



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 06:39 PM UTC

PDB ID : 8XEK / pdb_00008xek
EMDB ID : EMD-38292
Title : Cryo-EM structure of integrin ITGAV/ITGB3 complex, conformation 2
Authors : Xi, Z.
Deposited on : 2023-12-12
Resolution : 2.90 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.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

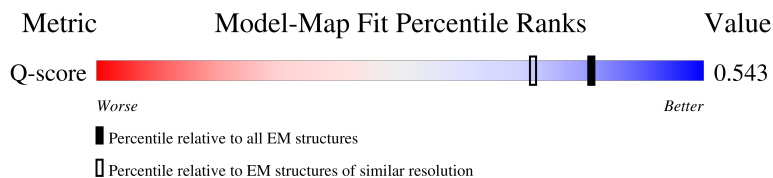
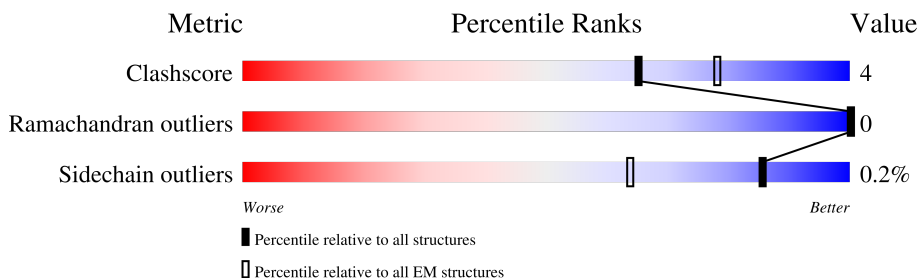
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	1048	 52% . 44%
2	B	788	 56% 5% 39%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10130 atoms, of which 1840 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	592	Total	C	H	N	O	S	0	0
			5600	2904	1016	779	880	21		

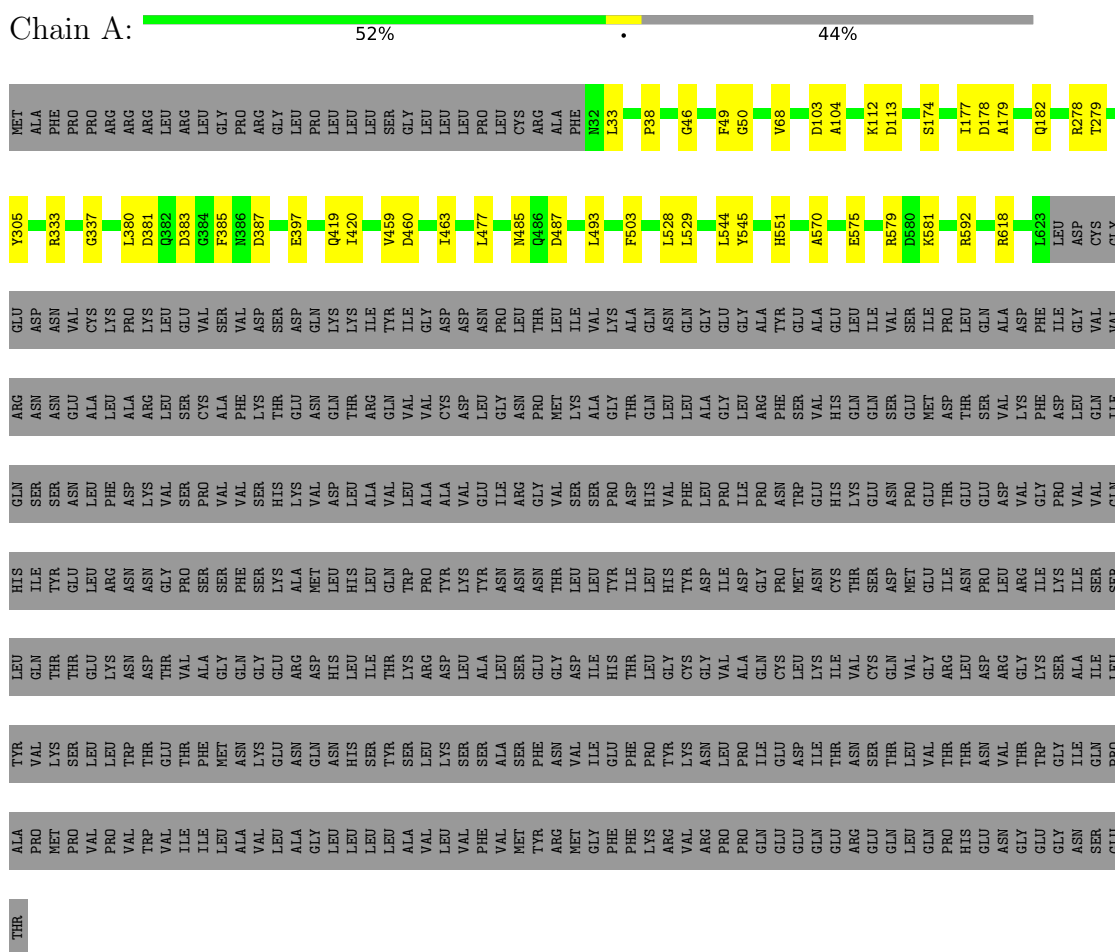
- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	481	Total	C	H	N	O	S	0	0
			4530	2303	824	632	736	35		

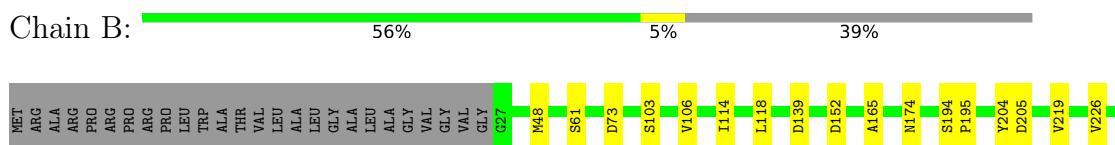
3 Residue-property plots

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: Integrin alpha-V



• Molecule 2: Integrin beta-3



Lys	Trp	Ile	Lys	Cys	Arg	E232
Leu	Trp	Leu	Lys	Asn	Gly	
Asp	Trp	Tyr	Phe	Cys	Leu	R240
Thr	Val	Val	Asp	Thr	Cys	
Ala	Val	Val	Arg	Thr	Leu	E260
Asn	Ala	Glj	Gly	Arg	Cys	
Asn	Ala	Ala	Leu	Thr	Gly	R265
Pro	Pro	Pro	Ala	Asp	Gln	
Leu	Leu	Glj	His	Thr	Cys	T275
Tyr	Cys	Cys	Asp	Cys	Val	
Lys	Pro	Pro	Glj	Met	Cys	A335
Glj	Lys	Lys	Asn	Ser	His	
Ala	Ala	Gly	Thr	Ser	Ser	V336
Pro	Pro	Pro	Cys	Asn	Ser	
Ser	Ser	Asp	Asn	Gly	Asp	Y344
Thr	Thr	Ile	Arg	Leu	Phe	Q345
Phe	Phe	Leu	Leu	Leu	Gly	
Thr	Thr	Val	Cys	Cys	Lys	V356
Asn	Val	Val	Arg	Ser	Ile	
Val	Val	Leu	Asp	Gly	Thr	V381
Ile	Leu	Leu	Asp	Gly	Gly	
Thr	Thr	Leu	Glj	Arg	Gly	E390
Tyr	Tyr	Ser	Ile	Gly	Lys	
Arg	Arg	Val	Leu	Lys	Tyr	L415
Gly	Gly	Met	Ser	Cys	Cys	
Thr	Thr	Met	Val	Glj	Glj	V429
	Ala	Ala	Lys	Cys	Asp	
Ile	Ile	Ile	Glj	Gly	Asp	Q434
Leu	Leu	Leu	Leu	Ser	Asp	E435
Leu	Leu	Leu	Lys	Cys	Phe	K436
Ile	Ile	Ile	Asp	Val	Ser	
Gly	Gly	Leu	Thr	Cys	Cys	L451
Leu	Leu	Leu	Gly	Ile	Val	
Ala	Ala	Ala	Lys	Gln	Arg	Q464
Ala	Ala	Ala	Asp	Pro	Tyr	
Leu	Leu	Leu	Ala	Gly	Lys	R473
Leu	Leu	Val	Val	Ser	Gly	
Ile	Ile	Ala	Asn	Tyr	Glj	V492
Trp	Trp	Lys	Cys	Gly	Met	
Lys	Lys	Lys	Thr	Asp	Cys	S500
Leu	Leu	Leu	Tyr	Thr	Ser	E501
Leu	Leu	Leu	Thr	Cys	Gly	E502
Ile	Ile	Ala	Asn	Glj	His	D503
Thr	Thr	Thr	Asp	Lys	Gly	
Ile	Ile	Ala	Glj	Cys	Gln	S507
Ile	Ile	His	Asp	Pro	Cys	
Asp	Asp	Asp	Cys	Thr	Ser	Gln
Arg	Arg	Arg	Val	Cys	Cys	Asp
Lys	Lys	Lys	Val	Pro	Gly	Glj
Glj	Glj	Glj	Arg	Asp	Asp	Glj
Phe	Phe	Phe	Phe	Ala	Cys	Cys
Ala	Ala	Ala	Gln	Cys	Leu	Ser
Lys	Lys	Lys	Thr	Thr	Cys	Pro
Phe	Phe	Phe	Tyr	Phe	Asp	Arg
Glj	Glj	Glj	Glj	Lys	Ser	Glj
Glj	Glj	Glj	Ser	Lys	Gly	Glj
Glj	Glj	Glj	Asp	Thr	Trp	Gln
Arg	Arg	Arg	Glj	Cys	Thr	Val
Ala	Ala	Ala	Gly	Val	Gly	Cys
Ala	Ala	Ala	Ser	Glj	Tyr	Ser
Ala	Ala	Ala	Ser	Cys	Tyr	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117205	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.407	Depositor
Minimum map value	-0.157	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.66, 0.66, 0.66	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	0.16	0/4687	0.32	0/6345
2	B	0.16	0/3775	0.35	2/5118 (0.0%)
All	All	0.16	0/8462	0.33	2/11463 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	GLU	CA-C-N	5.41	131.43	121.70
2	B	502	GLU	C-N-CA	5.41	131.43	121.70

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	4584	1016	4440	34	0
2	B	3706	824	3607	31	0
All	All	8290	1840	8047	65	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 65 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)
2:B:260:GLU:N	2:B:260:GLU:OE2	2.08	0.85
2:B:434:GLN:N	2:B:434:GLN:OE1	2.13	0.81
1:A:177:ILE:HD12	1:A:177:ILE:O	1.85	0.76
2:B:194:SER:OG	2:B:195:PRO:HD3	1.96	0.64
2:B:390:GLU:OE2	2:B:390:GLU:N	2.24	0.64

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	590/1048 (56%)	574 (97%)	16 (3%)	0	100	100
2	B	479/788 (61%)	464 (97%)	15 (3%)	0	100	100
All	All	1069/1836 (58%)	1038 (97%)	31 (3%)	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	485/890 (54%)	483 (100%)	2 (0%)	84	94
2	B	426/690 (62%)	426 (100%)	0	100	100
All	All	911/1580 (58%)	909 (100%)	2 (0%)	85	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	TYR
1	A	529	LEU

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

Mol	Chain	Res	Type
2	B	129	GLN
2	B	454	GLN
2	B	476	ASN
1	A	212	GLN
1	A	182	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 [i](#)

There are no chain breaks in this entry.

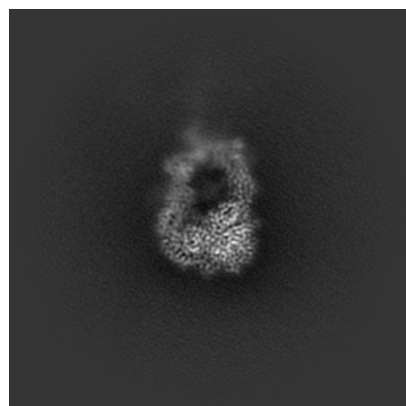
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38292. These allow visual inspection of the internal detail of the map and identification of artifacts.

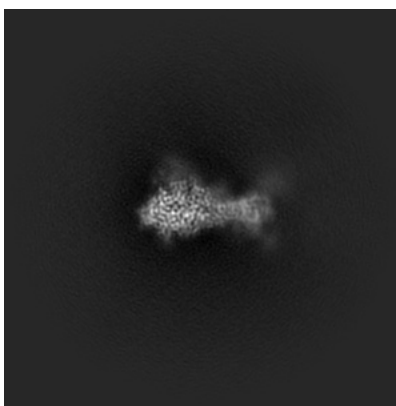
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

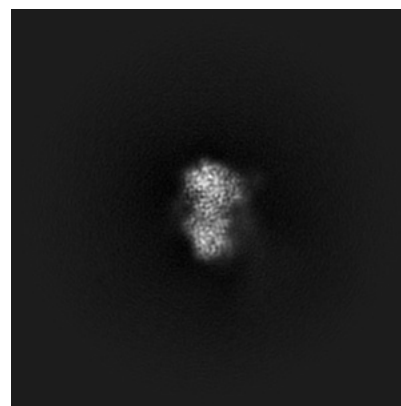
6.1.1 Primary map



X

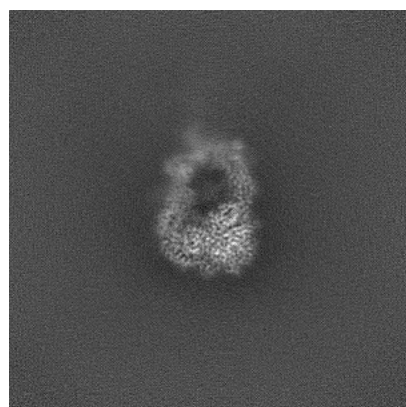


Y

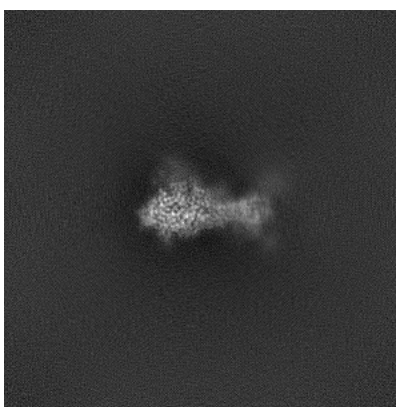


Z

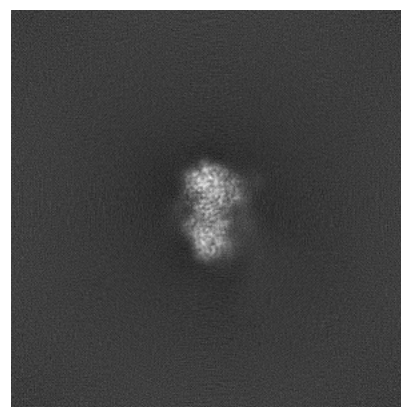
6.1.2 Raw map



X



Y

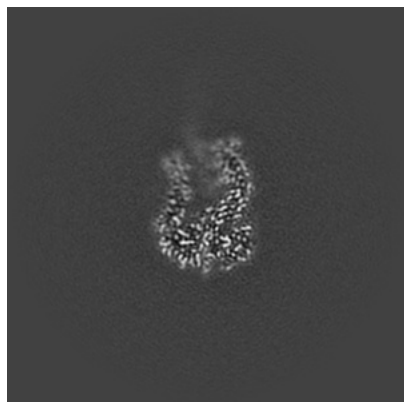


Z

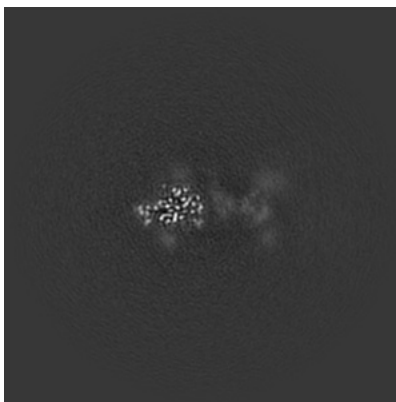
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

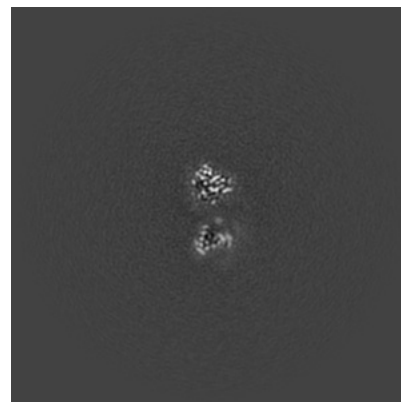
6.2.1 Primary map



X Index: 256

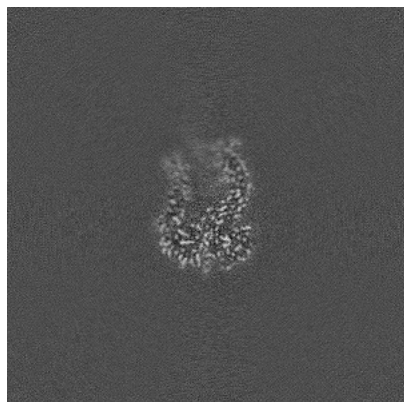


Y Index: 256

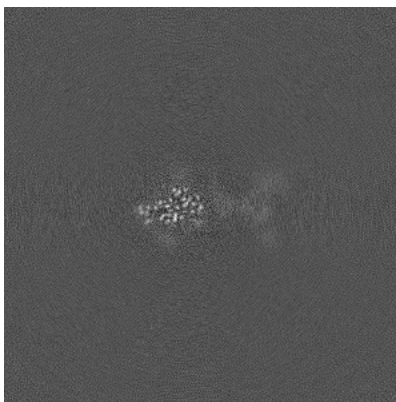


Z Index: 256

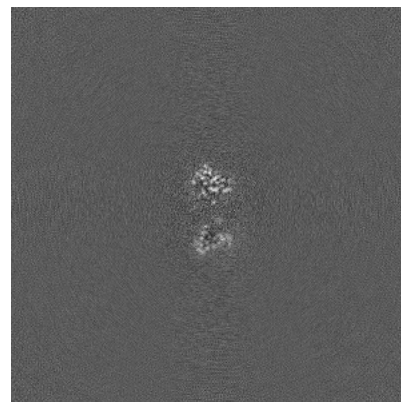
6.2.2 Raw map



X Index: 256



Y Index: 256

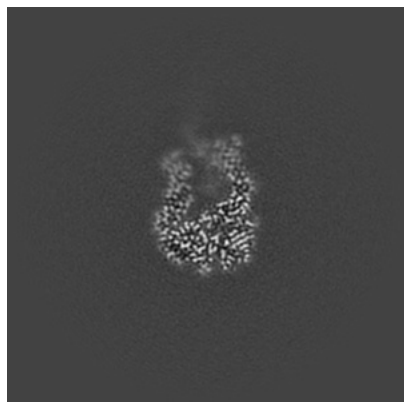


Z Index: 256

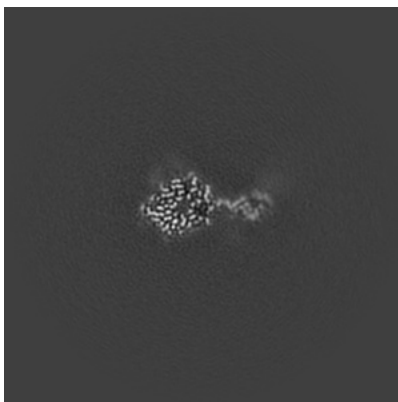
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

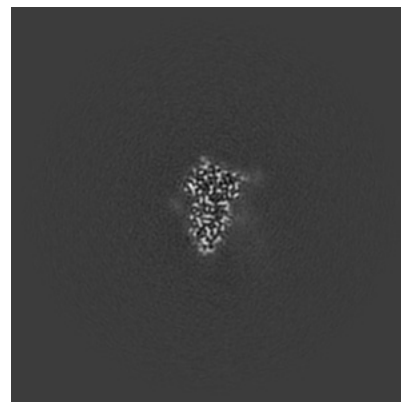
6.3.1 Primary map



X Index: 250

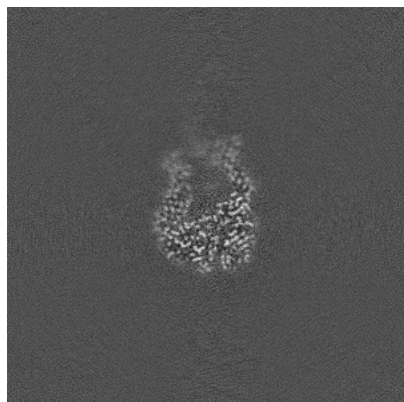


Y Index: 282

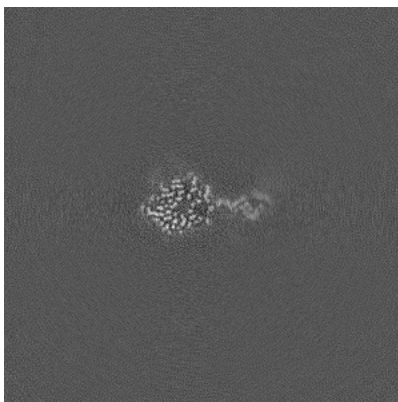


Z Index: 216

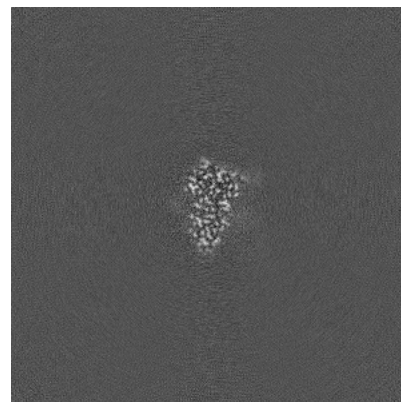
6.3.2 Raw map



X Index: 249



Y Index: 282

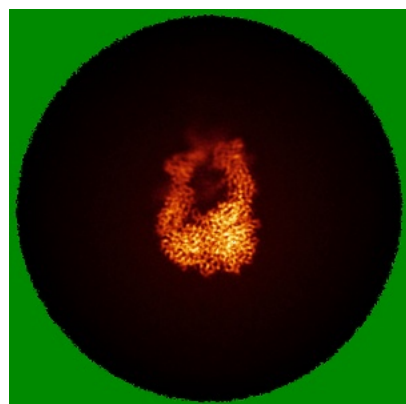


Z Index: 217

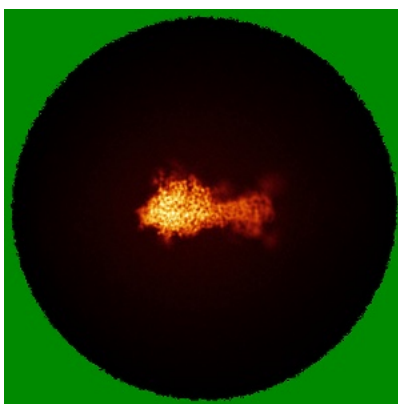
The images above show the largest variance slices of the map in three orthogonal directions.

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

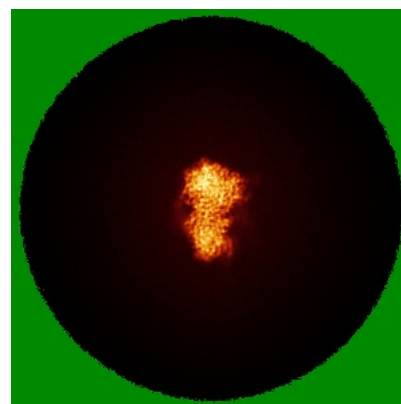
6.4.1 Primary map



X

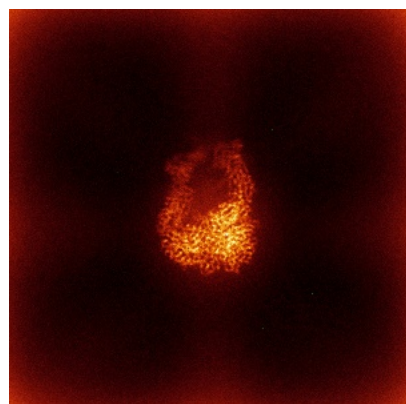


Y

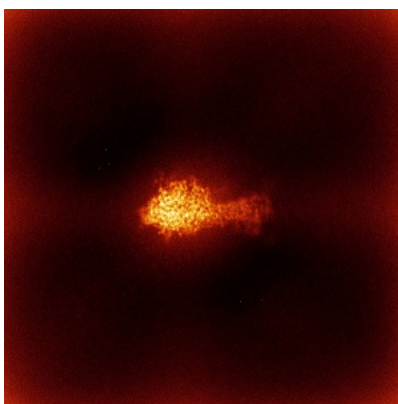


Z

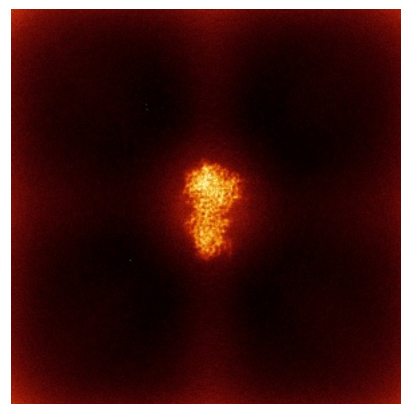
6.4.2 Raw map



X



Y

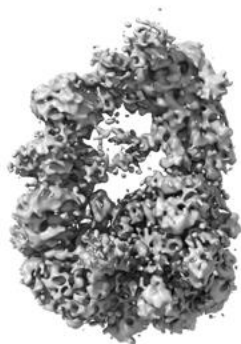


Z

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](#)

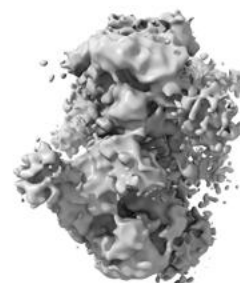
6.5.1 Primary map



X



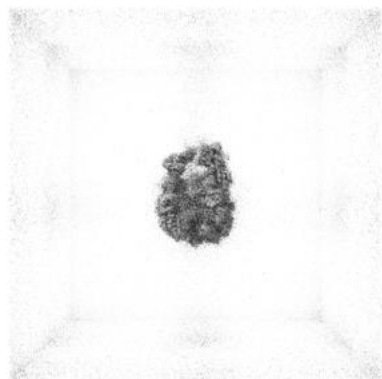
Y



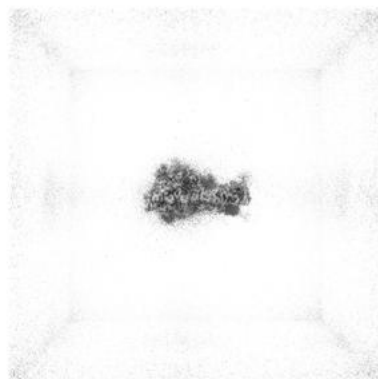
Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

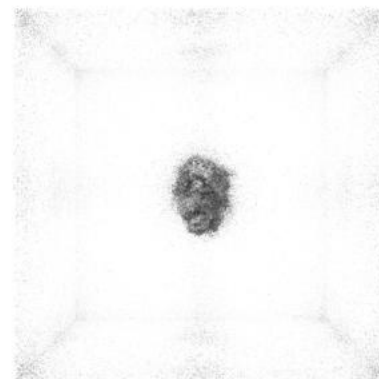
6.5.2 Raw map



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.

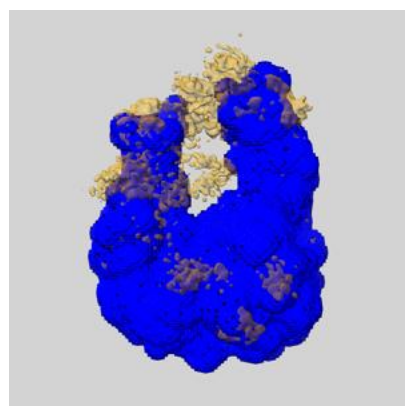
6.6 Mask visualisation [i](#)

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

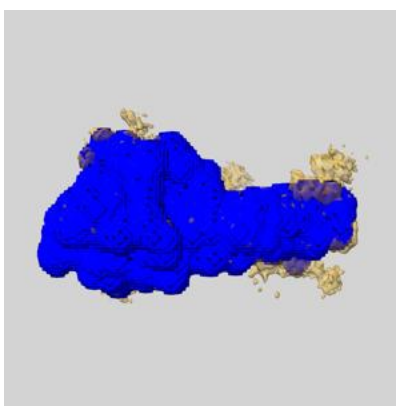
A mask typically either:

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

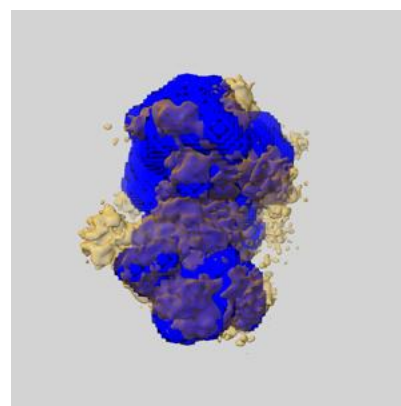
6.6.1 emd_38292_msk_1.map [i](#)



X



Y

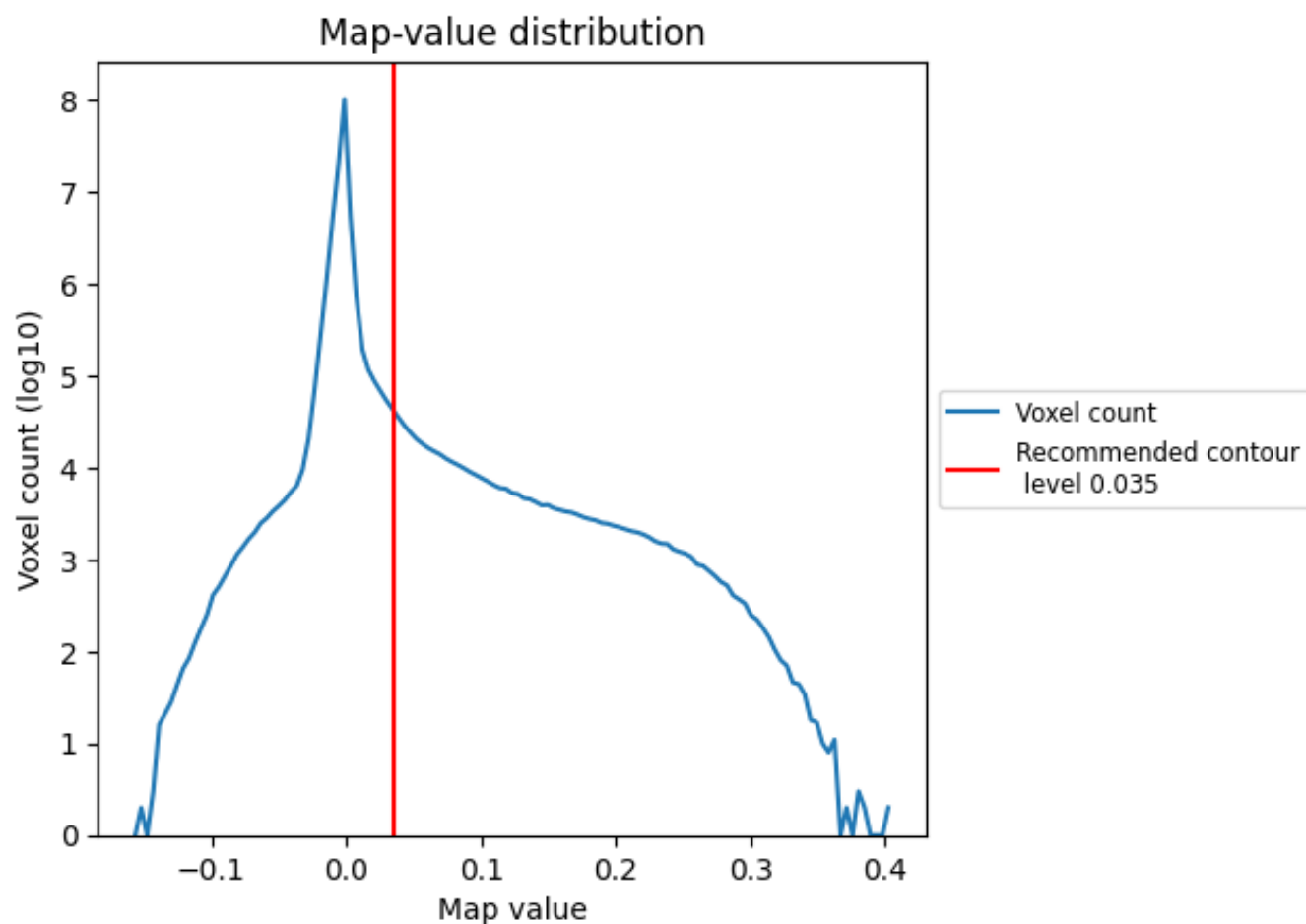


Z

7 Map analysis [i](#)

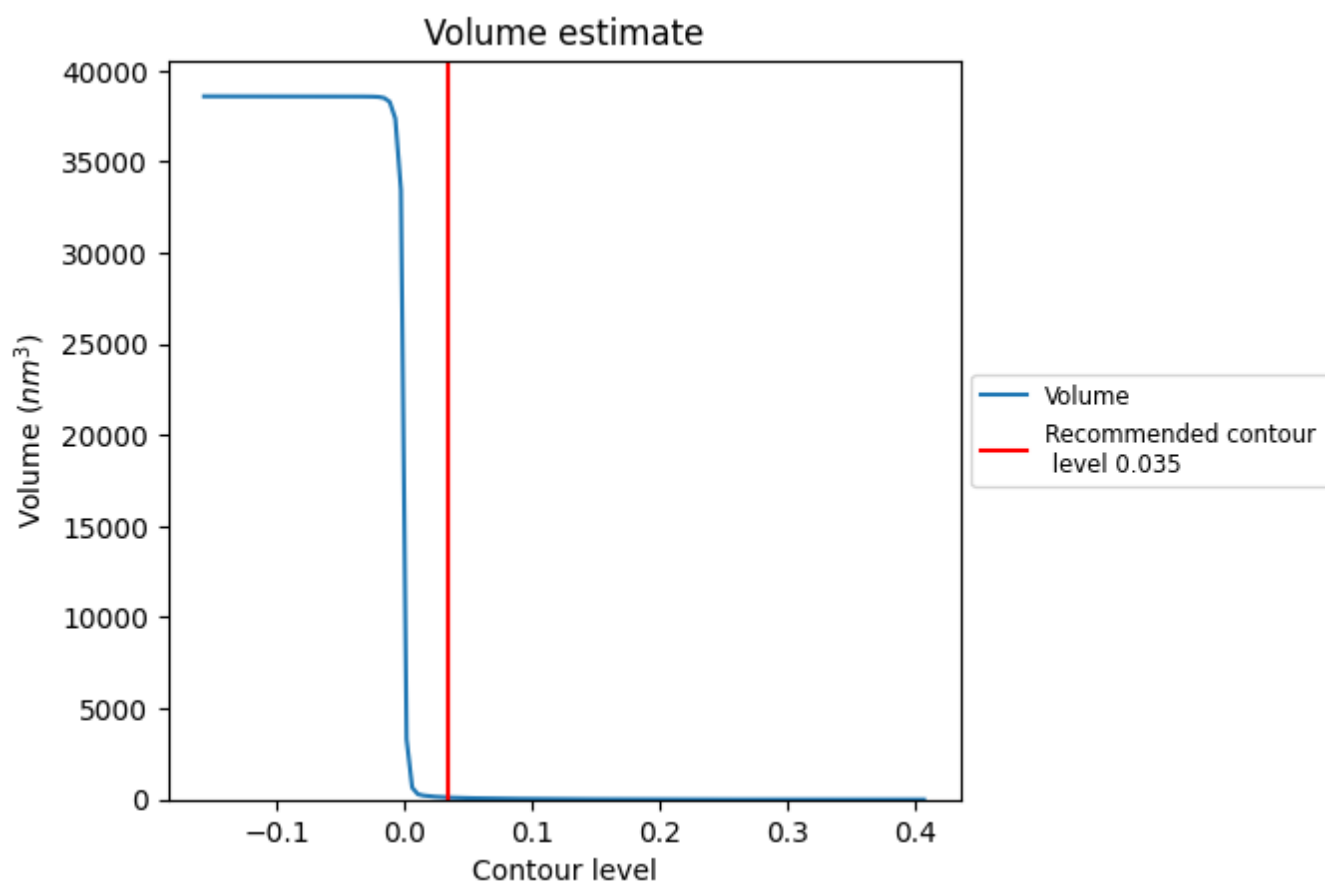
This section contains the results of statistical analysis of the map.

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.

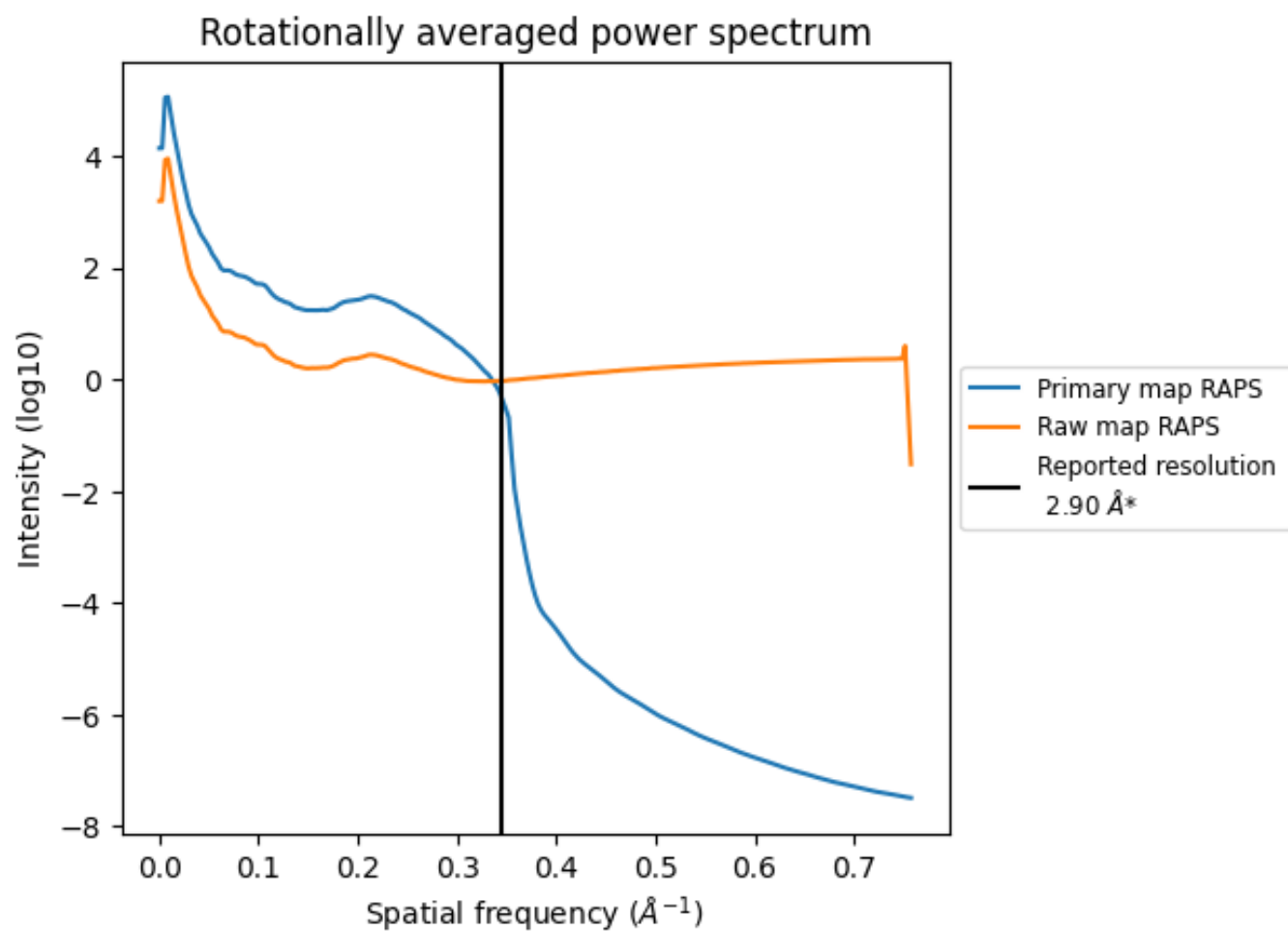
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm³; this corresponds to an approximate mass of 103 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 ⓘ

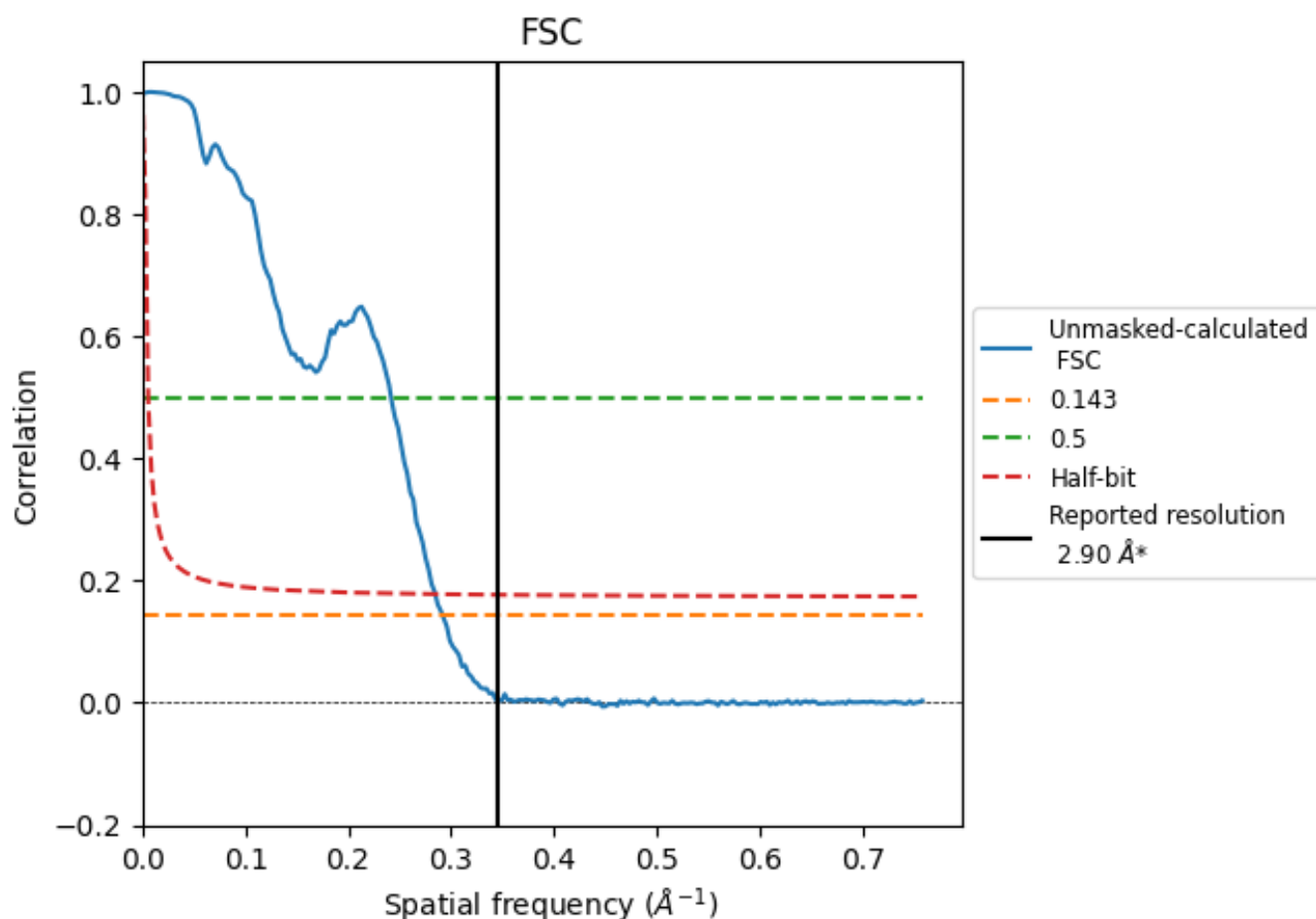


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

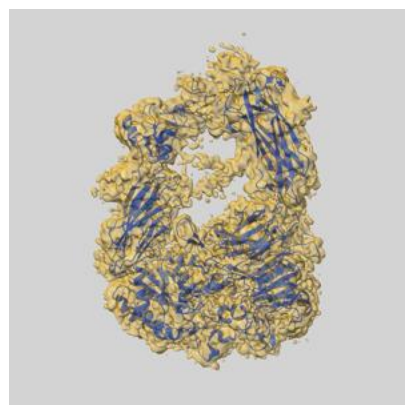
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.43	4.14	3.51

*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 3.43 differs from the reported value 2.9 by more than 10 %

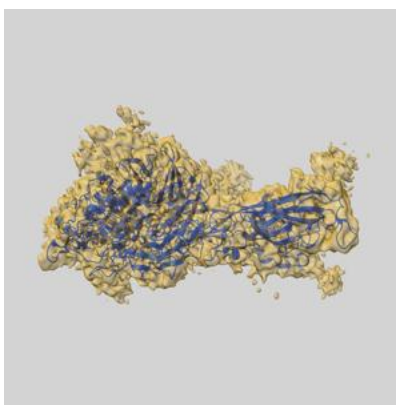
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38292 and PDB model 8XEK. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

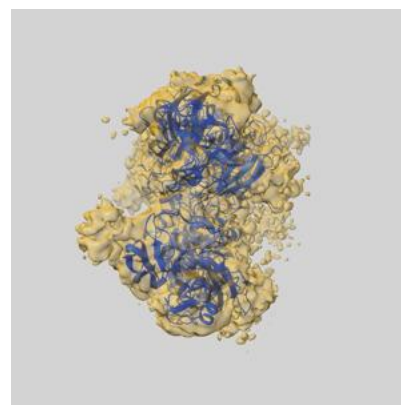
9.1 Map-model overlay [i](#)



X



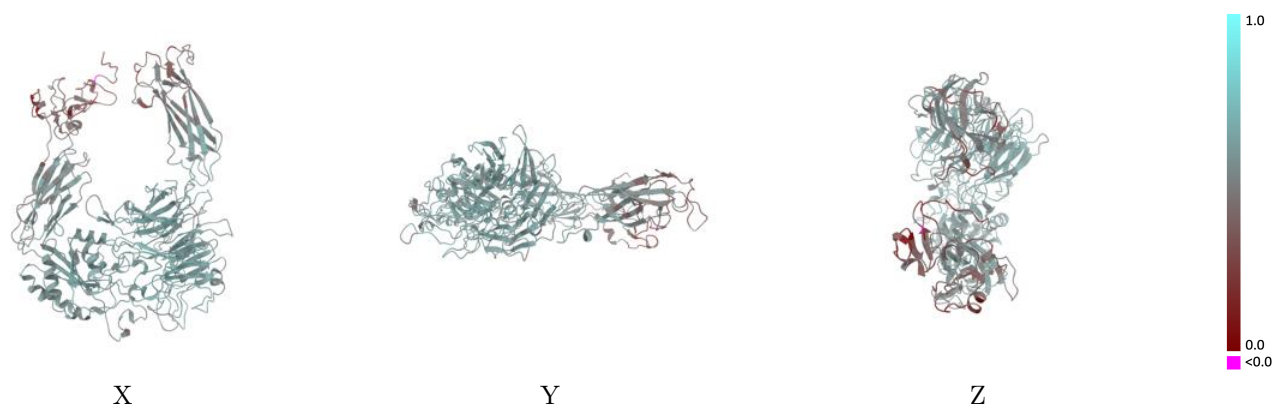
Y



Z

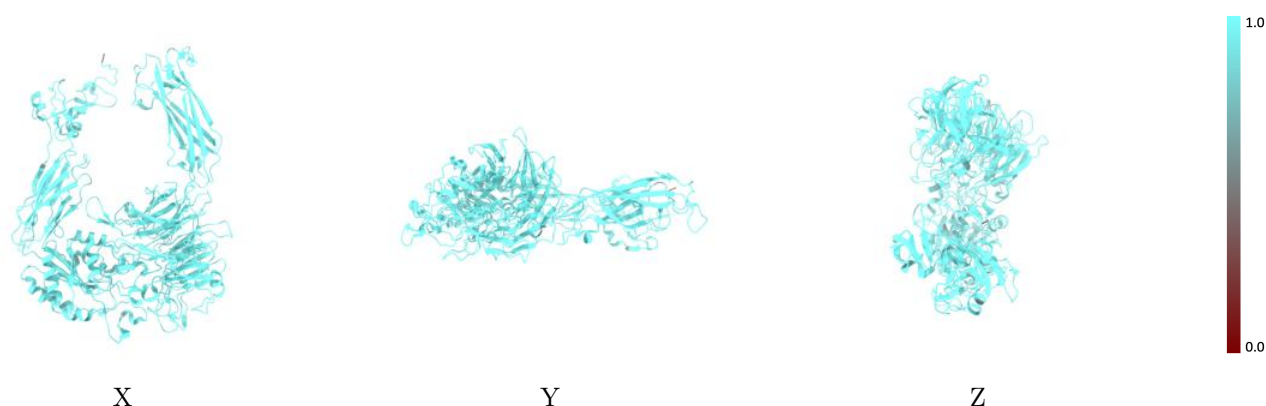
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



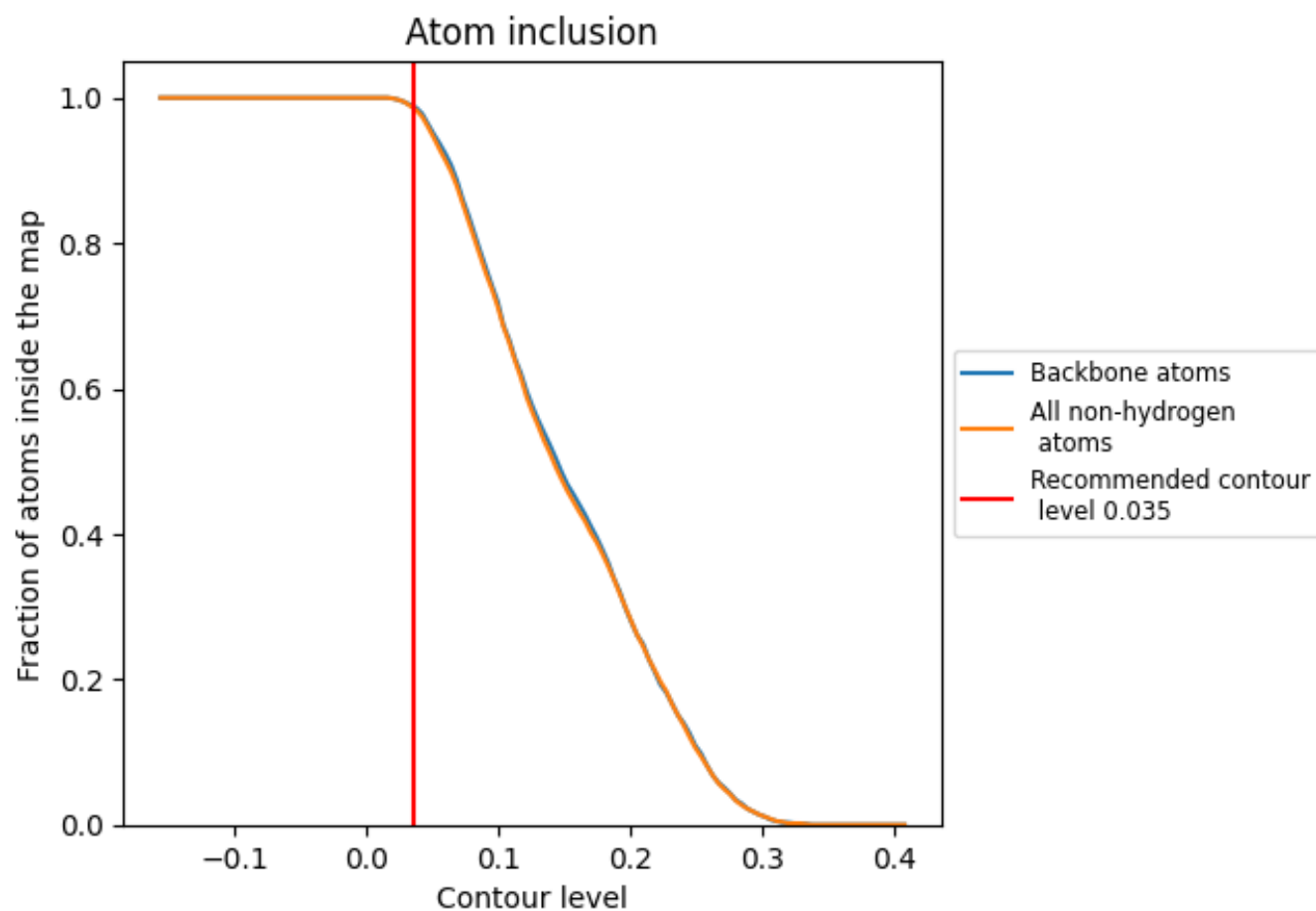
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9860	0.5430
A	0.9900	0.5640
B	0.9820	0.5180

