WORLDWIDE wwPDB
PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Aug 29, 2023 – 01:52 pm BST

PDB ID	:	8CE8
EMDB ID	:	EMD-16601
Title	:	Cytochrome c maturation complex CcmABCDE
Authors	:	Ilcu, L.; Zhang, L.; Einsle, O.
Deposited on	:	2023-02-01
Resolution	:	3.81 Å(reported)

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

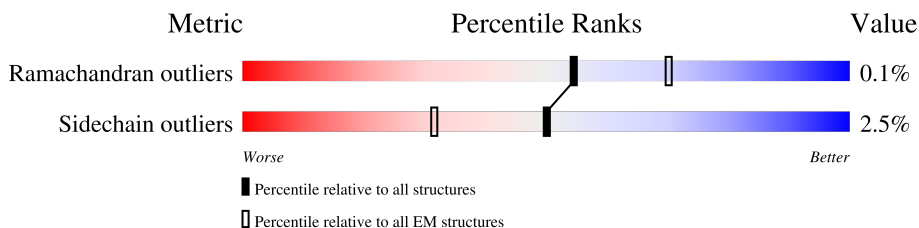|		
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)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

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.81 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	Percentile Ranks	Value
Ramachandran outliers		0.1%
Sidechain outliers		2.5%

Worse   *Better*

▊ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	218	5% 90% · 7%
1	a	218	· 89% 5% 7%
2	B	220	97% ·
2	b	220	97% ·
3	C	245	· 96% · ·
3	c	245	· 96% · ·
4	D	69	16% 97% ··
4	d	69	13% 96% · ·
5	E	159	75% 96% · ·

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 12674 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 Cytochrome c biogenesis ATP-binding export protein CcmA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	203	Total	C	N	O	S	0	0
			1595	999	296	295	5		
1	a	203	Total	C	N	O	S	0	0
			1595	999	296	295	5		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP P33931
A	-9	ALA	-	expression tag	UNP P33931
A	-8	SER	-	expression tag	UNP P33931
A	-7	TRP	-	expression tag	UNP P33931
A	-6	SER	-	expression tag	UNP P33931
A	-5	HIS	-	expression tag	UNP P33931
A	-4	PRO	-	expression tag	UNP P33931
A	-3	GLN	-	expression tag	UNP P33931
A	-2	PHE	-	expression tag	UNP P33931
A	-1	GLU	-	expression tag	UNP P33931
A	0	LYS	-	expression tag	UNP P33931
a	-10	MET	-	initiating methionine	UNP P33931
a	-9	ALA	-	expression tag	UNP P33931
a	-8	SER	-	expression tag	UNP P33931
a	-7	TRP	-	expression tag	UNP P33931
a	-6	SER	-	expression tag	UNP P33931
a	-5	HIS	-	expression tag	UNP P33931
a	-4	PRO	-	expression tag	UNP P33931
a	-3	GLN	-	expression tag	UNP P33931
a	-2	PHE	-	expression tag	UNP P33931
a	-1	GLU	-	expression tag	UNP P33931
a	0	LYS	-	expression tag	UNP P33931

- Molecule 2 is a protein called Heme exporter protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	219	Total 1656	C 1111	N 265	O 271	S 9	0	0
2	b	219	Total 1656	C 1111	N 265	O 271	S 9	0	0

• Molecule 3 is a protein called Heme exporter protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	241	Total 1930	C 1289	N 327	O 302	S 12	0	0
3	c	241	Total 1930	C 1289	N 327	O 302	S 12	0	0

• Molecule 4 is a protein called Heme exporter protein D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	68	Total 538	C 349	N 99	O 87	S 3	0	0
4	d	68	Total 538	C 349	N 99	O 87	S 3	0	0

• Molecule 5 is a protein called Cytochrome c-type biogenesis protein CcmE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	158	Total 1236	C 780	N 219	O 232	S 5	0	0

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: Cytochrome c biogenesis ATP-binding export protein CcmA

Chain A:
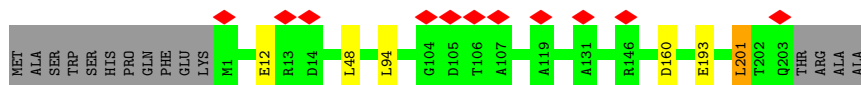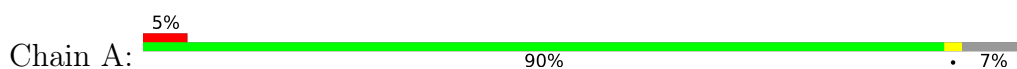
• Molecule 1: Cytochrome c biogenesis ATP-binding export protein CcmA

Chain a:
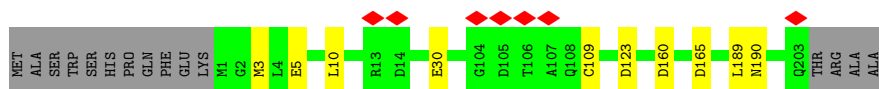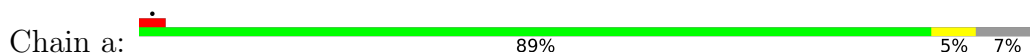
• Molecule 2: Heme exporter protein B

Chain B:

• Molecule 2: Heme exporter protein B

Chain b:

• Molecule 3: Heme exporter protein C
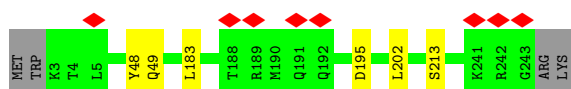
Chain C:

• Molecule 3: Heme exporter protein C

Chain c:

96%

MET TRP K3 L14 Y15 Q16 F21 Y54 H147 D150 L154 S187 T188 R189 M190 E237 K241 R242 G243 ARG LYS

• Molecule 4: Heme exporter protein D

Chain D:

16%

97%

MET T2 F11 E57 A58 R59 L60 R61 A62 A63 Q64 Q65 Q66 E67 A68 A69

• Molecule 4: Heme exporter protein D

Chain d:

13%

96%

MET T2 S7 M27 R61 A62 A63 Q64 Q65 Q66 E67 A68 A69
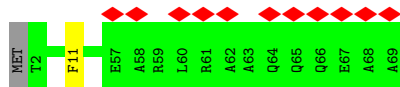
• Molecule 5: Cytochrome c-type biogenesis protein CcmE

Chain E:

75%

96%

MET N2 I3 W10 C13 L19 L27 N33 I34 D35 L36 F37 Y38 T39 P40 G41 E42 I43 L44 Y45 G46 K47 R48 E49 T50 Q51 Q52 M53 P54 E55 V56 G57 Q58 R59 L60 R61 V62 G63 G64 M65 V66 M67 P68 G69 S70 V71 Q72 R73 D74 P75 N76 S77 L78 K79 V80

T81 F82 T83 I84 Y85 D86 A87 E88 G89 S90 S94 Y95 E96 G97 I98 L99 P100 D101 L102 F103 R104 E105 G106 Q107 G108 V109 Q112 G113 E114 L115 E116 K117 G118 N119 H120 I121 L122 A123 K124 E125 V126 L127 A128 K129 H130 D131 E132 N133 Y134 T135 P136 P137 E138 V139 E140 K141 A142 M143

E144 A145 N146 H147 R148 R149 P150 A151 S152 V153 Y154 K155 D156 P157 A158 S159

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135175	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.185	Depositor
Minimum map value	-1.441	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.086	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	208.8, 208.8, 208.8	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.35	0/1624	0.75	2/2204 (0.1%)
1	a	0.35	0/1624	0.80	3/2204 (0.1%)
2	B	0.32	0/1696	0.73	3/2322 (0.1%)
2	b	0.32	0/1696	0.72	1/2322 (0.0%)
3	C	0.33	0/1994	0.72	3/2726 (0.1%)
3	c	0.33	0/1994	0.70	5/2726 (0.2%)
4	D	0.30	0/551	0.60	0/747
4	d	0.36	0/551	0.76	1/747 (0.1%)
5	E	0.29	0/1259	0.65	0/1703
All	All	0.33	0/12989	0.72	18/17701 (0.1%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	195	ASP	CB-CG-OD1	8.22	125.70	118.30
1	A	201	LEU	CA-CB-CG	6.98	131.36	115.30
1	a	165	ASP	CB-CG-OD1	6.93	124.54	118.30
3	C	202	LEU	CA-CB-CG	6.64	130.57	115.30
3	c	16	GLN	CA-CB-CG	6.56	127.84	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	201/218 (92%)	192 (96%)	9 (4%)	0	100	100
1	a	201/218 (92%)	193 (96%)	8 (4%)	0	100	100
2	B	217/220 (99%)	213 (98%)	4 (2%)	0	100	100
2	b	217/220 (99%)	210 (97%)	7 (3%)	0	100	100
3	C	239/245 (98%)	233 (98%)	6 (2%)	0	100	100
3	c	239/245 (98%)	231 (97%)	8 (3%)	0	100	100
4	D	66/69 (96%)	65 (98%)	1 (2%)	0	100	100
4	d	66/69 (96%)	66 (100%)	0	0	100	100
5	E	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	62
All	All	1602/1663 (96%)	1554 (97%)	47 (3%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	34	ILE

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	A	168/180 (93%)	163 (97%)	5 (3%)	41	66
1	a	168/180 (93%)	161 (96%)	7 (4%)	30	58
2	B	175/176 (99%)	171 (98%)	4 (2%)	50	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	175/176 (99%)	171 (98%)	4 (2%)	50	71
3	C	196/200 (98%)	193 (98%)	3 (2%)	65	80
3	c	196/200 (98%)	193 (98%)	3 (2%)	65	80
4	D	52/53 (98%)	51 (98%)	1 (2%)	57	76
4	d	52/53 (98%)	51 (98%)	1 (2%)	57	76
5	E	132/133 (99%)	127 (96%)	5 (4%)	33	60
All	All	1314/1351 (97%)	1281 (98%)	33 (2%)	50	70

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	27	LEU
5	E	33	ASN
5	E	143	MET
4	D	11	PHE
3	C	213	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	101	HIS
3	c	85	GLN
5	E	2	ASN
3	c	169	ASN
4	D	38	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-16601. 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 ⓘ
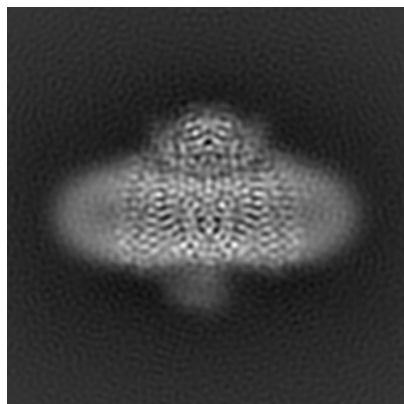
6.1.1 Primary map

X
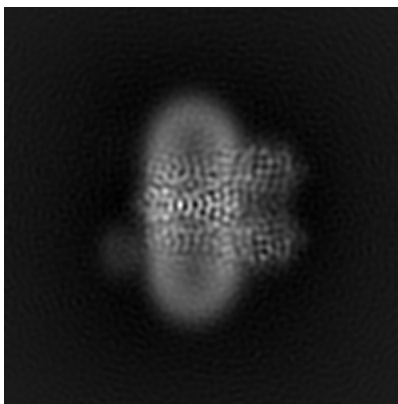
Y
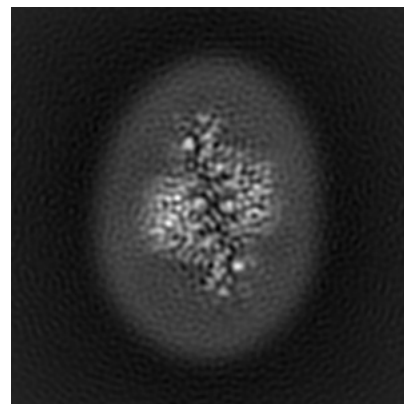
Z

6.1.2 Raw map

X

Y

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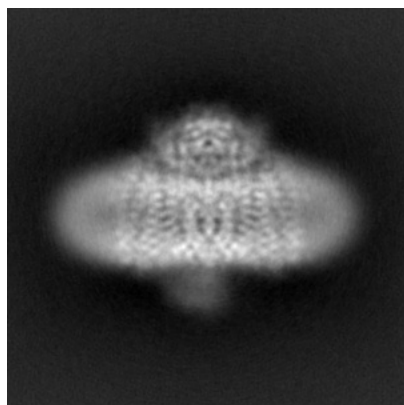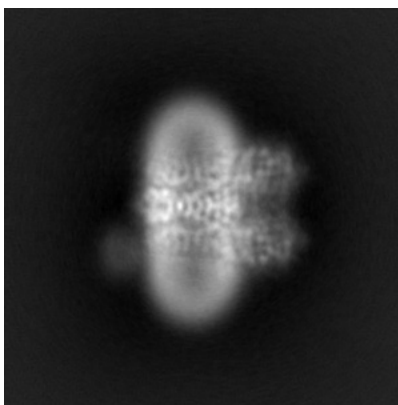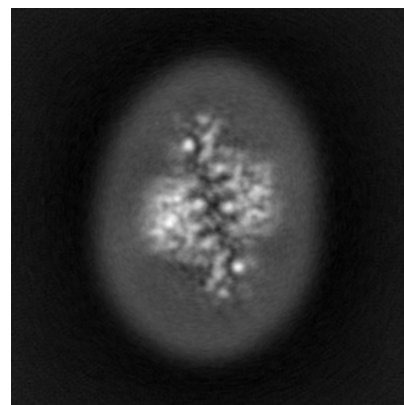
The images above show the map projected vl in three orthogonal directions.

6.2 Central slices ⓘ
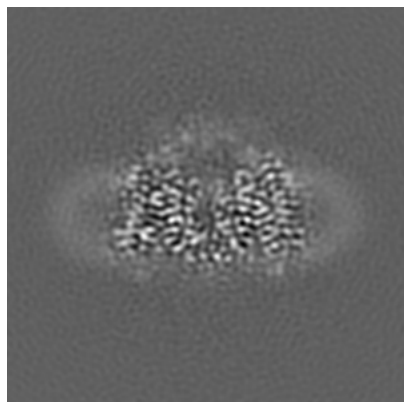
6.2.1 Primary map
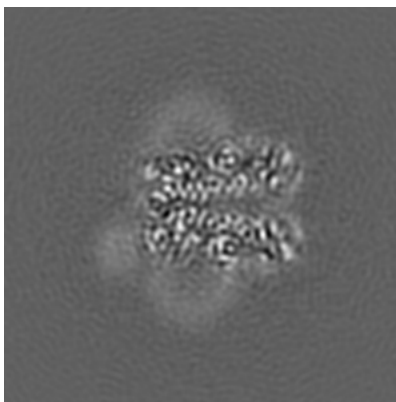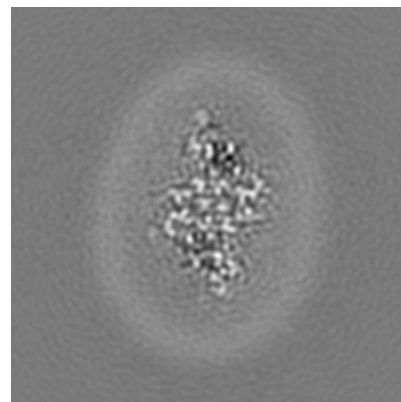
| X Index: 120 | Y Index: 120 | Z Index: 120 |

6.2.2 Raw map
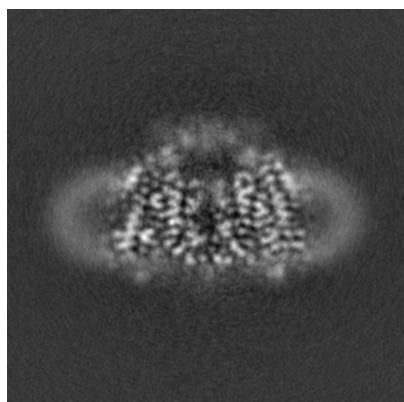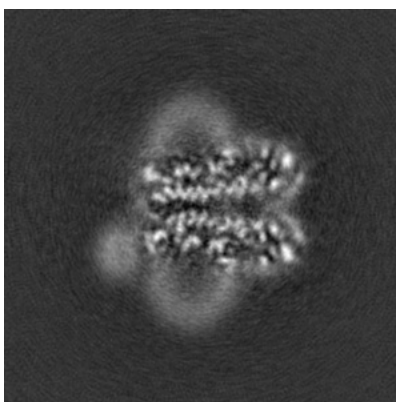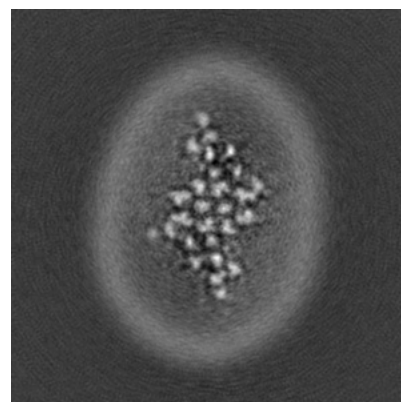
| X Index: 120 | Y Index: 120 | Z Index: 120 |

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

6.3   Largest variance slices   ⓘ
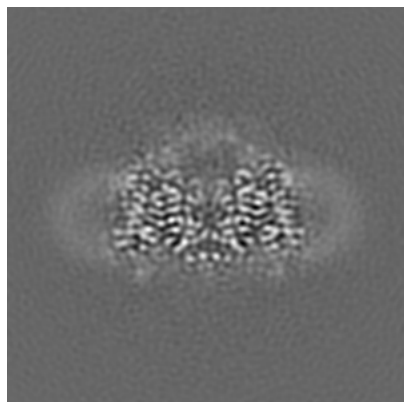
6.3.1   Primary map
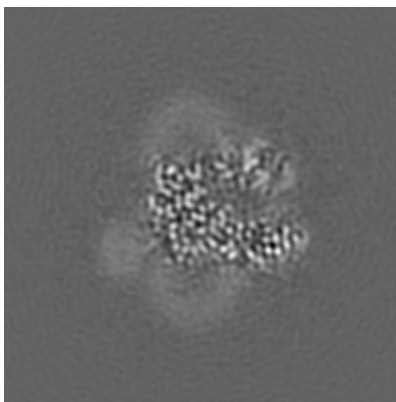
| X Index: 121 | Y Index: 110 | Z Index: 97 |
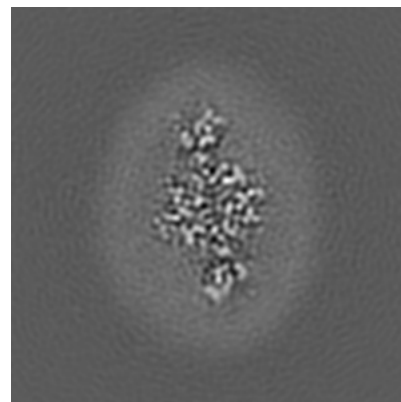
6.3.2   Raw map
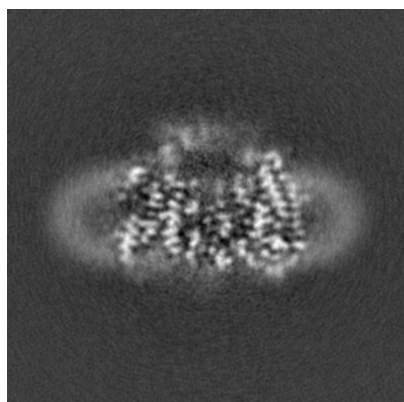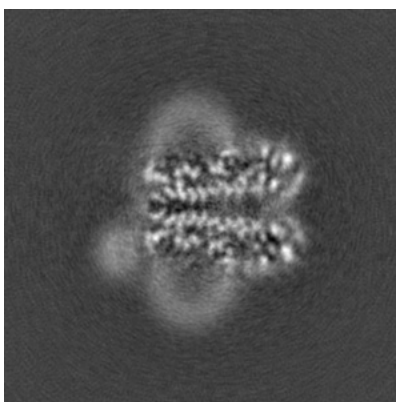
| X Index: 118 | Y Index: 121 | Z Index: 97 |
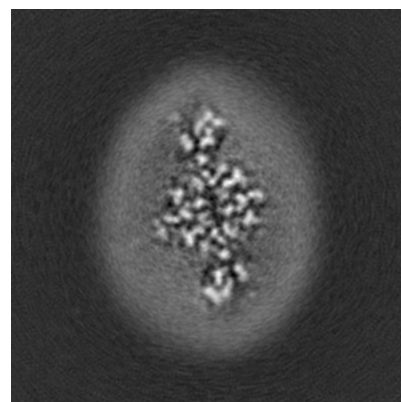
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
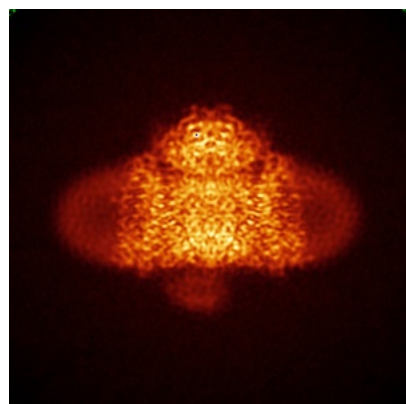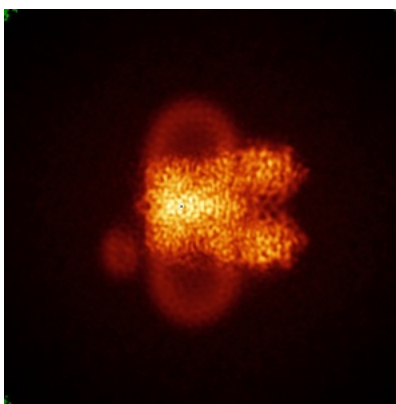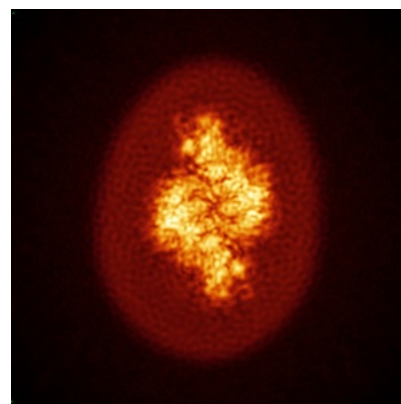
X	Y	Z

6.4.2 Raw map

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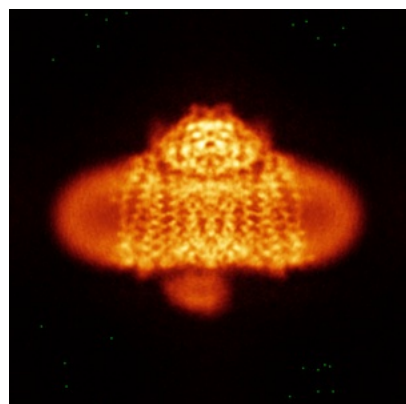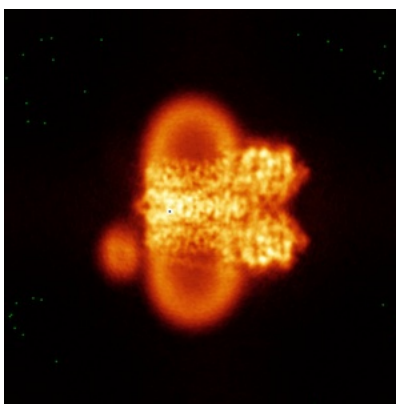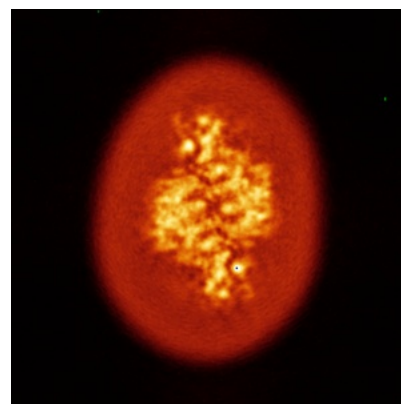
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5   Orthogonal surface views   ⓘ

6.5.1   Primary map

X   Y   Z
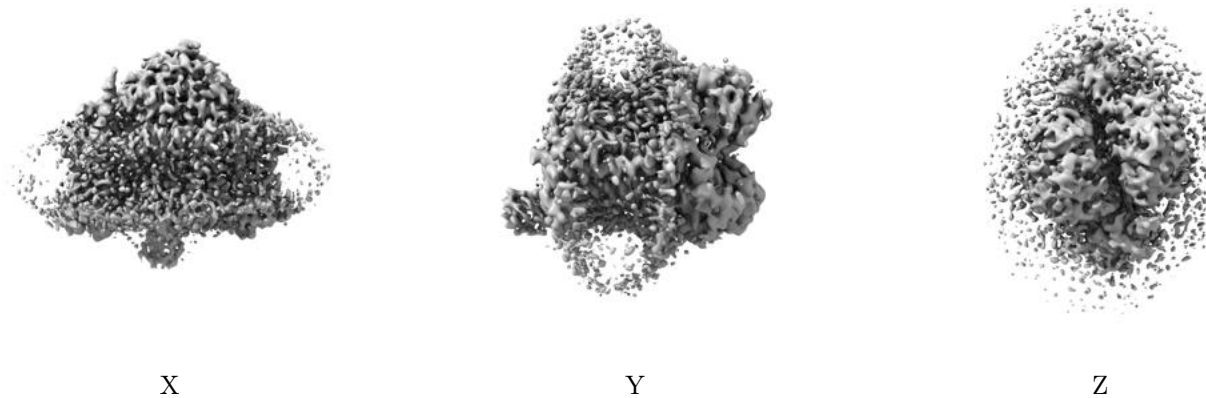
The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2   Raw map

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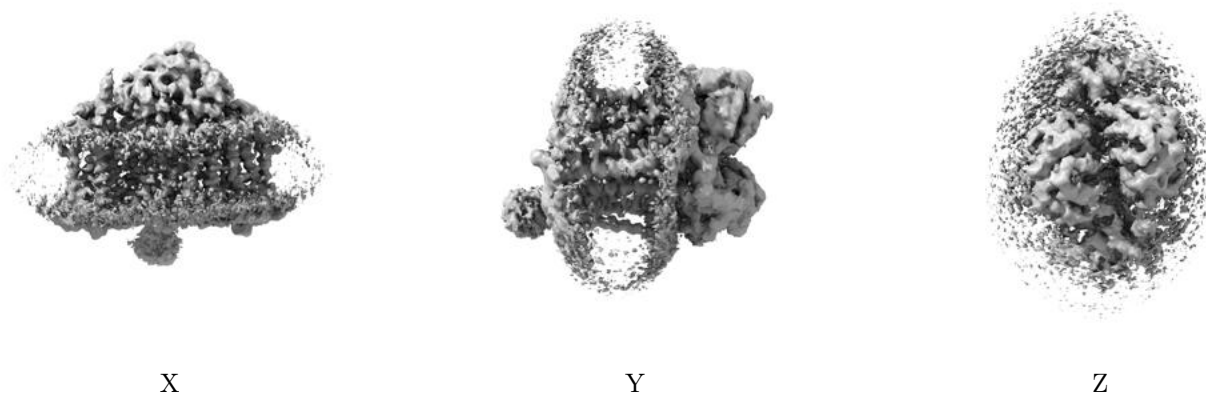
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6   Mask visualisation   ⓘ

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

7 Map analysis ⓘ

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

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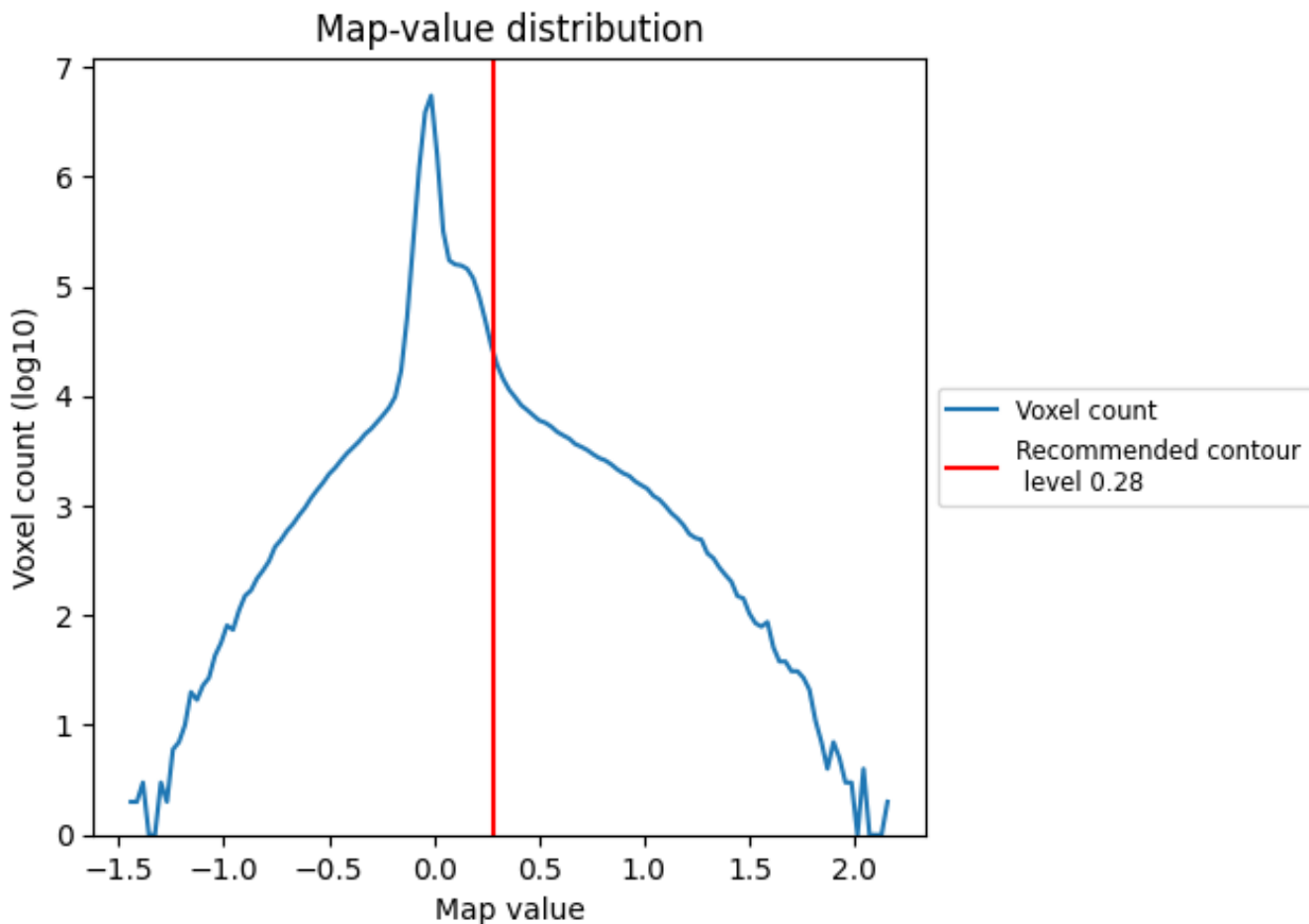
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
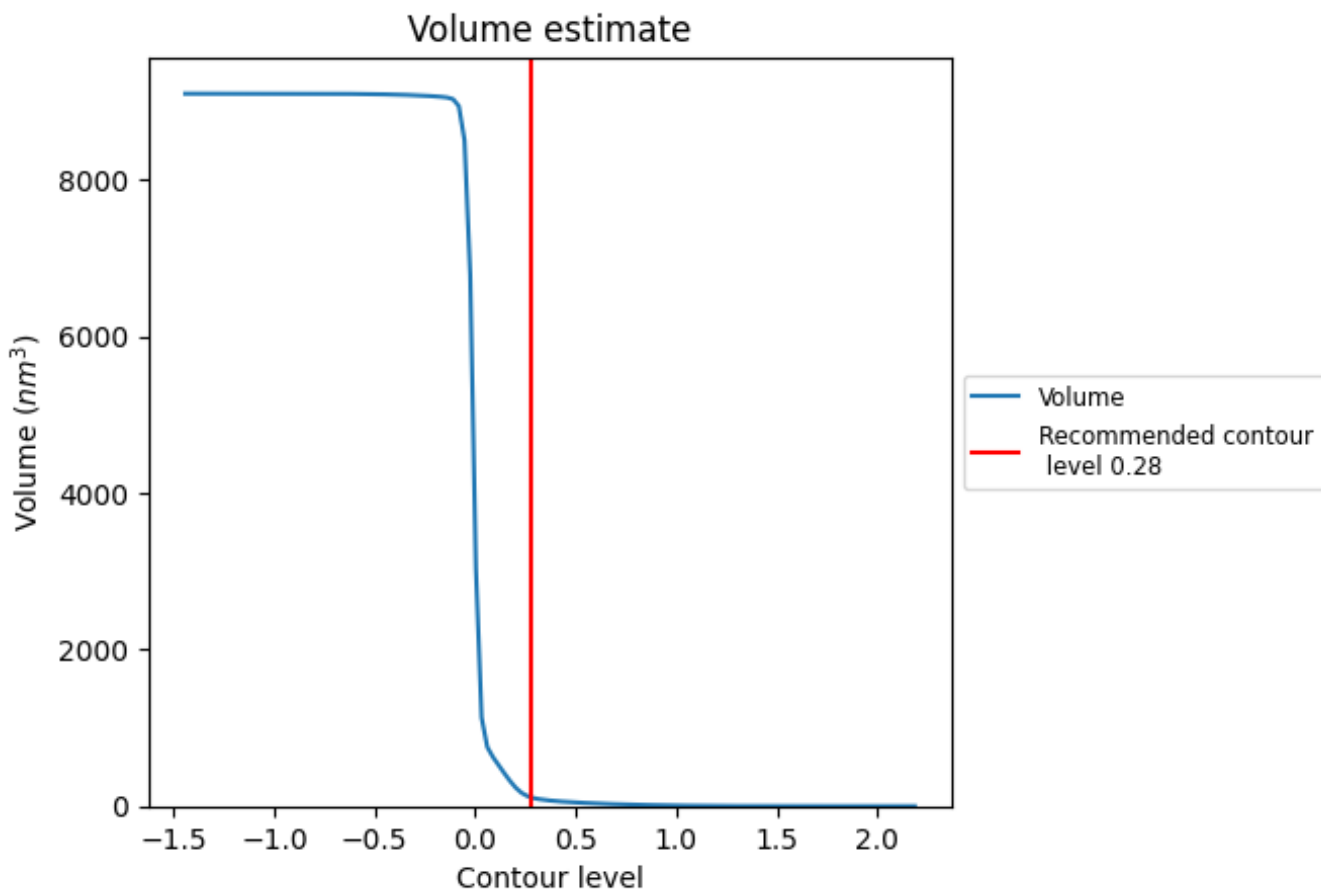
The volume at the recommended contour level is 111 nm^3; this corresponds to an approximate mass of 101 kDa.

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 ⓘ
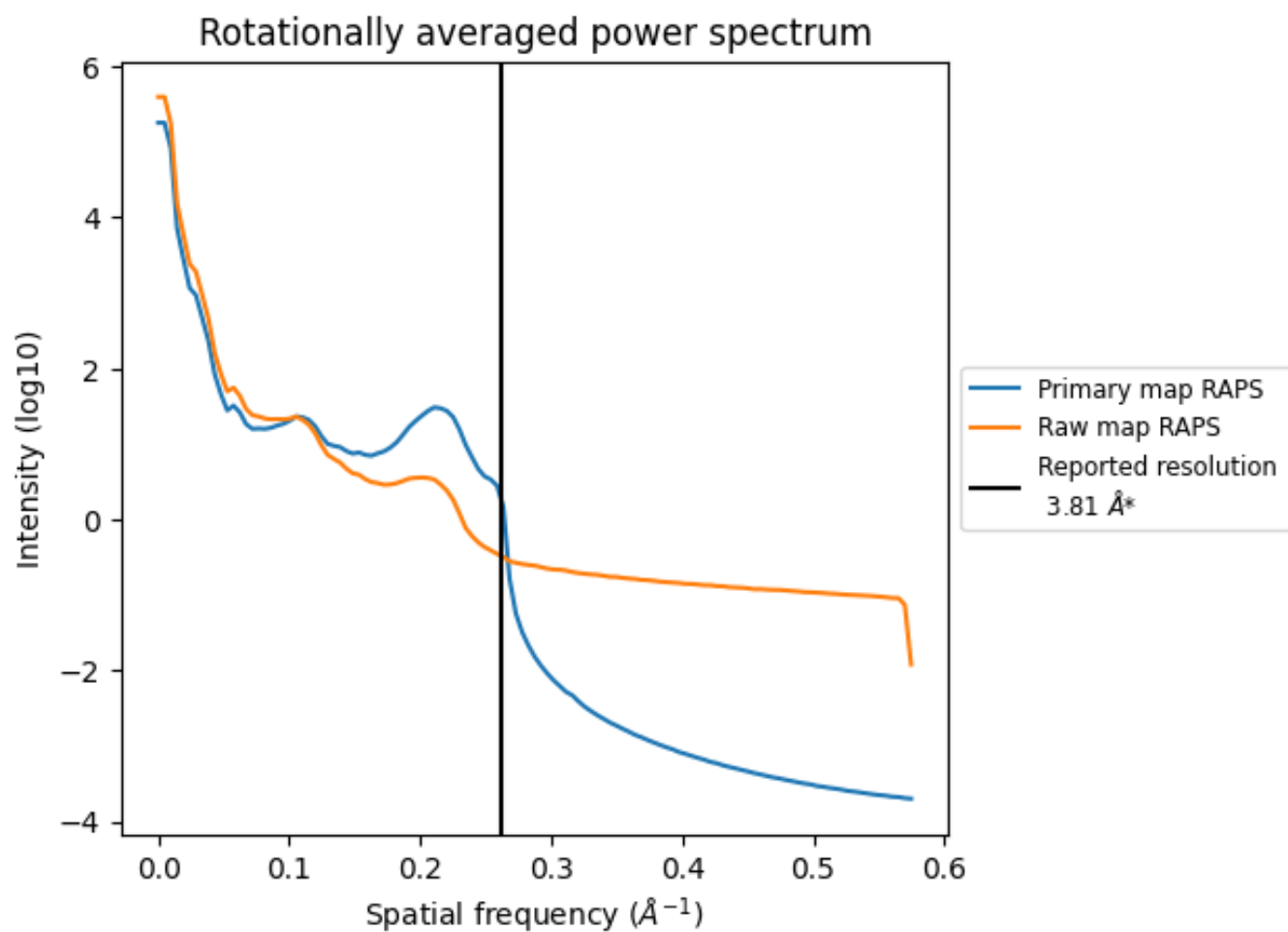
*Reported resolution corresponds to spatial frequency of 0.262 Å^{-1}

8   Fourier-Shell correlation ⓘ

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 ⓘ
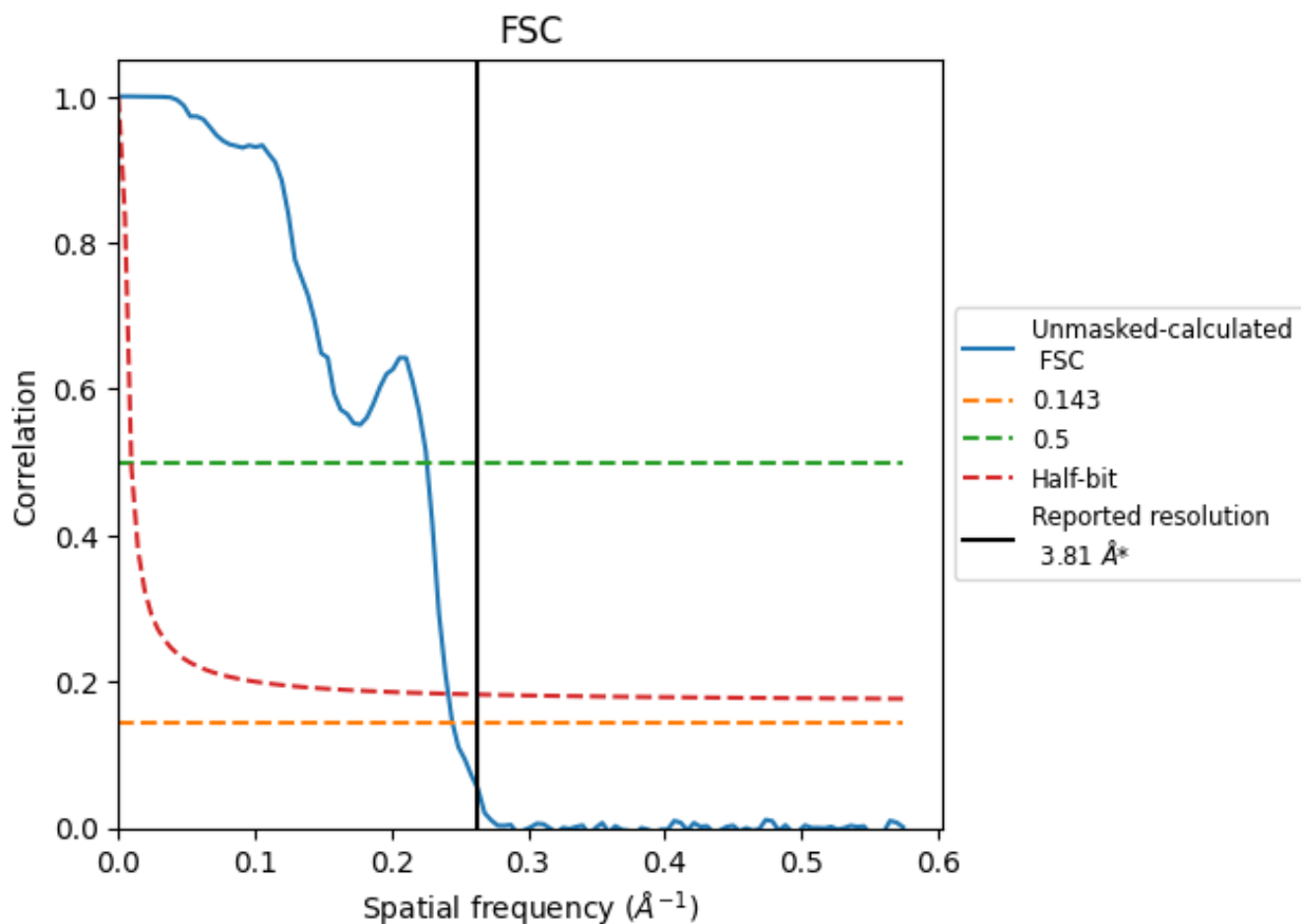
*Reported resolution corresponds to spatial frequency of 0.262 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.81	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.09	4.43	4.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-16601 and PDB model 8CE8. Per-residue inclusion information can be found in section 3 on page 5.

9.1   Map-model overlay ⓘ

X   Y   Z
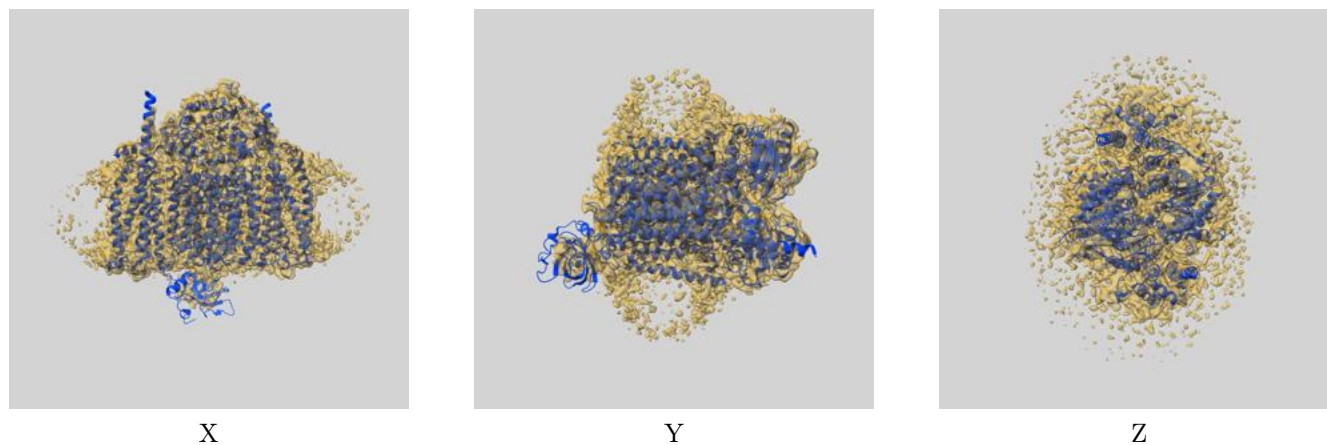
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

The images above show the model with each residue coloured according 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 ⓘ
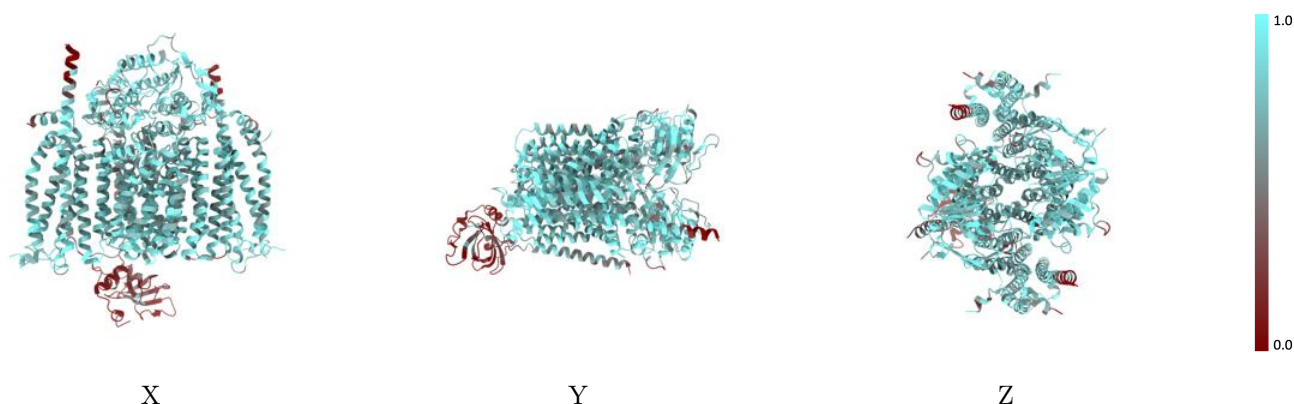
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.28).

9.4 Atom inclusion (i)
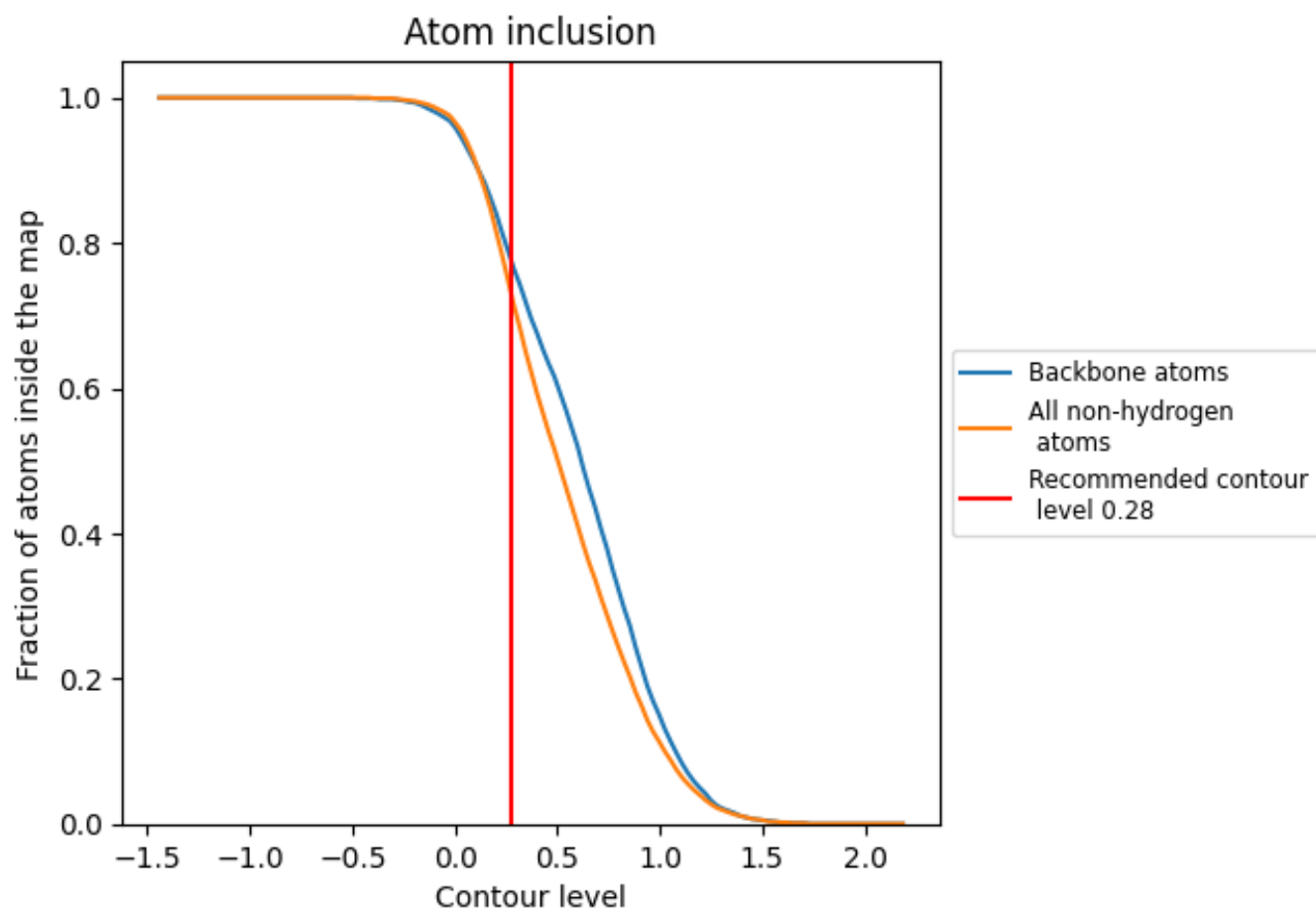
At the recommended contour level, 77% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7230	0.3780
A	0.7780	0.3900
B	0.7990	0.4360
C	0.7730	0.4010
D	0.6920	0.3420
E	0.2060	0.1320
a	0.7870	0.3930
b	0.7870	0.4400
c	0.7980	0.4060
d	0.7080	0.3420

1.0

0.0
<0.0