



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 08:43 PM UTC

PDB ID : 9BGJ / pdb_00009bgj
EMDB ID : EMD-44514
Title : SgrAI mutant K242A endonuclease DNA-bound dimer with Mg²⁺ and intact primary site DNA
Authors : Shan, Z.; Lyumkis, D.; Horton, N.C.
Deposited on : 2024-04-18
Resolution : 3.34 Å(reported)
Based on initial model : 6OBJ

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:

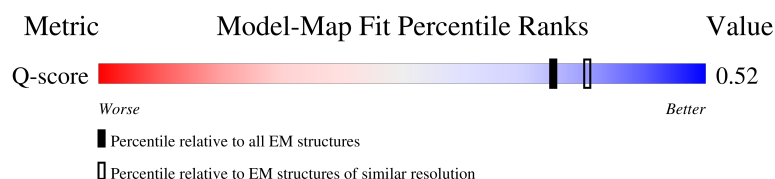
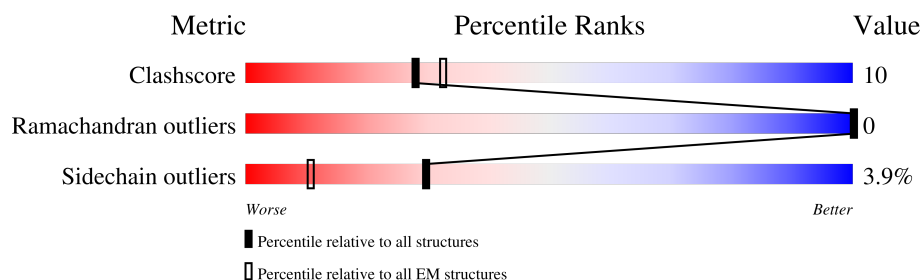
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.34 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14446 (2.84 - 3.84)

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	352	6% 72% 24% • •
1	B	352	5% 71% 23% • 5%
2	C	80	9% 22% 69%
2	D	80	8% 15% 18% 68%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6361 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 SgraIR restriction enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	338	Total	C	N	O	S	0	0
			2669	1686	479	495	9		
1	B	334	Total	C	N	O	S	0	0
			2640	1670	472	489	9		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	ASP	ASN	conflict	UNP Q9F6L0
A	242	ALA	LYS	engineered mutation	UNP Q9F6L0
A	336	LYS	LEU	conflict	UNP Q9F6L0
A	340	GLU	-	expression tag	UNP Q9F6L0
A	341	ASN	-	expression tag	UNP Q9F6L0
A	342	LEU	-	expression tag	UNP Q9F6L0
A	343	TYR	-	expression tag	UNP Q9F6L0
A	344	PHE	-	expression tag	UNP Q9F6L0
A	345	GLN	-	expression tag	UNP Q9F6L0
A	346	SER	-	expression tag	UNP Q9F6L0
A	347	HIS	-	expression tag	UNP Q9F6L0
A	348	HIS	-	expression tag	UNP Q9F6L0
A	349	HIS	-	expression tag	UNP Q9F6L0
A	350	HIS	-	expression tag	UNP Q9F6L0
A	351	HIS	-	expression tag	UNP Q9F6L0
A	352	HIS	-	expression tag	UNP Q9F6L0
B	63	ASP	ASN	conflict	UNP Q9F6L0
B	242	ALA	LYS	engineered mutation	UNP Q9F6L0
B	336	LYS	LEU	conflict	UNP Q9F6L0
B	340	GLU	-	expression tag	UNP Q9F6L0
B	341	ASN	-	expression tag	UNP Q9F6L0
B	342	LEU	-	expression tag	UNP Q9F6L0
B	343	TYR	-	expression tag	UNP Q9F6L0
B	344	PHE	-	expression tag	UNP Q9F6L0
B	345	GLN	-	expression tag	UNP Q9F6L0
B	346	SER	-	expression tag	UNP Q9F6L0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	347	HIS	-	expression tag	UNP Q9F6L0
B	348	HIS	-	expression tag	UNP Q9F6L0
B	349	HIS	-	expression tag	UNP Q9F6L0
B	350	HIS	-	expression tag	UNP Q9F6L0
B	351	HIS	-	expression tag	UNP Q9F6L0
B	352	HIS	-	expression tag	UNP Q9F6L0

- Molecule 2 is a DNA chain called 40-1 DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	25	Total	C	N	O	P	0	0
			517	244	95	153	25		
2	D	26	Total	C	N	O	P	0	0
			524	249	99	151	25		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	4	Total	O	0
			4	4	
4	B	5	Total	O	0
			5	5	

A20	A21	G22	A23	C24	C25	C26	DA	DC	DG	DC	DA	DT	DC
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4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-86.2°, rise=20.9 Å, axial sym=C2	Depositor
Number of segments used	357489	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 ($e^-/\text{Å}^2$)	42.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.640	Depositor
Minimum map value	-1.189	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.14	0/2728	0.30	0/3703
1	B	0.14	0/2698	0.29	0/3662
2	C	0.19	0/579	0.36	0/893
2	D	0.19	0/587	0.32	0/902
All	All	0.15	0/6592	0.31	0/9160

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	2669	0	2634	51	0
1	B	2640	0	2606	49	0
2	C	517	0	282	16	0
2	D	524	0	291	15	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	0	2	0
4	B	5	0	0	1	0
All	All	6361	0	5813	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 117 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:147:VAL:HG22	1:A:191:VAL:HG22	1.71	0.72
1:A:232:PRO:HB3	1:A:268:LEU:HD13	1.74	0.69
1:B:147:VAL:HG22	1:B:191:VAL:HG22	1.76	0.66
1:B:147:VAL:HG13	1:B:189:LEU:HD21	1.78	0.66
1:A:276:GLU:OE2	1:A:278:HIS:NE2	2.30	0.62

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	336/352 (96%)	308 (92%)	28 (8%)	0	100	100
1	B	330/352 (94%)	310 (94%)	20 (6%)	0	100	100
All	All	666/704 (95%)	618 (93%)	48 (7%)	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	281/295 (95%)	269 (96%)	12 (4%)	26	54
1	B	279/295 (95%)	269 (96%)	10 (4%)	31	58
All	All	560/590 (95%)	538 (96%)	22 (4%)	30	56

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	VAL
1	B	167	VAL
1	B	161	VAL
1	B	203	MET
1	A	156	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	21	GLN
1	B	74	ASN
1	B	258	ASN
1	A	112	ASN
1	A	21	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

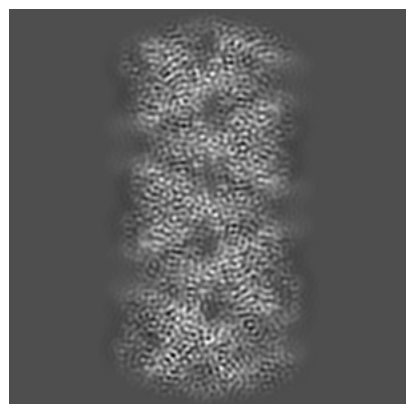
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44514. These allow visual inspection of the internal detail of the map and identification of artifacts.

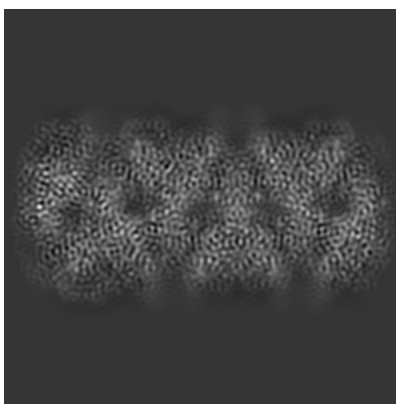
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

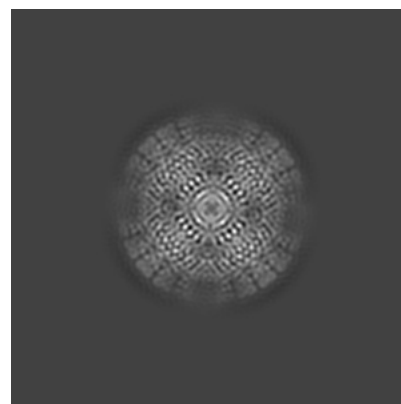
6.1.1 Primary map



X

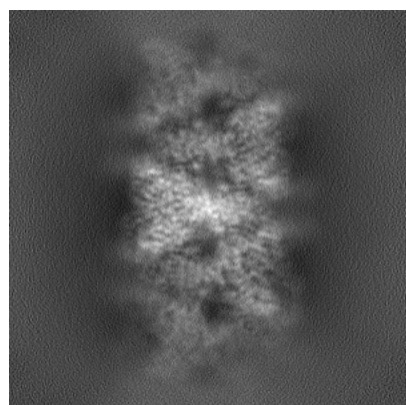


Y

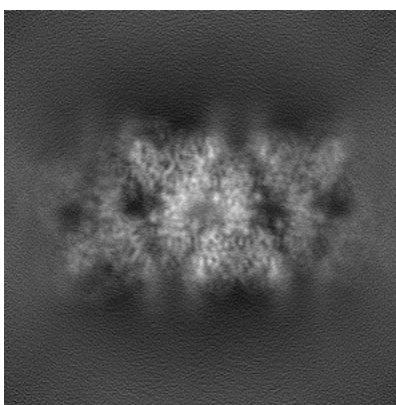


Z

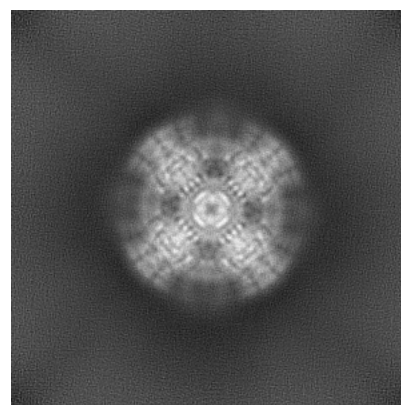
6.1.2 Raw map



X



Y

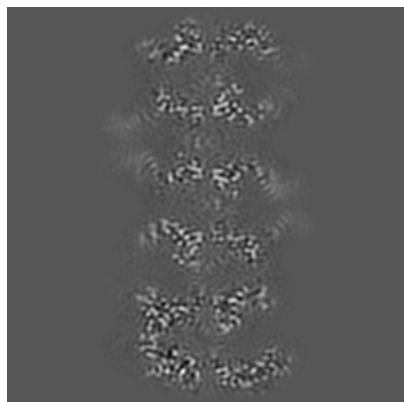


Z

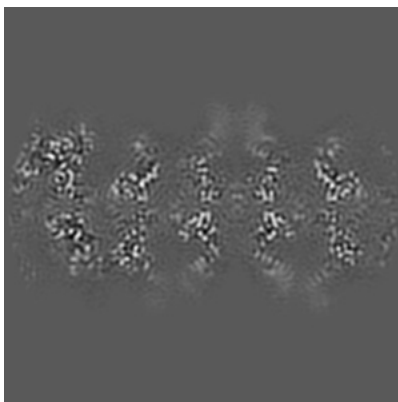
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160

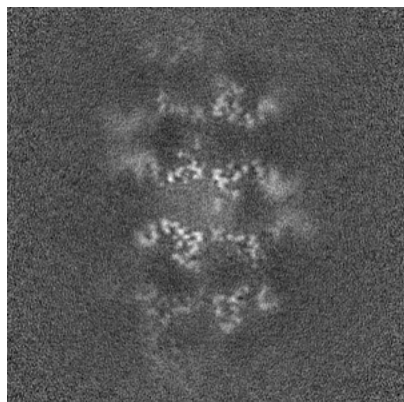


Y Index: 160

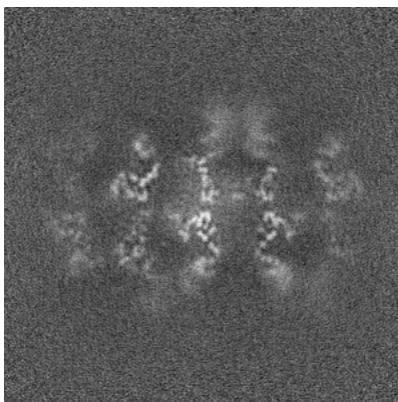


Z Index: 160

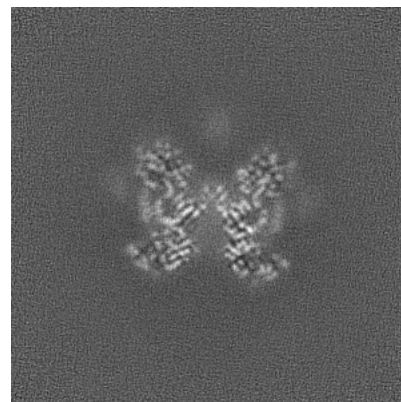
6.2.2 Raw map



X Index: 160



Y Index: 160

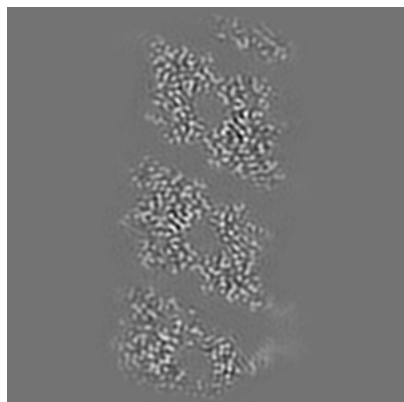


Z Index: 160

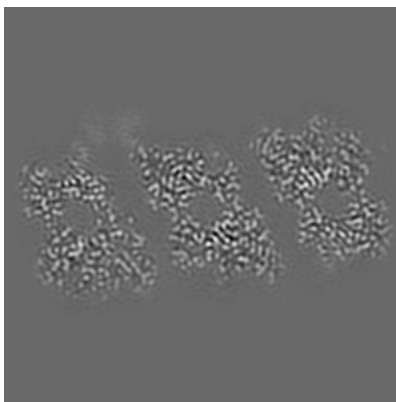
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

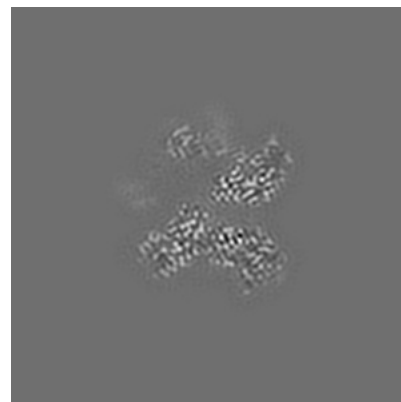
6.3.1 Primary map



X Index: 183

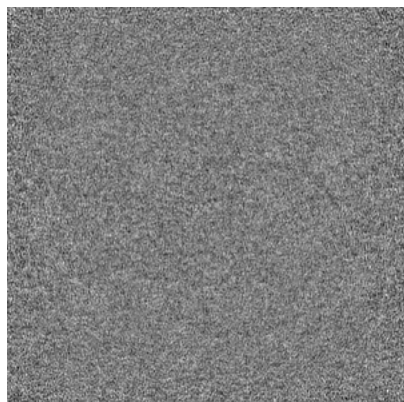


Y Index: 136

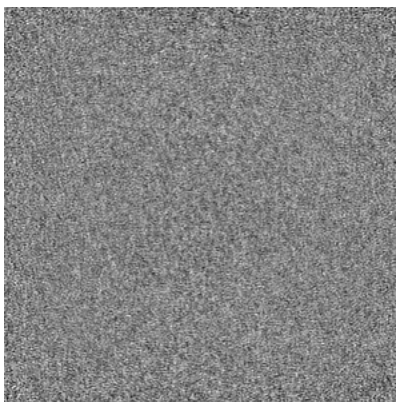


Z Index: 143

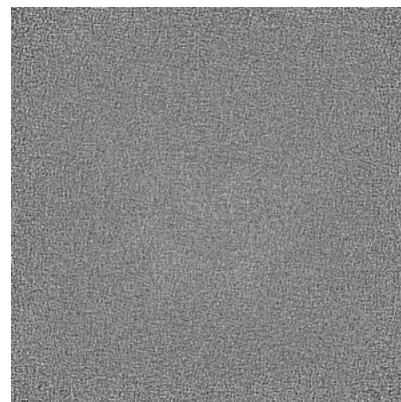
6.3.2 Raw map



X Index: 0



Y Index: 0

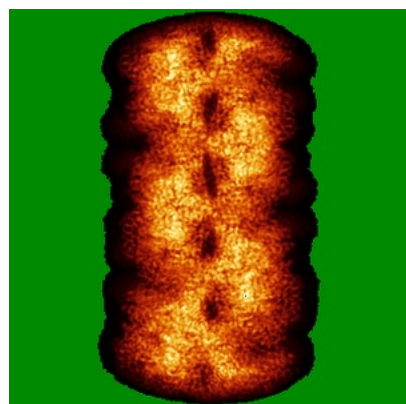


Z Index: 0

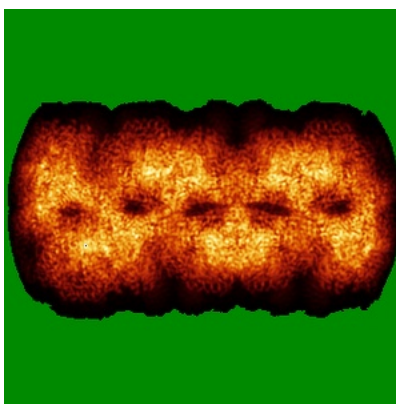
The images above show the largest variance slices of the map in three orthogonal directions.

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

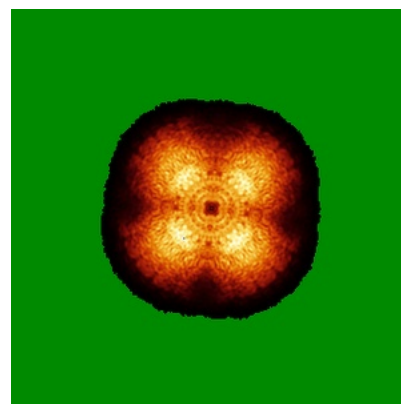
6.4.1 Primary map



X

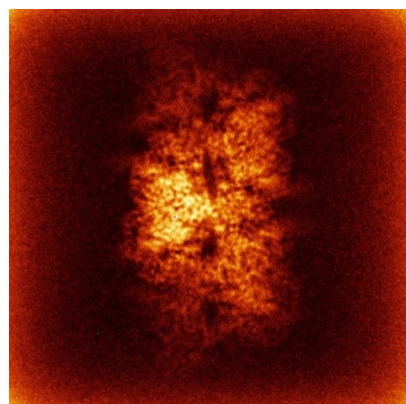


Y

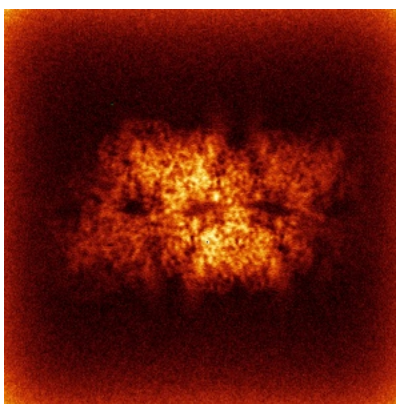


Z

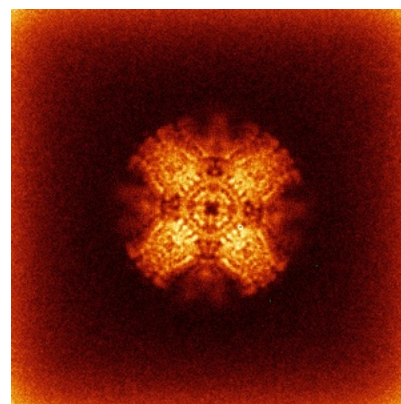
6.4.2 Raw map



X



Y

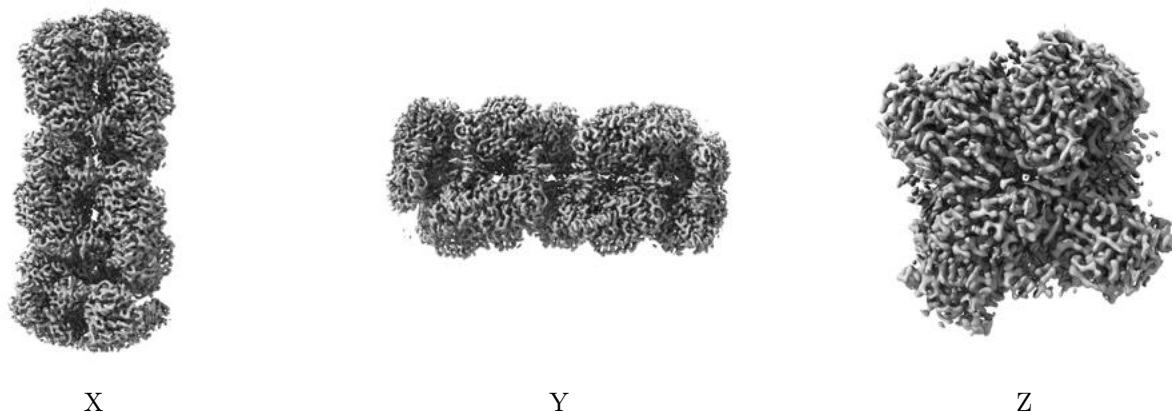


Z

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

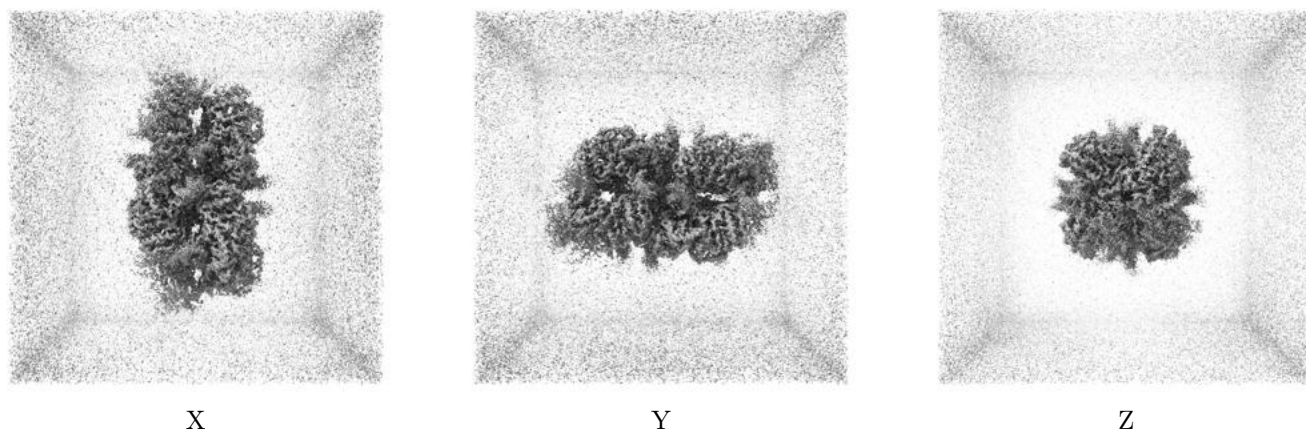
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.17. 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.

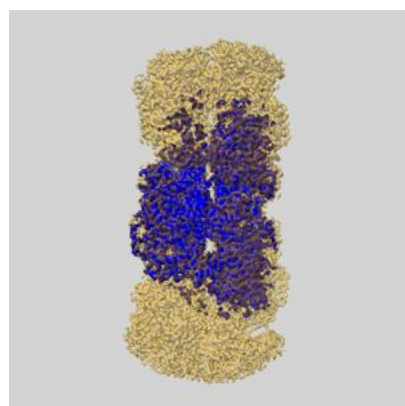
6.6 Mask visualisation [i](#)

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

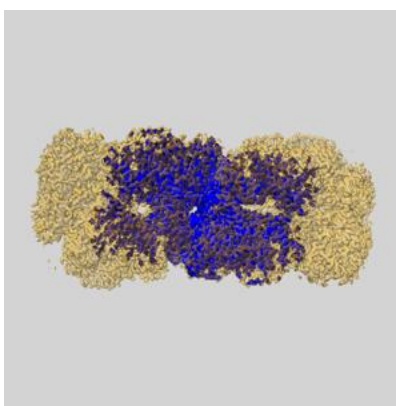
A mask typically either:

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

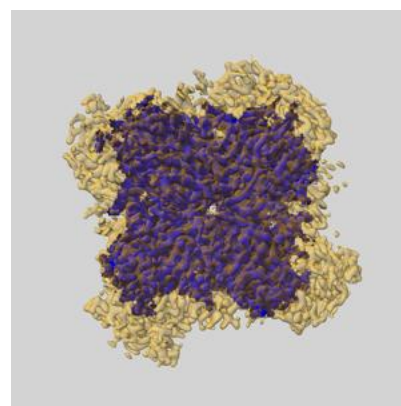
6.6.1 emd_44514_msk_1.map [i](#)



X



Y

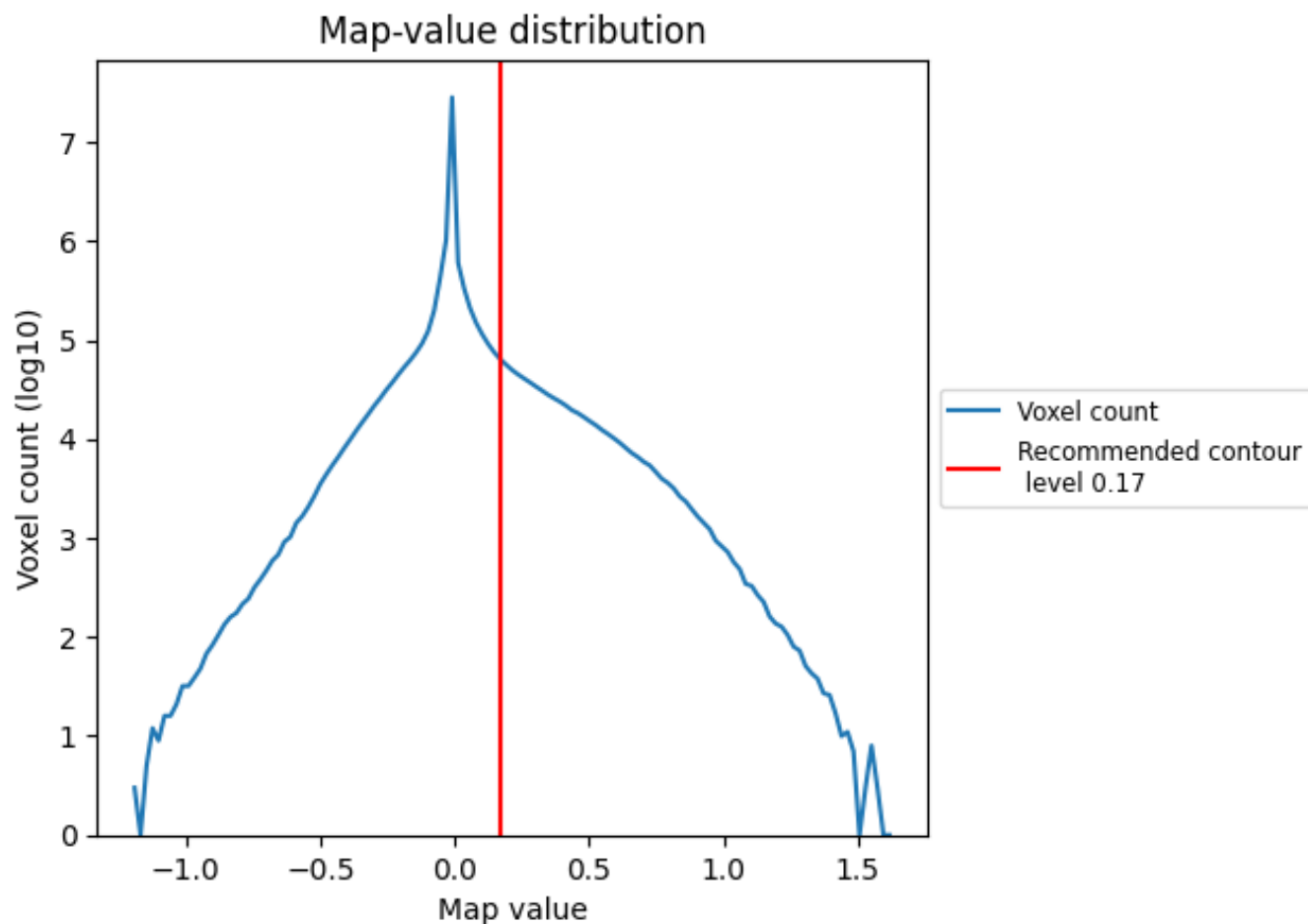


Z

7 Map analysis [i](#)

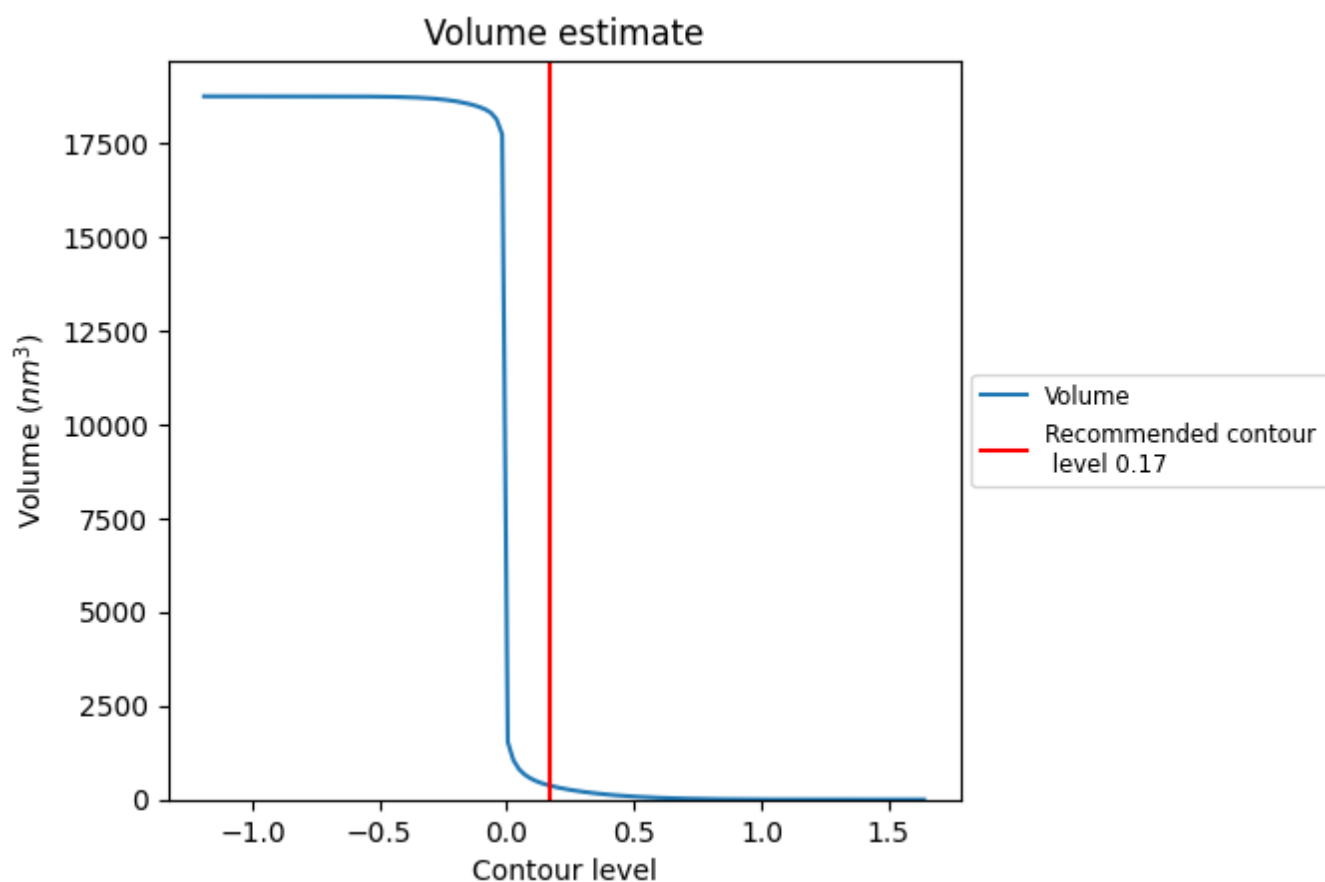
This section contains the results of statistical analysis of the map.

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.

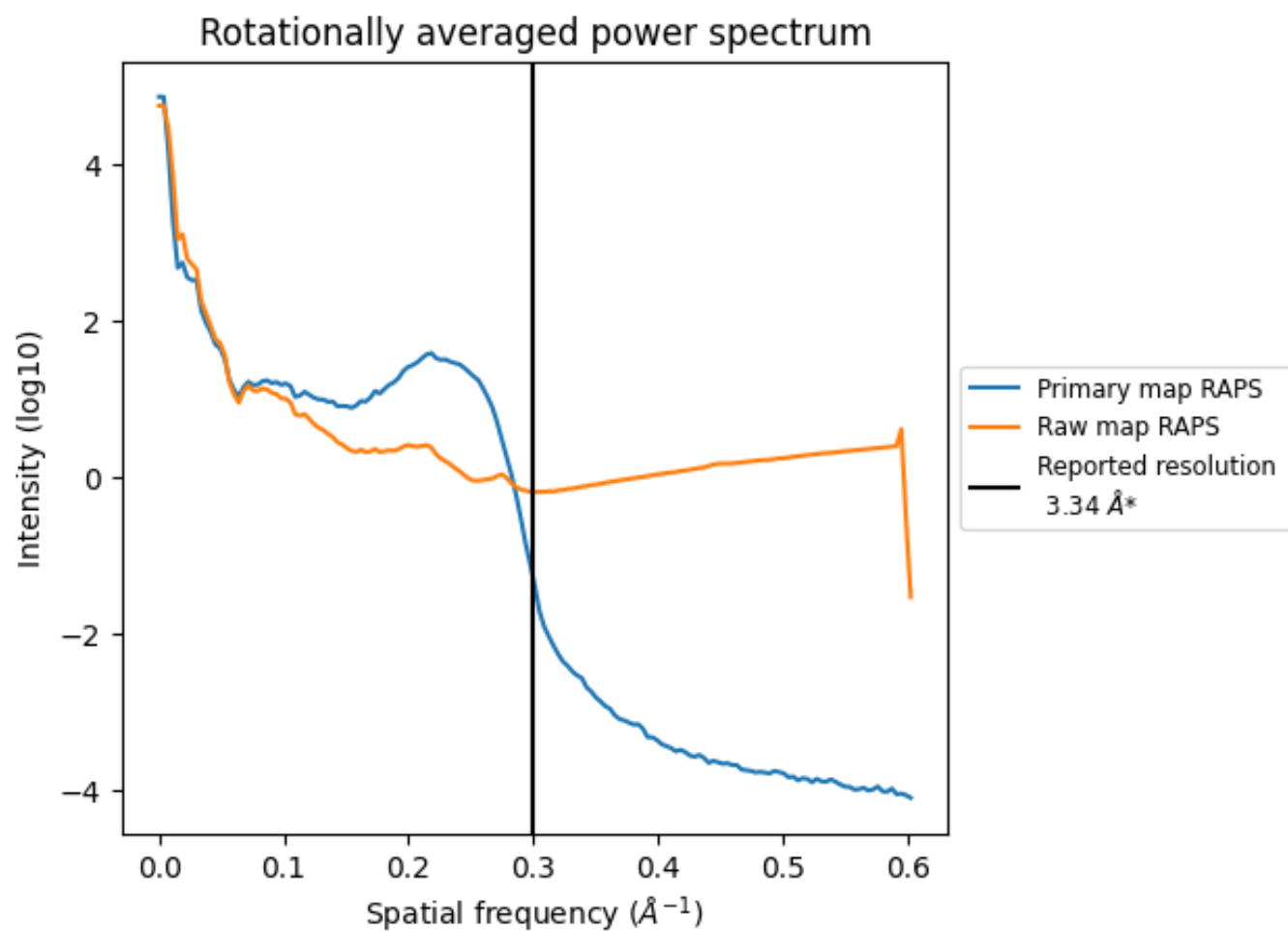
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 371 nm³; this corresponds to an approximate mass of 335 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 ⓘ

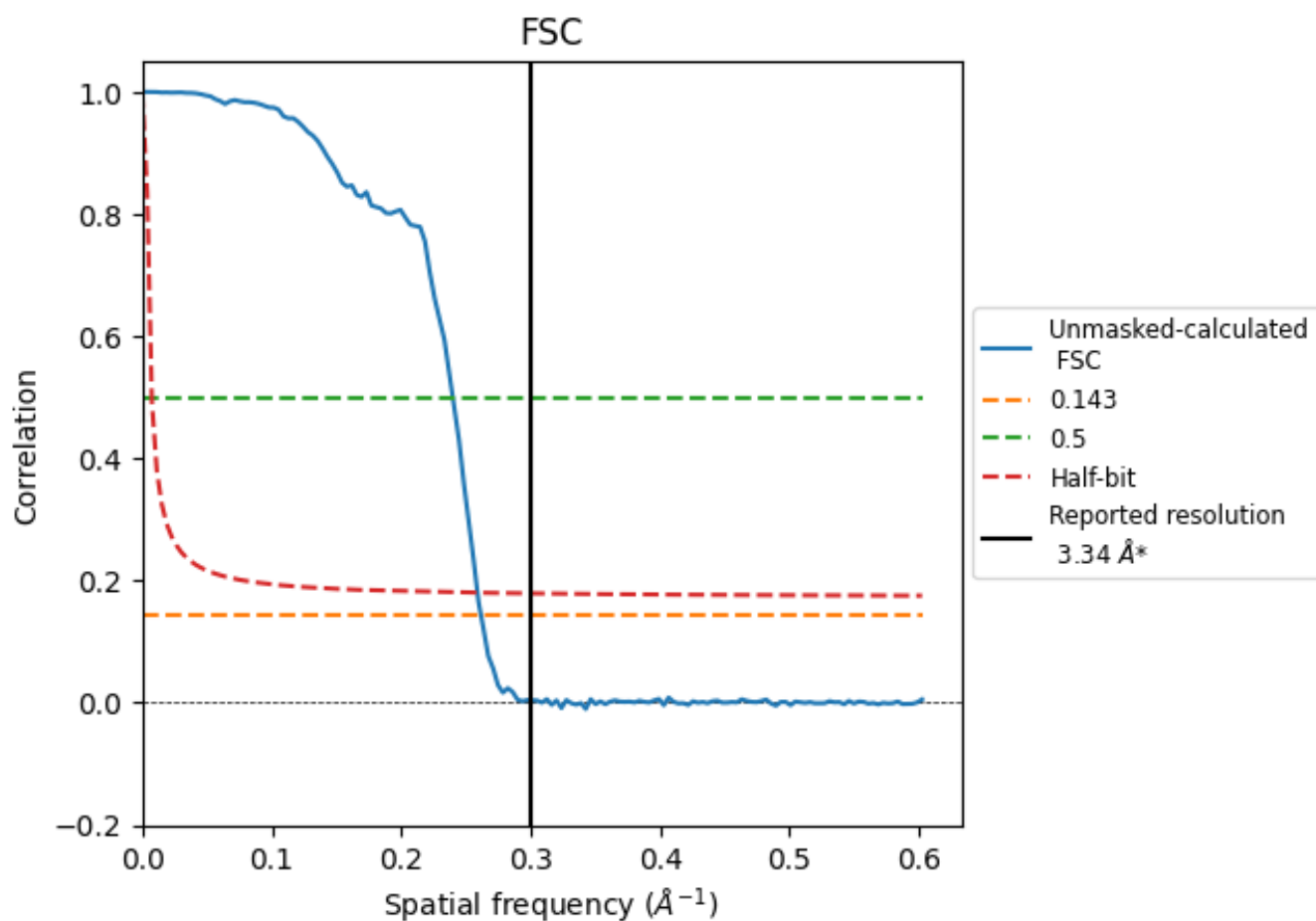


*Reported resolution corresponds to spatial frequency of 0.299 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

8.2 Resolution estimates [i](#)

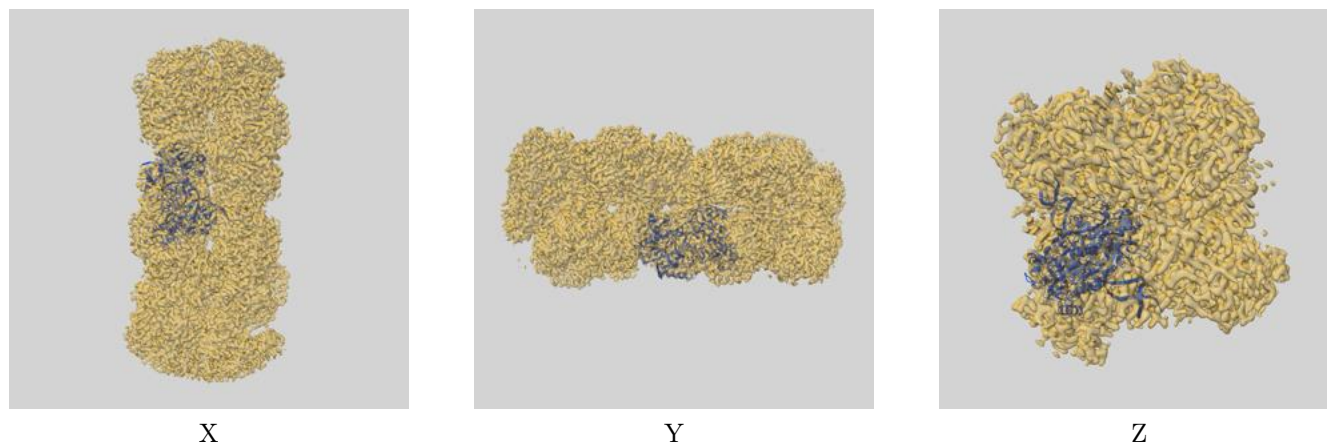
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	4.16	3.86

*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 3.82 differs from the reported value 3.34 by more than 10 %

9 Map-model fit [i](#)

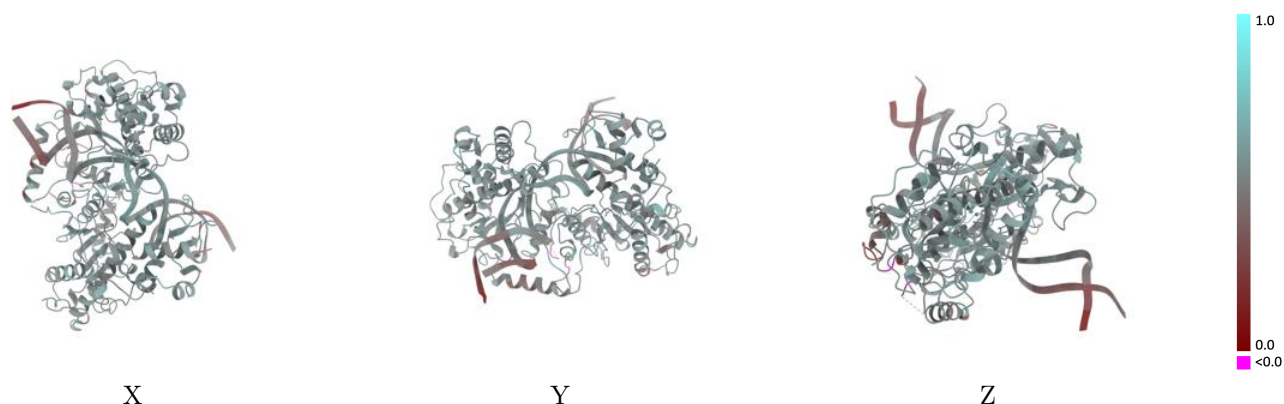
This section contains information regarding the fit between EMDB map EMD-44514 and PDB model 9BGJ. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



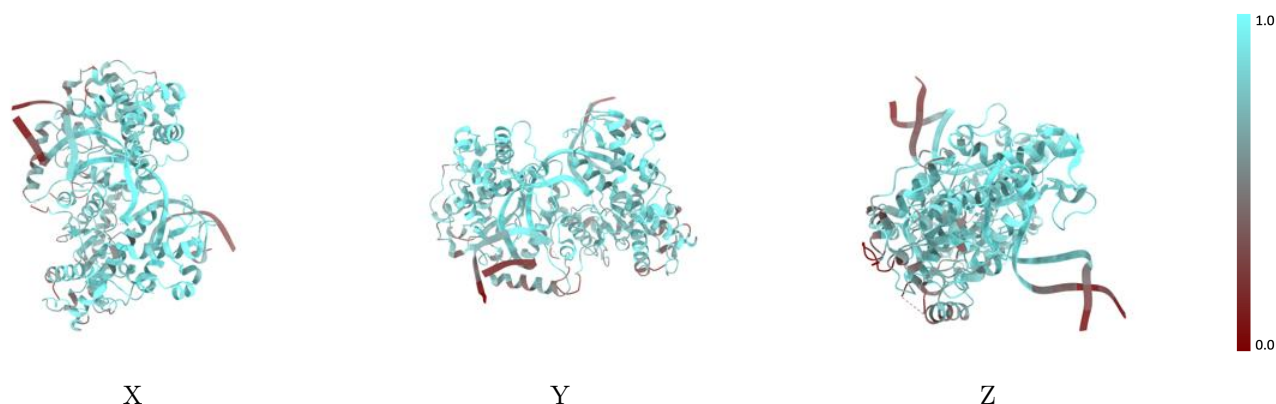
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



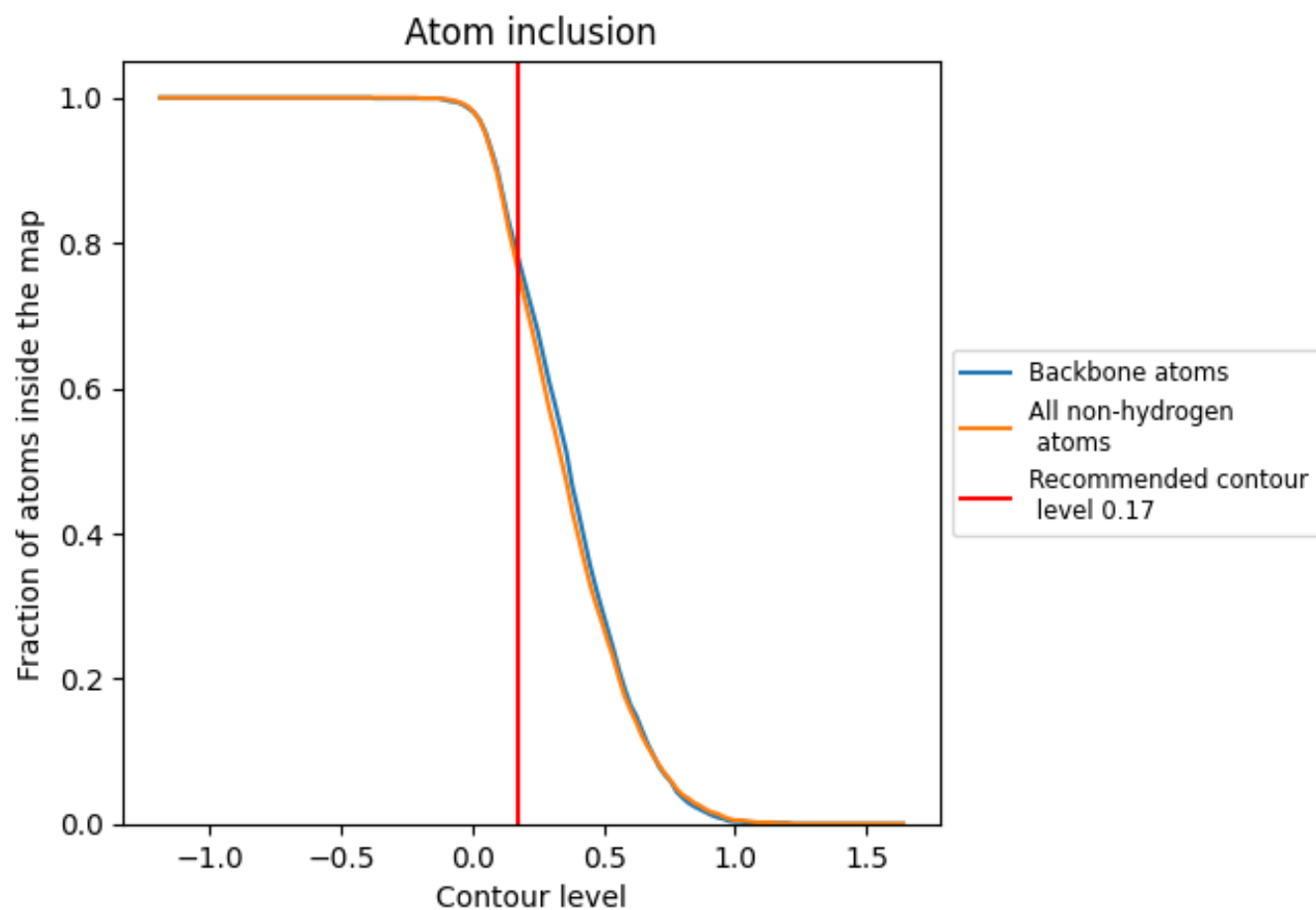
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.17).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7680	0.5200
A	0.7800	0.5300
B	0.7900	0.5310
C	0.6850	0.4650
D	0.6870	0.4660

