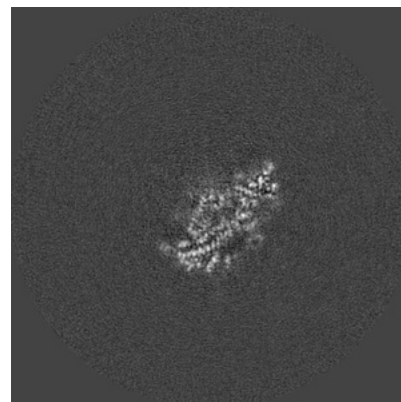
6.3.2 Raw map



X Index: 146



Y Index: 168

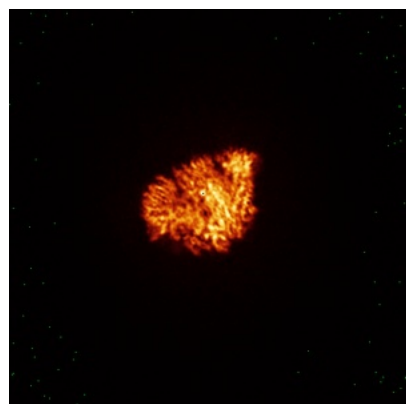


Z Index: 152

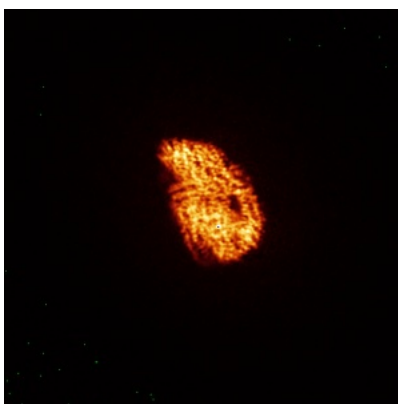
The images above show the largest variance slices of the map in three orthogonal directions.

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

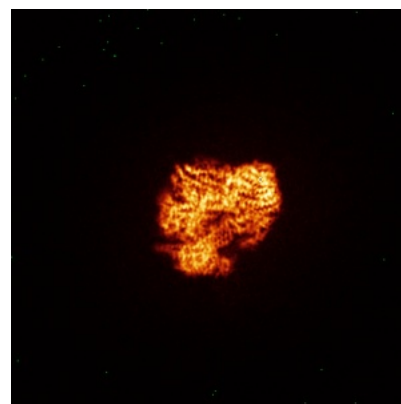
6.4.1 Primary map



X

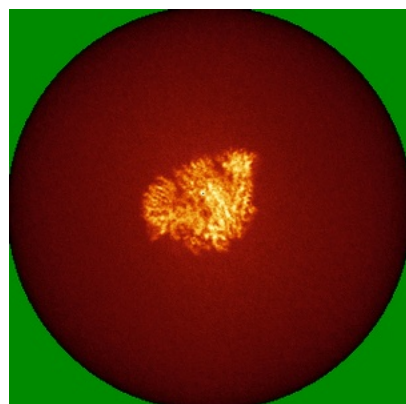


Y

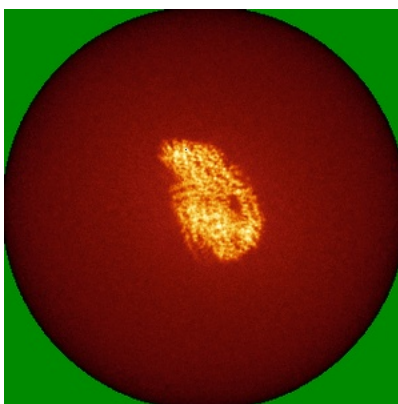


Z

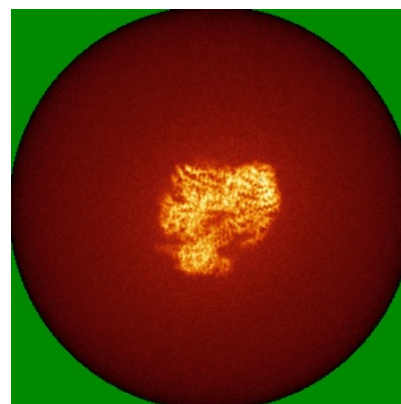
6.4.2 Raw map



X



Y

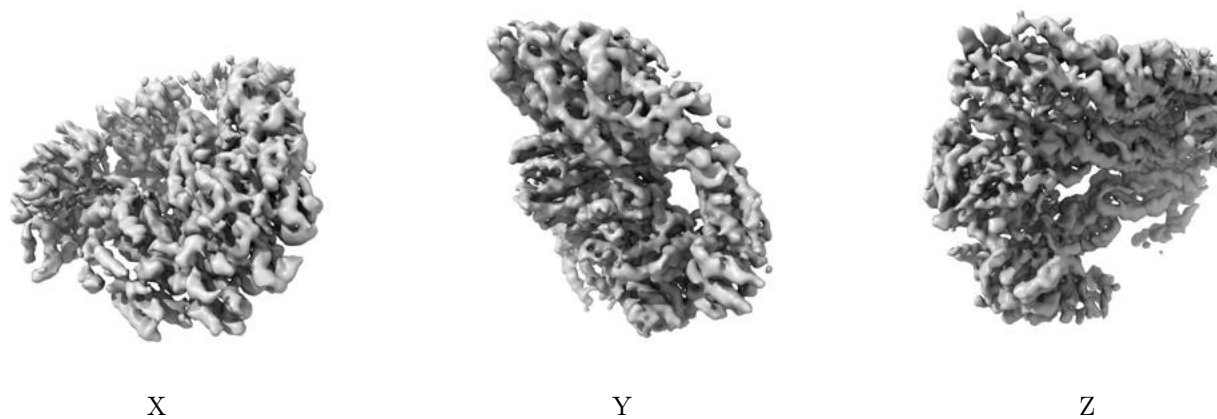


Z

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.

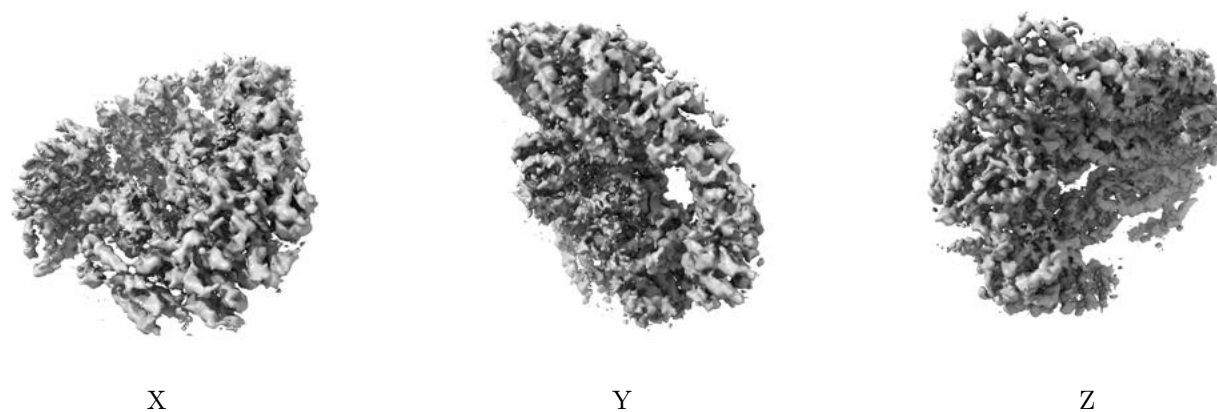
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0075. 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.

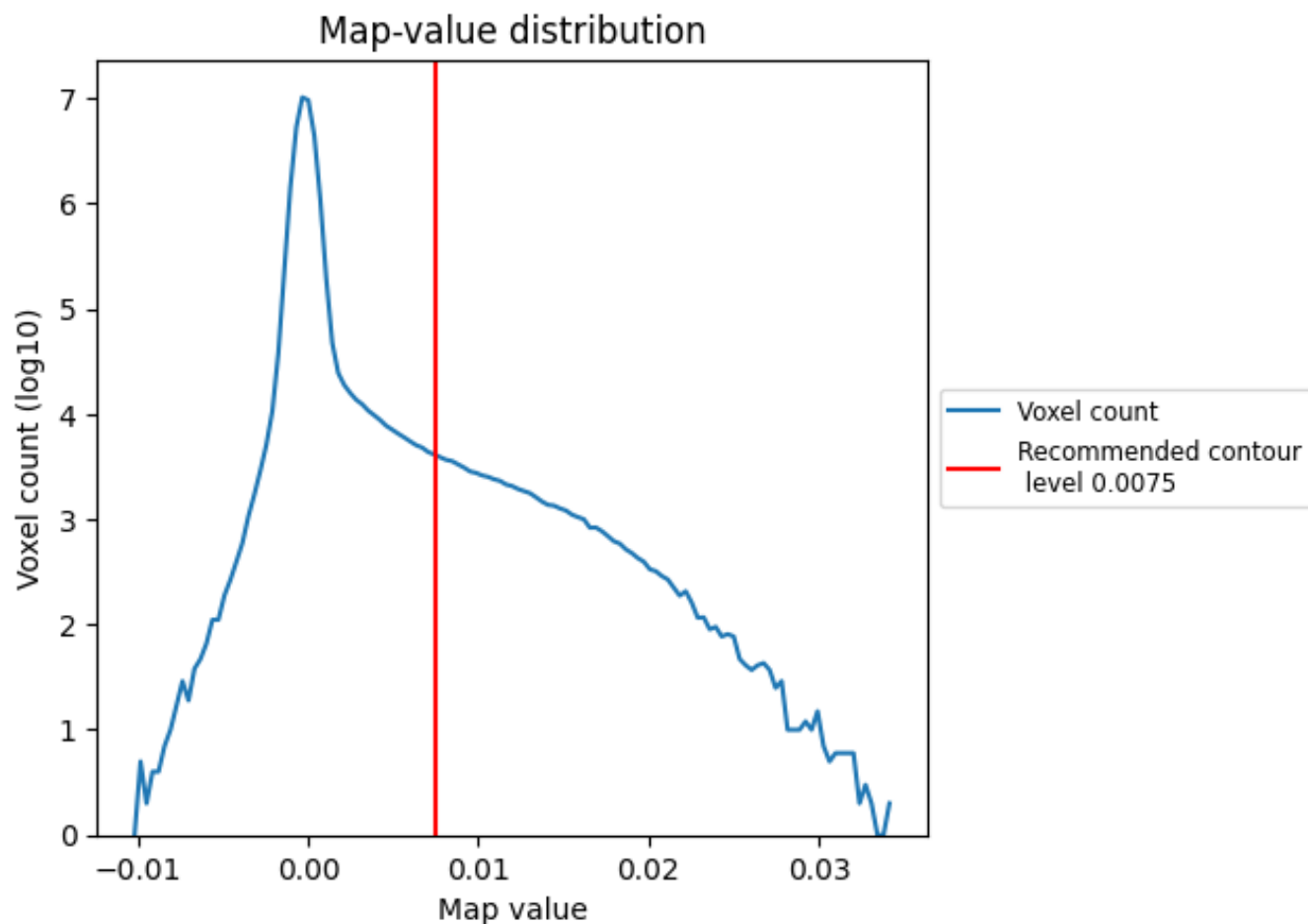
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

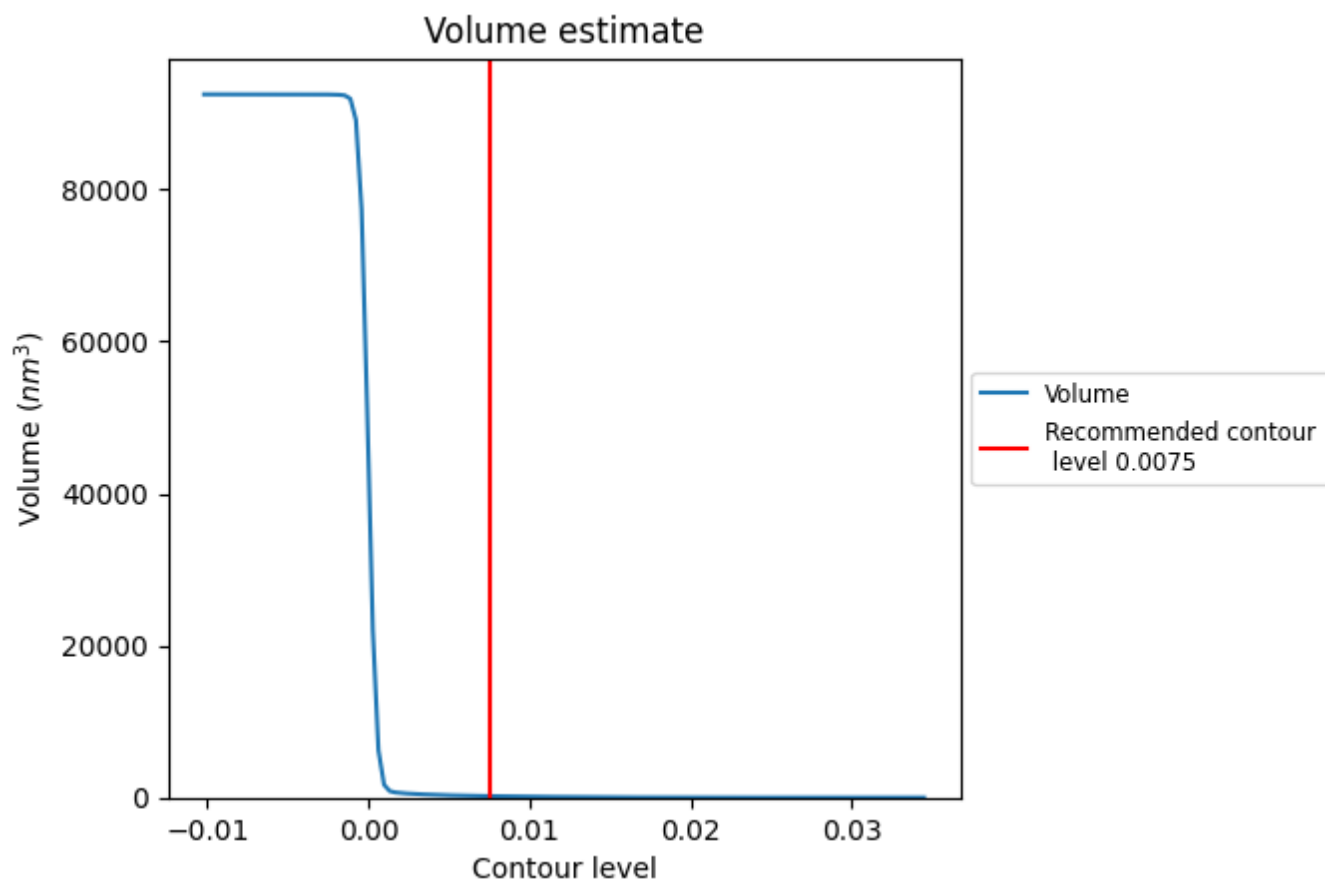
This section contains the results of statistical analysis of the map.

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.

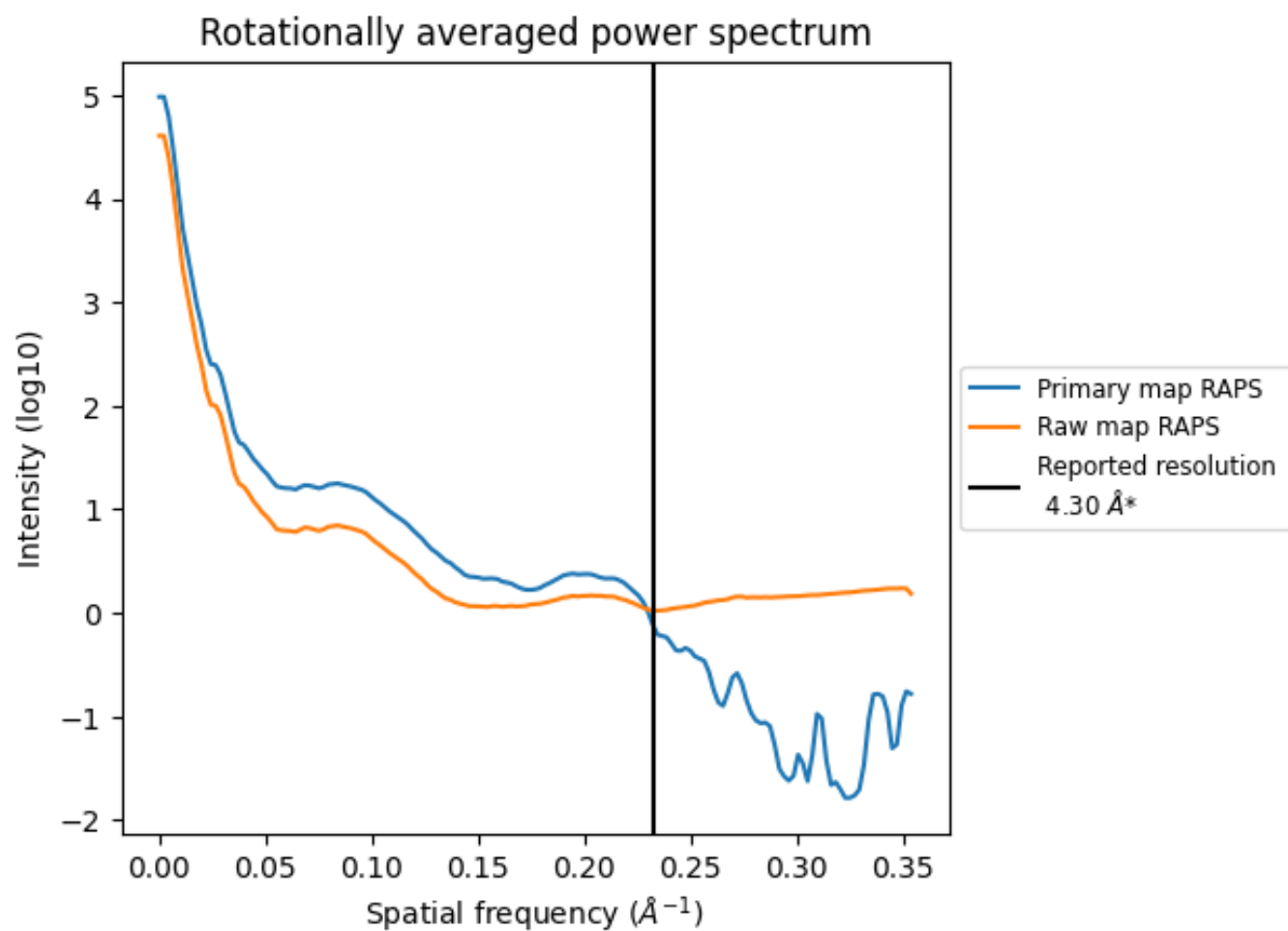
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm³; this corresponds to an approximate mass of 169 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 ⓘ

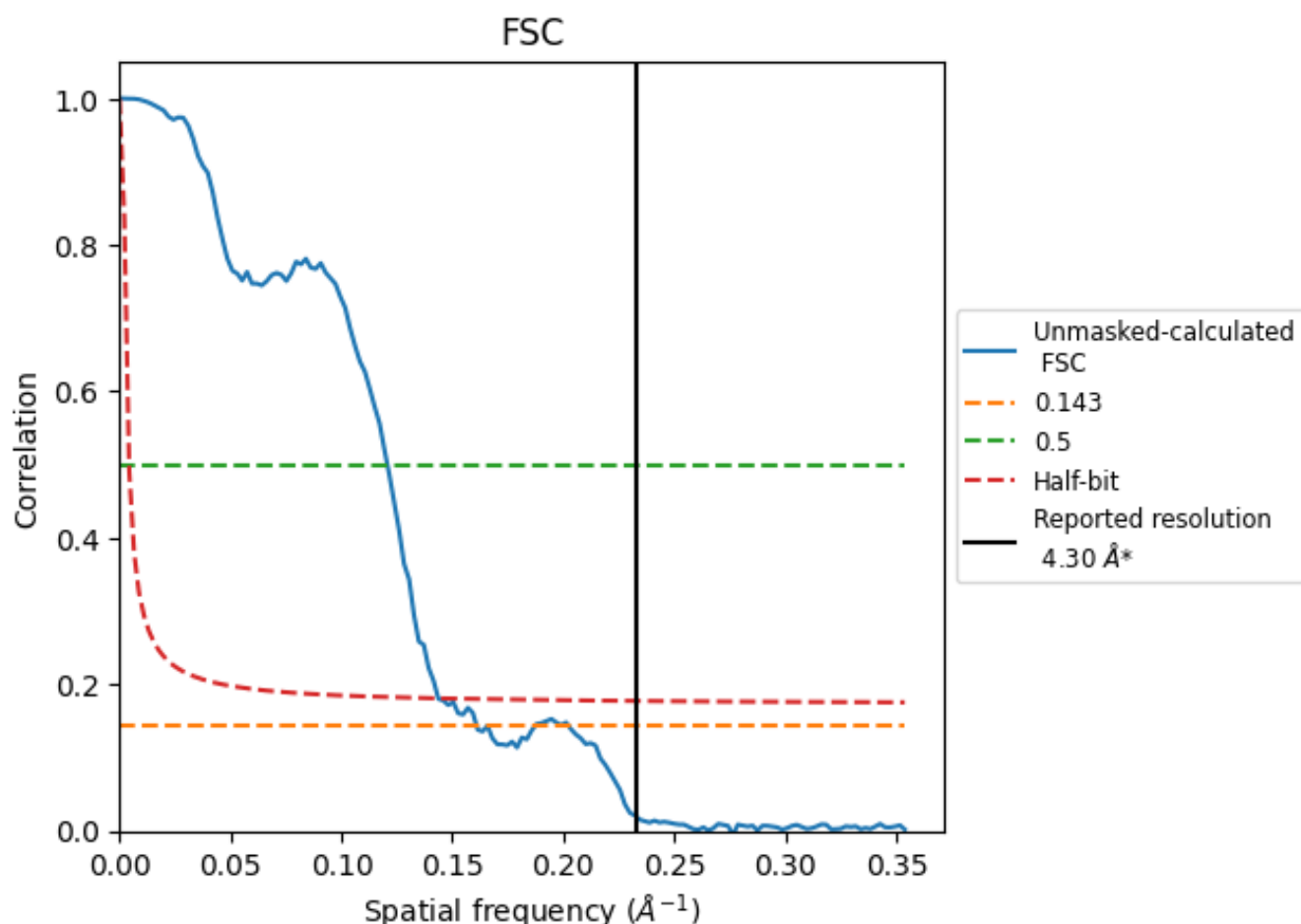


*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

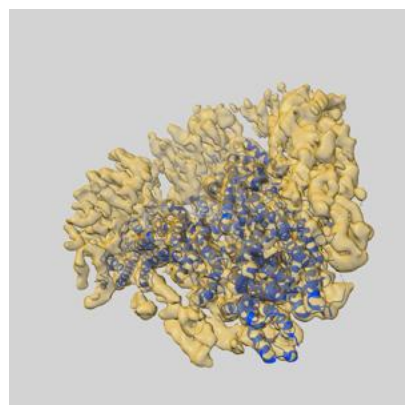
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.22	8.29	6.96

*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 6.22 differs from the reported value 4.3 by more than 10 %

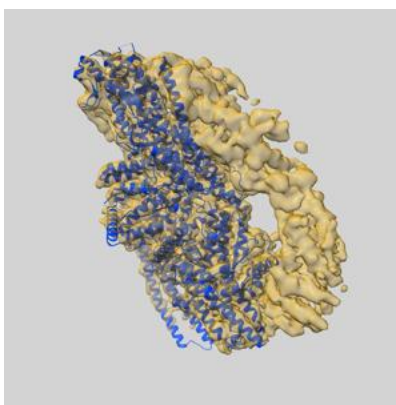
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51020 and PDB model 9G40. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

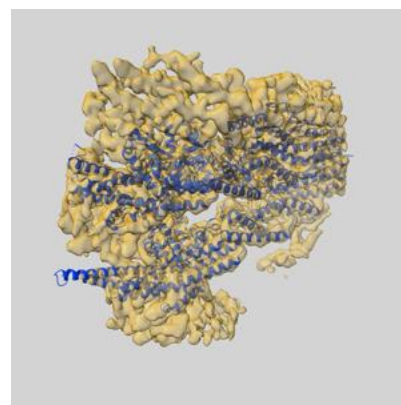
9.1 Map-model overlay [i](#)



X



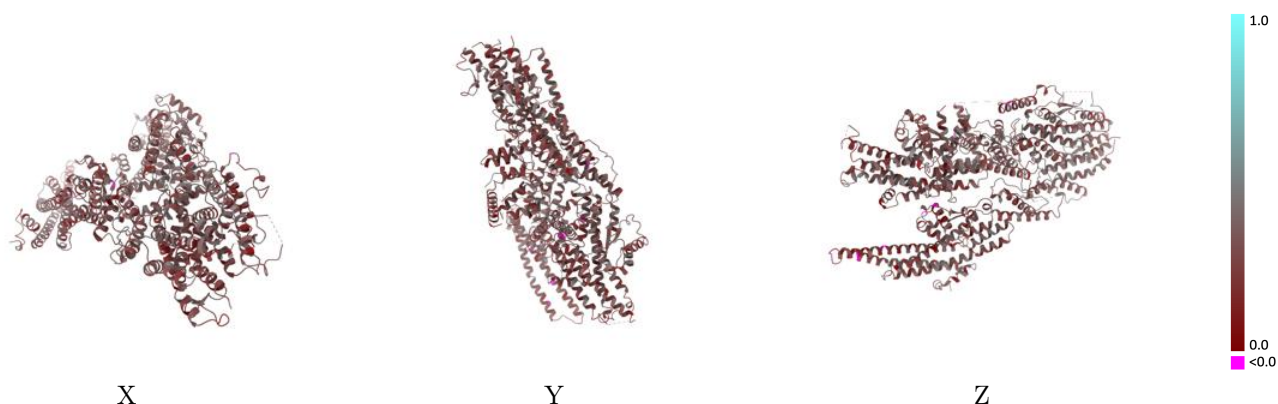
Y



Z

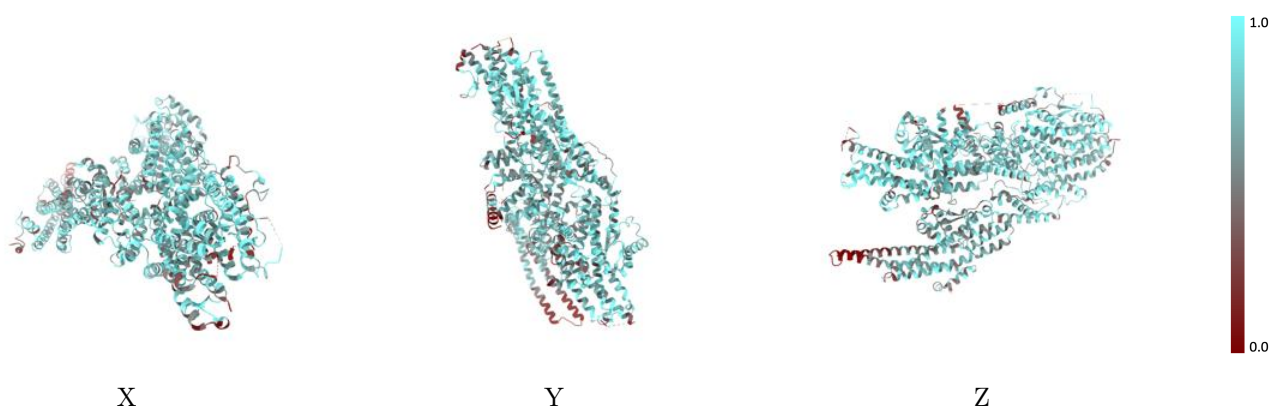
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



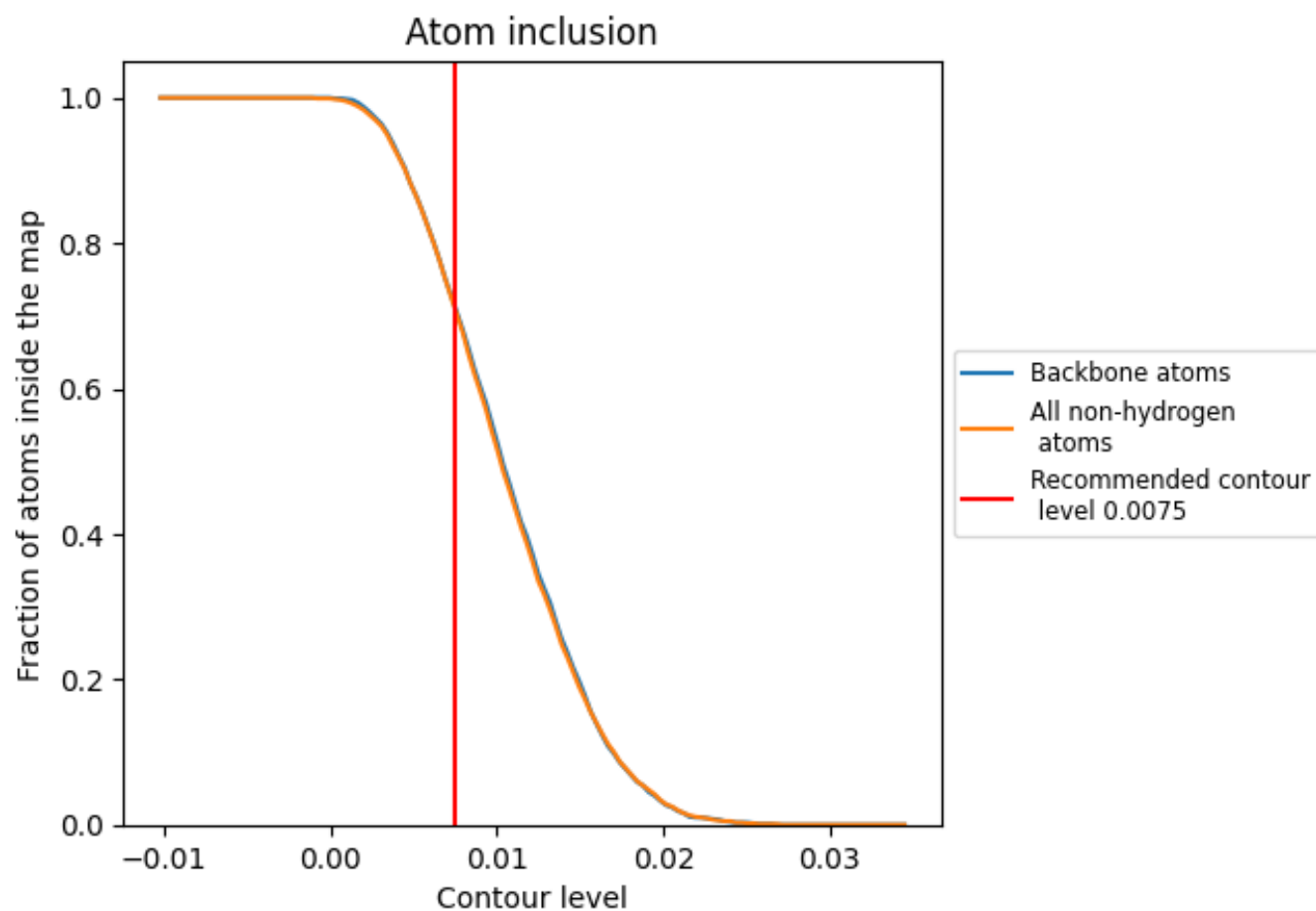
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0075).

9.4 Atom inclusion ⓘ



At the recommended contour level, 71% of all backbone atoms, 71% 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 (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7090	<div></div> 0.3040
F	<div></div> 0.6660	<div></div> 0.2910
G	<div></div> 0.7440	<div></div> 0.3130
X	<div></div> 0.6730	<div></div> 0.2980
u	<div></div> 0.7690	<div></div> 0.3360
v	<div></div> 0.7660	<div></div> 0.3250

