



# wwPDB EM Validation Summary Report ⓘ

Aug 30, 2023 – 12:14 PM JST

PDB ID : 7Y5V  
EMDB ID : EMD-33626  
Title : Cryo-EM structure of the dimeric human CAF1LC-H3-H4 complex  
Authors : Liu, C.P.; Yu, C.; Yu, Z.Y.; Xu, R.M.  
Deposited on : 2022-06-17  
Resolution : 6.10 Å (reported)  
Based on initial model : 7Y5U

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

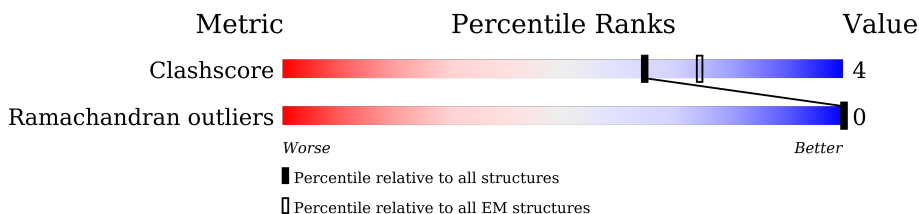
EMDB validation analysis : 0.0.1.dev50  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.10 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

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  $\geq 3$ , 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	412	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 6%, orange 6%, yellow 6%, green 42%, grey 57%);"></span> 6%                      42%                      57%
1	F	412	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 7%, orange 7%, yellow 7%, green 42%, grey 57%);"></span> 7%                      42%                      57%
2	D	136	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 5%, orange 5%, yellow 5%, green 79%, grey 20%);"></span> 5%                      79%                      20%
2	I	136	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 5%, orange 5%, yellow 5%, green 80%, grey 20%);"></span> 5%                      80%                      20%
3	E	103	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 5%, orange 5%, yellow 5%, green 77%, grey 21%);"></span> 5%                      77%                      21%
3	J	103	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 5%, orange 5%, yellow 5%, green 77%, grey 21%);"></span> 5%                      77%                      21%
4	C	425	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 5%, orange 5%, yellow 5%, green 89%, yellow 5%, grey 6%);"></span> 5%                      89%                      5% 6%
4	H	425	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 5%, orange 5%, yellow 5%, green 90%, yellow 5%, grey 6%);"></span> 5%                      90%                      5% 6%
5	B	419	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 5%, orange 5%, yellow 5%, green 84%, yellow 5%, grey 11%);"></span> 5%                      84%                      5% 11%

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Mol	Chain	Length	Quality of chain
5	G	419	 84% 5% 11%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9104 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 Chromatin assembly factor 1 subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	176	Total	C	N	O	0	0
			704	352	176	176		
1	F	176	Total	C	N	O	0	0
			704	352	176	176		

- Molecule 2 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	109	Total	C	N	O	0	0
			436	218	109	109		
2	I	109	Total	C	N	O	0	0
			436	218	109	109		

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	E	81	Total	C	N	O	0	0
			324	162	81	81		
3	J	81	Total	C	N	O	0	0
			324	162	81	81		

- Molecule 4 is a protein called Histone-binding protein RBBP4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	C	401	Total	C	N	O	0	0
			1604	802	401	401		
4	H	401	Total	C	N	O	0	0
			1604	802	401	401		

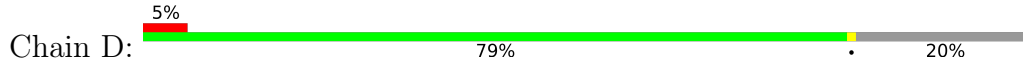
- Molecule 5 is a protein called Chromatin assembly factor 1 subunit B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	B	371	1484	742	371	371	0	0
5	G	371	1484	742	371	371	0	0



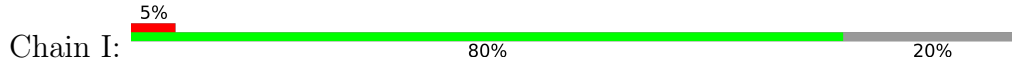
MET CYS TRP TYR VAL HIS PRO VAL LEU GLN SER PHE GLN GLN HIS LEU VAL PRO CYS TRP TYR VAL SER VAL PRO ALA GLN LYS THR VAL VAL PRO ALA THR GLN LYS GLU ASP SER

● Molecule 2: Histone H3.1



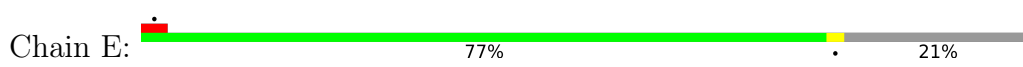
MET A1 R2 T3 K4 Q5 T6 T11 GLY GLY LYS ALA PRO ARG LYS LEU ALA THR LYS ALA ARG LYS SER ALA PRO ALA THR GLY VAL K36 G110 A114 E133 ARG ALA

● Molecule 2: Histone H3.1



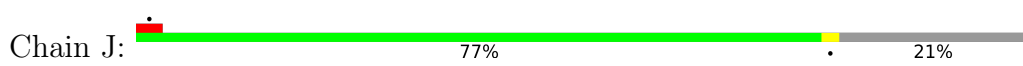
MET A1 R2 T3 K4 Q5 T6 T11 GLY GLY LYS ALA PRO ARG LYS LEU ALA THR LYS ALA ARG LYS SER ALA PRO ALA THR GLY VAL K36 E133 ARG ALA

● Molecule 3: Histone H4



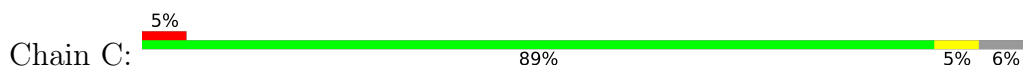
MET SER GLY ARG LYS LYS LYS LYS LEU GLY LYS LYS LYS ALA ALA LYS ARG HIS ARG LYS V21 L22 R23 Y72 A76 G101 GLY

● Molecule 3: Histone H4



MET SER ARG LYS LYS LYS LYS LEU GLY LYS LYS LYS ALA ALA LYS ARG HIS ARG LYS V21 L22 R23 D24 Y72 A76 G101 GLY

● Molecule 4: Histone-binding protein RBBP4



MET ALA ASP LYS ALA PHE ASP ASP A11 V12 L34 V35 M36 L40 P43 S62 L66 H71 T72 S73 D74 A82 L86 E101 G106 V111 P163 S164 G165 R174 A209 K212 E213 V217 H260 L300 L310 H311

L342 G351 E352 E353 Q354 S355 P356 E360 H370 S378 V393 N397 V401 W402 Q403 E411 GLU ASP PRO GLU SER VAL ASP PRO GLU GLY CLN SER

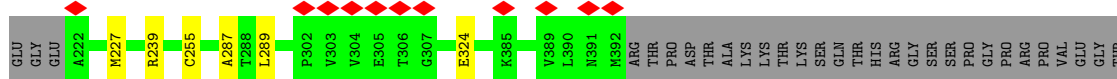
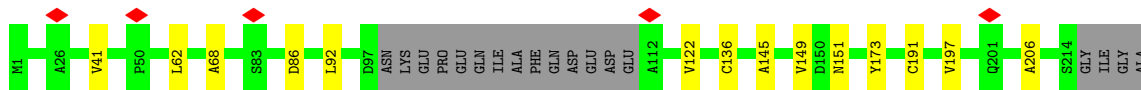
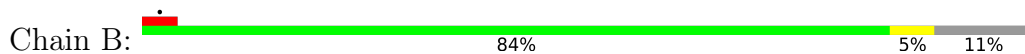
● Molecule 4: Histone-binding protein RBBP4



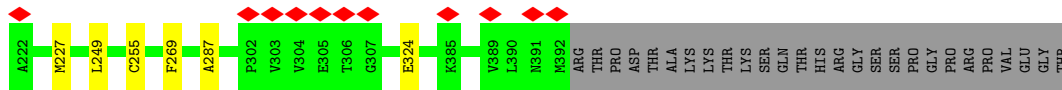
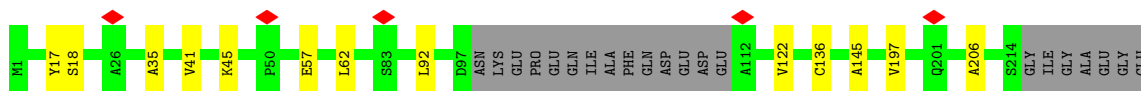
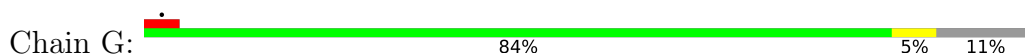
MET ALA ASP LYS ALA PHE ASP ASP A11 R36 L40 P43 S62 L66 H71 T72 S73 D74 A82 L86 E101 G106 V111 P163 S164 G165 A209 E213 H260 V298 A299 L300 L310 H311 F313 L342 G351 E352



• Molecule 5: Chromatin assembly factor 1 subunit B



• Molecule 5: Chromatin assembly factor 1 subunit B





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	24904	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.225	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.07	Depositor
Map size ( $\text{\AA}$ )	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0, 1.0, 1.0	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	A	0.24	0/702	0.49	0/874
1	F	0.24	0/702	0.48	0/874
2	D	0.28	0/434	0.51	0/539
2	I	0.28	0/434	0.51	0/539
3	E	0.29	0/323	0.52	0/402
3	J	0.31	0/323	0.53	0/402
4	C	0.28	0/1603	0.52	0/2002
4	H	0.27	0/1603	0.51	0/2002
5	B	0.28	0/1481	0.53	0/1846
5	G	0.28	0/1481	0.53	0/1846
All	All	0.27	0/9086	0.52	0/11326

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	A	704	0	189	1	0
1	F	704	0	189	1	0
2	D	436	0	112	1	0
2	I	436	0	112	0	0
3	E	324	0	95	1	0
3	J	324	0	95	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1604	0	422	13	0
4	H	1604	0	422	12	0
5	B	1484	0	400	10	0
5	G	1484	0	400	10	0
All	All	9104	0	2436	48	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 4.

The worst 5 of 48 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:C:62:SER:N	4:C:86:LEU:O	2.13	0.78
5:B:227:MET:O	5:B:255:CYS:N	2.23	0.70
4:H:62:SER:N	4:H:86:LEU:O	2.15	0.70
5:B:92:LEU:O	5:B:122:VAL:N	2.19	0.69
5:G:92:LEU:O	5:G:122:VAL:N	2.18	0.68

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	172/412 (42%)	168 (98%)	4 (2%)	0	100	100
1	F	172/412 (42%)	167 (97%)	5 (3%)	0	100	100
2	D	105/136 (77%)	100 (95%)	5 (5%)	0	100	100
2	I	105/136 (77%)	97 (92%)	8 (8%)	0	100	100
3	E	79/103 (77%)	76 (96%)	3 (4%)	0	100	100
3	J	79/103 (77%)	75 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	399/425 (94%)	384 (96%)	15 (4%)	0	100	100
4	H	399/425 (94%)	383 (96%)	16 (4%)	0	100	100
5	B	365/419 (87%)	348 (95%)	17 (5%)	0	100	100
5	G	365/419 (87%)	347 (95%)	18 (5%)	0	100	100
All	All	2240/2990 (75%)	2145 (96%)	95 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

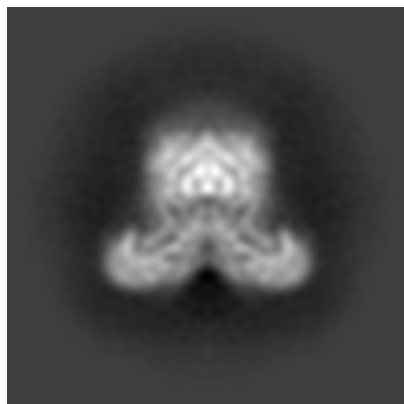
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33626. These allow visual inspection of the internal detail of the map and identification of artifacts.

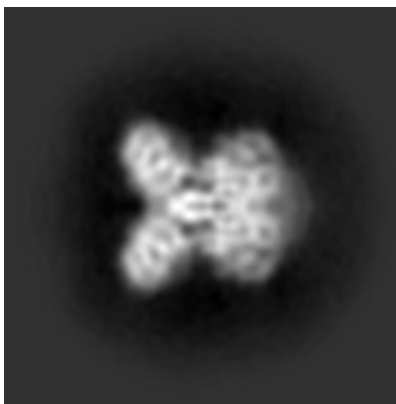
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

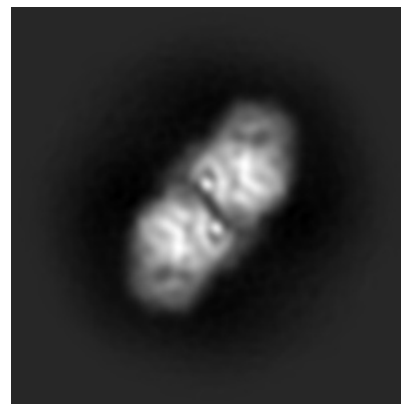
#### 6.1.1 Primary map



X

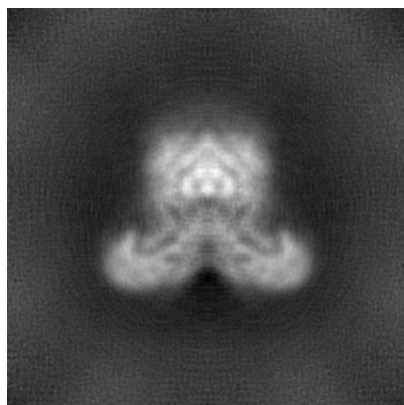


Y

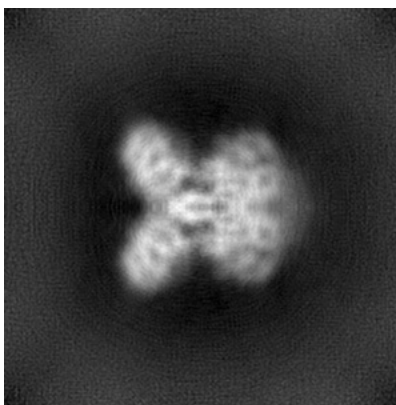


Z

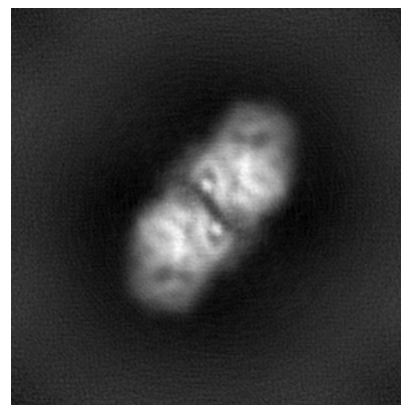
#### 6.1.2 Raw map



X



Y

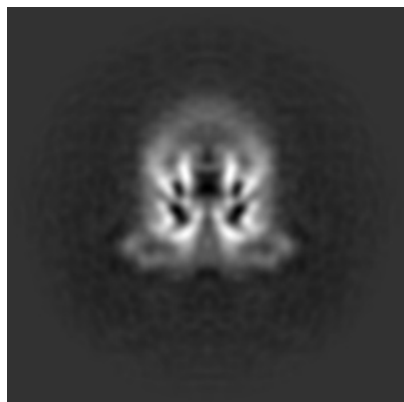


Z

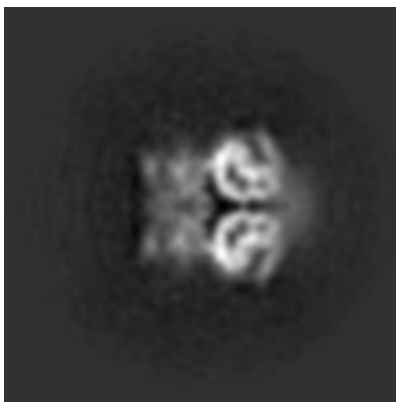
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

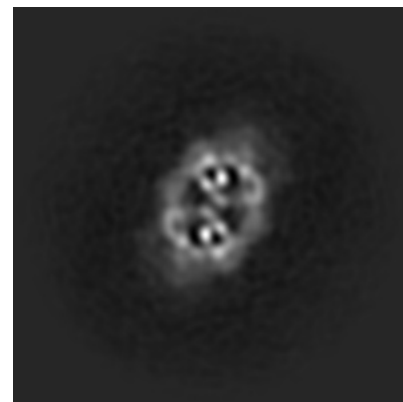
### 6.2.1 Primary map



X Index: 128

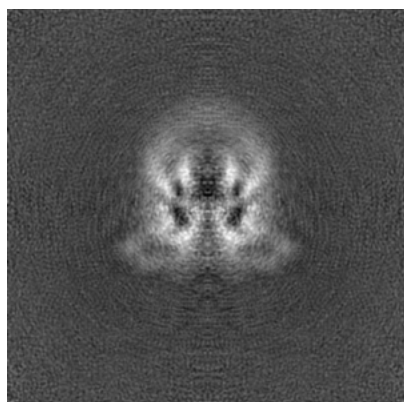


Y Index: 128

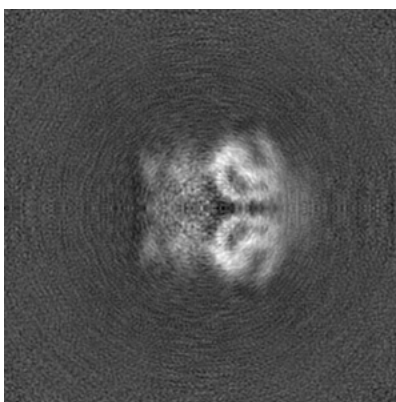


Z Index: 128

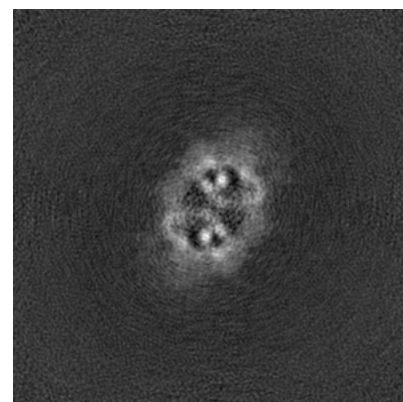
### 6.2.2 Raw map



X Index: 128



Y Index: 128

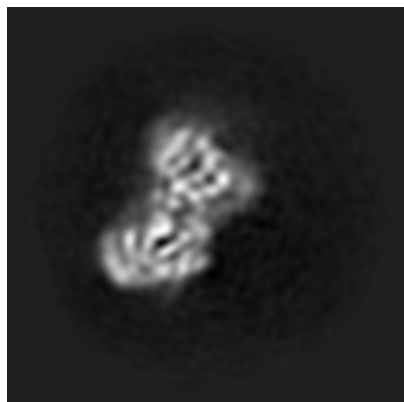


Z Index: 128

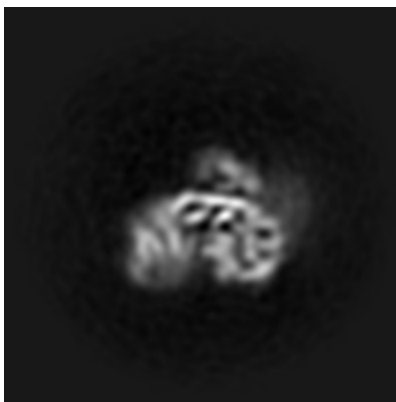
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

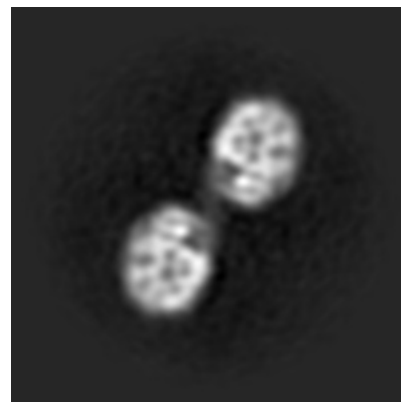
### 6.3.1 Primary map



X Index: 106

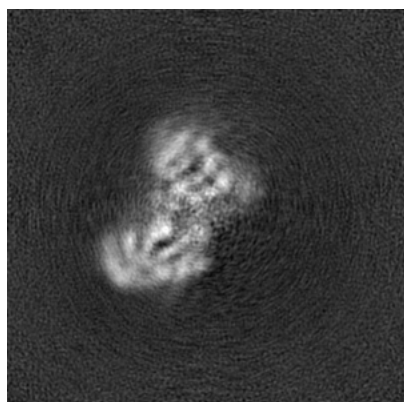


Y Index: 114

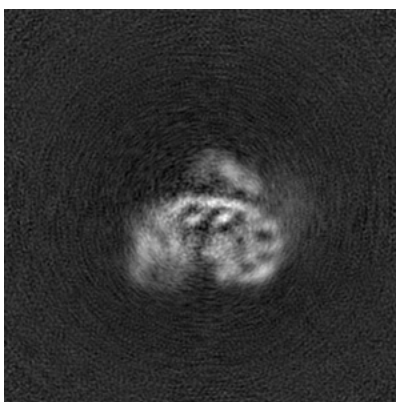


Z Index: 91

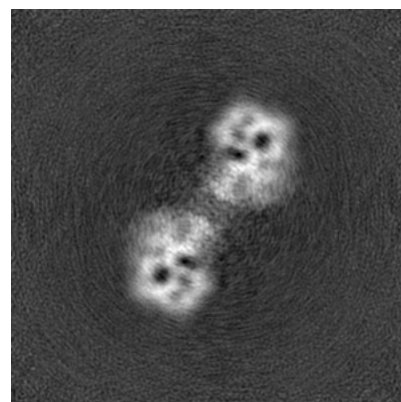
### 6.3.2 Raw map



X Index: 106



Y Index: 115

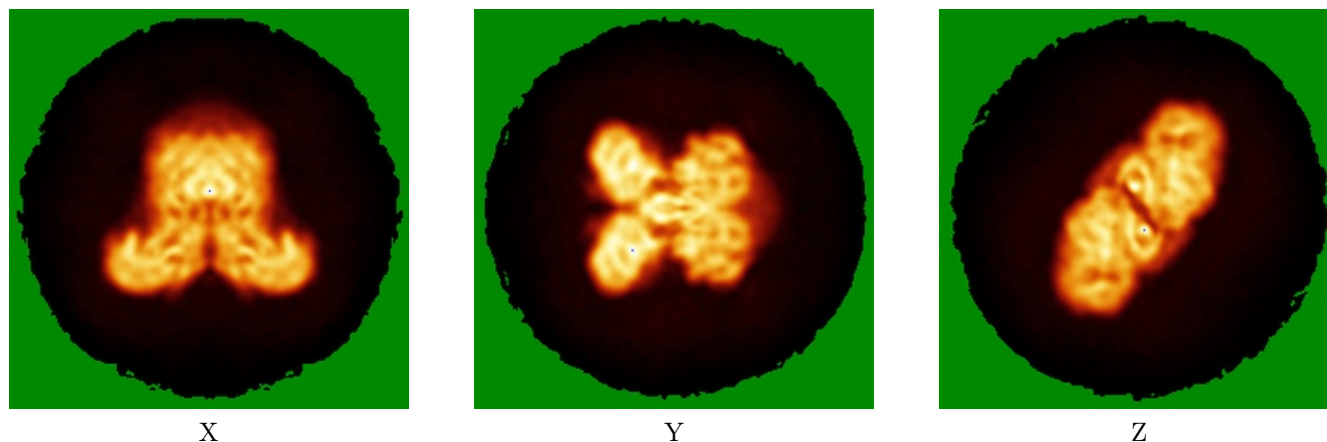


Z Index: 100

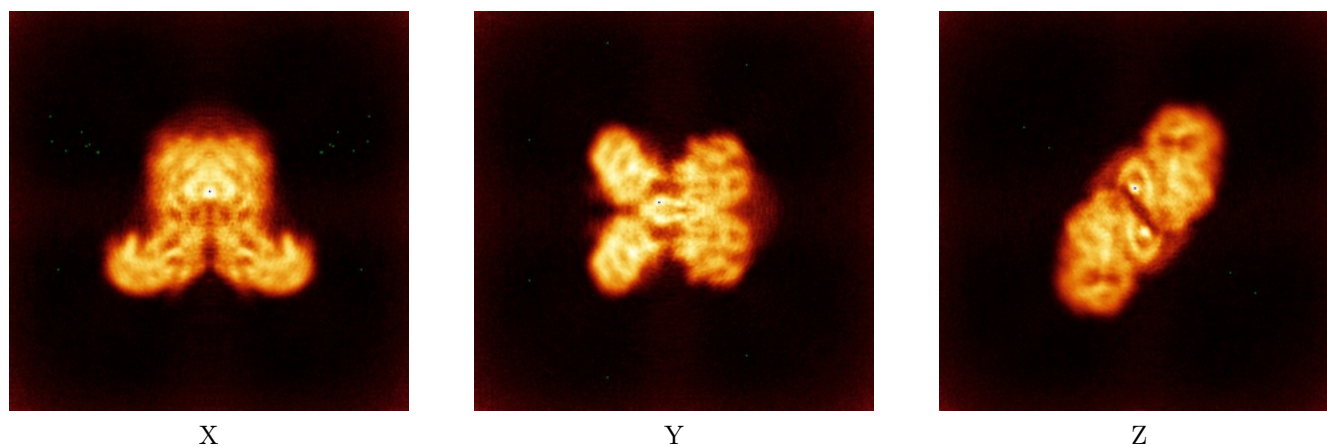
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map

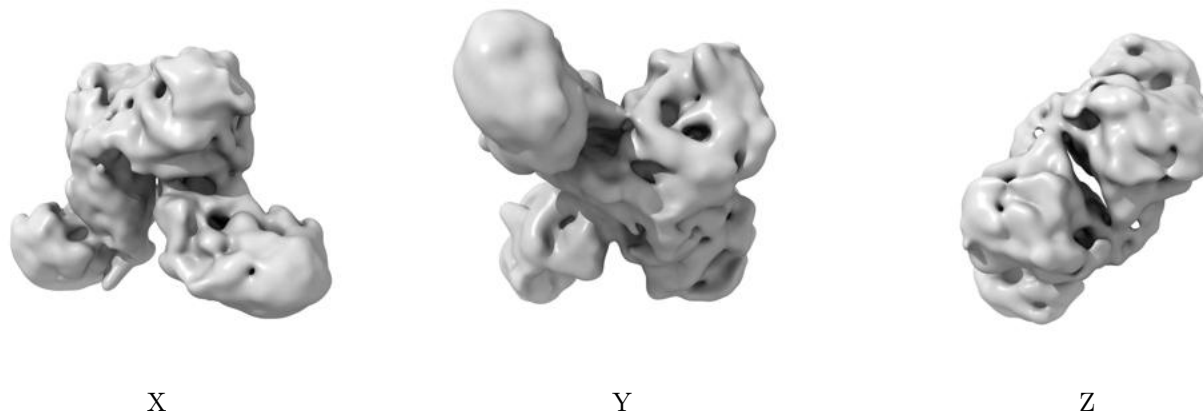


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



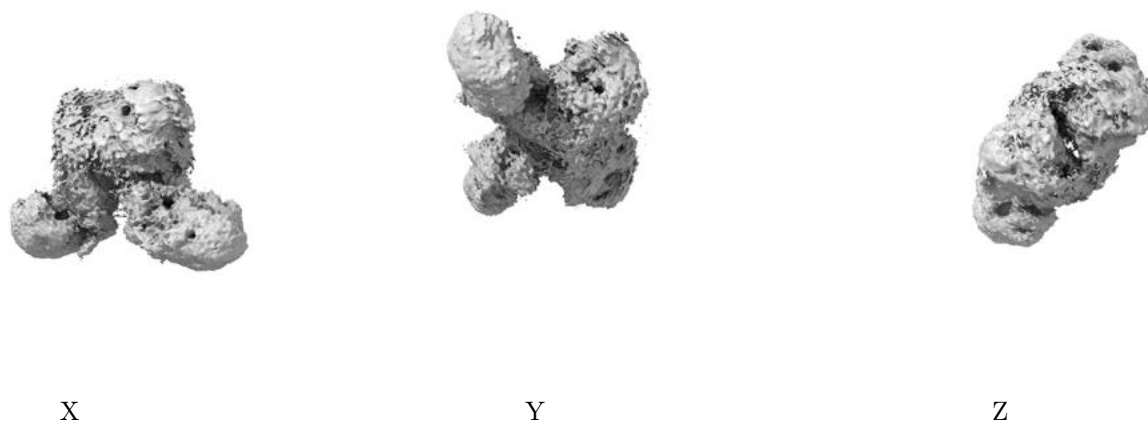
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

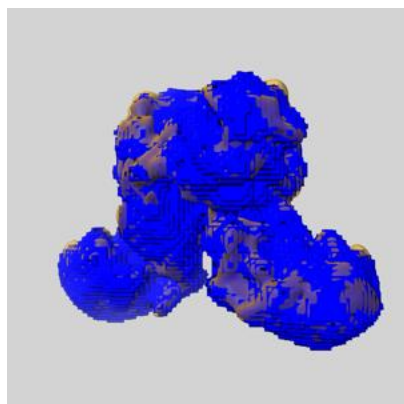
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

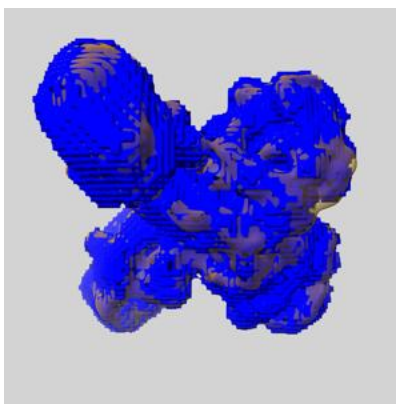
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

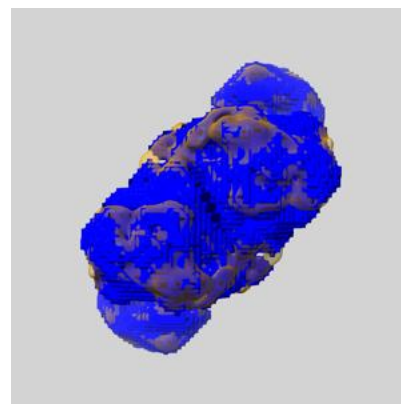
### 6.6.1 emd\_33626\_msk\_1.map [i](#)



X



Y

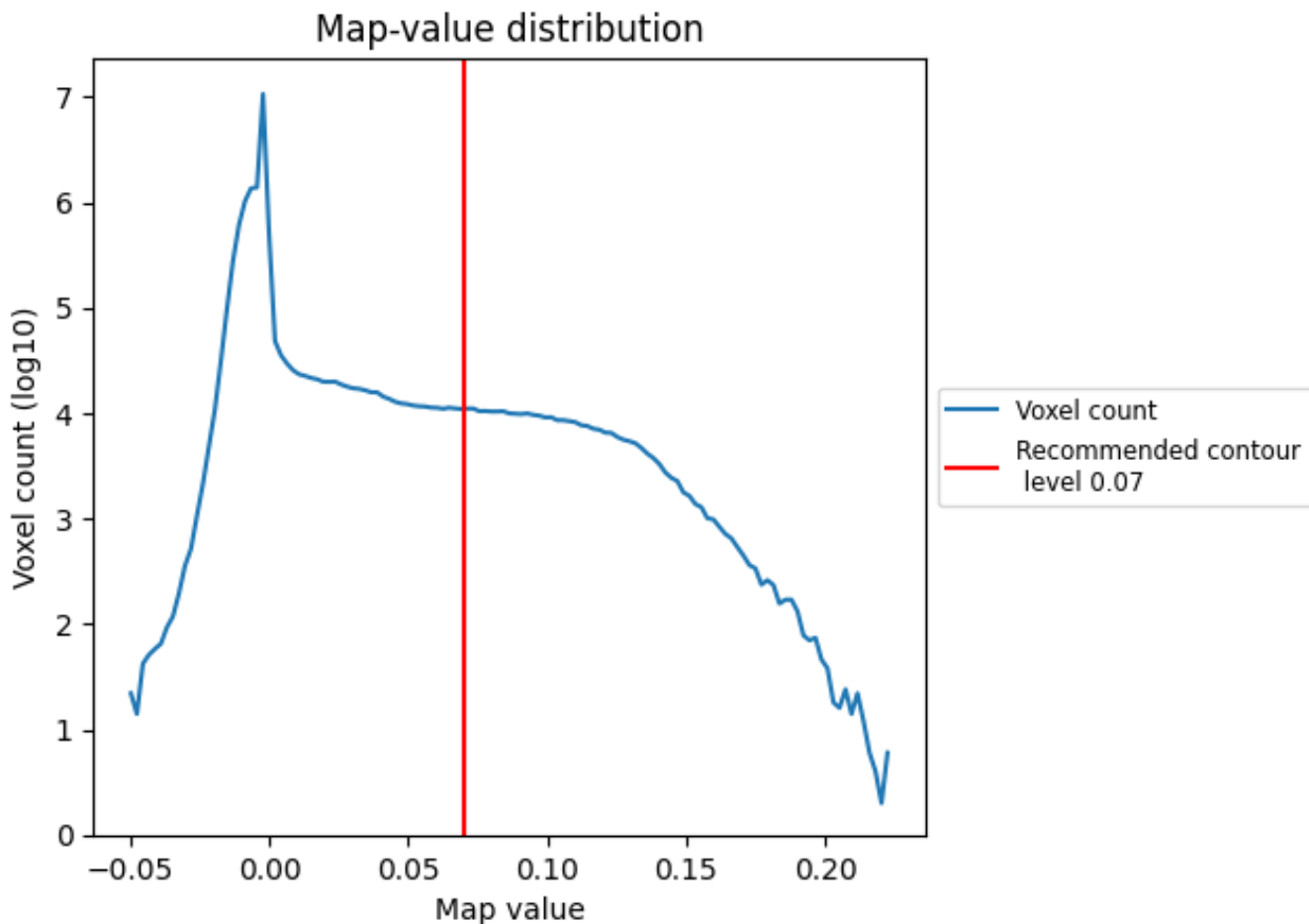


Z

## 7 Map analysis [i](#)

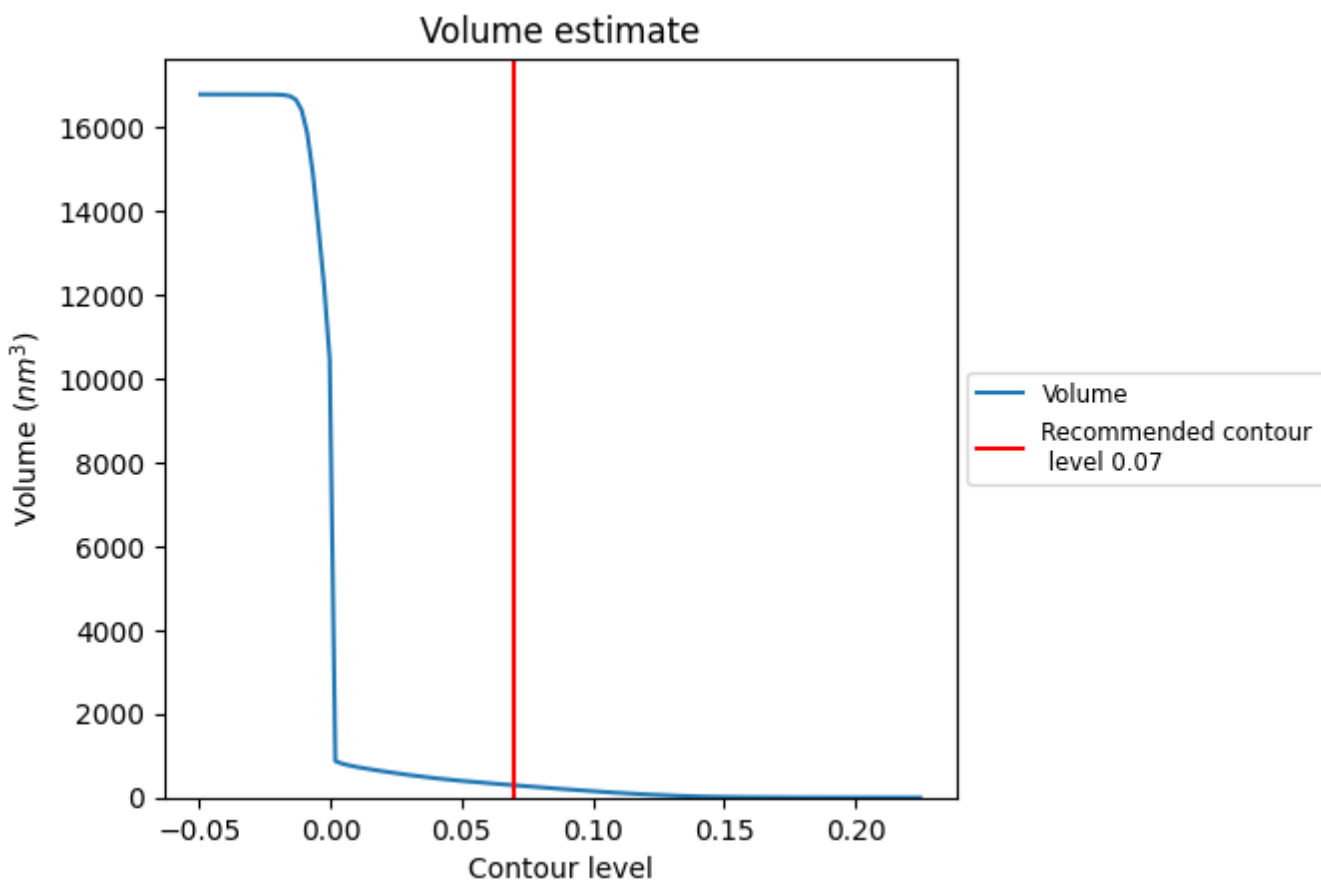
This section contains the results of statistical analysis of the map.

### 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.

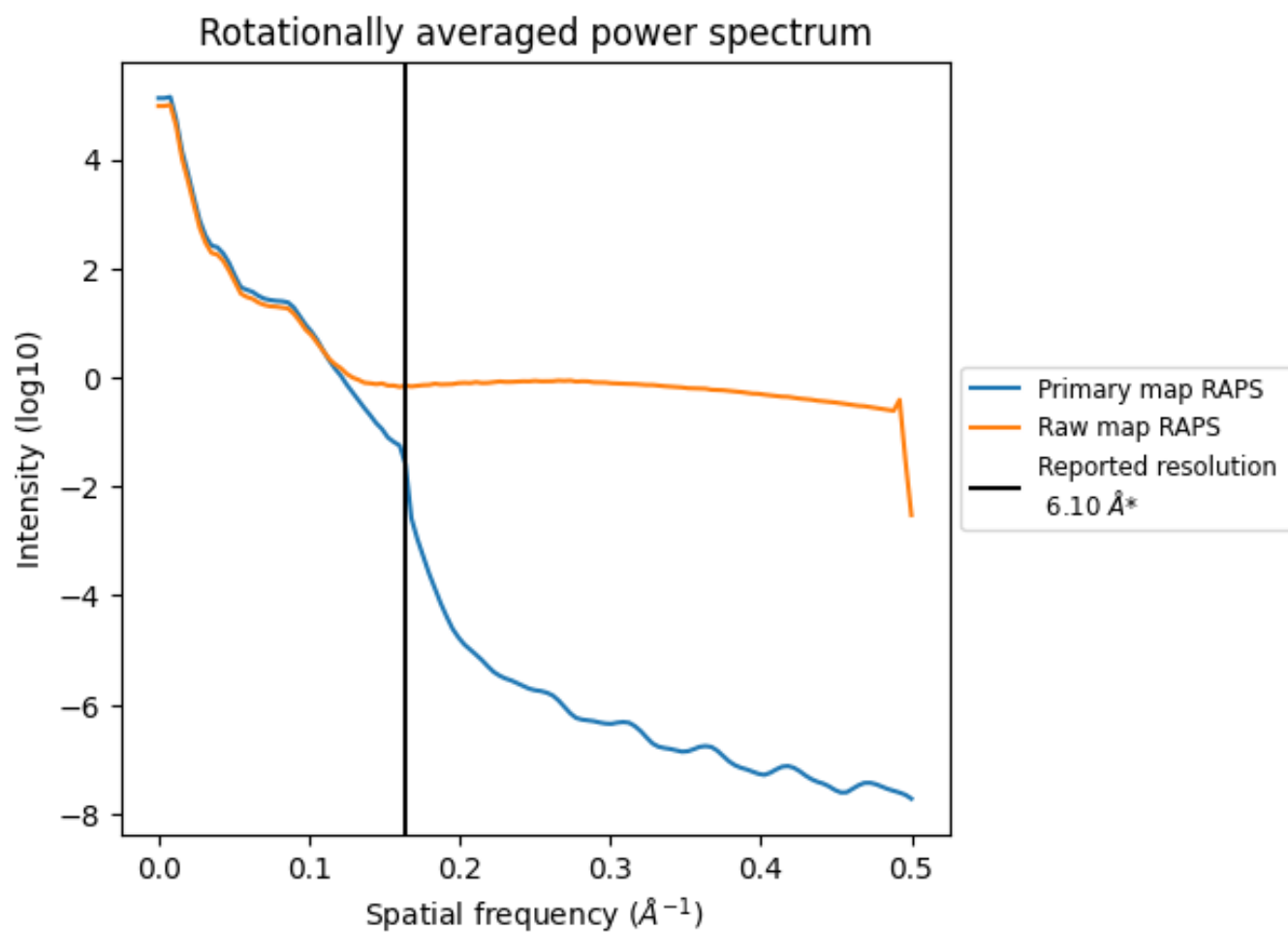
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 293 nm<sup>3</sup>; this corresponds to an approximate mass of 264 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

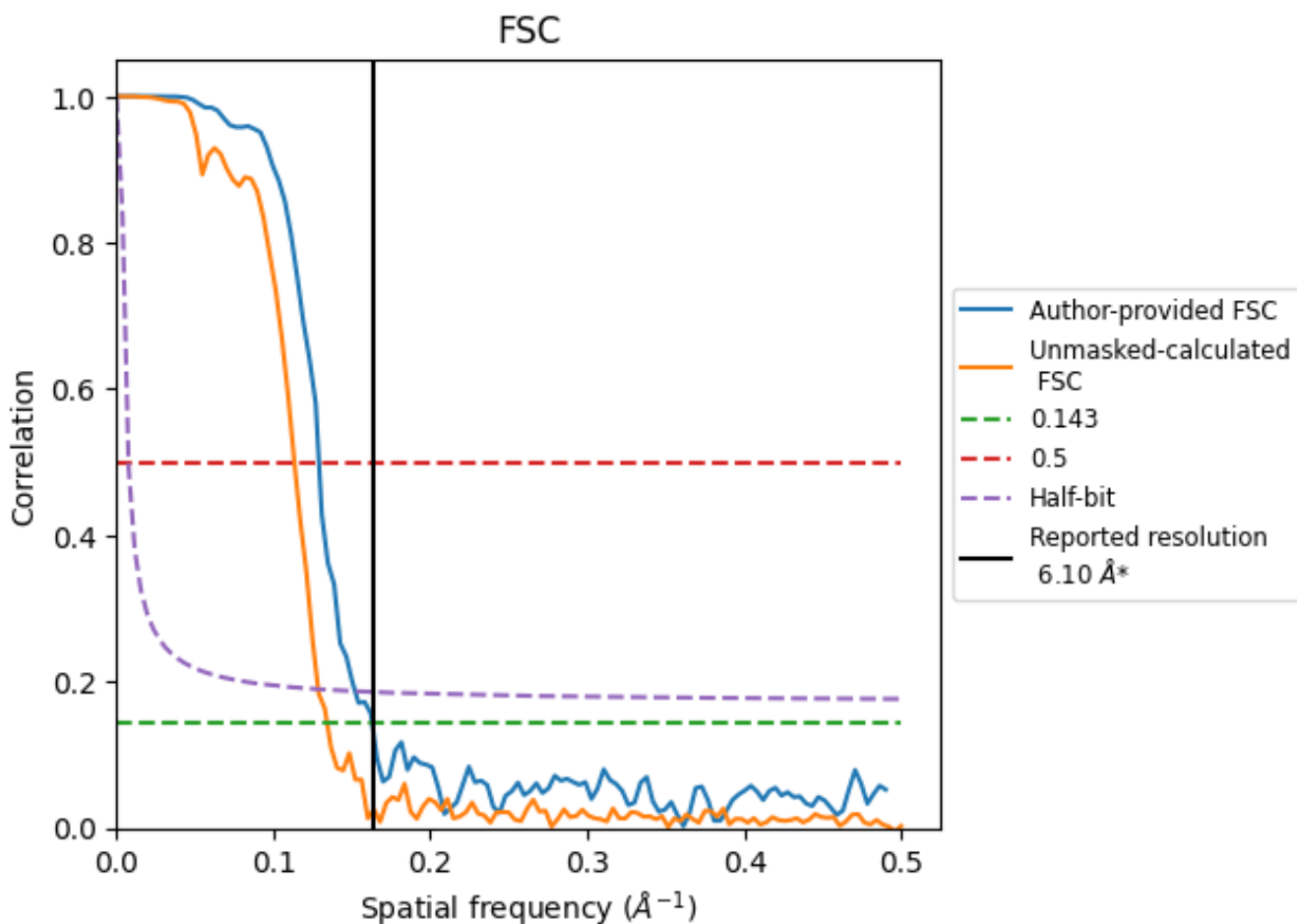


\*Reported resolution corresponds to spatial frequency of 0.164 Å<sup>-1</sup>

## 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 0.164 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

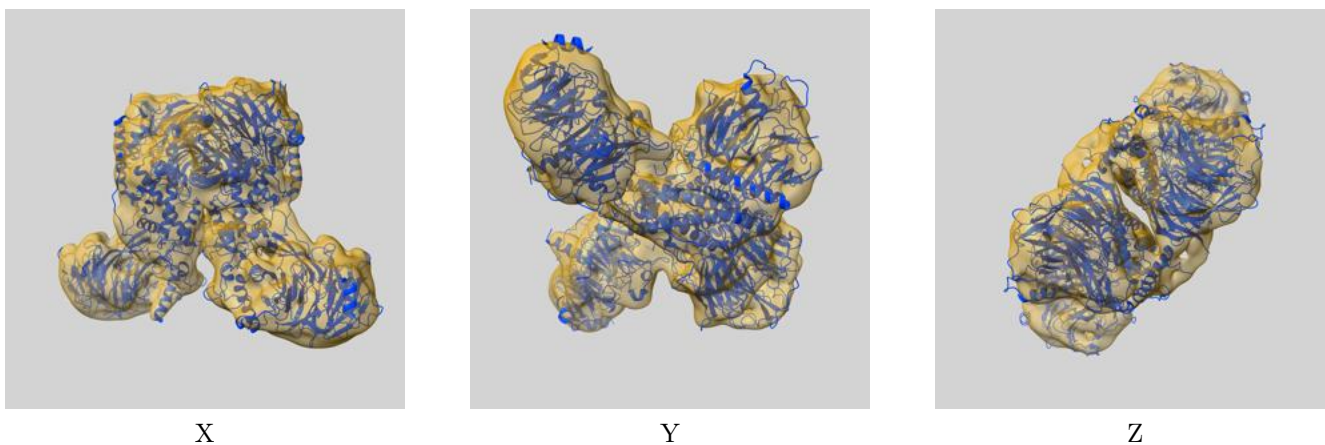
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.10	-	-
Author-provided FSC curve	6.13	7.75	6.57
Unmasked-calculated*	7.45	8.82	7.78

\*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 7.45 differs from the reported value 6.1 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33626 and PDB model 7Y5V. Per-residue inclusion information can be found in section 3 on page 6.

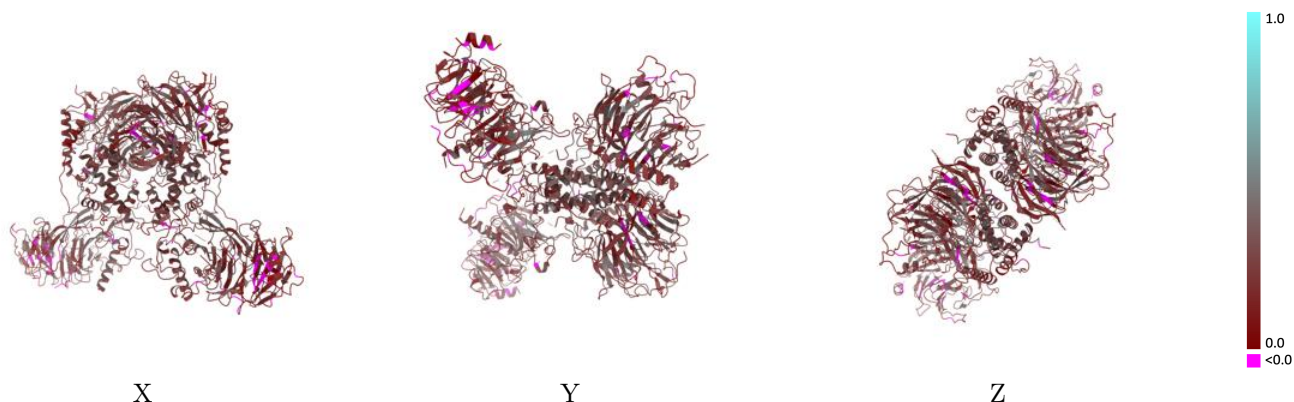
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

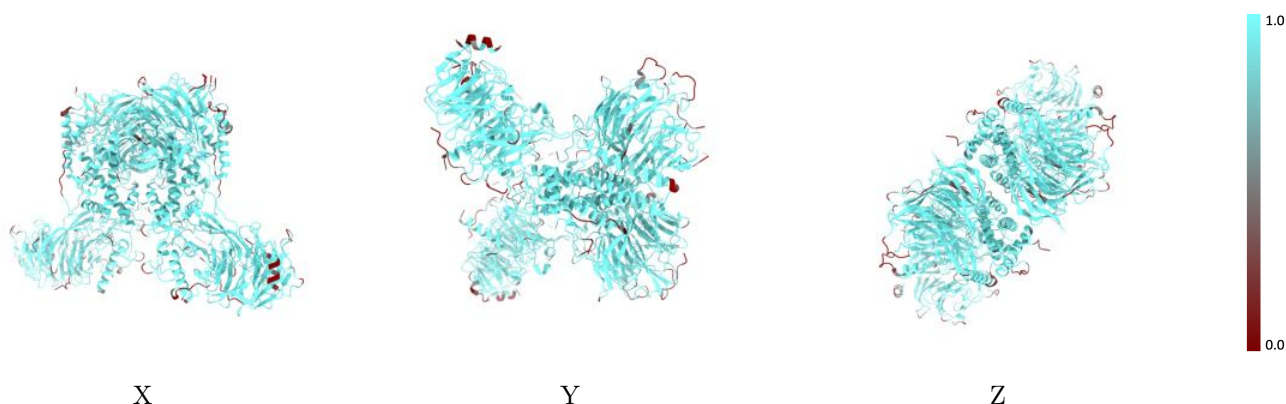


## 9.2 Q-score mapped to coordinate model [i](#)



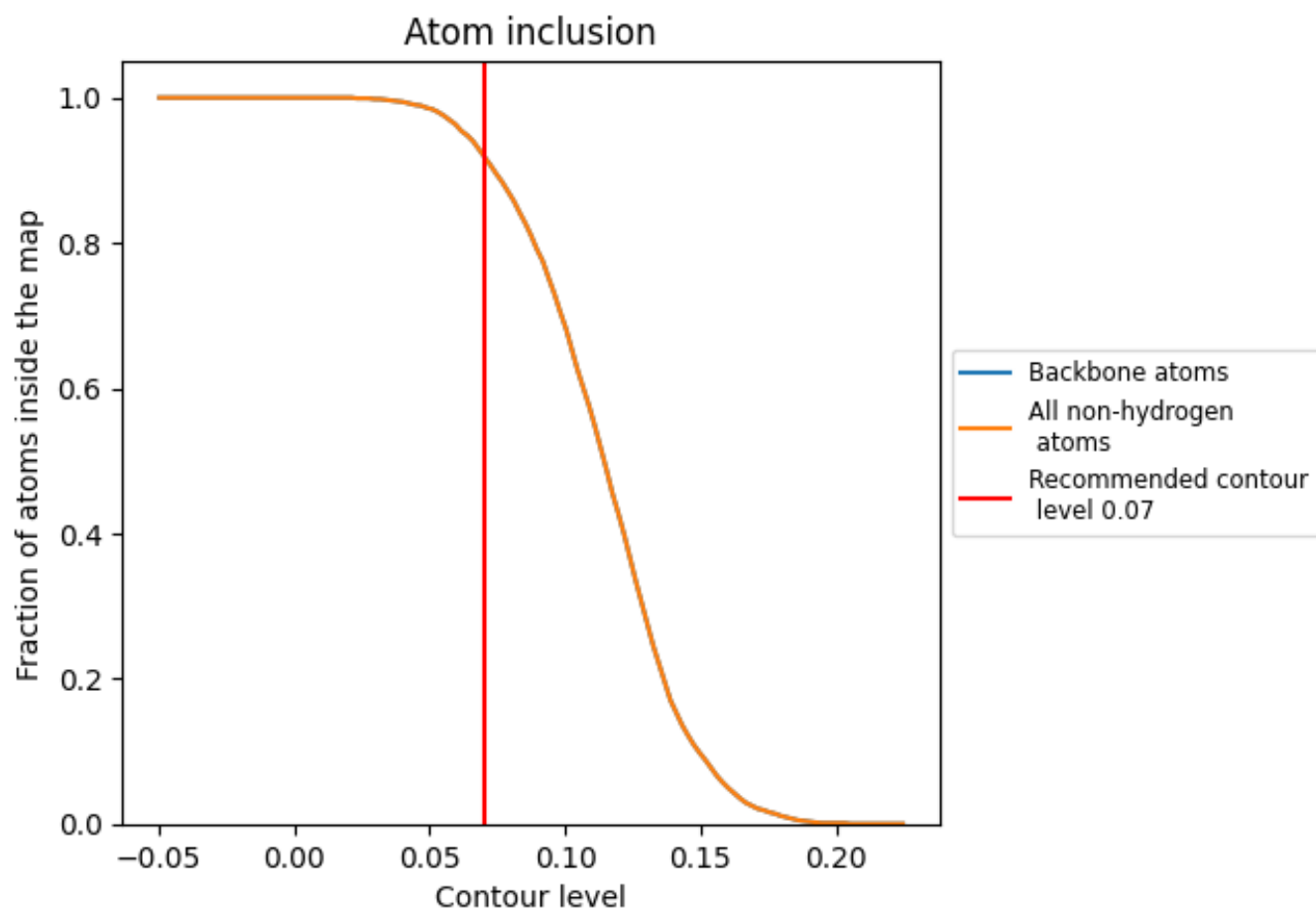
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

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

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9200	 0.2220
A	 0.8270	 0.1870
B	 0.9350	 0.2300
C	 0.9450	 0.2110
D	 0.9150	 0.2640
E	 0.9570	 0.2750
F	 0.8120	 0.1870
G	 0.9360	 0.2280
H	 0.9460	 0.2110
I	 0.9130	 0.2630
J	 0.9540	 0.2730

