



## Full wwPDB EM Validation Report ⓘ

Feb 4, 2024 – 01:46 PM EST

PDB ID : 8CSL  
EMDB ID : EMD-26965  
Title : Sub-tomogram averaging of erythrocyte ankyrin-1 complex  
Authors : Vallese, F.; Kim, K.; Yen, L.Y.; Johnston, J.D.; Noble, A.J.; Cali, T.; Clarke, O.B.  
Deposited on : 2022-05-12  
Resolution : 25.00 Å (reported)  
Based on initial model : 8CS9

This is a Full wwPDB EM Validation 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:

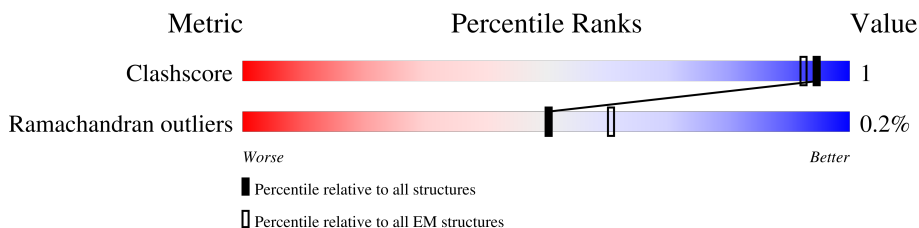
EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 25.00 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.



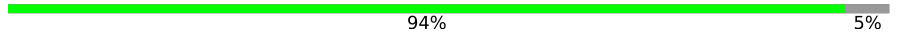
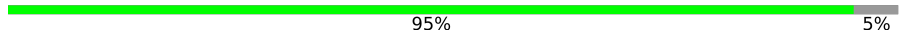
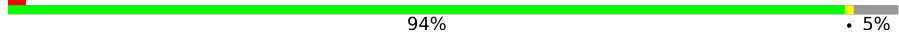







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	1881	
2	V	911	
2	W	911	
2	Y	911	
2	Z	911	
2	e	911	
2	f	911	
2	g	911	
3	K	417	

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Mol	Chain	Length	Quality of chain
4	L	409	 94% 5%
4	Q	409	 95% 5%
5	X	691	 94% 5%
6	P	91	 36% 64%
7	R	150	 24% 76%
7	S	150	 22% 78%
7	T	150	 25% 75%
7	a	150	 25% 75%
7	b	150	 25% 75%
7	c	150	 22% 78%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 30720 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 Ankyrin-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	796	3184	1592	796	796	0	0

- Molecule 2 is a protein called Band 3 anion transport protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	W	30	120	60	30	30	0	0
2	V	810	3240	1620	810	810	0	0
2	e	804	3216	1608	804	804	0	0
2	Y	786	3144	1572	786	786	0	0
2	f	802	3208	1604	802	802	0	0
2	Z	798	3192	1596	798	798	0	0
2	g	790	3160	1580	790	790	0	0

- Molecule 3 is a protein called Blood group Rh(CE) polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	K	380	1529	764	382	383	2	0

- Molecule 4 is a protein called Ammonium transporter Rh type A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	L	388	1553	776	388	389	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	Q	390	Total	C	N	O	0	0
			1561	780	390	391		

- Molecule 5 is a protein called Protein 4.2.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	X	656	Total	C	N	O	0	0
			2624	1312	656	656		

- Molecule 6 is a protein called Glycophorin-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	33	Total	C	N	O	0	0
			133	66	33	34		

- Molecule 7 is a protein called Glycophorin-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	R	36	Total	C	N	O	0	0
			144	72	36	36		
7	a	37	Total	C	N	O	0	0
			148	74	37	37		
7	S	33	Total	C	N	O	0	0
			132	66	33	33		
7	b	38	Total	C	N	O	0	0
			152	76	38	38		
7	T	37	Total	C	N	O	0	0
			148	74	37	37		
7	c	33	Total	C	N	O	0	0
			132	66	33	33		

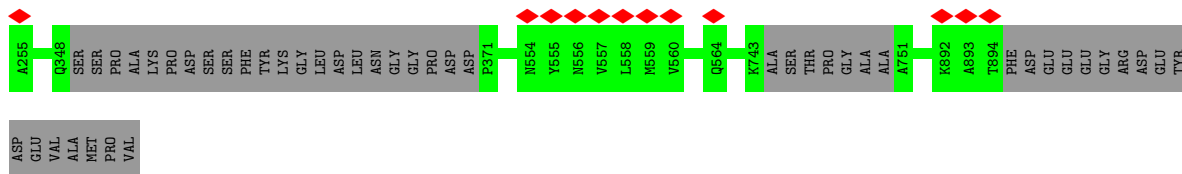




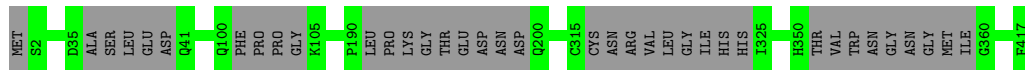




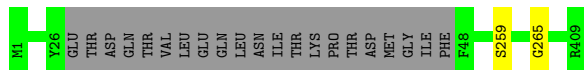




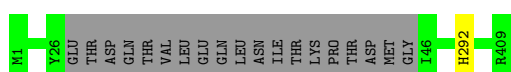
• Molecule 3: Blood group Rh(CE) polypeptide



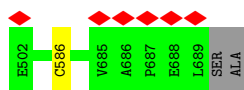
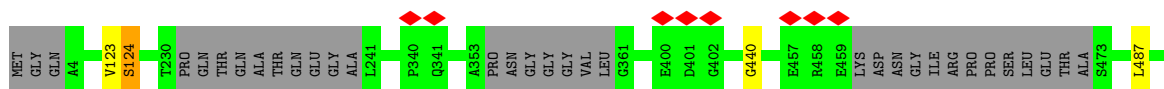
• Molecule 4: Ammonium transporter Rh type A



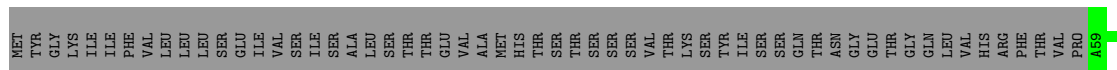
• Molecule 4: Ammonium transporter Rh type A



• Molecule 5: Protein 4.2



• Molecule 6: Glycophorin-B



• Molecule 7: Glycophorin-A





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	1596	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Warp	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	113	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.676	Depositor
Minimum map value	-0.223	Depositor
Average map value	0.030	Depositor
Map value standard deviation	0.136	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	320.0, 320.0, 320.0	wwPDB
Map dimensions	80, 80, 80	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.0, 4.0, 4.0	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	0.44	0/3182	0.64	0/3974
2	V	0.34	0/3235	0.55	0/4035
2	W	0.37	0/119	0.64	0/147
2	Y	0.37	0/3139	0.56	0/3915
2	Z	0.34	0/3188	0.55	0/3978
2	e	0.34	0/3212	0.54	0/4008
2	f	0.34	0/3204	0.53	0/3998
2	g	0.29	0/3155	0.51	0/3935
3	K	0.32	0/1523	0.48	0/1892
4	L	0.32	0/1551	0.50	0/1934
4	Q	0.40	0/1559	0.56	0/1944
5	X	0.43	0/2620	0.61	0/3268
6	P	0.25	0/132	0.37	0/162
7	R	0.24	0/143	0.48	0/177
7	S	0.25	0/131	0.48	0/162
7	T	0.25	0/147	0.47	0/182
7	a	0.24	0/147	0.47	0/182
7	b	0.26	0/151	0.48	0/187
7	c	0.55	0/131	0.59	0/162
All	All	0.36	0/30669	0.55	0/38242

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	3184	0	872	5	0
2	V	3240	0	863	2	0
2	W	120	0	27	0	0
2	Y	3144	0	839	6	0
2	Z	3192	0	853	1	0
2	e	3216	0	855	0	0
2	f	3208	0	857	0	0
2	g	3160	0	843	0	0
3	K	1529	0	412	0	0
4	L	1553	0	460	1	0
4	Q	1561	0	462	0	0
5	X	2624	0	704	3	0
6	P	133	0	35	0	0
7	R	144	0	42	0	0
7	S	132	0	39	0	0
7	T	148	0	43	0	0
7	a	148	0	43	0	0
7	b	152	0	44	0	0
7	c	132	0	39	0	0
All	All	30720	0	8332	17	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 1.

All (17) 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:L:259:SER:O	4:L:265:GLY:HA2	1.98	0.64
1:A:436:LYS:O	1:A:438:GLU:N	2.30	0.62
2:Z:181:SER:O	2:Z:183:ASP:N	2.32	0.57
2:Y:150:ARG:O	2:Y:153:LEU:N	2.40	0.55
2:V:428:GLY:O	2:V:429:GLU:C	2.47	0.53
2:V:31:MET:O	2:V:32:GLU:C	2.45	0.53
5:X:123:VAL:O	5:X:124:SER:C	2.55	0.44
1:A:468:LYS:C	1:A:470:ASP:N	2.69	0.44
2:Y:142:GLU:O	2:Y:143:ASP:C	2.57	0.43
1:A:382:ASN:O	5:X:440:GLY:HA3	2.19	0.43
1:A:468:LYS:C	1:A:470:ASP:H	2.21	0.43
2:Y:490:ARG:C	2:Y:492:TRP:N	2.71	0.42
2:Y:431:THR:O	2:Y:432:ARG:C	2.57	0.42
5:X:487:LEU:N	5:X:586:CYS:O	2.49	0.41
2:Y:140:ILE:O	2:Y:143:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LEU:O	1:A:458:GLN:C	2.59	0.41
2:Y:164:ALA:O	2:Y:165:GLY:C	2.60	0.41

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	792/1881 (42%)	758 (96%)	29 (4%)	5 (1%)	25	66
2	V	800/911 (88%)	779 (97%)	20 (2%)	1 (0%)	51	86
2	W	28/911 (3%)	24 (86%)	4 (14%)	0	100	100
2	Y	776/911 (85%)	754 (97%)	22 (3%)	0	100	100
2	Z	790/911 (87%)	770 (98%)	18 (2%)	2 (0%)	41	77
2	e	796/911 (87%)	776 (98%)	18 (2%)	2 (0%)	41	77
2	f	794/911 (87%)	766 (96%)	24 (3%)	4 (0%)	29	69
2	g	780/911 (86%)	763 (98%)	17 (2%)	0	100	100
3	K	370/417 (89%)	363 (98%)	7 (2%)	0	100	100
4	L	384/409 (94%)	379 (99%)	5 (1%)	0	100	100
4	Q	386/409 (94%)	376 (97%)	9 (2%)	1 (0%)	41	77
5	X	648/691 (94%)	637 (98%)	10 (2%)	1 (0%)	47	81
6	P	31/91 (34%)	31 (100%)	0	0	100	100
7	R	34/150 (23%)	34 (100%)	0	0	100	100
7	S	31/150 (21%)	31 (100%)	0	0	100	100
7	T	35/150 (23%)	35 (100%)	0	0	100	100
7	a	35/150 (23%)	35 (100%)	0	0	100	100
7	b	36/150 (24%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	c	31/150 (21%)	31 (100%)	0	0	100 100
All	All	7577/11175 (68%)	7378 (97%)	183 (2%)	16 (0%)	50 81

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	ASN
2	e	165	GLY
2	f	432	ARG
1	A	437	VAL
5	X	124	SER
2	V	31	MET
2	f	181	SER
2	Z	757	LYS
2	f	472	GLU
1	A	461	ALA
2	e	83	GLN
2	Z	185	SER
1	A	658	GLN
1	A	167	GLY
2	f	491	VAL
4	Q	292	HIS

### 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.

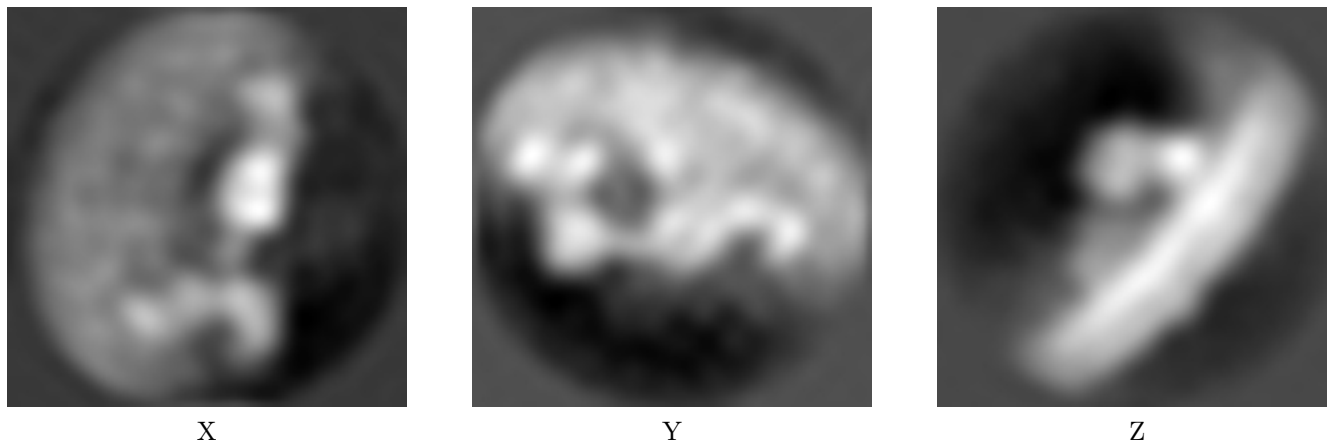
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26965. These allow visual inspection of the internal detail of the map and identification of artifacts.

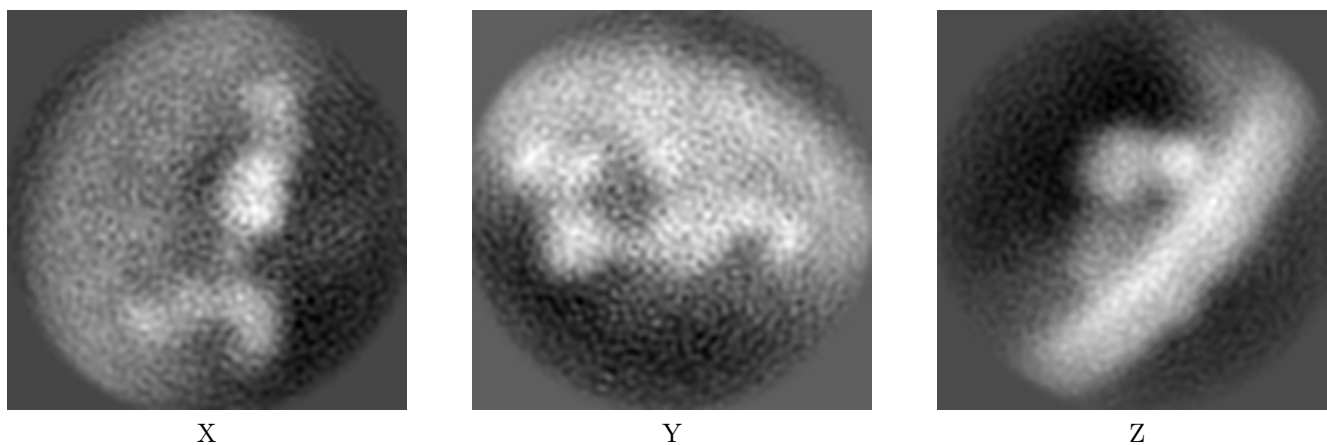
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



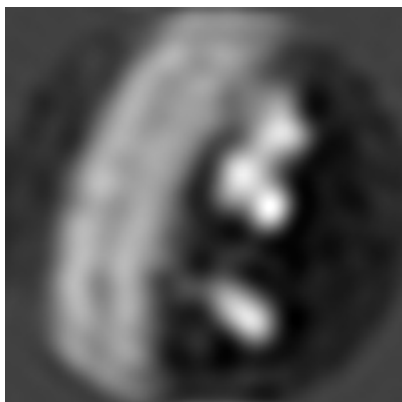
#### 6.1.2 Raw map



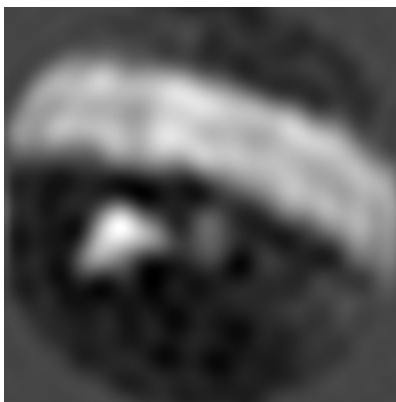
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

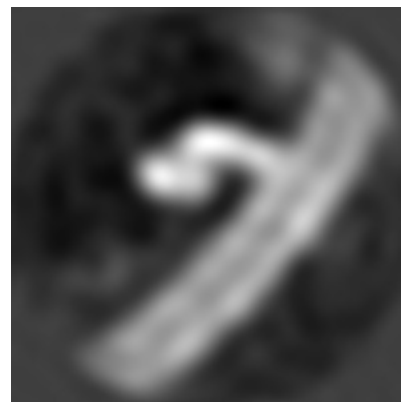
### 6.2.1 Primary map



X Index: 40

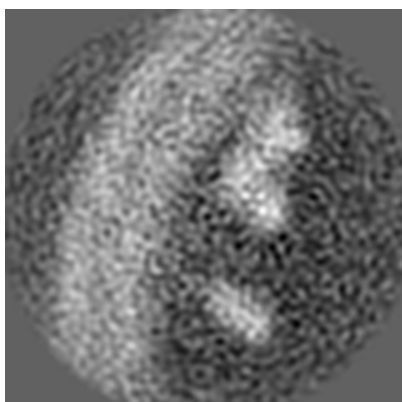


Y Index: 40

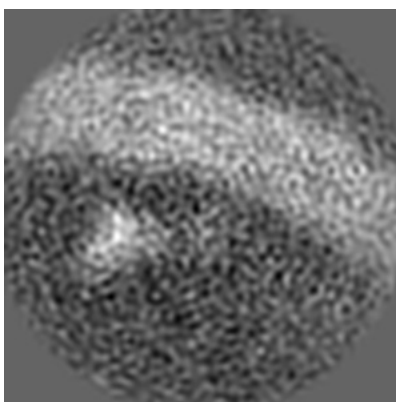


Z Index: 40

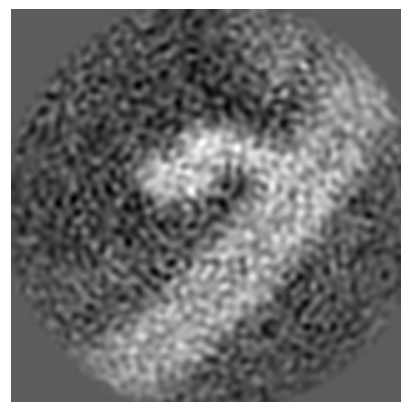
### 6.2.2 Raw map



X Index: 40



Y Index: 40

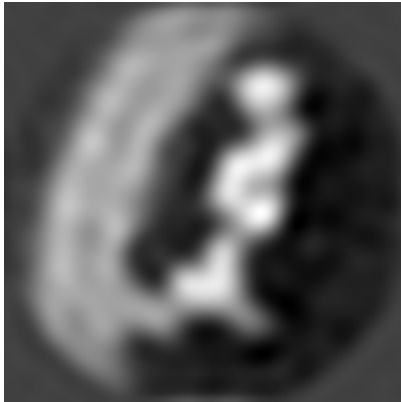


Z Index: 40

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

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

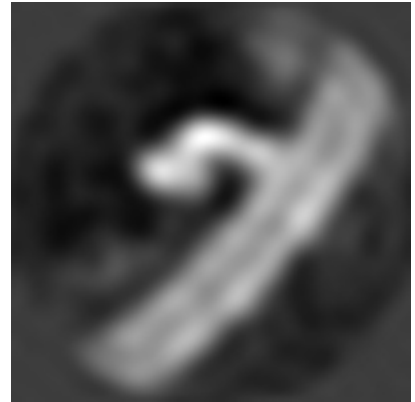
### 6.3.1 Primary map



X Index: 35

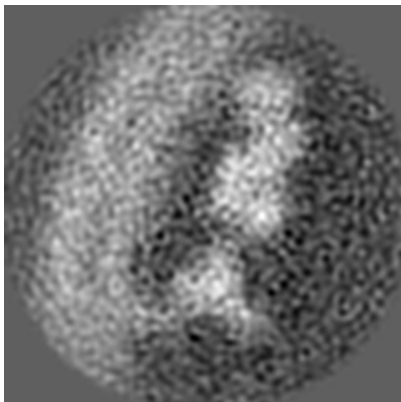


Y Index: 50

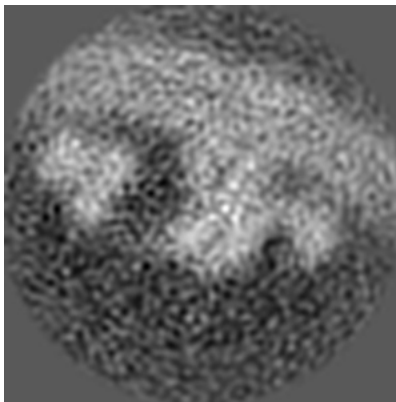


Z Index: 39

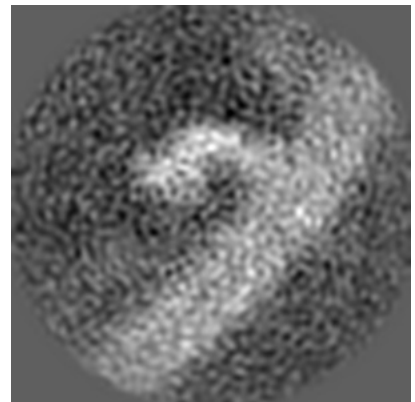
### 6.3.2 Raw map



X Index: 36



Y Index: 49

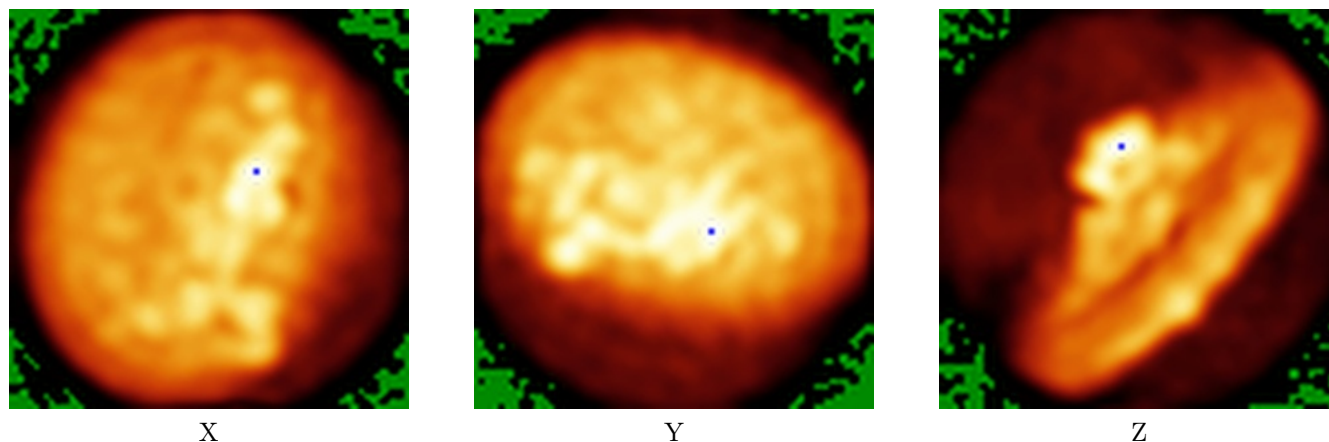


Z Index: 39

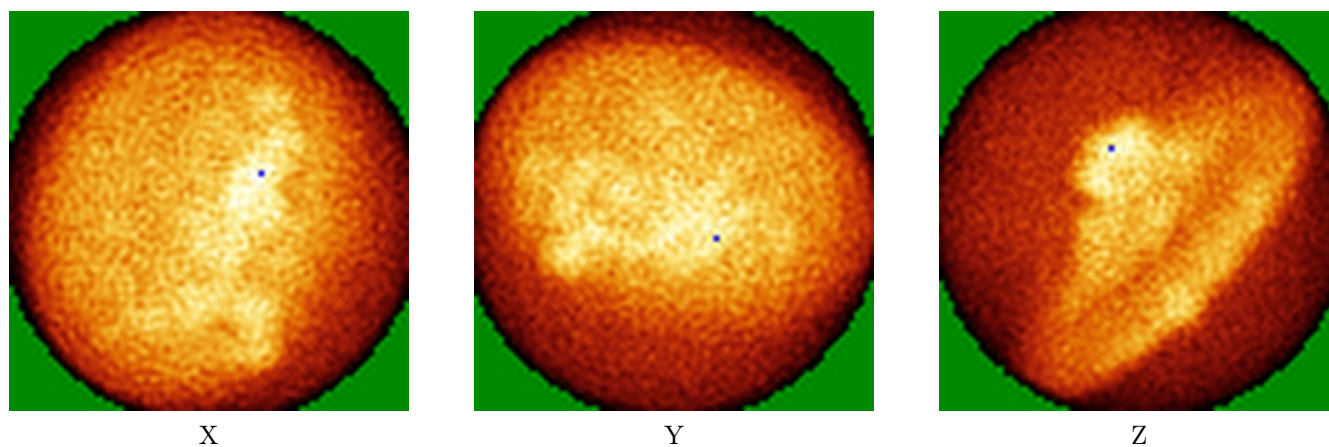
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



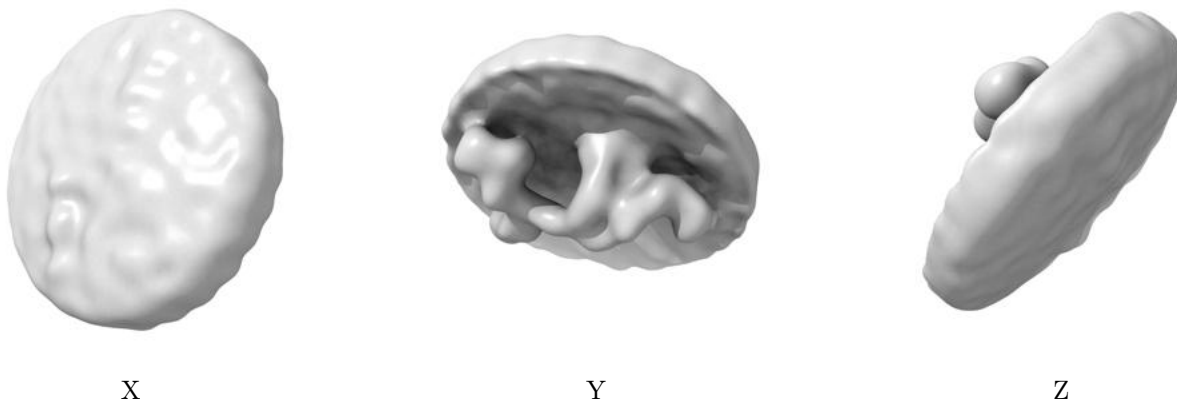
### 6.4.2 Raw map



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.

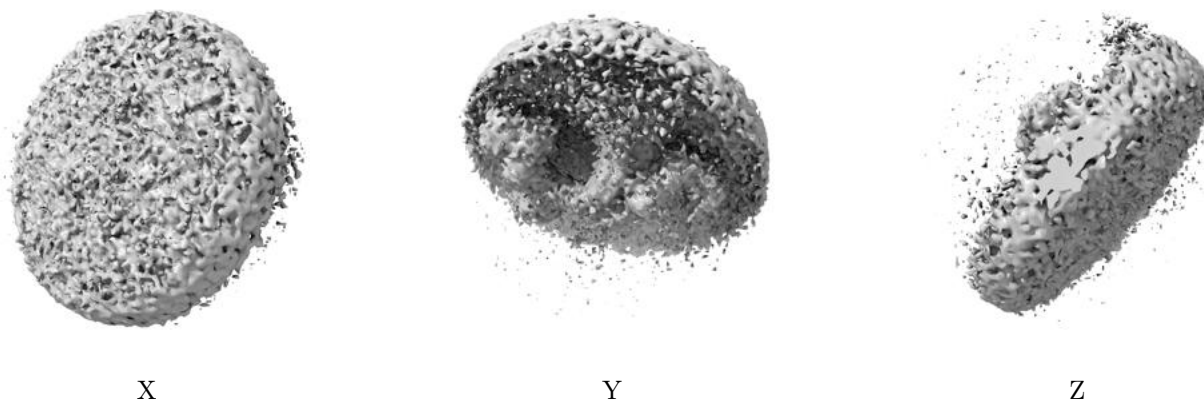
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

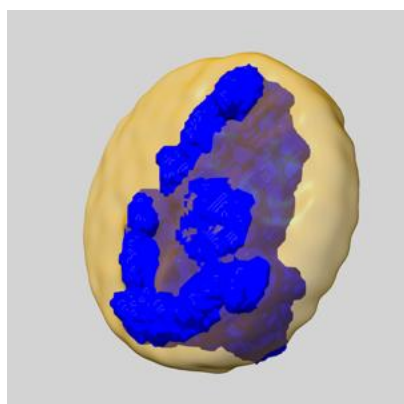
## 6.6 Mask visualisation [i](#)

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

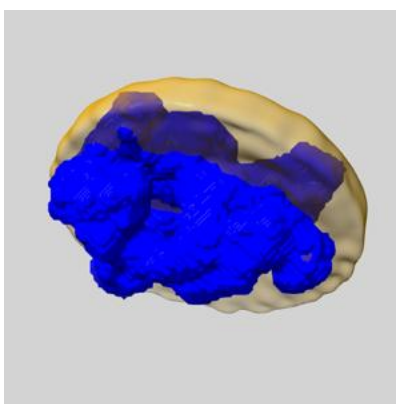
A mask typically either:

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

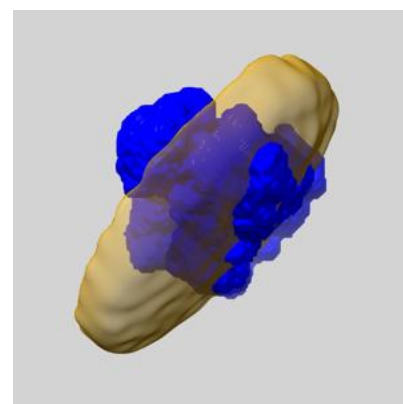
### 6.6.1 emd\_26965\_msk\_1.map [i](#)



X



Y



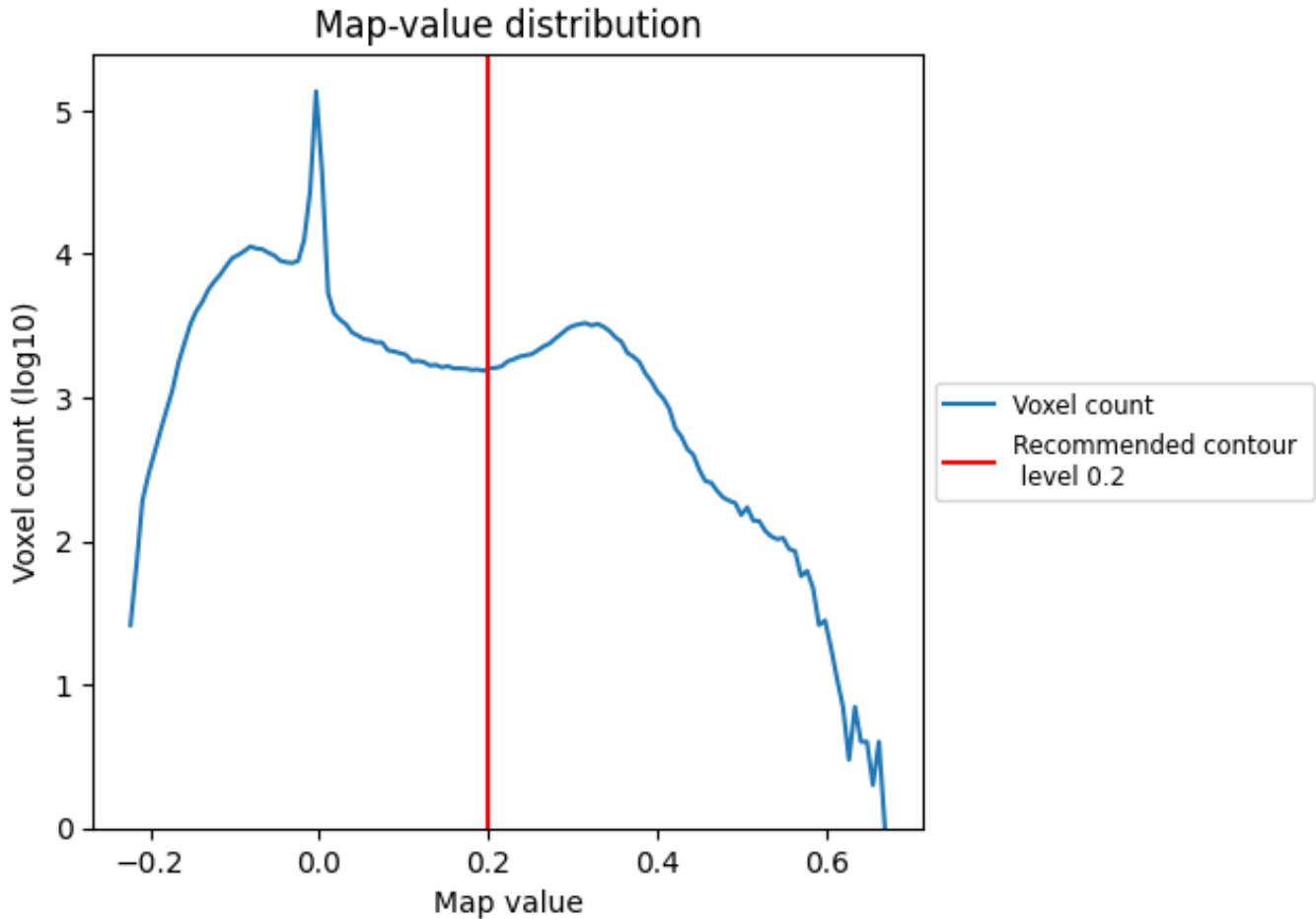
Z



## 7 Map analysis [i](#)

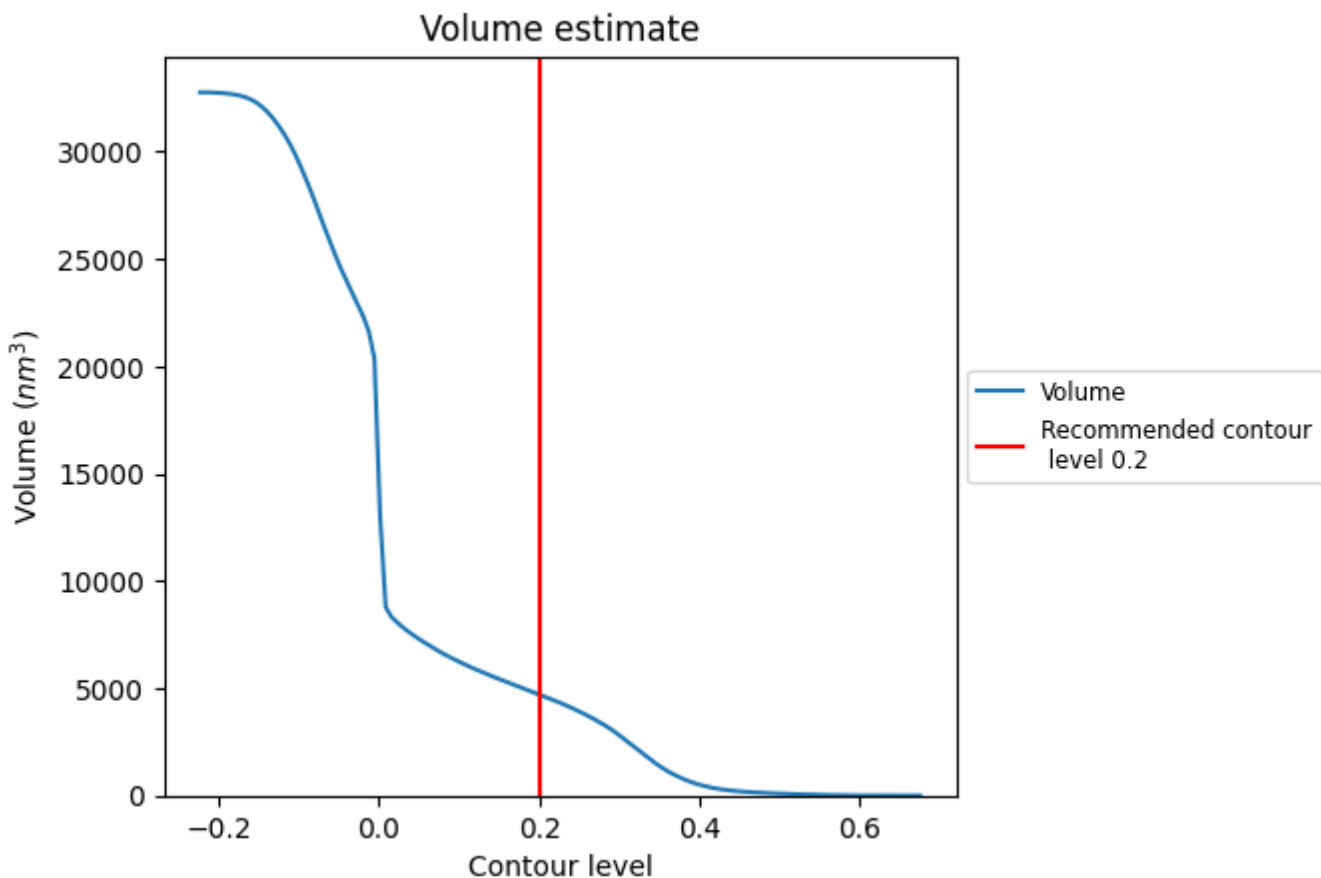
This section contains the results of statistical analysis of the map.

### 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.

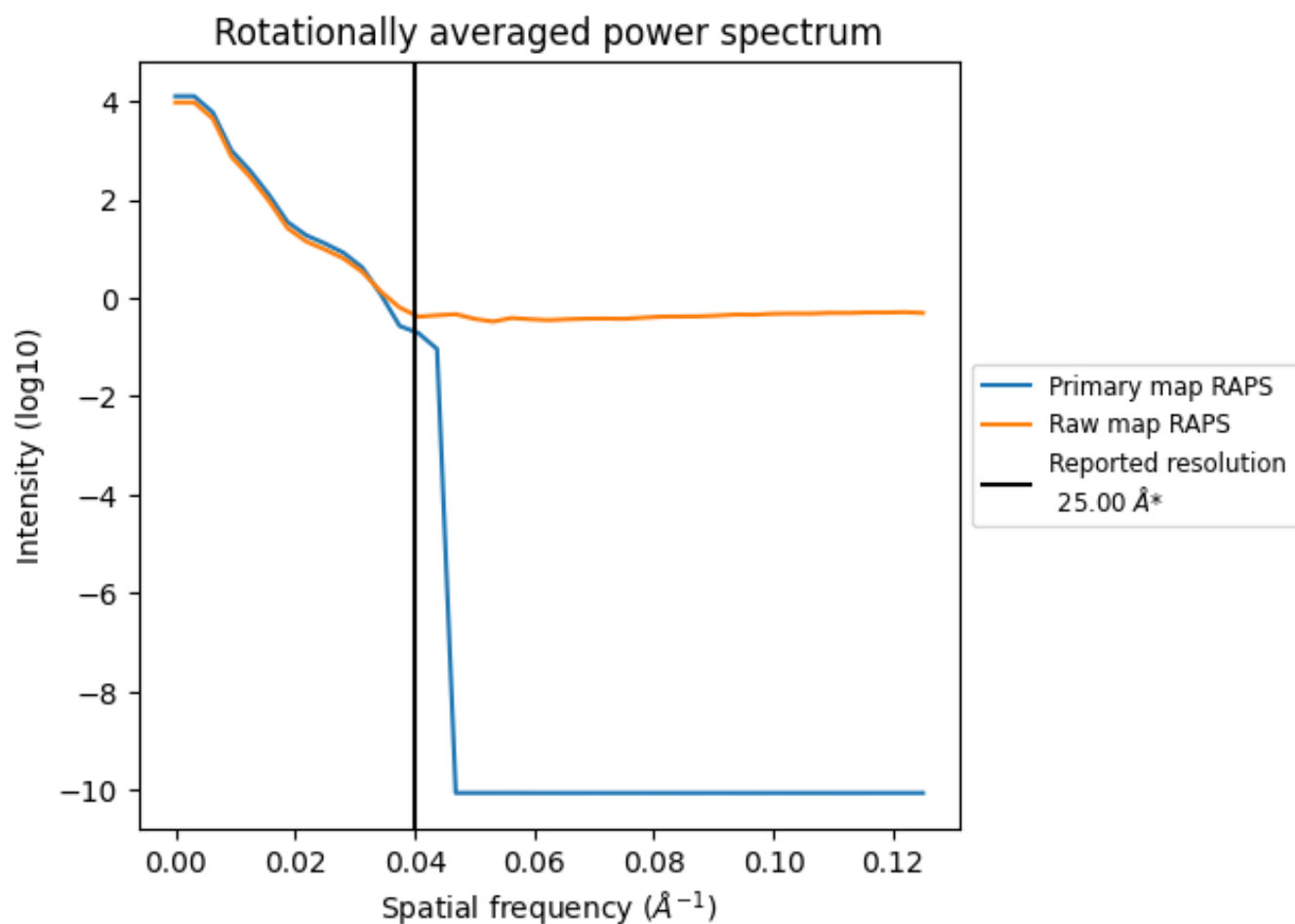
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4716 nm<sup>3</sup>; this corresponds to an approximate mass of 4260 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 [\(i\)](#)

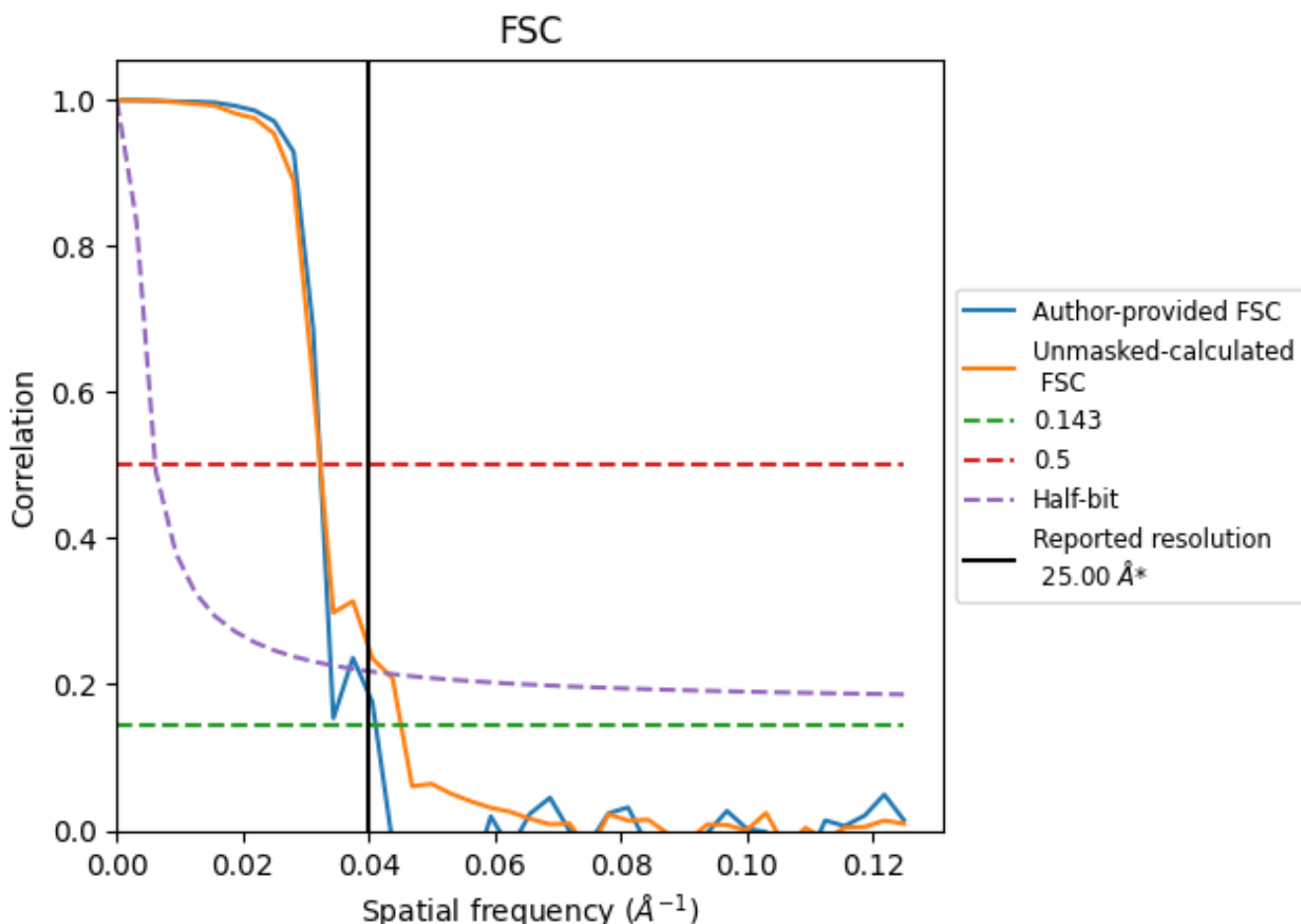


\*Reported resolution corresponds to spatial frequency of 0.040 Å<sup>-1</sup>

## 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 0.040 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

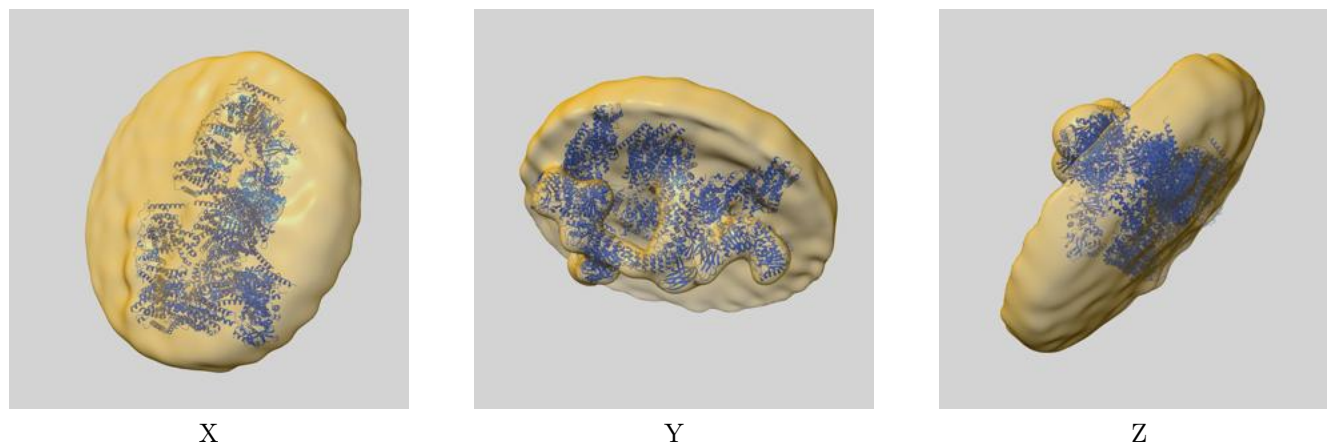
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	25.00	-	-
Author-provided FSC curve	24.33	30.96	29.41
Unmasked-calculated*	22.17	30.86	23.26

\*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 22.17 differs from the reported value 25.0 by more than 10 %

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

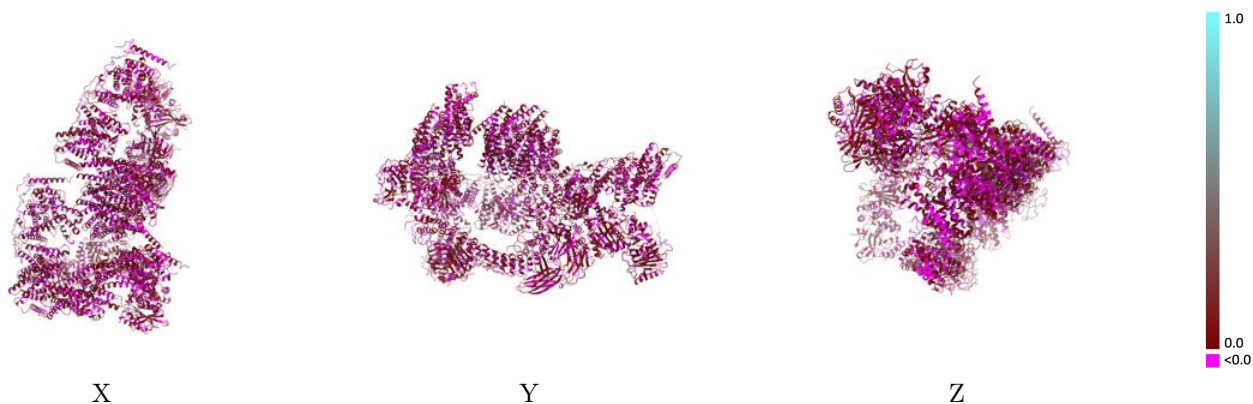
This section contains information regarding the fit between EMDB map EMD-26965 and PDB model 8CSL. Per-residue inclusion information can be found in section 3 on page 6.

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



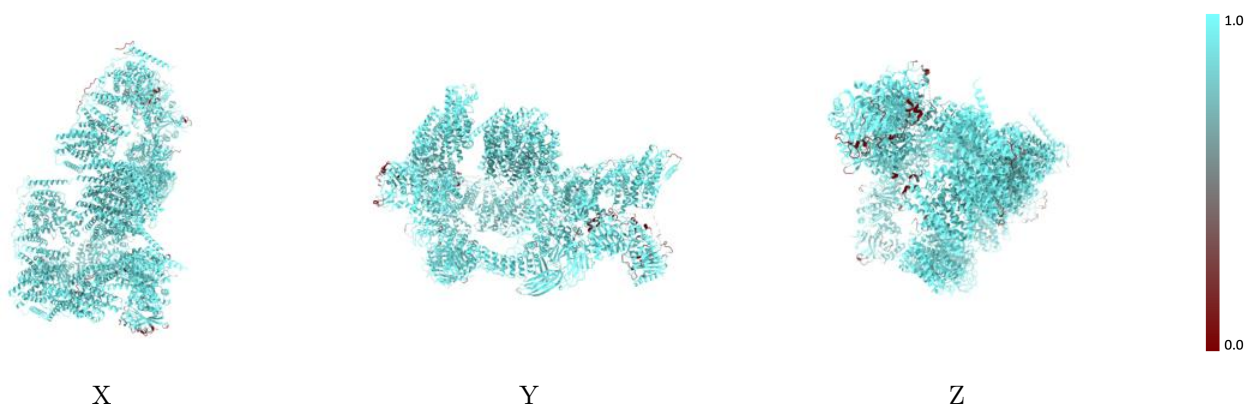
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



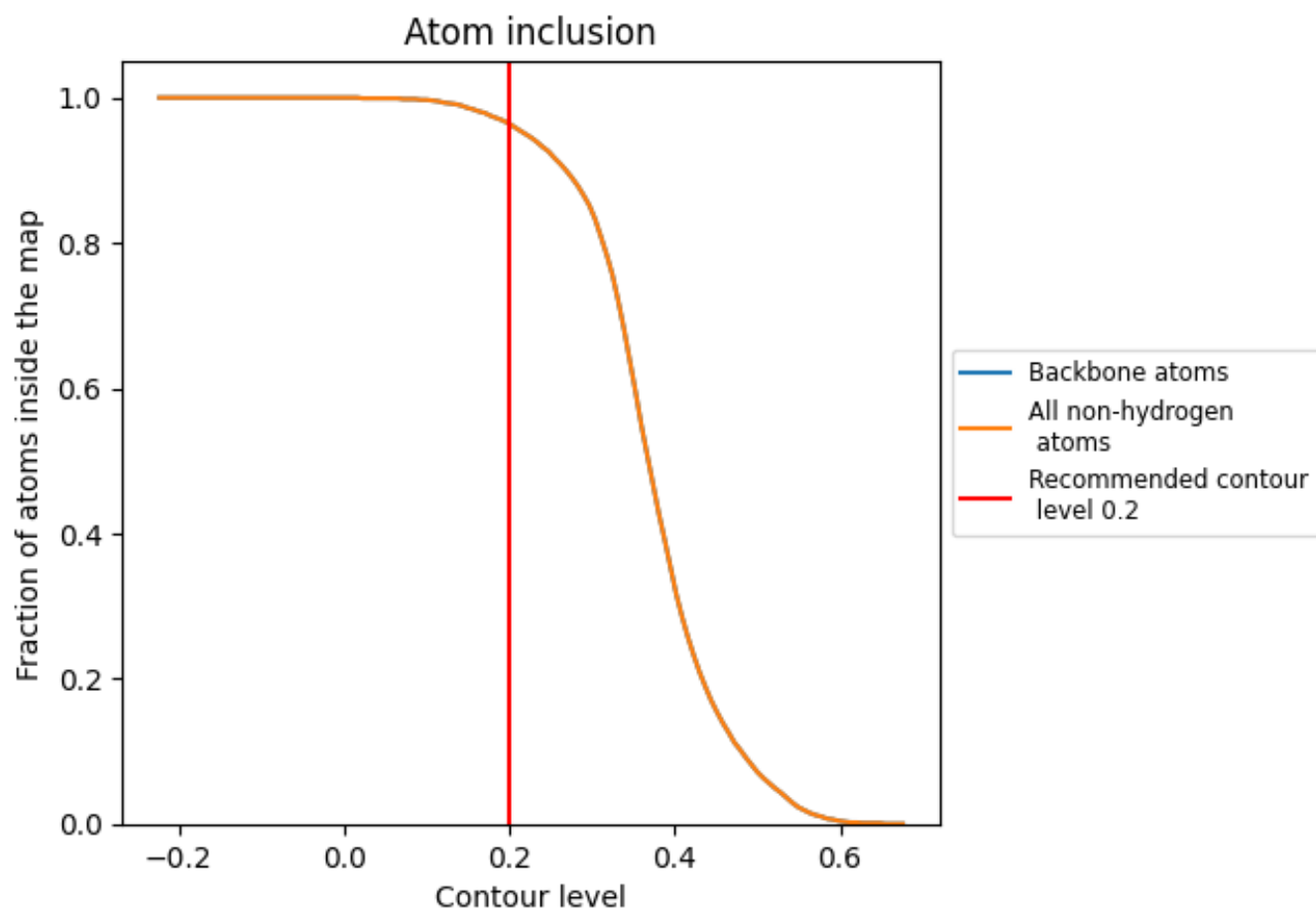
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

## 9.4 Atom inclusion [i](#)











































At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.0460
A	 0.9870	 0.0710
K	 1.0000	 0.0380
L	 1.0000	 0.0390
P	 1.0000	 0.0190
Q	 0.9980	 0.0360
R	 0.9650	 0.0300
S	 1.0000	 0.0190
T	 0.9730	 0.0340
V	 0.9410	 0.0410
W	 0.9500	 0.0330
X	 0.9760	 0.0510
Y	 0.9710	 0.0490
Z	 0.9650	 0.0460
a	 0.8310	 -0.0110
b	 1.0000	 0.0050
c	 1.0000	 -0.0250
e	 0.9030	 0.0440
f	 0.9790	 0.0520
g	 0.9400	 0.0440

