



wwPDB EM Validation Summary Report ⓘ

Dec 30, 2024 – 03:50 PM EST

PDB ID : 8E2E
EMDB ID : EMD-27833
Title : Cryo-EM structure of helical arch of BIRC6 (from local refinement 1)
Authors : Hunkeler, M.; Fischer, E.S.
Deposited on : 2022-08-15
Resolution : 1.98 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

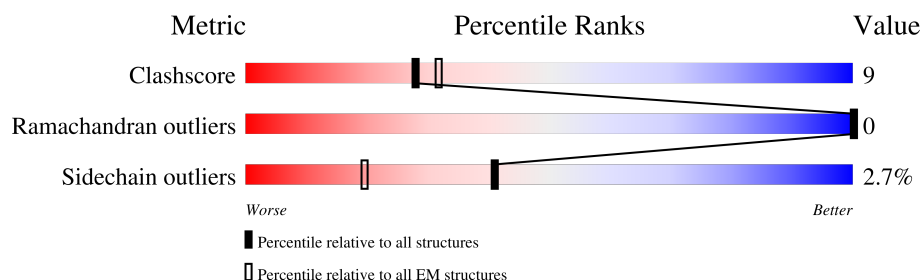
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.98 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	A	4888	
1	B	4888	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26633 atoms, of which 13332 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 Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	827	Total	C	H	N	O	S	23	0
			13128	4144	6666	1091	1178	49		
1	B	827	Total	C	H	N	O	S	23	0
			13128	4144	6666	1091	1178	49		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	expression tag	UNP Q9NR09
A	-29	ASP	-	expression tag	UNP Q9NR09
A	-28	TYR	-	expression tag	UNP Q9NR09
A	-27	LYS	-	expression tag	UNP Q9NR09
A	-26	ASP	-	expression tag	UNP Q9NR09
A	-25	ASP	-	expression tag	UNP Q9NR09
A	-24	ASP	-	expression tag	UNP Q9NR09
A	-23	ASP	-	expression tag	UNP Q9NR09
A	-22	LYS	-	expression tag	UNP Q9NR09
A	-21	LEU	-	expression tag	UNP Q9NR09
A	-20	ALA	-	expression tag	UNP Q9NR09
A	-19	ALA	-	expression tag	UNP Q9NR09
A	-18	ALA	-	expression tag	UNP Q9NR09
A	-17	ASN	-	expression tag	UNP Q9NR09
A	-16	SER	-	expression tag	UNP Q9NR09
A	-15	SER	-	expression tag	UNP Q9NR09
A	-14	ILE	-	expression tag	UNP Q9NR09
A	-13	ASP	-	expression tag	UNP Q9NR09
A	-12	LEU	-	expression tag	UNP Q9NR09
A	-11	ILE	-	expression tag	UNP Q9NR09
A	-10	SER	-	expression tag	UNP Q9NR09
A	-9	THR	-	expression tag	UNP Q9NR09
A	-8	SER	-	expression tag	UNP Q9NR09
A	-7	LEU	-	expression tag	UNP Q9NR09
A	-6	TYR	-	expression tag	UNP Q9NR09
A	-5	LYS	-	expression tag	UNP Q9NR09

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	LYS	-	expression tag	UNP Q9NR09
A	-3	ALA	-	expression tag	UNP Q9NR09
A	-2	GLY	-	expression tag	UNP Q9NR09
A	-1	LEU	-	expression tag	UNP Q9NR09
A	0	THR	-	expression tag	UNP Q9NR09
A	1332	VAL	LEU	conflict	UNP Q9NR09
B	-30	MET	-	expression tag	UNP Q9NR09
B	-29	ASP	-	expression tag	UNP Q9NR09
B	-28	TYR	-	expression tag	UNP Q9NR09
B	-27	LYS	-	expression tag	UNP Q9NR09
B	-26	ASP	-	expression tag	UNP Q9NR09
B	-25	ASP	-	expression tag	UNP Q9NR09
B	-24	ASP	-	expression tag	UNP Q9NR09
B	-23	ASP	-	expression tag	UNP Q9NR09
B	-22	LYS	-	expression tag	UNP Q9NR09
B	-21	LEU	-	expression tag	UNP Q9NR09
B	-20	ALA	-	expression tag	UNP Q9NR09
B	-19	ALA	-	expression tag	UNP Q9NR09
B	-18	ALA	-	expression tag	UNP Q9NR09
B	-17	ASN	-	expression tag	UNP Q9NR09
B	-16	SER	-	expression tag	UNP Q9NR09
B	-15	SER	-	expression tag	UNP Q9NR09
B	-14	ILE	-	expression tag	UNP Q9NR09
B	-13	ASP	-	expression tag	UNP Q9NR09
B	-12	LEU	-	expression tag	UNP Q9NR09
B	-11	ILE	-	expression tag	UNP Q9NR09
B	-10	SER	-	expression tag	UNP Q9NR09
B	-9	THR	-	expression tag	UNP Q9NR09
B	-8	SER	-	expression tag	UNP Q9NR09
B	-7	LEU	-	expression tag	UNP Q9NR09
B	-6	TYR	-	expression tag	UNP Q9NR09
B	-5	LYS	-	expression tag	UNP Q9NR09
B	-4	LYS	-	expression tag	UNP Q9NR09
B	-3	ALA	-	expression tag	UNP Q9NR09
B	-2	GLY	-	expression tag	UNP Q9NR09
B	-1	LEU	-	expression tag	UNP Q9NR09
B	0	THR	-	expression tag	UNP Q9NR09
B	1332	VAL	LEU	conflict	UNP Q9NR09

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		AltConf
2	A	195	Total 195	O 195	0
2	B	182	Total 182	O 182	0







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

- Molecule 1: Baculoviral IAP repeat-containing protein 6

[illegible]







[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	1116480	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.167	Depositor
Minimum map value	-4.035	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	1.33	Depositor
Map size (Å)	422.4, 422.4, 422.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	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	0.35	0/6659	0.52	0/9058
1	B	0.35	0/6659	0.52	0/9058
All	All	0.35	0/13318	0.52	0/18116

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	6462	6666	6577	134	0
1	B	6462	6666	6577	131	0
2	A	195	0	0	5	0
2	B	182	0	0	5	0
All	All	13301	13332	13154	247	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 9.

The worst 5 of 247 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2830:GLN:NE2	1:B:2830:GLN:OE1	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3352:ALA:O	1:A:3355:THR:HG22	1.84	0.78
1:B:3352:ALA:O	1:B:3355:THR:HG22	1.84	0.77
1:B:2384:LEU:HD12	1:B:2642[A]:CYS:SG	2.24	0.76
1:A:2384:LEU:HD12	1:A:2642[A]:CYS:SG	2.25	0.76

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	820/4888 (17%)	791 (96%)	29 (4%)	0	100	100
1	B	820/4888 (17%)	790 (96%)	30 (4%)	0	100	100
All	All	1640/9776 (17%)	1581 (96%)	59 (4%)	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	A	751/4242 (18%)	731 (97%)	20 (3%)	40	30
1	B	751/4242 (18%)	731 (97%)	20 (3%)	40	30
All	All	1502/8484 (18%)	1462 (97%)	40 (3%)	41	30

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3093	ASP
1	B	3407	SER
1	B	3208	CYS
1	B	3276	SER
1	B	3455	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2830	GLN
1	B	3388	GLN
1	B	3503	HIS
1	B	3226	GLN
1	A	3069	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 ⓘ

There are no chain breaks in this entry.

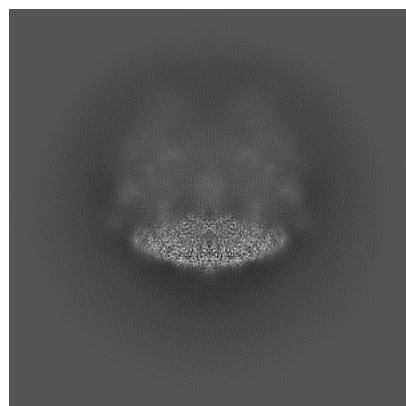
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27833. These allow visual inspection of the internal detail of the map and identification of artifacts.

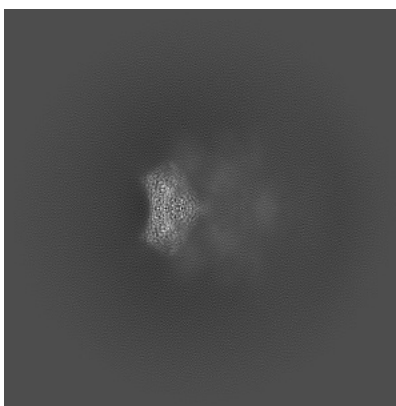
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

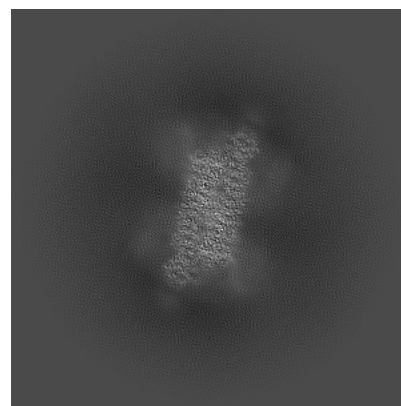
6.1.1 Primary map



X

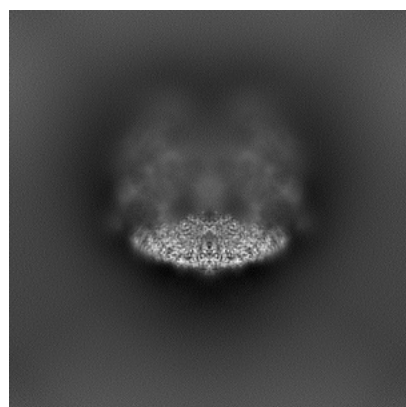


Y

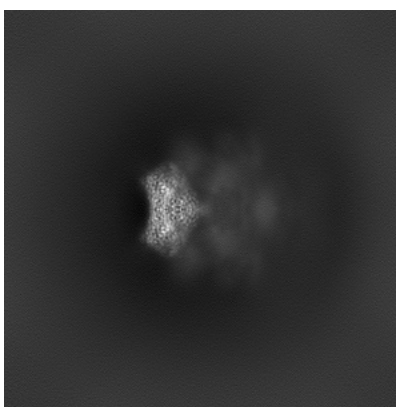


Z

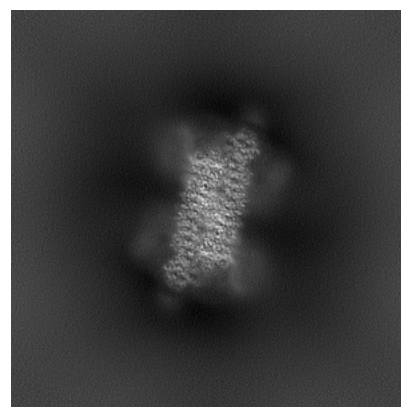
6.1.2 Raw map



X



Y

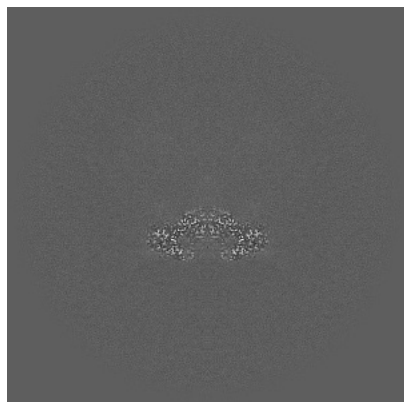


Z

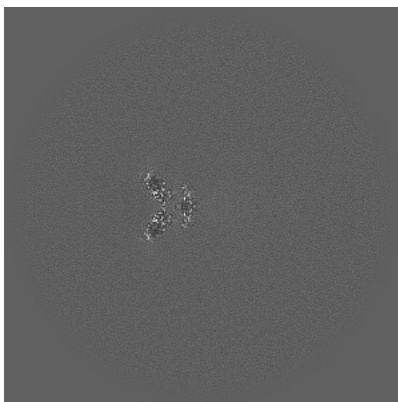
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

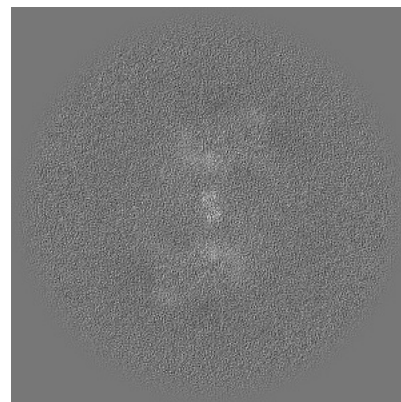
6.2.1 Primary map



X Index: 240

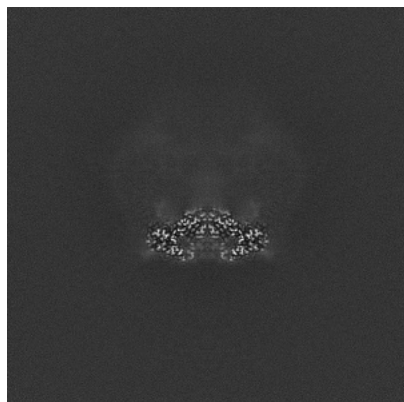


Y Index: 240

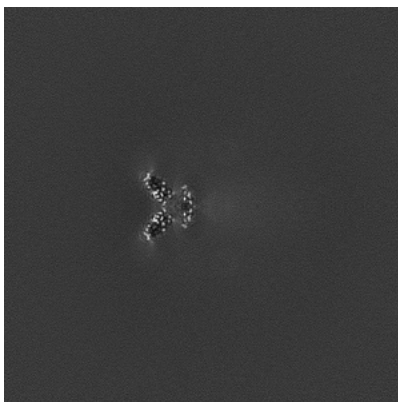


Z Index: 240

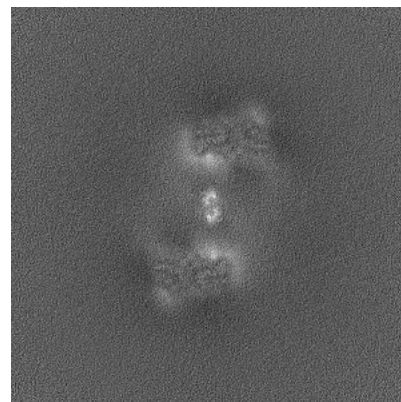
6.2.2 Raw map



X Index: 240



Y Index: 240

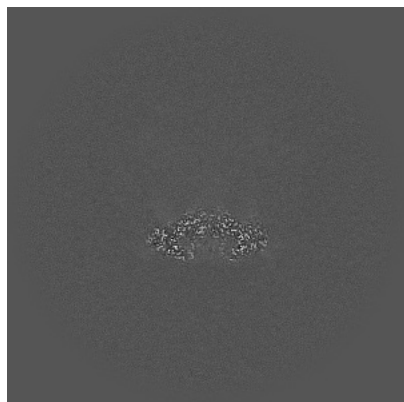


Z Index: 240

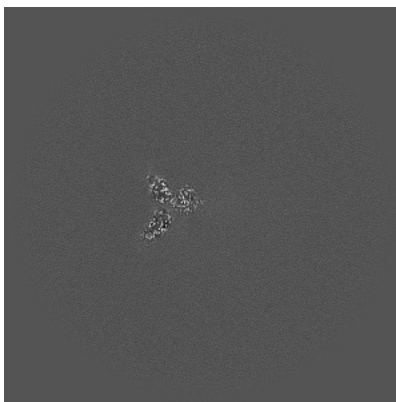
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

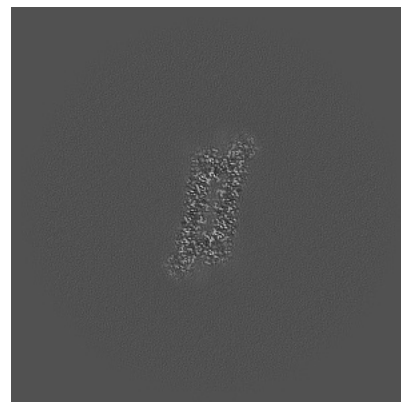
6.3.1 Primary map



X Index: 241

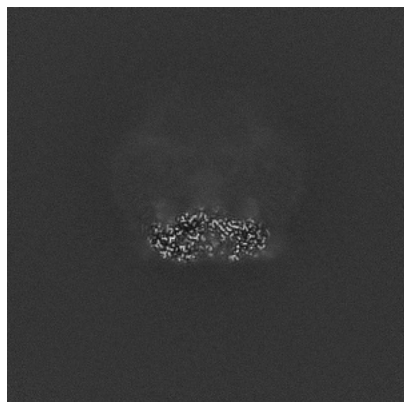


Y Index: 234

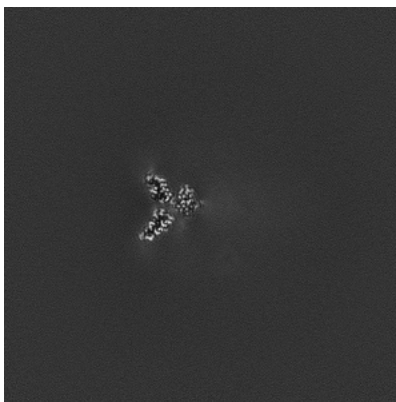


Z Index: 192

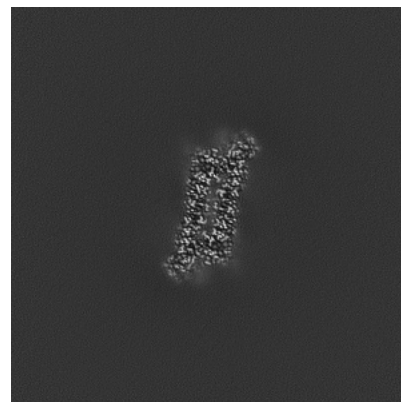
6.3.2 Raw map



X Index: 244



Y Index: 235

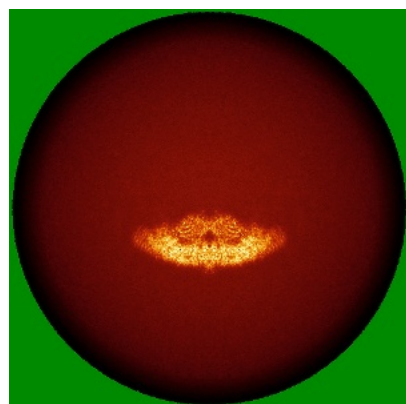


Z Index: 192

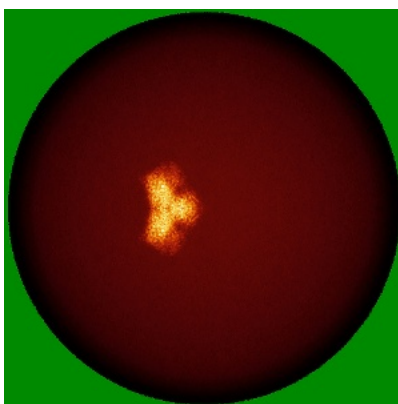
The images above show the largest variance slices of the map in three orthogonal directions.

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

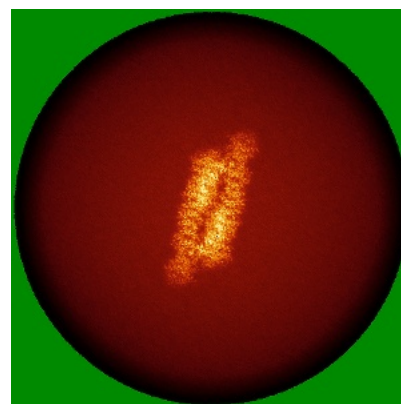
6.4.1 Primary map



X

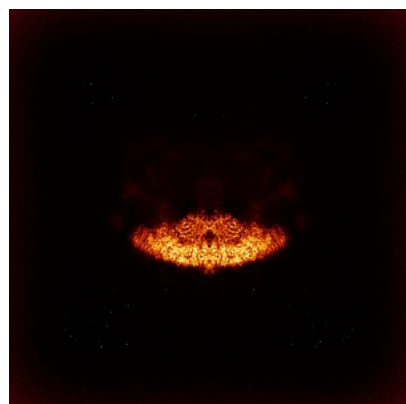


Y

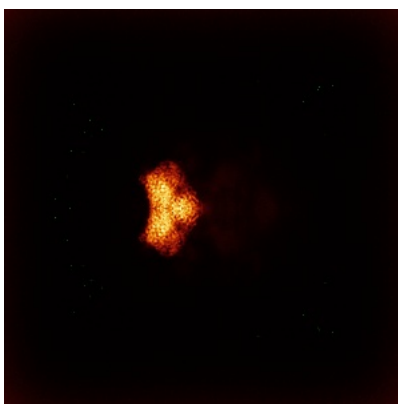


Z

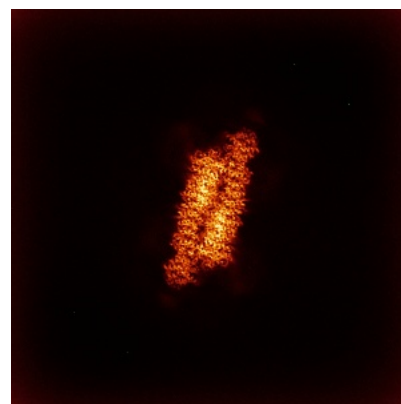
6.4.2 Raw map



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.

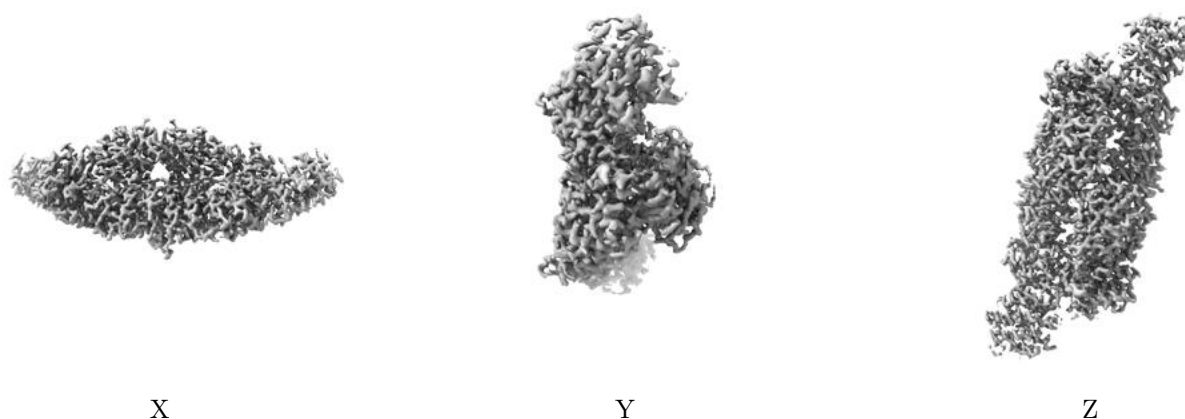
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.33. 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.

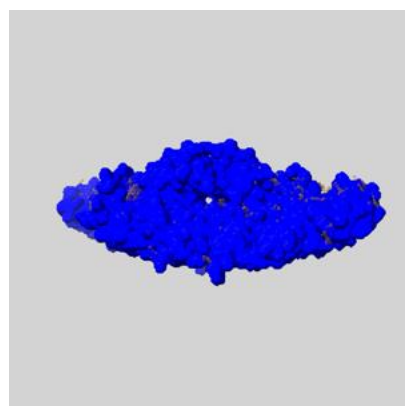
6.6 Mask visualisation [i](#)

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

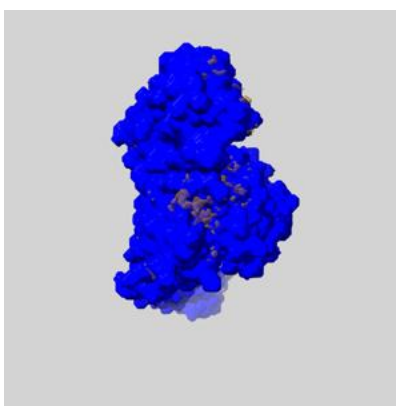
A mask typically either:

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

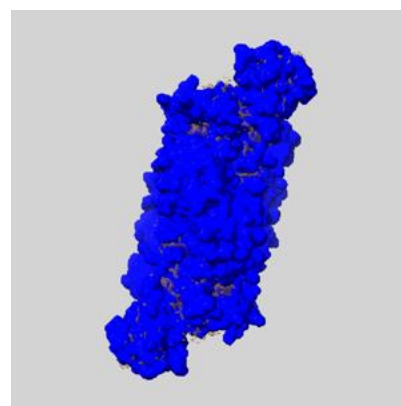
6.6.1 emd_27833_msk_1.map [i](#)



X



Y

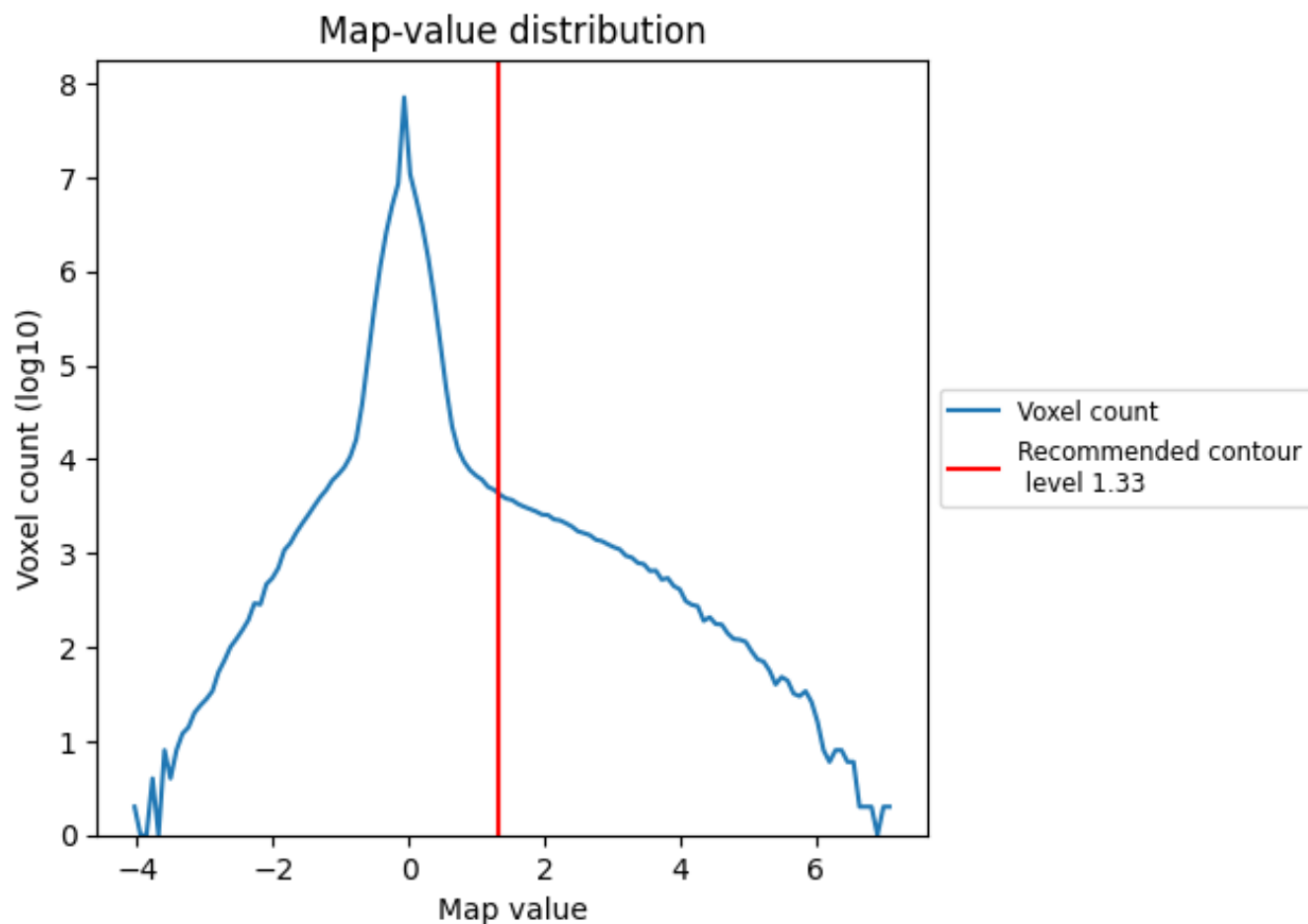


Z

7 Map analysis [i](#)

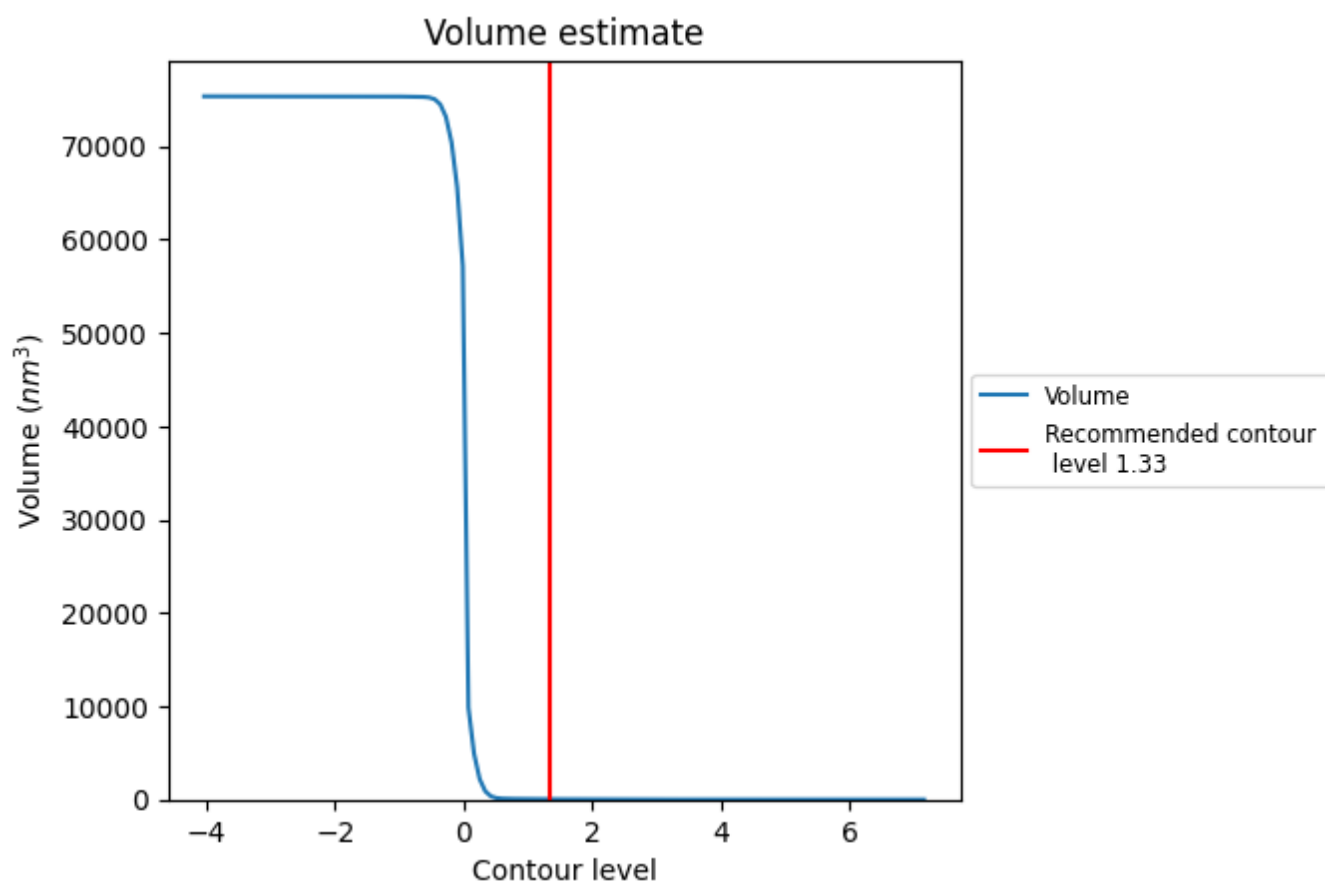
This section contains the results of statistical analysis of the map.

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.

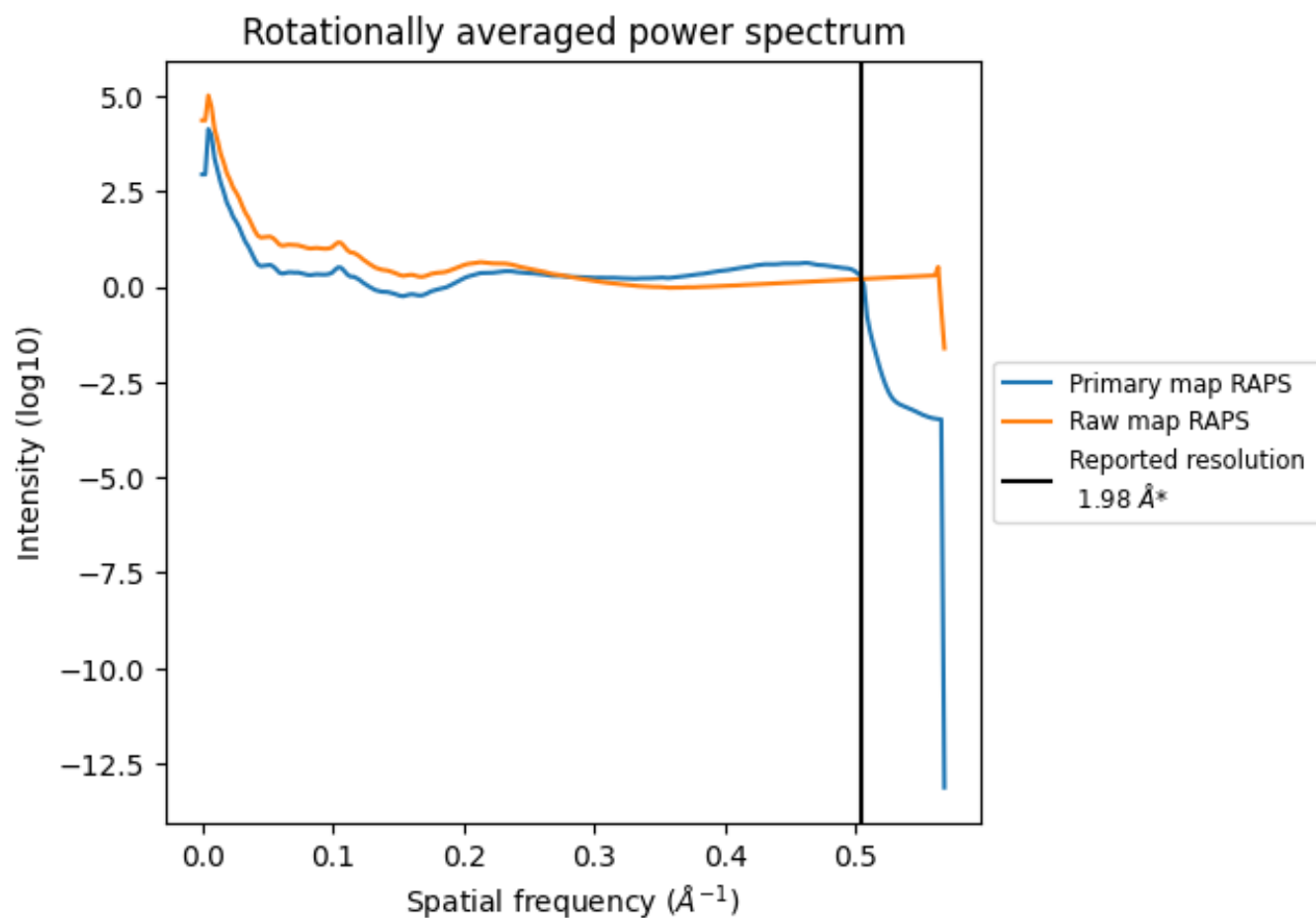
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40 nm³; this corresponds to an approximate mass of 36 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 ⓘ

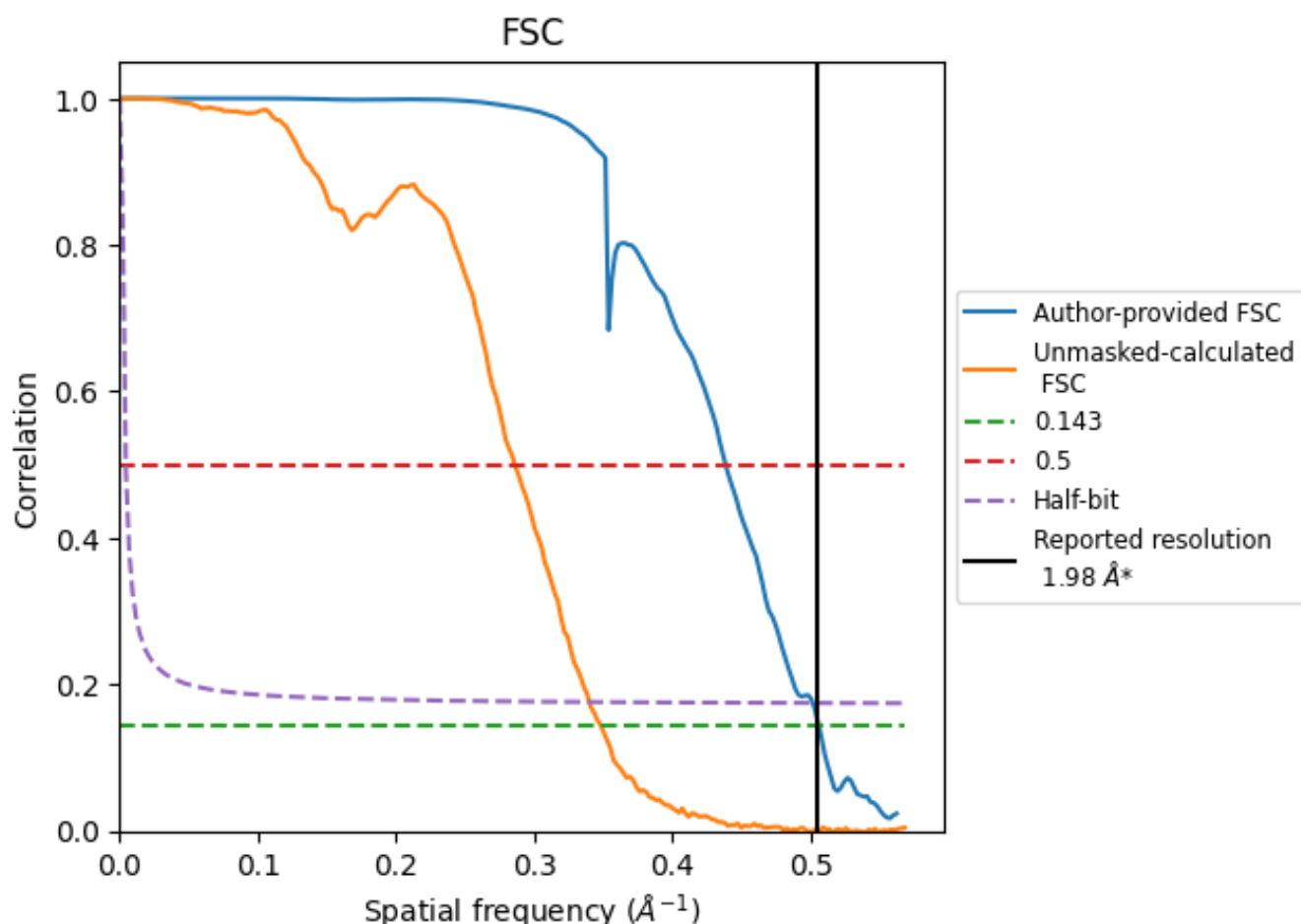


*Reported resolution corresponds to spatial frequency of 0.505 Å⁻¹

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 0.505 Å⁻¹

8.2 Resolution estimates [i](#)

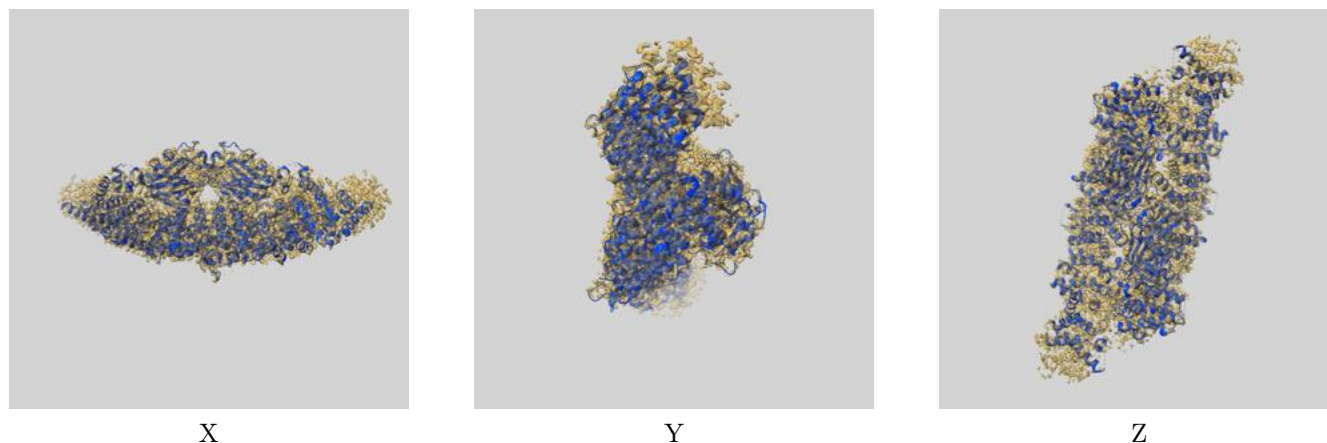
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.98	-	-
Author-provided FSC curve	1.98	2.28	1.99
Unmasked-calculated*	2.87	3.50	2.94

*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 2.87 differs from the reported value 1.98 by more than 10 %

9 Map-model fit [i](#)

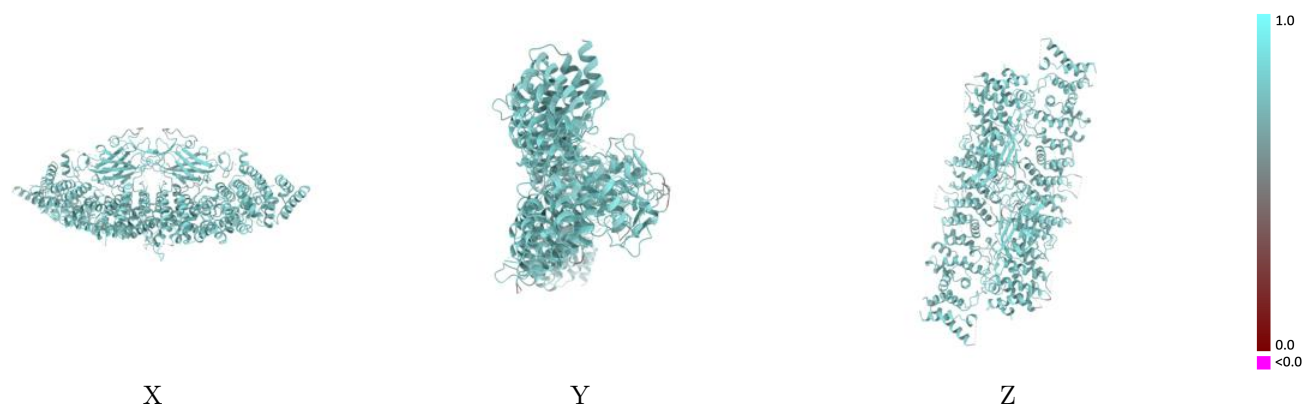
This section contains information regarding the fit between EMDB map EMD-27833 and PDB model 8E2E. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



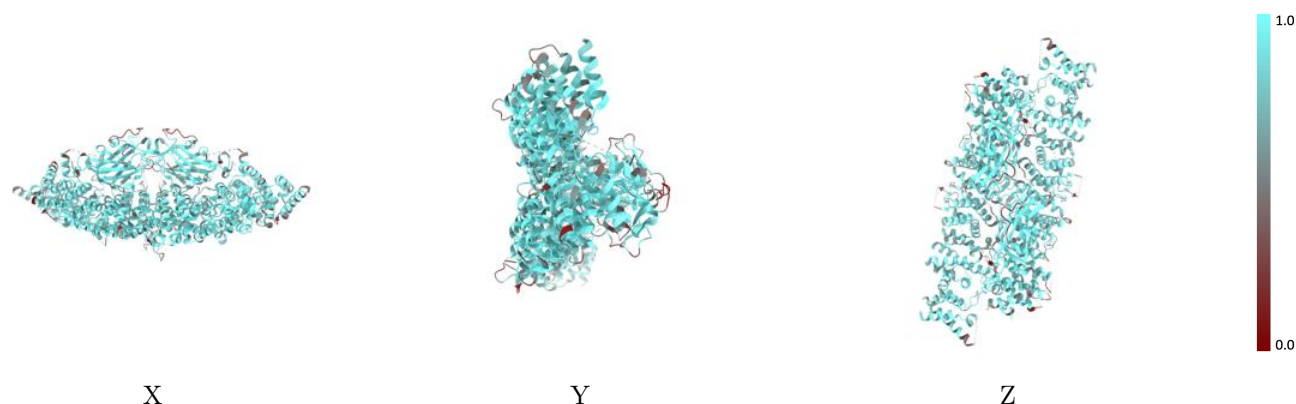
The images above show the 3D surface view of the map at the recommended contour level 1.33 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



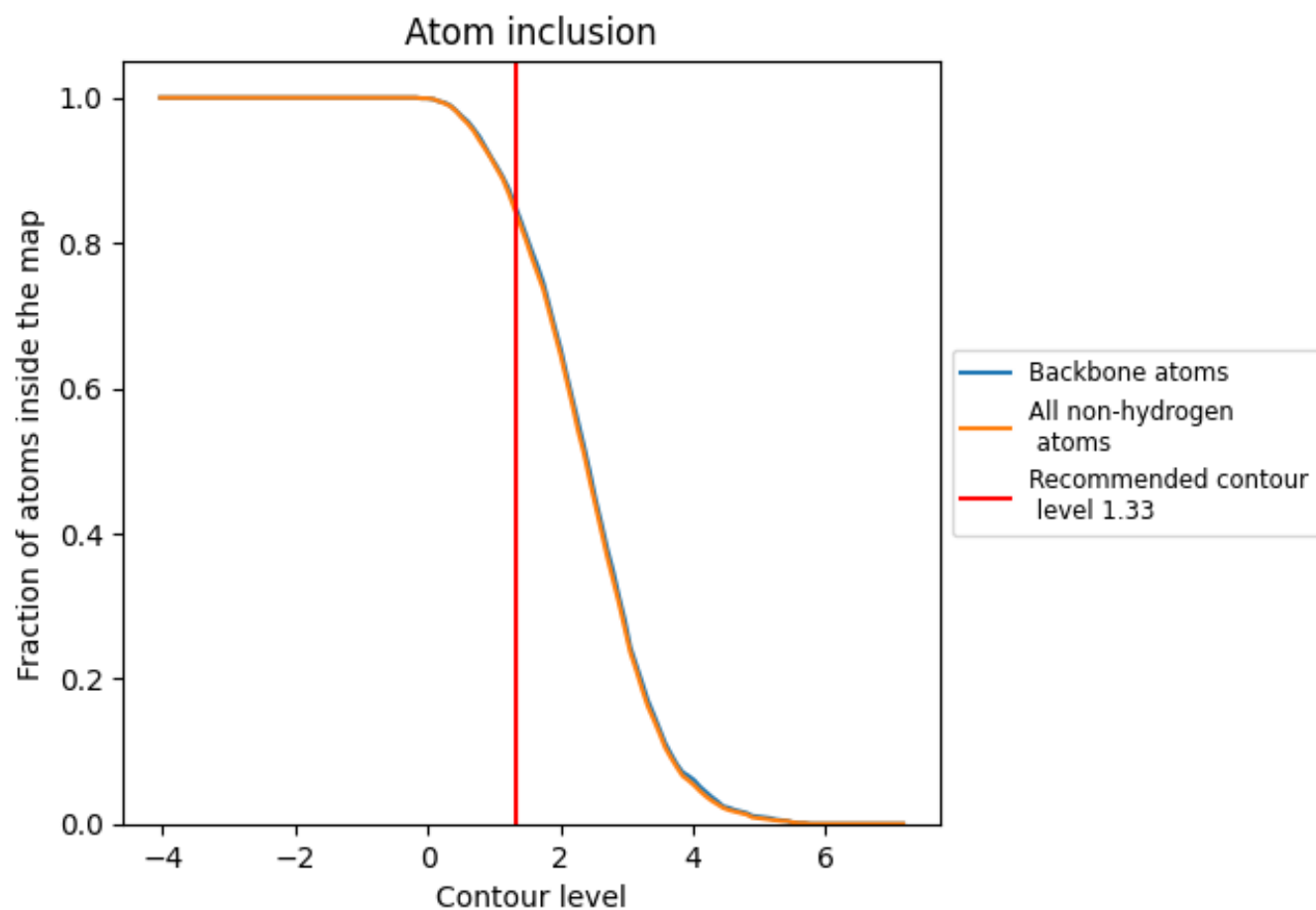
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.33).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (1.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8410	<div></div> 0.7430
A	<div></div> 0.8420	<div></div> 0.7430
B	<div></div> 0.8420	<div></div> 0.7430

