



wwPDB EM Validation Summary Report ⓘ

Oct 15, 2025 – 01:44 am BST

PDB ID : 9QWX / pdb_00009qwx
EMDB ID : EMD-53430
Title : Cryo-EM structure of the human UBR4/KCMF1/CALM1 complex (N-term focused refinement)
Authors : Grabarczyk, D.B.; Clausen, T.
Deposited on : 2025-04-15
Resolution : 3.60 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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

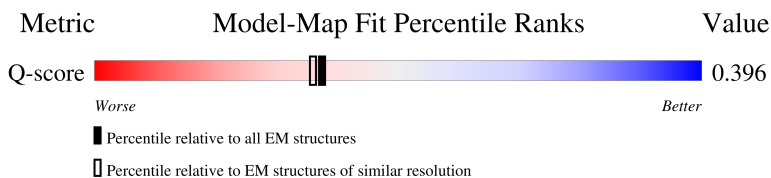
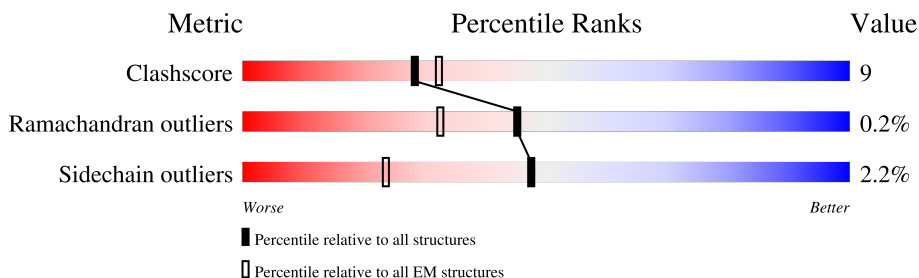
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	5193	 20% 6% 74%
1	B	5193	 20% 5% 74%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20114 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 E3 ubiquitin-protein ligase UBR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1351	Total	C	N	O	S	0	0
			10057	6388	1719	1904	46		
1	B	1351	Total	C	N	O	S	0	0
			10057	6388	1719	1904	46		

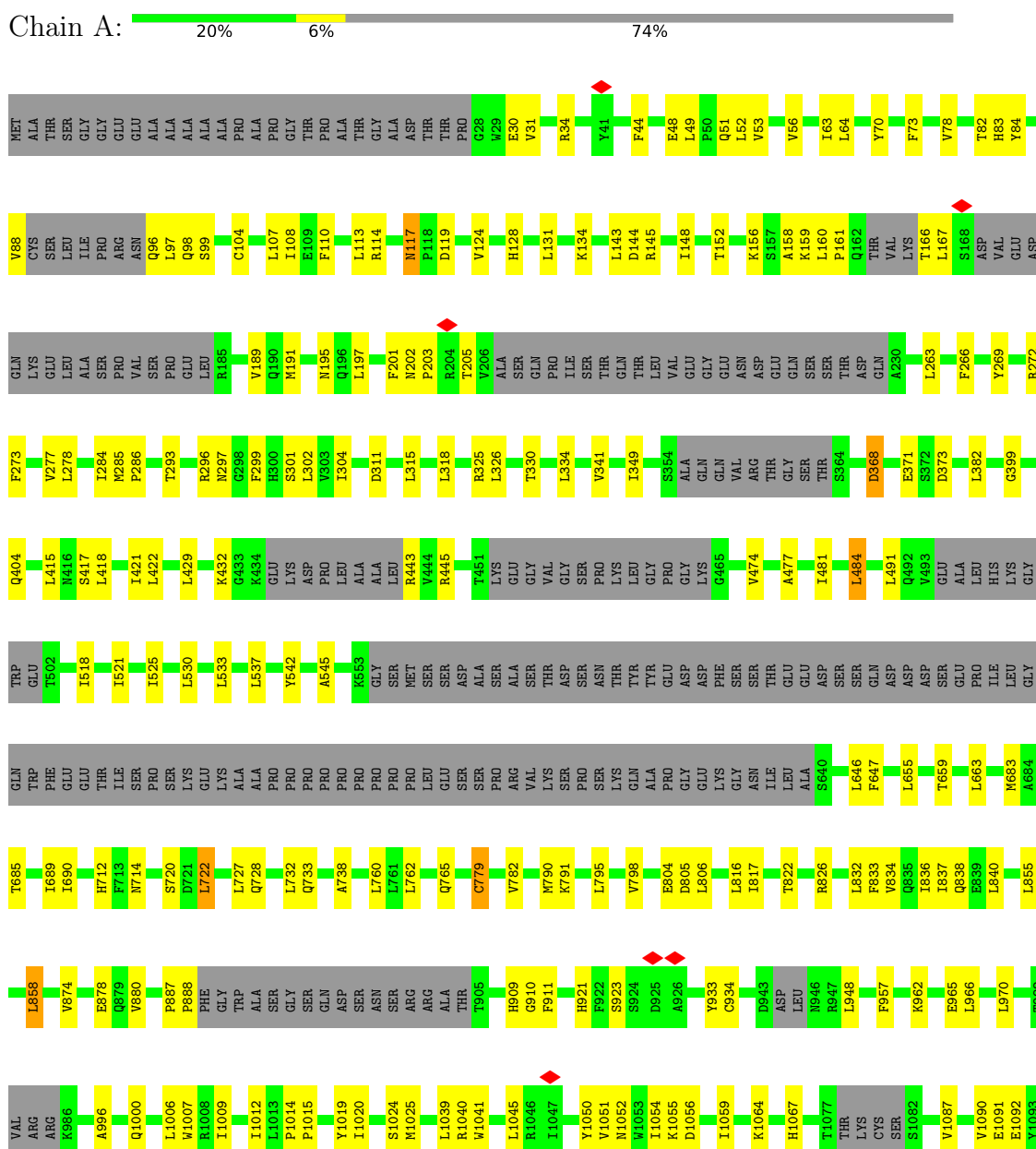
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5184	HIS	-	expression tag	UNP Q5T4S7
A	5185	HIS	-	expression tag	UNP Q5T4S7
A	5186	HIS	-	expression tag	UNP Q5T4S7
A	5187	HIS	-	expression tag	UNP Q5T4S7
A	5188	HIS	-	expression tag	UNP Q5T4S7
A	5189	HIS	-	expression tag	UNP Q5T4S7
A	5190	HIS	-	expression tag	UNP Q5T4S7
A	5191	HIS	-	expression tag	UNP Q5T4S7
A	5192	HIS	-	expression tag	UNP Q5T4S7
A	5193	HIS	-	expression tag	UNP Q5T4S7
B	5184	HIS	-	expression tag	UNP Q5T4S7
B	5185	HIS	-	expression tag	UNP Q5T4S7
B	5186	HIS	-	expression tag	UNP Q5T4S7
B	5187	HIS	-	expression tag	UNP Q5T4S7
B	5188	HIS	-	expression tag	UNP Q5T4S7
B	5189	HIS	-	expression tag	UNP Q5T4S7
B	5190	HIS	-	expression tag	UNP Q5T4S7
B	5191	HIS	-	expression tag	UNP Q5T4S7
B	5192	HIS	-	expression tag	UNP Q5T4S7
B	5193	HIS	-	expression tag	UNP Q5T4S7

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: E3 ubiquitin-protein ligase UBR4

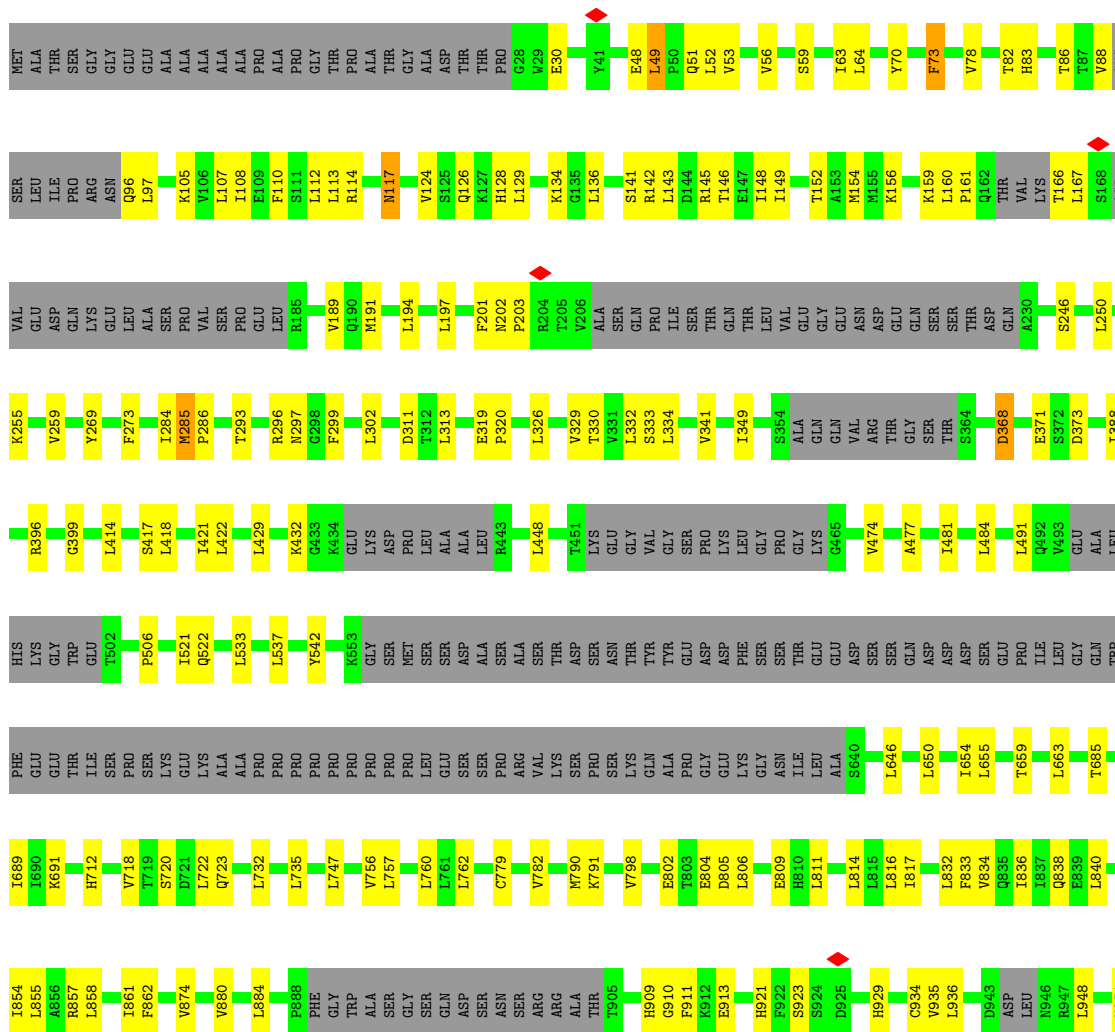








- Molecule 1: E3 ubiquitin-protein ligase UBR4









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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	75153	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00397	Depositor
Map size (Å)	486.912, 486.912, 486.912	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.268, 1.268, 1.268	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	0.13	0/10223	0.36	0/13903
1	B	0.14	0/10223	0.37	0/13903
All	All	0.13	0/20446	0.36	0/27806

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ASN	Peptide
1	B	117	ASN	Peptide
1	B	285	MET	Peptide

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	10057	0	9639	191	0
1	B	10057	0	9639	183	0
All	All	20114	0	19278	365	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 365 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:B:790:MET:HE3	1:B:854:ILE:HG23	1.57	0.87
1:A:272:ARG:HD3	1:A:285:MET:HE2	1.61	0.83
1:B:811:LEU:HD11	1:B:861:ILE:HD11	1.65	0.78
1:A:124:VAL:HG13	1:A:128:HIS:HB2	1.70	0.73
1:B:1119:GLN:O	1:B:1123:THR:HG23	1.90	0.72

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	1311/5193 (25%)	1265 (96%)	44 (3%)	2 (0%)	44	73
1	B	1311/5193 (25%)	1260 (96%)	49 (4%)	2 (0%)	44	73
All	All	2622/10386 (25%)	2525 (96%)	93 (4%)	4 (0%)	45	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	923	SER
1	B	923	SER
1	B	1223	PRO

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Mol	Chain	Res	Type
1	A	1223	PRO

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	1036/4531 (23%)	1015 (98%)	21 (2%)	50	72
1	B	1036/4531 (23%)	1011 (98%)	25 (2%)	44	67
All	All	2072/9062 (23%)	2026 (98%)	46 (2%)	47	69

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	368	ASP
1	B	1000	GLN
1	B	481	ILE
1	B	929	HIS
1	B	1029	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1227	GLN
1	B	1164	GLN
1	B	237	ASN
1	B	990	ASN
1	B	83	HIS

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.

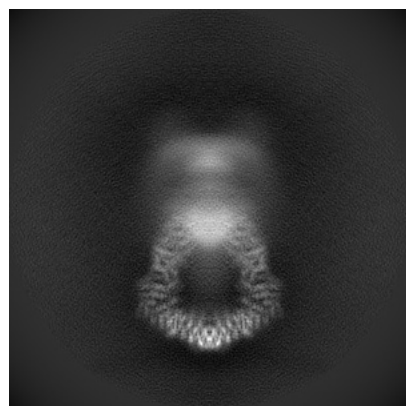
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53430. These allow visual inspection of the internal detail of the map and identification of artifacts.

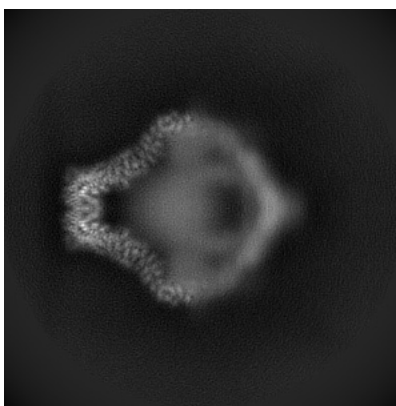
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

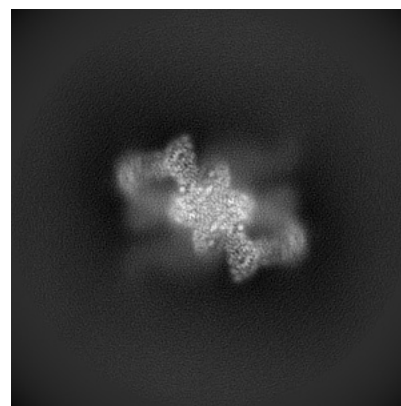
6.1.1 Primary map



X

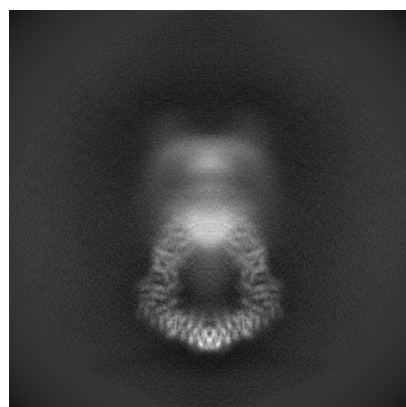


Y

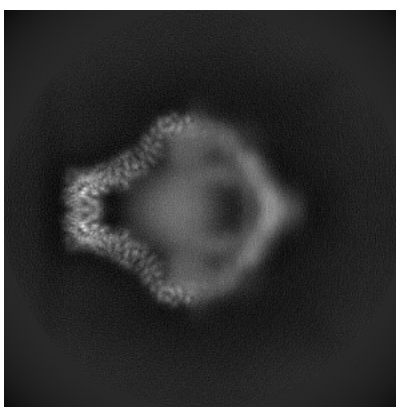


Z

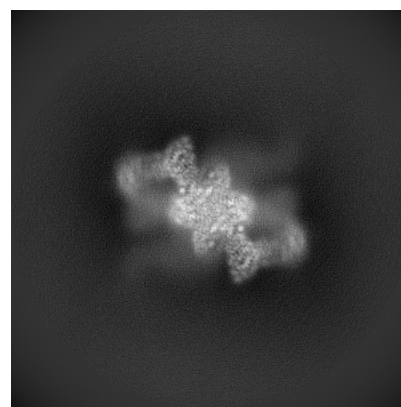
6.1.2 Raw map



X



Y

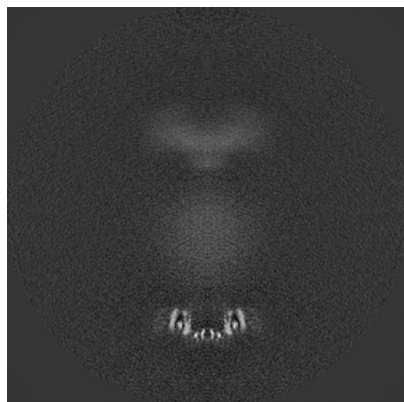


Z

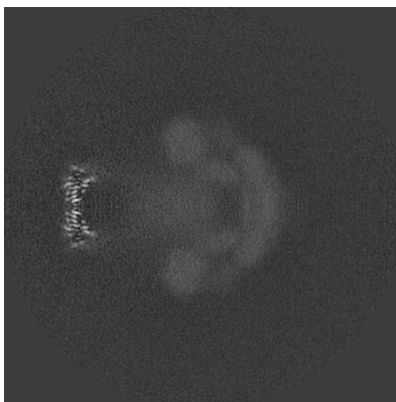
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

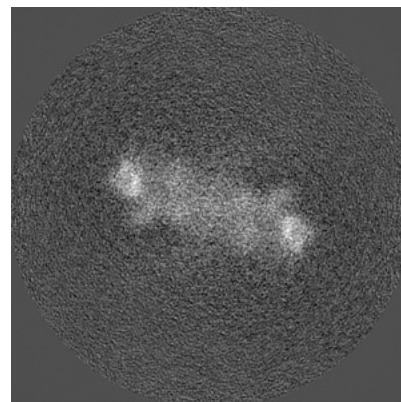
6.2.1 Primary map



X Index: 192

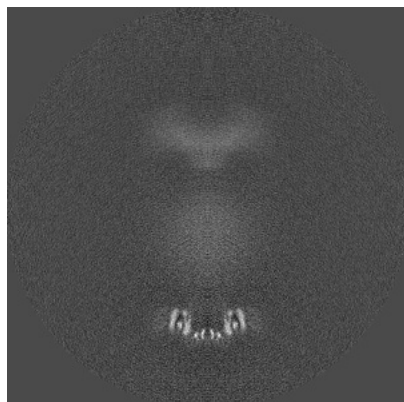


Y Index: 192

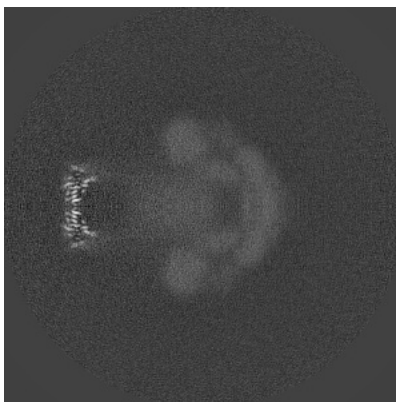


Z Index: 192

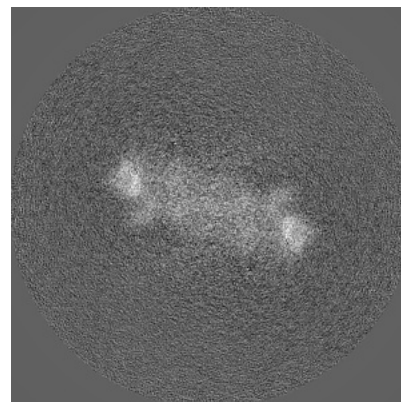
6.2.2 Raw map



X Index: 192



Y Index: 192

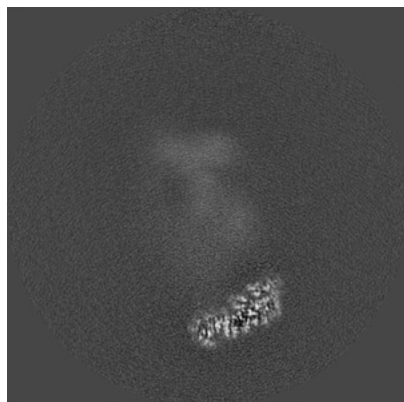


Z Index: 192

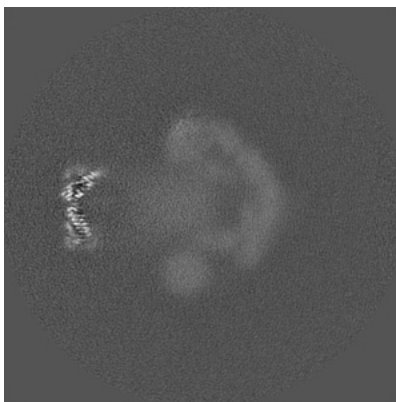
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

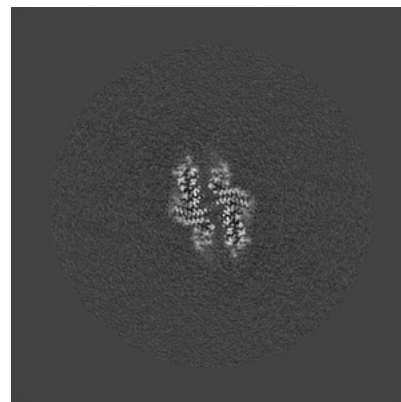
6.3.1 Primary map



X Index: 165

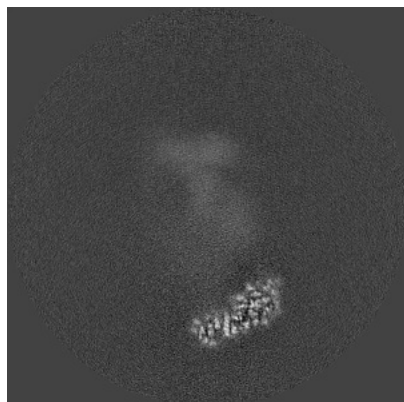


Y Index: 184

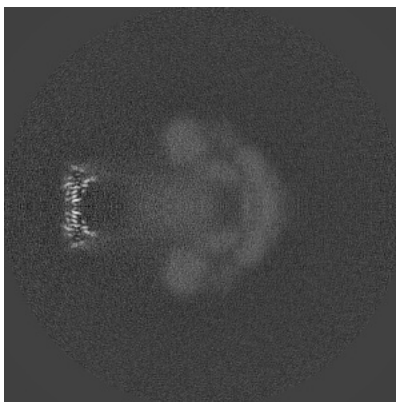


Z Index: 75

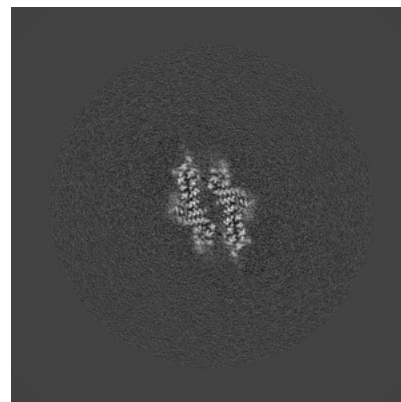
6.3.2 Raw map



X Index: 164



Y Index: 192

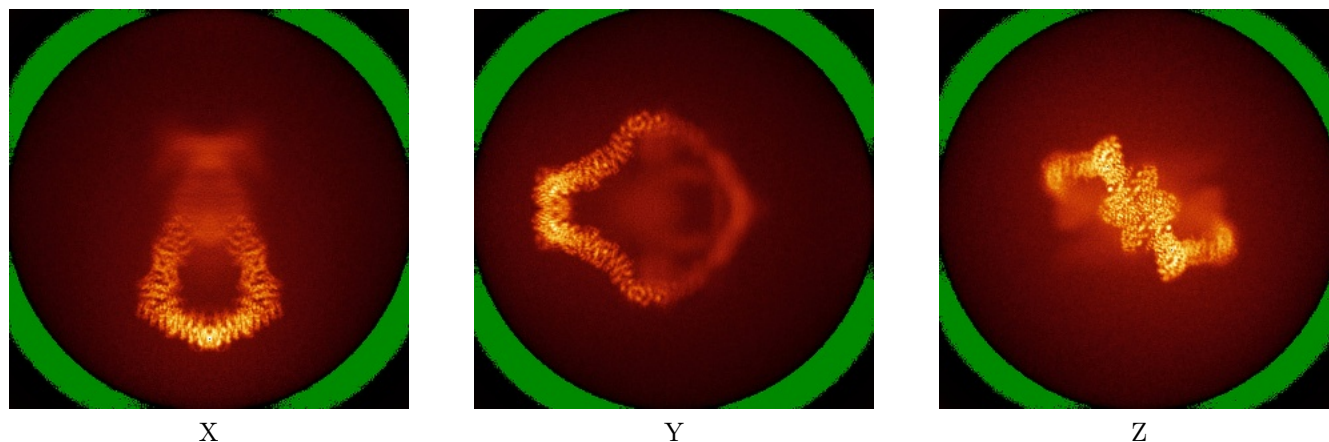


Z Index: 76

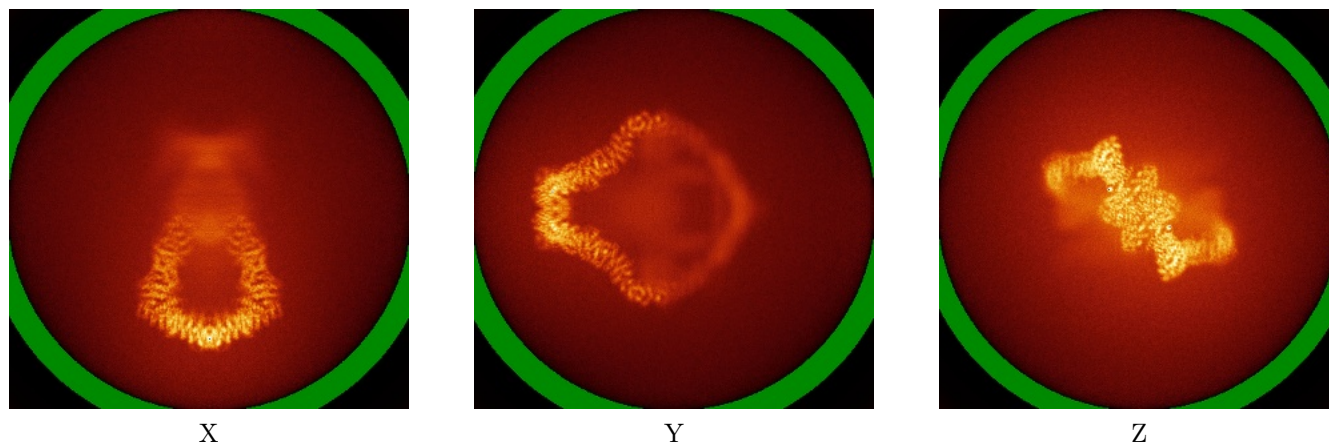
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



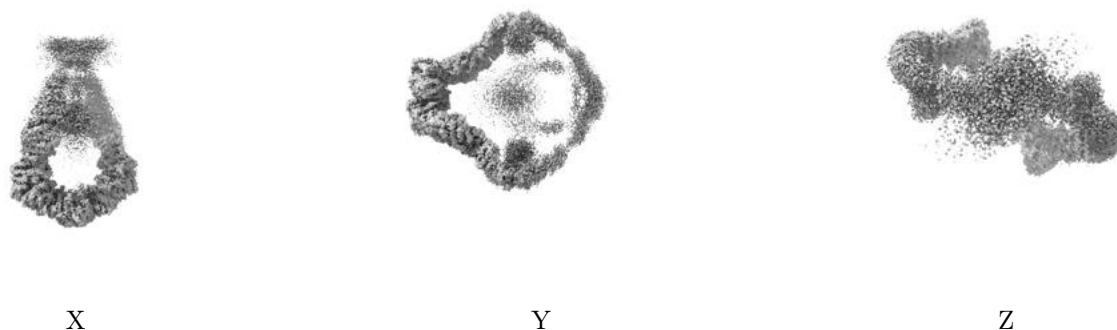
6.4.2 Raw map



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

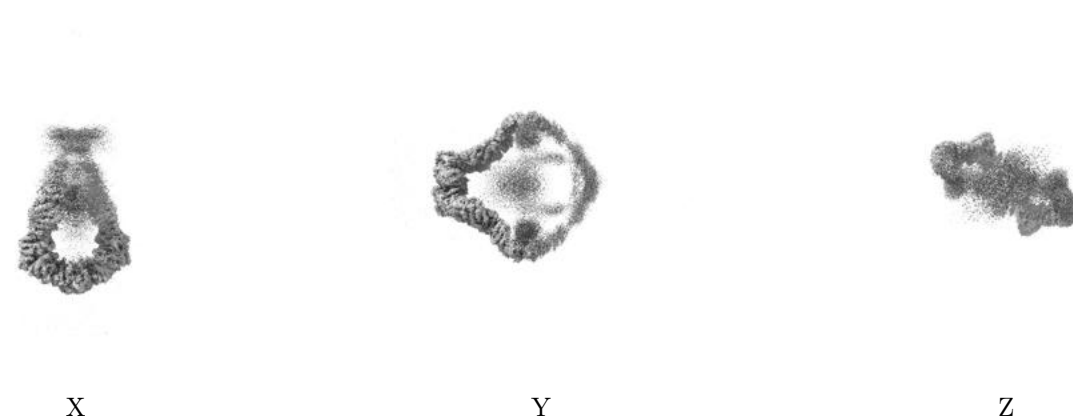
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00397. 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

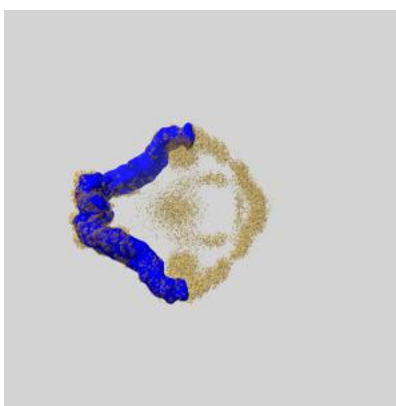
A mask typically either:

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

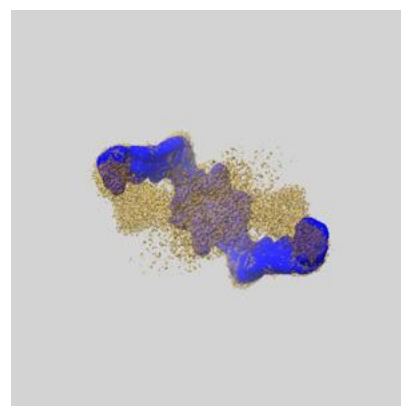
6.6.1 emd_53430_msk_1.map [i](#)



X



Y

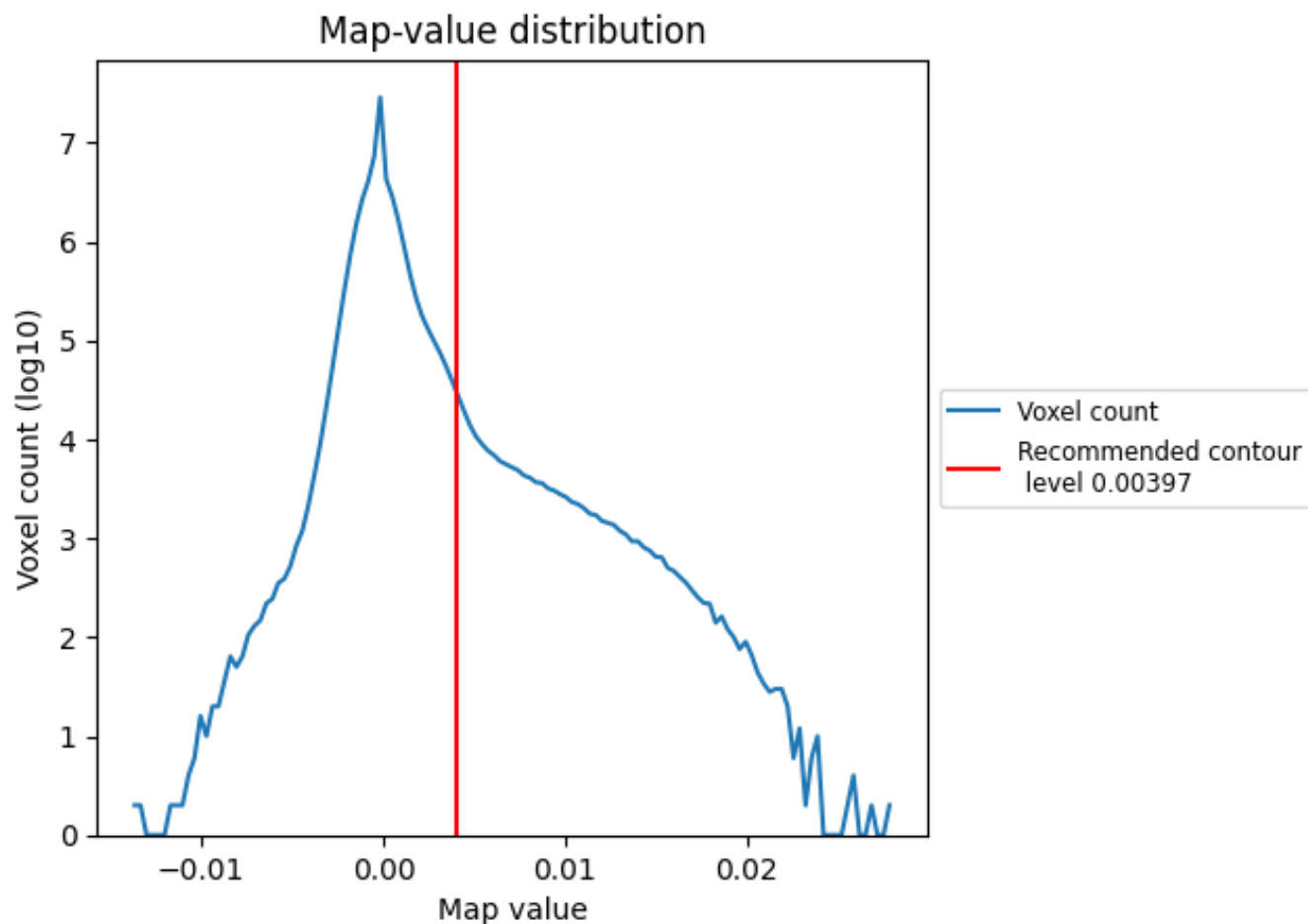


Z

7 Map analysis [i](#)

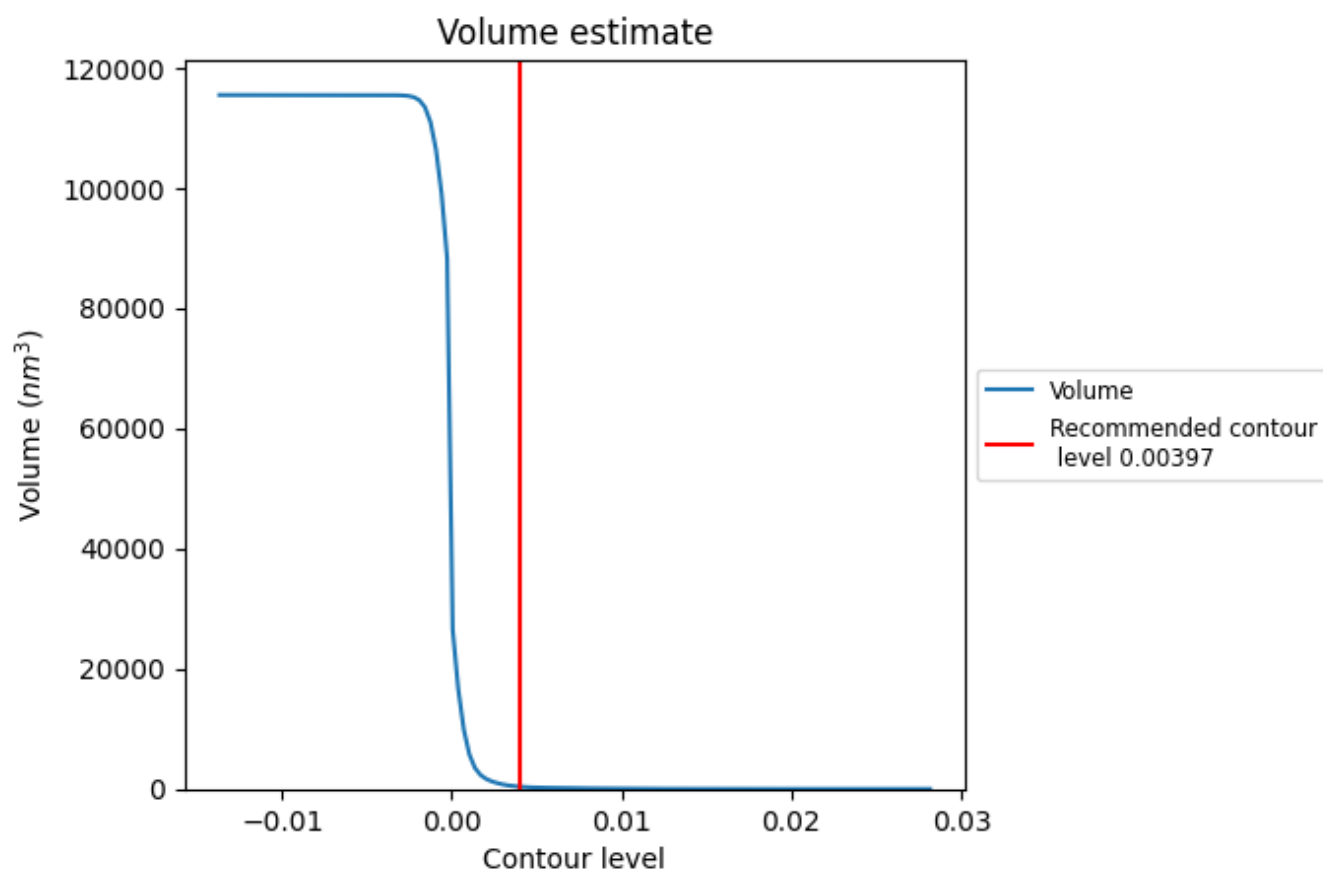
This section contains the results of statistical analysis of the map.

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.

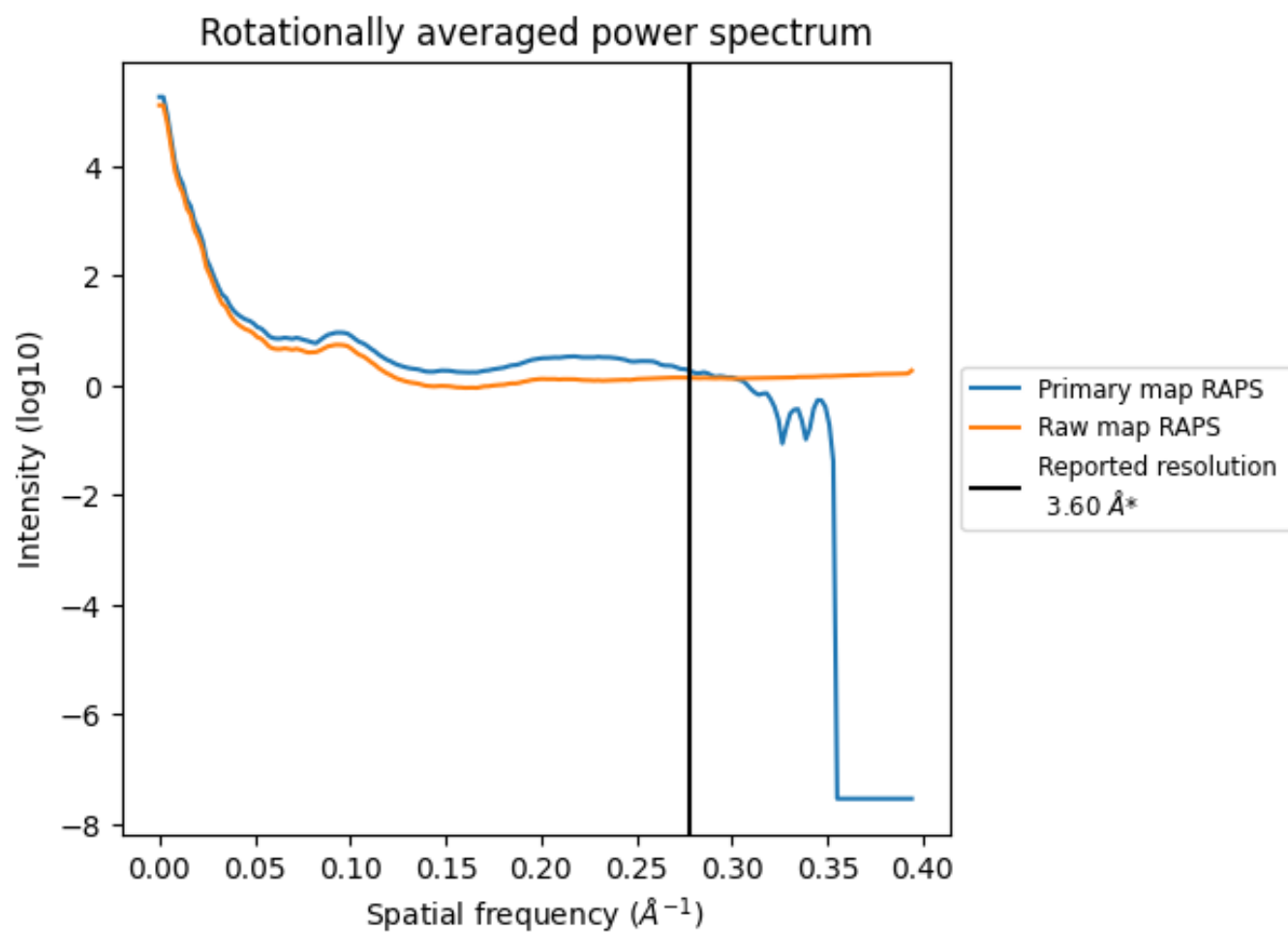
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 376 nm³; this corresponds to an approximate mass of 340 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 ⓘ

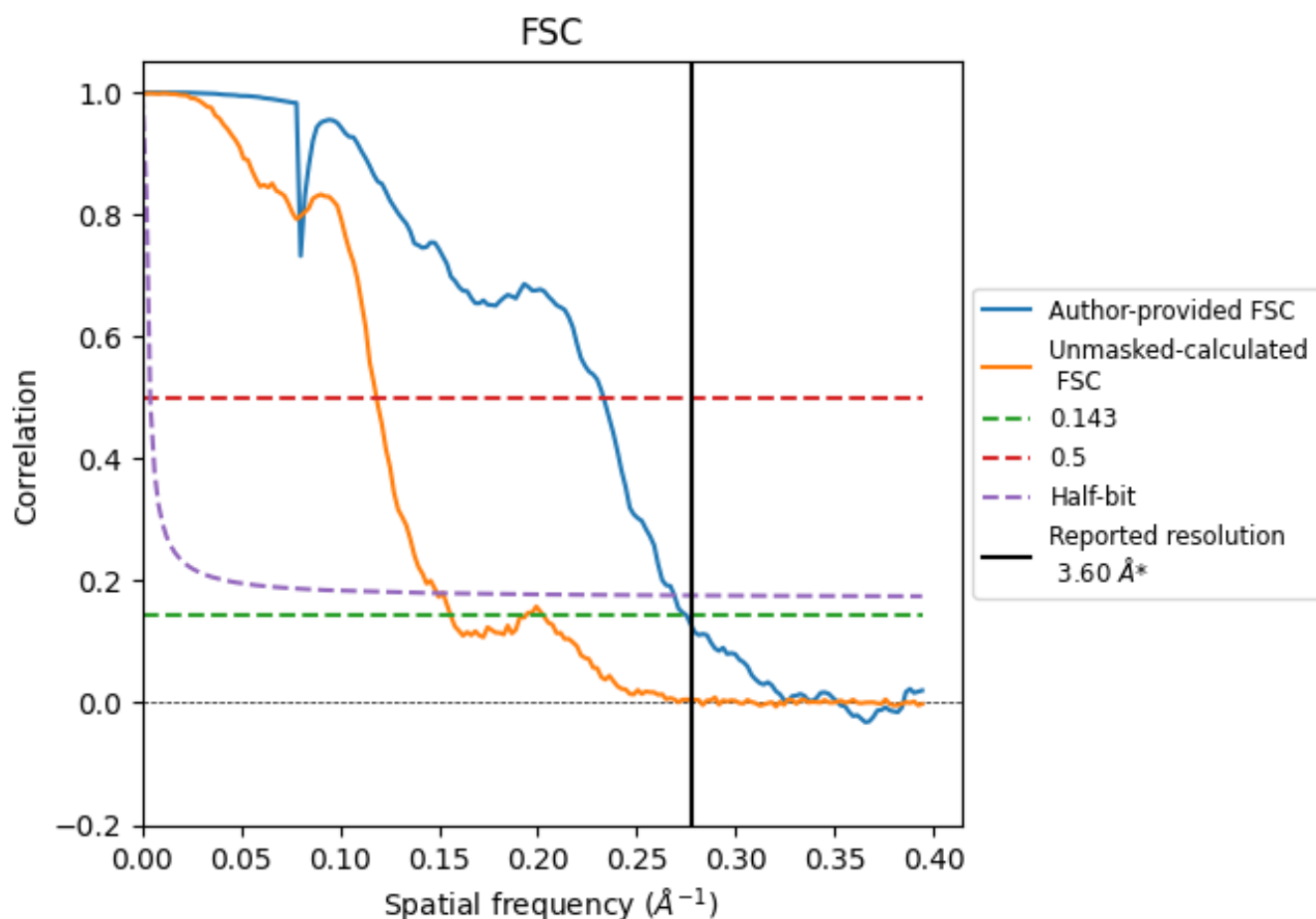


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

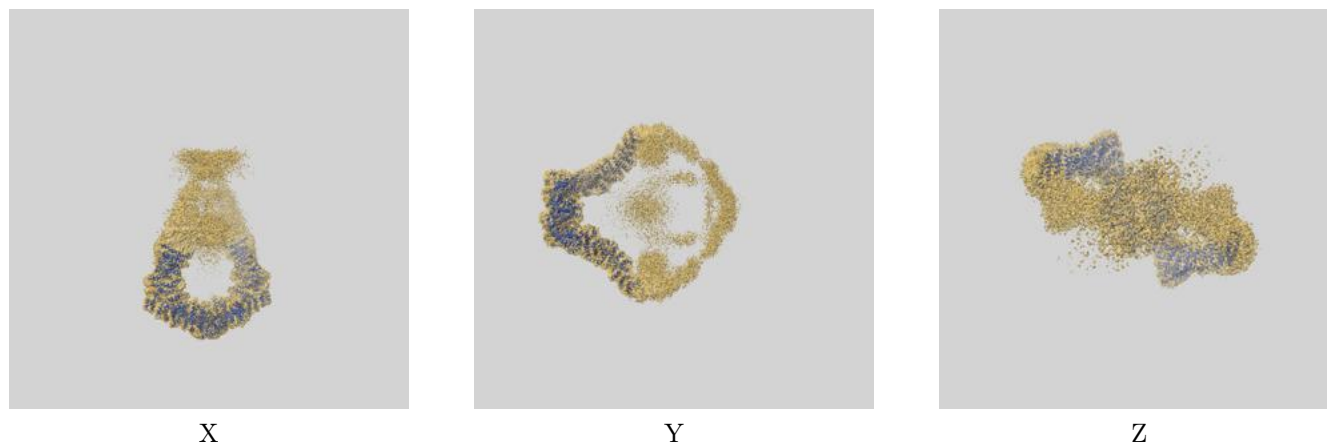
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.63	4.29	3.72
Unmasked-calculated*	6.41	8.45	6.71

*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 6.41 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

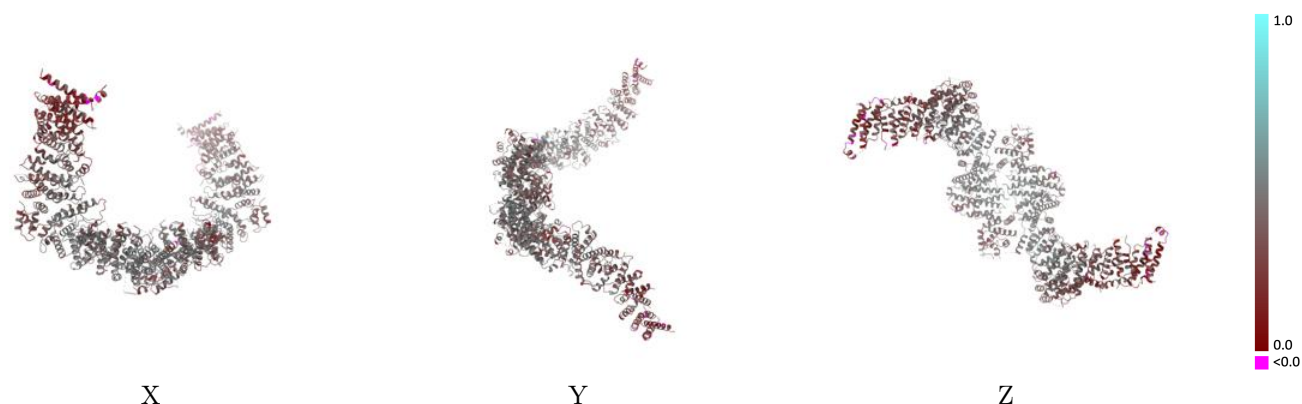
This section contains information regarding the fit between EMDB map EMD-53430 and PDB model 9QWX. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



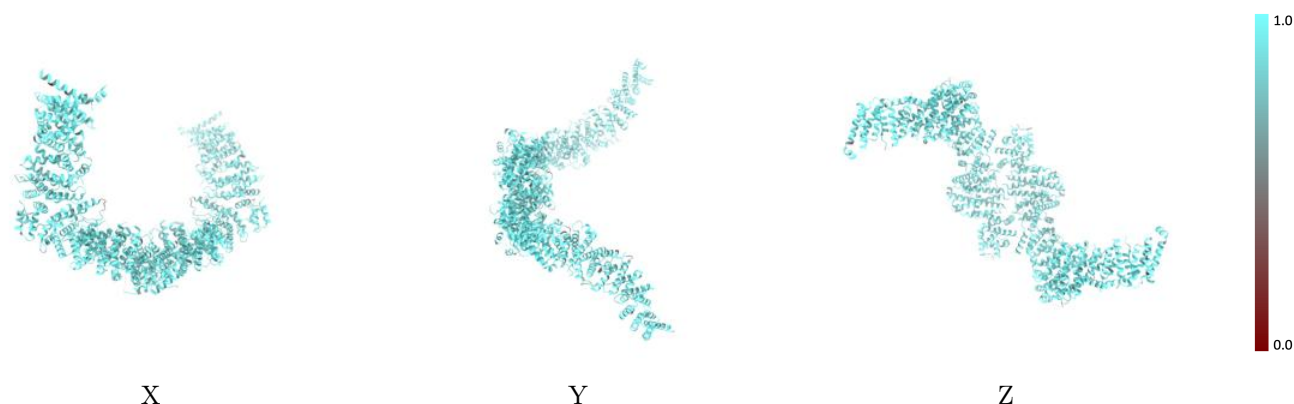
The images above show the 3D surface view of the map at the recommended contour level 0.00397 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



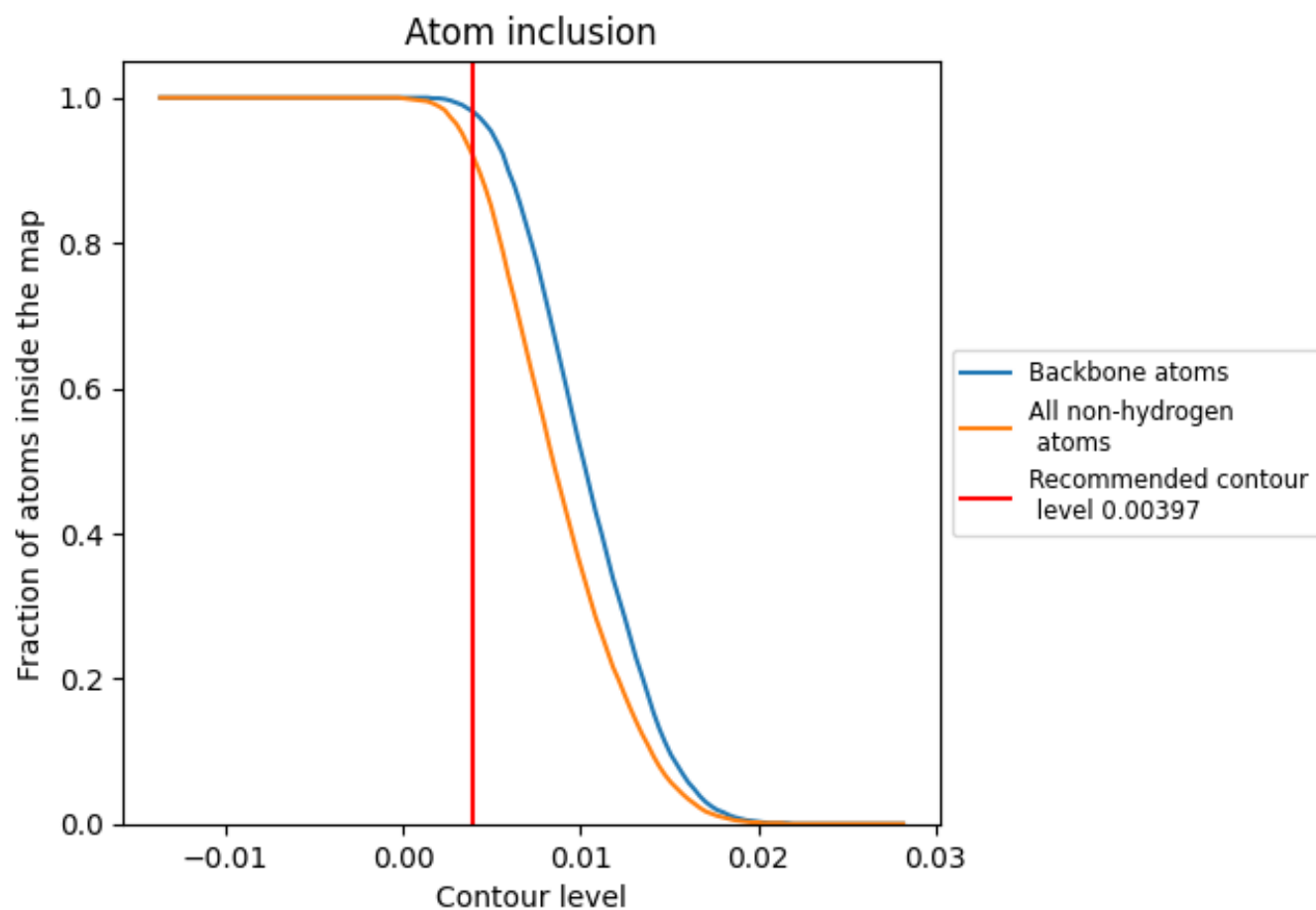
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00397).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 92% 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 (0.00397) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9180	<div></div> 0.3960
A	<div></div> 0.9200	<div></div> 0.3980
B	<div></div> 0.9160	<div></div> 0.3950

