



wwPDB EM Validation Summary Report ⓘ

Mar 4, 2026 – 10:08 PM UTC

PDB ID : 9KEN / pdb_00009ken
EMDB ID : EMD-62292
Title : cryo-EM structure of TRIP12 in complex with K29/48 branched-triUb
Authors : Ai, H.S.; Wu, X.W.; Liu, L.
Deposited on : 2024-11-05
Resolution : 3.63 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:

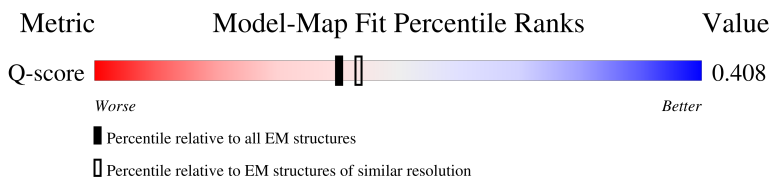
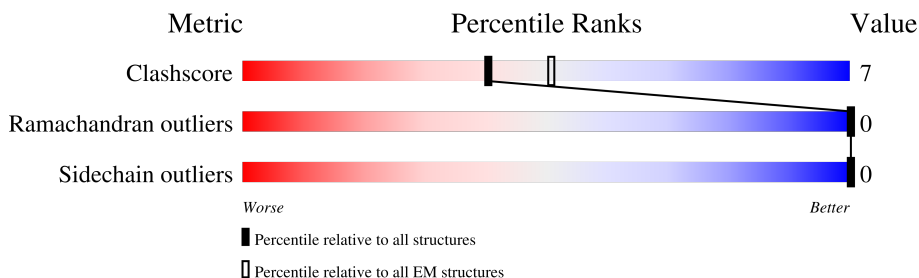
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.63 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	11696 (3.13 - 4.13)

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	C	76	 71% 29%
2	D	76	 71% 26%
3	A	1609	 57% 12% 30%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10083 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 Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	76	Total	C	N	O	S	0	0
			597	376	105	115	1		

- Molecule 2 is a protein called Ubiquitin K29C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	74	Total	C	N	O	S	0	0
			581	366	99	115	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	CYS	LYS	engineered mutation	UNP P62979

- Molecule 3 is a protein called E3 ubiquitin-protein ligase TRIP12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1124	Total	C	N	O	S	0	0
			8905	5696	1504	1644	61		

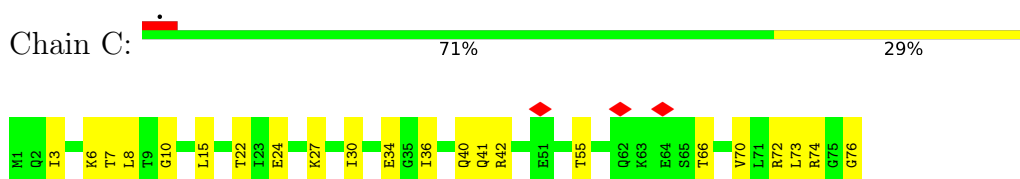
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	384	ASP	-	expression tag	UNP Q14669
A	385	TYR	-	expression tag	UNP Q14669
A	386	LYS	-	expression tag	UNP Q14669
A	387	ASP	-	expression tag	UNP Q14669
A	388	ASP	-	expression tag	UNP Q14669
A	389	ASP	-	expression tag	UNP Q14669
A	390	ASP	-	expression tag	UNP Q14669
A	391	LYS	-	expression tag	UNP Q14669
A	392	GLY	-	expression tag	UNP Q14669
A	393	THR	-	expression tag	UNP Q14669

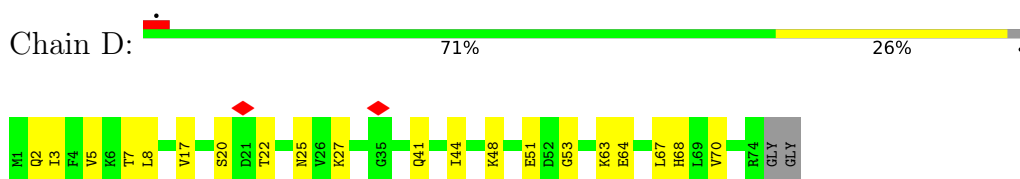
3 Residue-property plots

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.

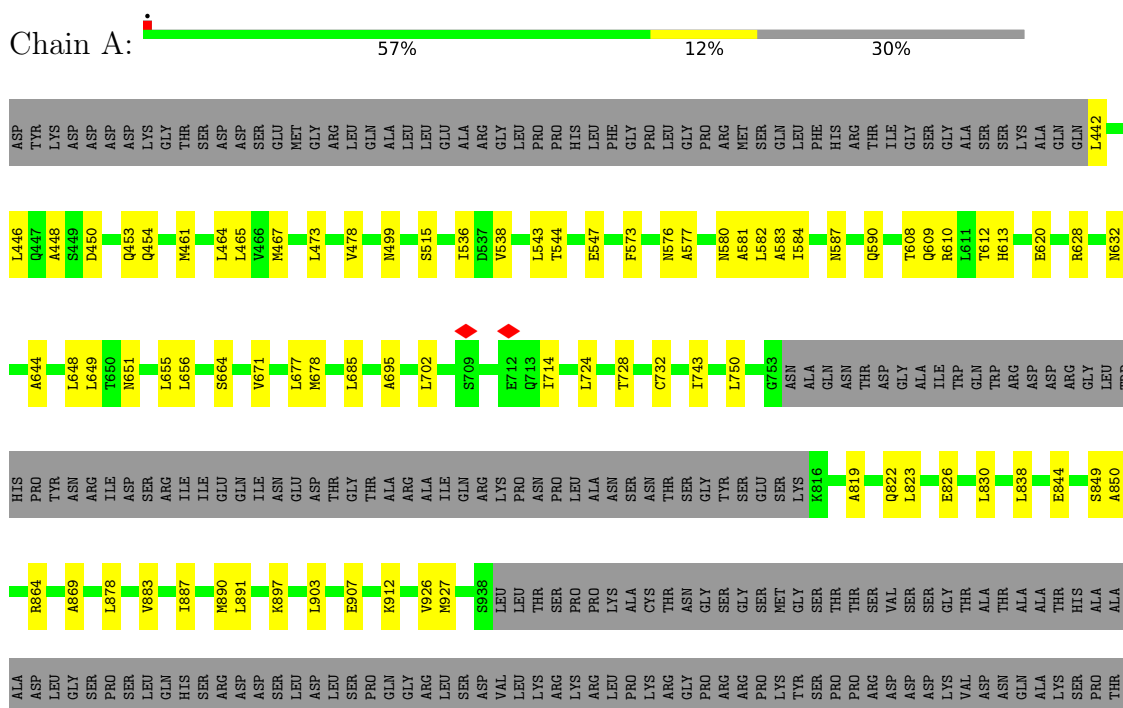
- Molecule 1: Ubiquitin



- Molecule 2: Ubiquitin K29C



- Molecule 3: E3 ubiquitin-protein ligase TRIP12



A1871	D1872	T1873	H1887	R1894	A1895	L1899	I1902	R1912	L1915	T1919	R1923	L1936	K1941	T1942	V1956	M1957	Y1962	L1963	P1966	S1969	G1985	GLN	GLN	SER	PHE	HIS	LEU	SER																
F1711	R1712	P1721	K1724	W1725	E1730	D1737	I1741	V1749	I1755	K1759	D1765	SER	GLN	THR	LYS	GLU	SER	L1777	M1782	C1785	G1808	I1811	I1815	L1822	I1826	F1827	W1828	A1829	L1830	N1831	E1832	F1838	F1841	E1861	S1869	LYS								
F1540	R1547	R1560	A1561	M1562	H1569	M1573	GLN	SER	ASP	GLN	ASP	ARG	VAL	K1583	K1590	R1591	E1603	I1618	V1624	G1625	T1626	F1634	E1641	R1644	A1645	D1646	L1647	M1672	G1675	F1681	G1682	R1683	K1686	P1687	V1693	K1696	M1709	D1710						
GLY	GLY	LYS	ARG	GLY	ARG	ALA	PRO	THR	LYS	THR	PRO	SER	ARG	ASN	ALA	K1432	D1435	E1436	G1441	E1451	P1459	I1462	D1466	L1469	L1475	L1478	H1479	S1482	M1491	A1492	M1493	I1497	I1498	F1503	I1504	N1505	S1506	K1507	L1508	K1511	M1523			
LEU	PRO	TYR	ASN	MET	THR	VAL	TYR	GLN	ALA	ALA	VAL	GLN	PHE	ILE	GLN	ALA	GLU	ASP	GLU	ASP	GLY	ASN	PRO	GLU	ILE	GLY	ALA	ASP	GLY	THR	ILE	TRP	LYS	ASP	GLU	LEU	GLN	VAL	GLY	GLY	PRO	LEU		
ALA	LEU	VAL	GLN	ALA	ILE	GLU	ARG	TYR	GLY	THR	GLY	ARG	VAL	VAL	GLN	ASP	GLU	ASP	ASP	ASP	GLY	SER	ASN	THR	GLU	GLY	ALA	ASP	GLY	THR	ALA	CYS	ASP	ALA	ASN	VAL	LYS	GLN	TRP	LYS	GLY	PRO	LEU	
K1099	F1105	E1108	ASN	MET	ASP	GLY	SER	ASN	PRO	ALA	L1117	L1123	E1128	L1141	I1144	I1147	S1154	E1157	H1160	F1163	S1173	V1180	S1181	R1182	E1183	I1184	R1185	R1188	F1193	P1199	G1200	E1201	G1205	R1206	M1212	L1215	V1219	E1095						
THR	THR	GLN	SER	PRO	LYS	SER	PHE	LEU	ALA	SER	LEU	ASN	PRO	LYS	THR	TRP	GLY	ARG	LEU	SER	THR	GLN	ASN	SER	ASN	ASN	GLY	ILE	GLU	PRO	ALA	ALA	LYS	ASP	T1081	E1087	K1088	I1089	K1090	G1091	W1092	I1093	K1094	E1095

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	259711	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	206.848, 206.848, 206.848	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.808, 0.808, 0.808	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	C	0.28	0/603	0.63	0/811
2	D	0.37	0/587	0.59	0/793
3	A	0.40	0/9082	0.57	0/12289
All	All	0.39	0/10272	0.57	0/13893

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
3	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1128	GLU	Peptide
3	A	1160	HIS	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	C	597	0	625	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	581	0	597	14	0
3	A	8905	0	8955	122	0
All	All	10083	0	10177	141	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 7.

The worst 5 of 141 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)
3:A:1497:ILE:HG22	3:A:1498:ILE:HG13	1.72	0.71
3:A:1618:ILE:HG21	3:A:1634:PHE:HB2	1.80	0.62
3:A:1466:ASP:HB3	3:A:1469:LEU:HB2	1.82	0.61
3:A:1560:ARG:NH1	3:A:1709:MET:O	2.35	0.60
3:A:1725:TRP:HZ2	3:A:1831:ASN:HA	1.66	0.60

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	C	74/76 (97%)	64 (86%)	10 (14%)	0	100	100
2	D	72/76 (95%)	64 (89%)	8 (11%)	0	100	100
3	A	1108/1609 (69%)	1045 (94%)	63 (6%)	0	100	100
All	All	1254/1761 (71%)	1173 (94%)	81 (6%)	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	C	67/68 (98%)	67 (100%)	0	100	100
2	D	66/68 (97%)	66 (100%)	0	100	100
3	A	993/1412 (70%)	993 (100%)	0	100	100
All	All	1126/1548 (73%)	1126 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	856	HIS
3	A	881	HIS
3	A	1689	HIS
3	A	1515	GLN
3	A	1643	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.

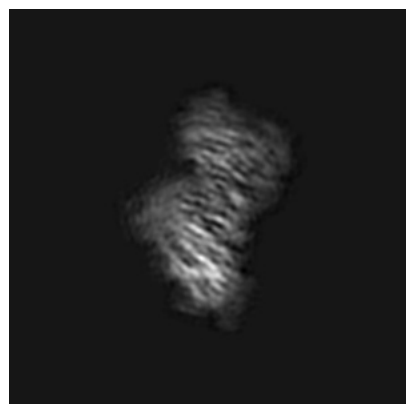
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62292. These allow visual inspection of the internal detail of the map and identification of artifacts.

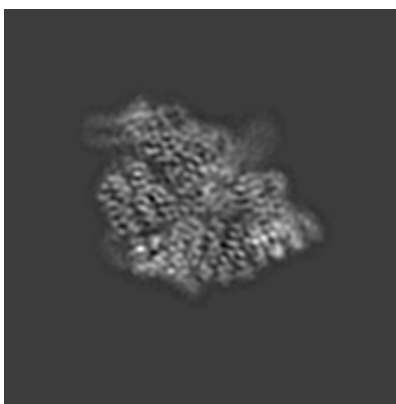
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

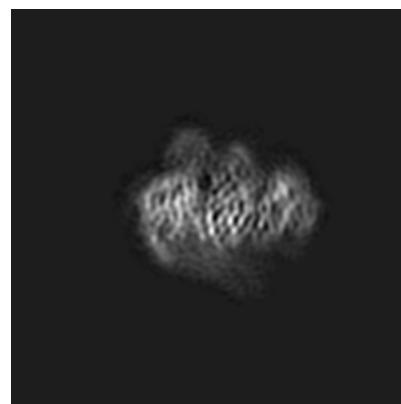
6.1.1 Primary map



X

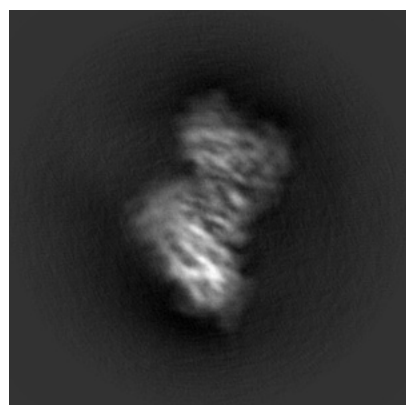


Y

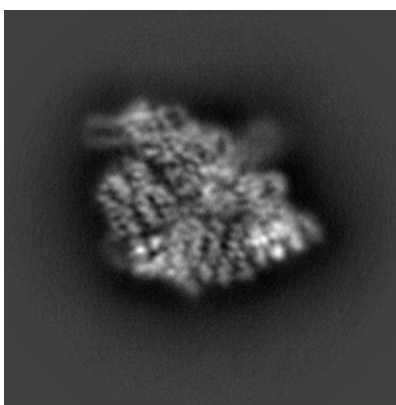


Z

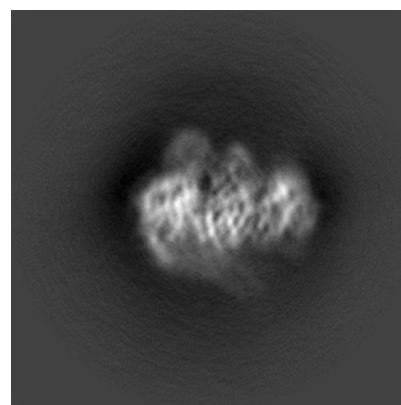
6.1.2 Raw map



X



Y



Z

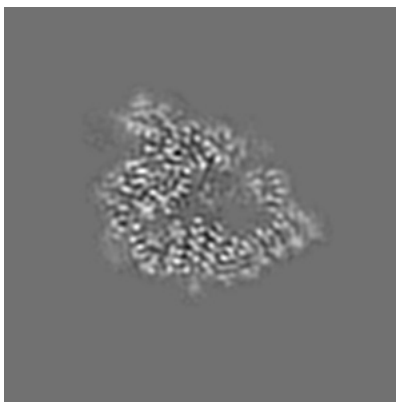
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

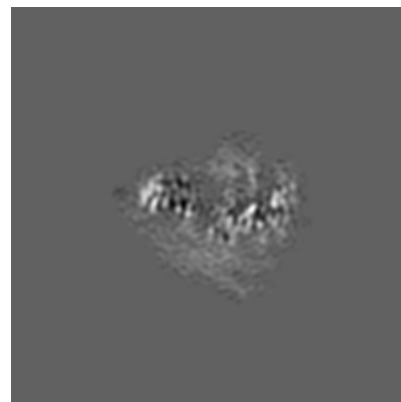
6.2.1 Primary map



X Index: 128

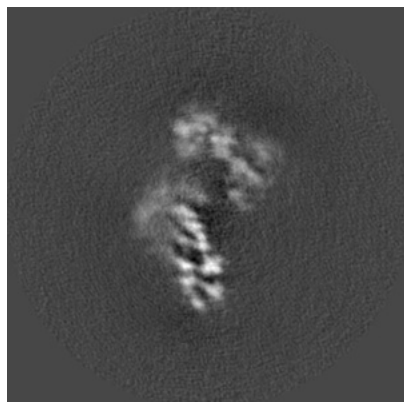


Y Index: 128

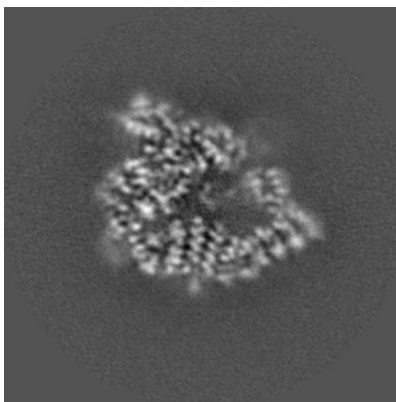


Z Index: 128

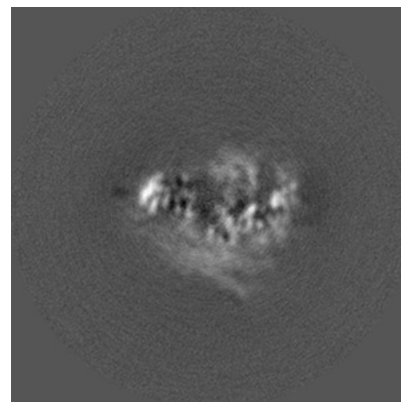
6.2.2 Raw map



X Index: 128



Y Index: 128

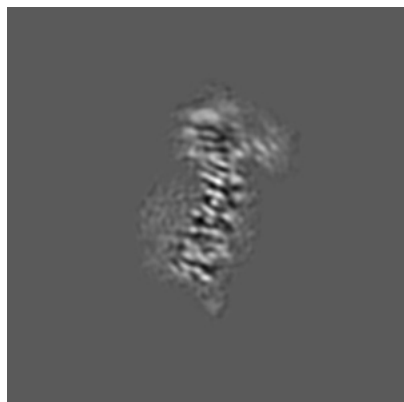


Z Index: 128

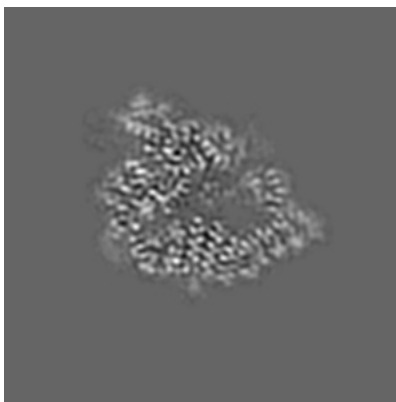
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 106

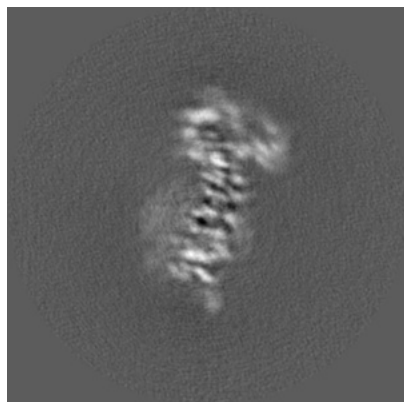


Y Index: 129

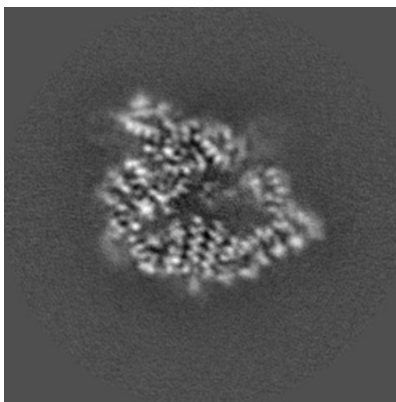


Z Index: 88

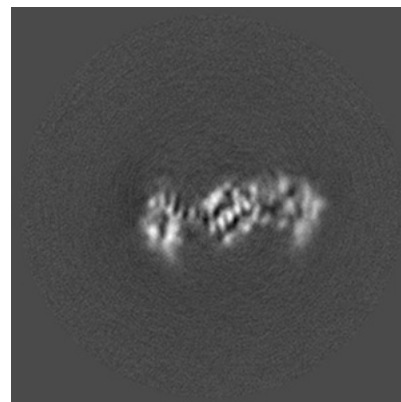
6.3.2 Raw map



X Index: 107



Y Index: 129

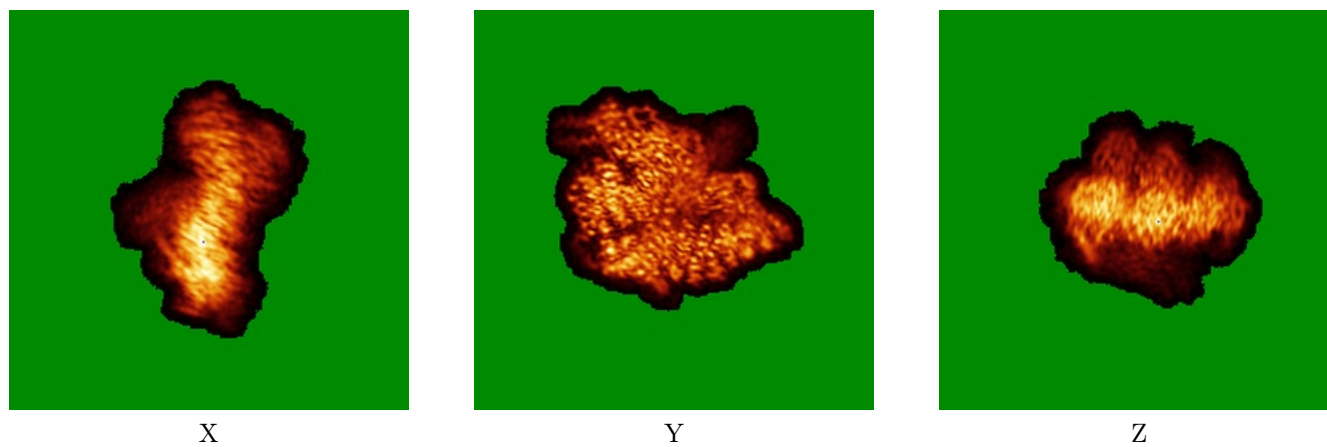


Z Index: 88

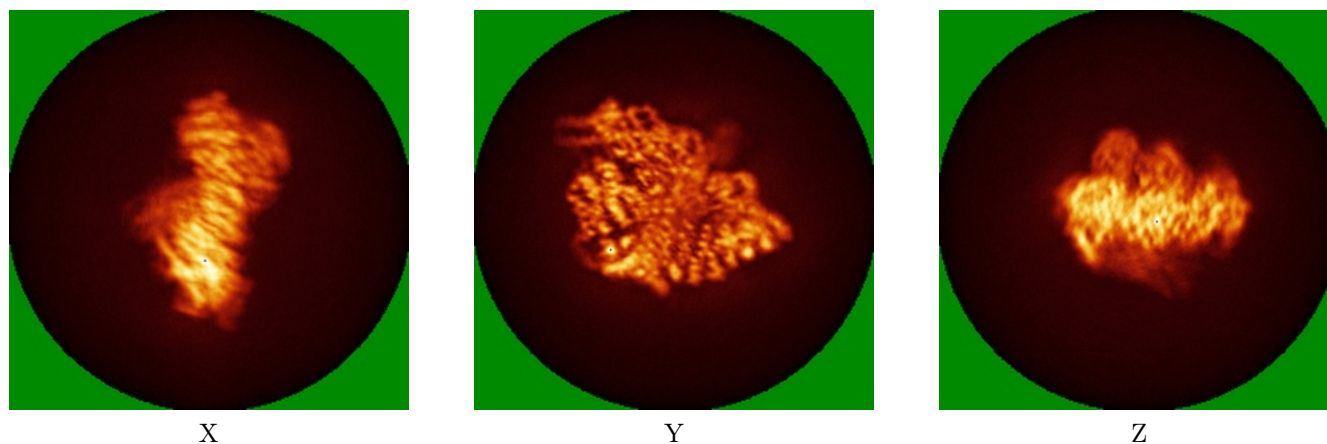
The images above show the largest variance slices of the map in three orthogonal directions.

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](#)

This section was not generated.

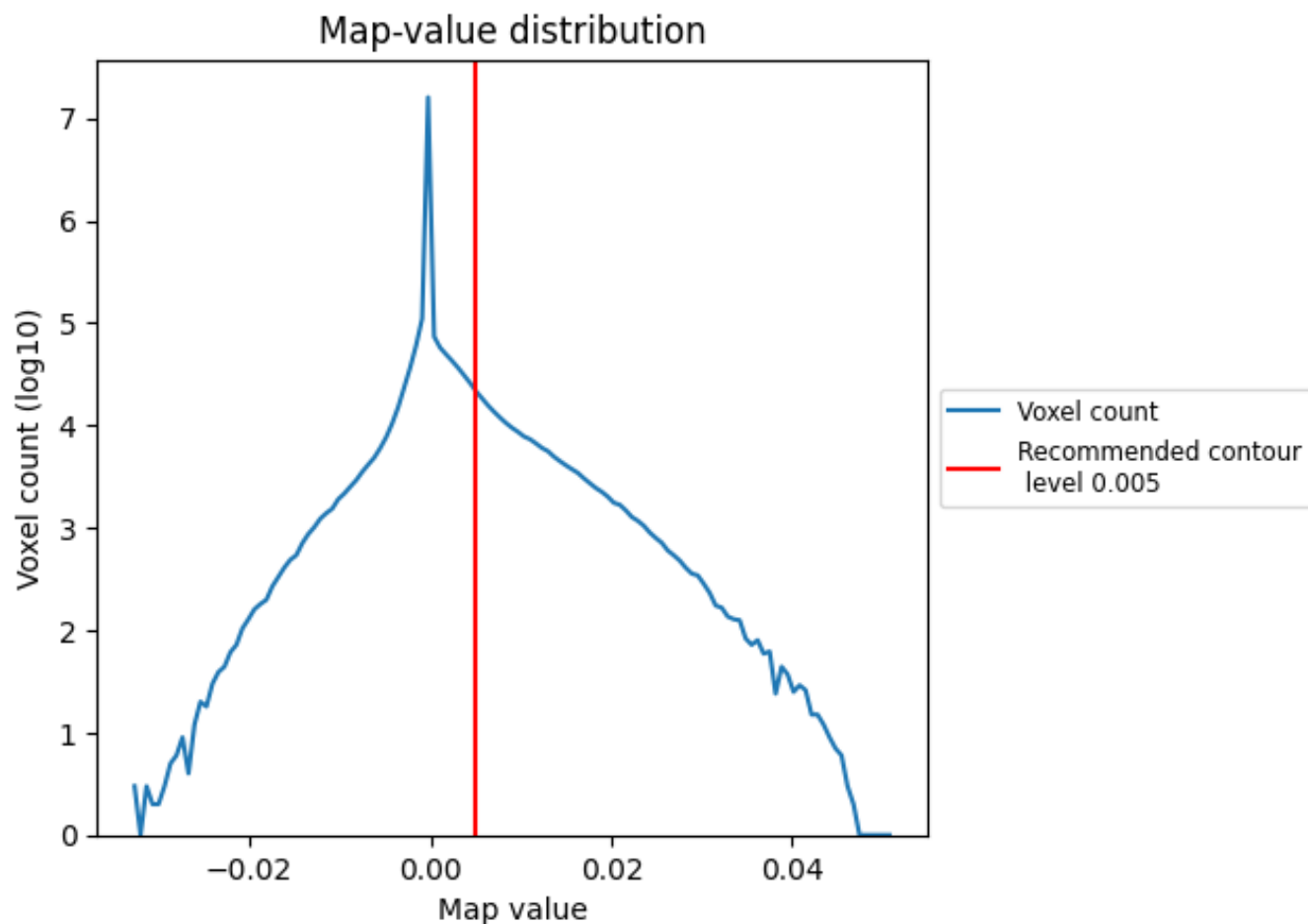
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

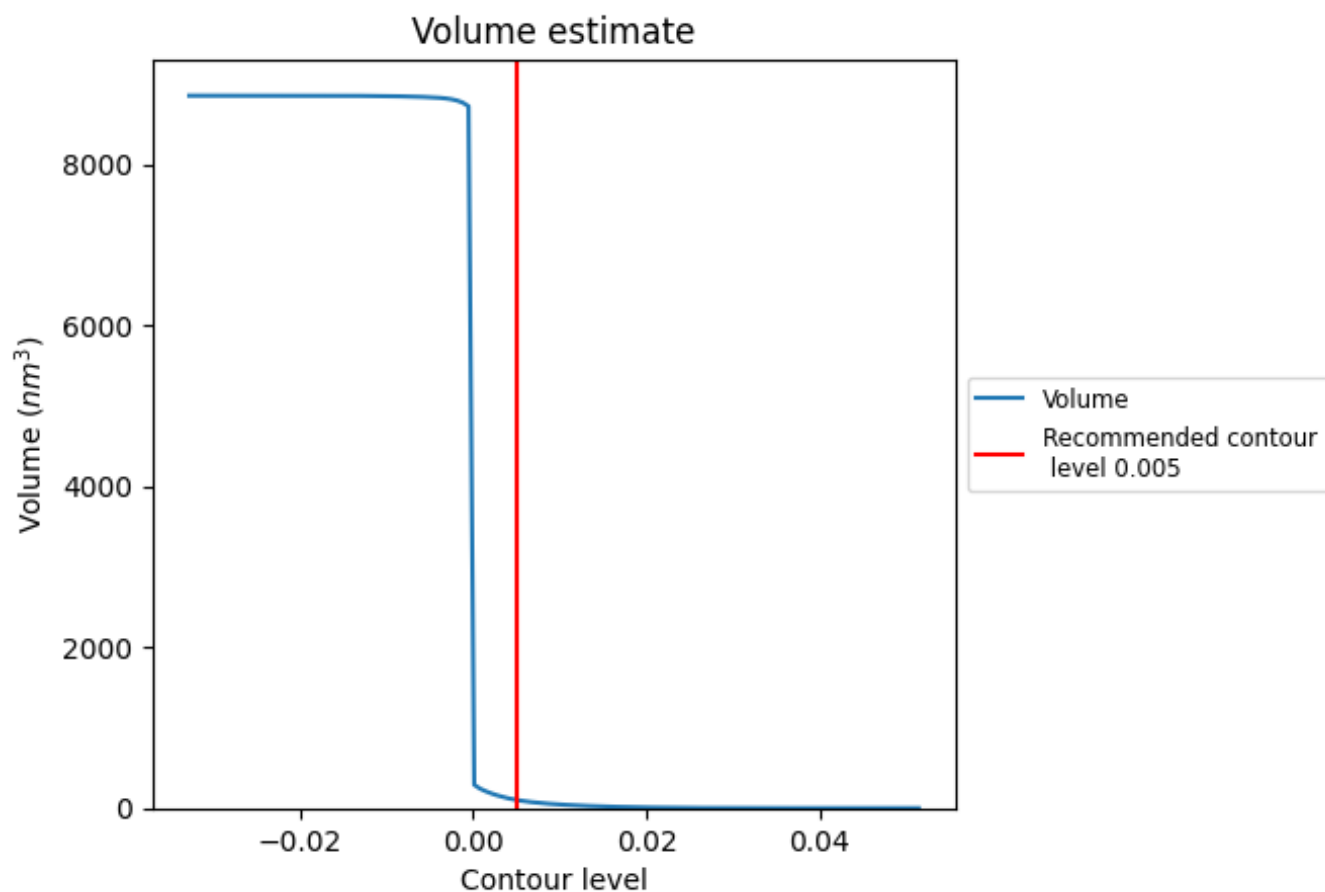
This section contains the results of statistical analysis of the map.

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.

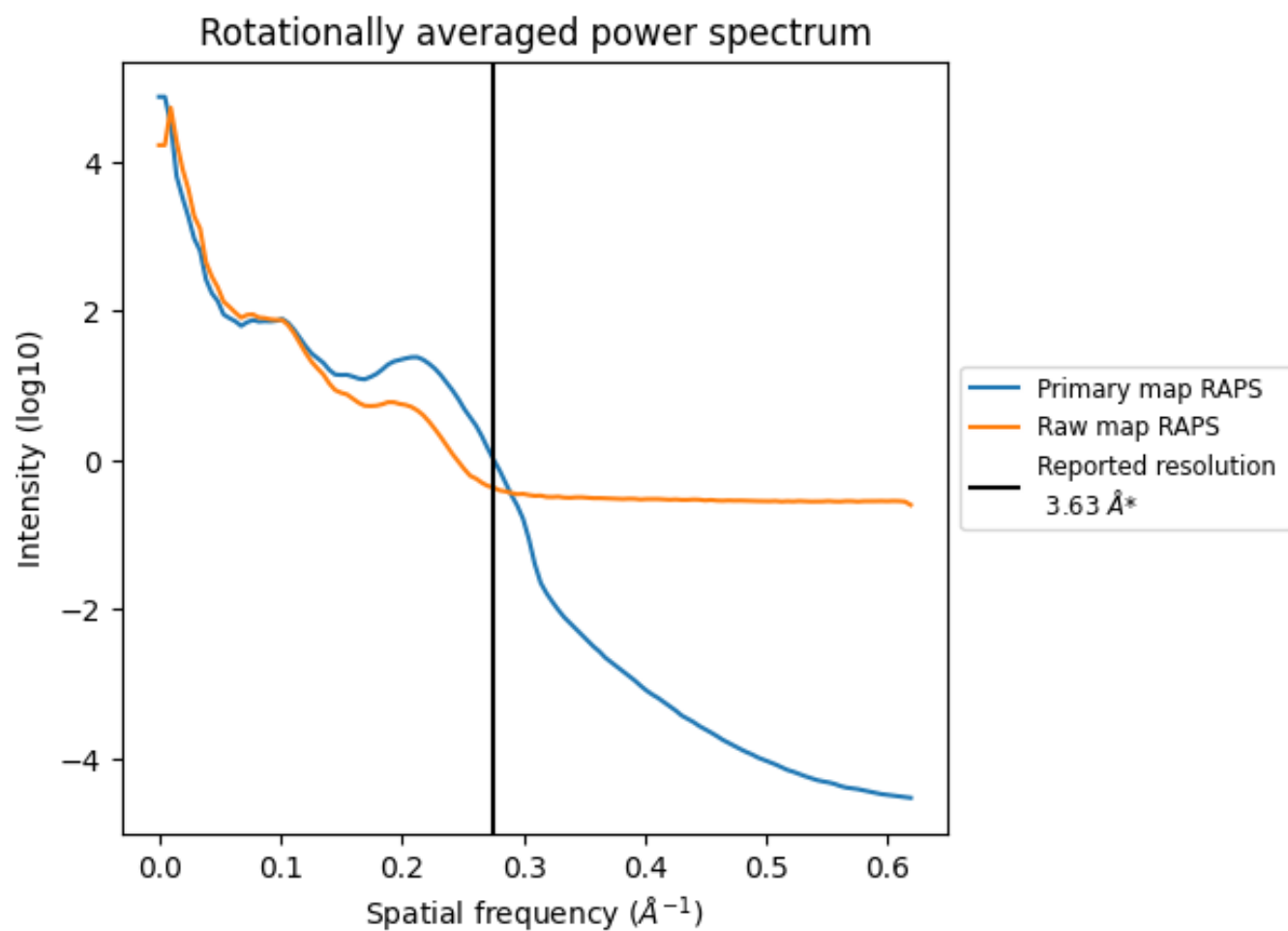
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm³; this corresponds to an approximate mass of 92 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 [i](#)

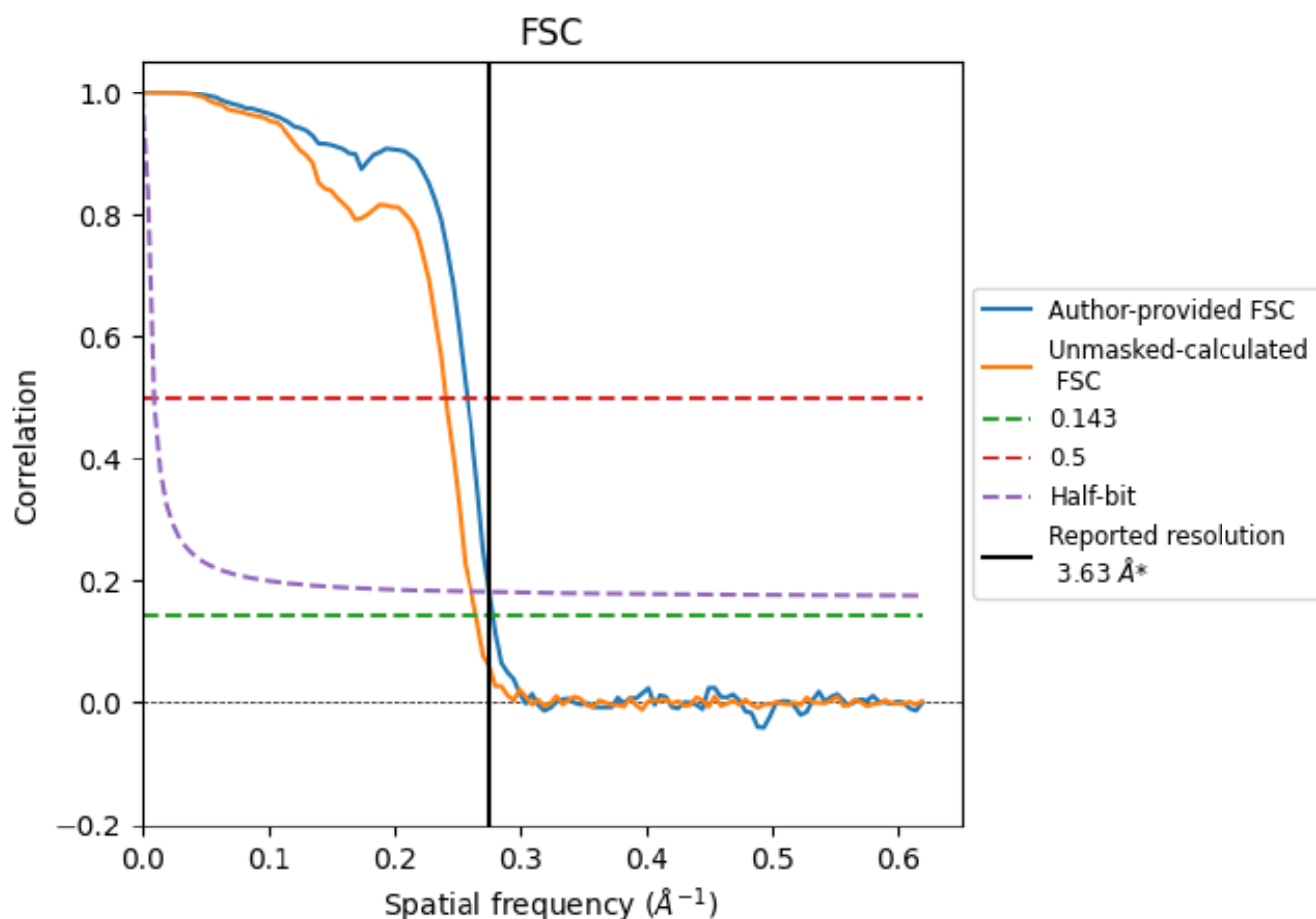


*Reported resolution corresponds to spatial frequency of 0.275 Å⁻¹

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 $0.275 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.63	-	-
Author-provided FSC curve	3.59	3.88	3.63
Unmasked-calculated*	3.77	4.15	3.83

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

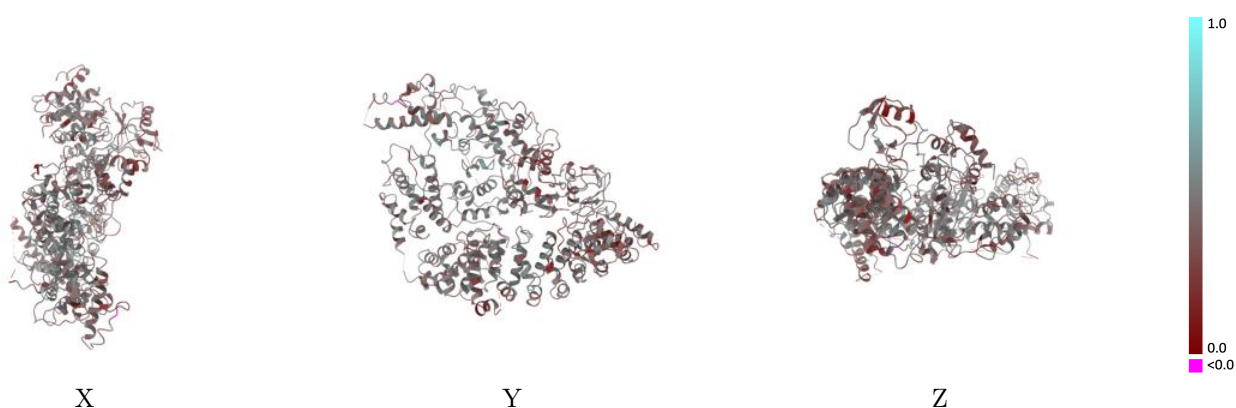
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-62292 and PDB model 9KEN. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

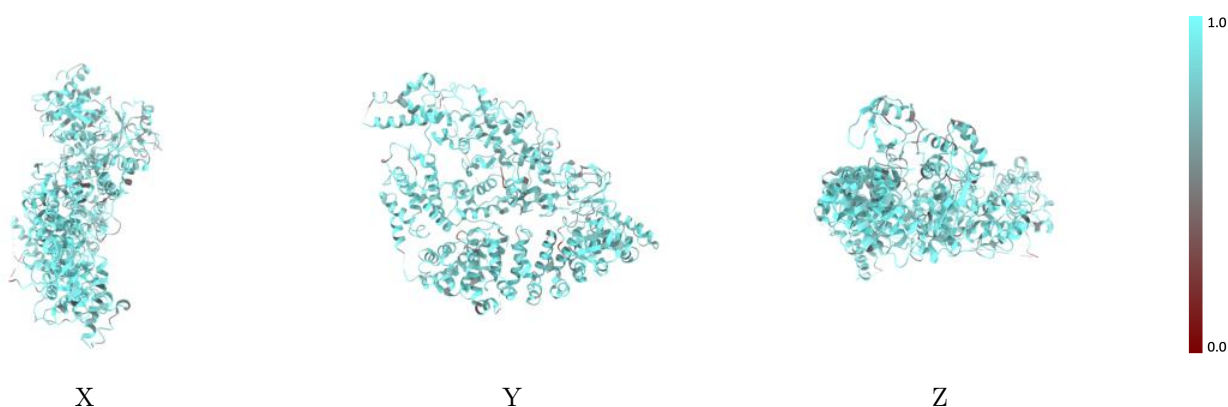
This section was not generated.

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



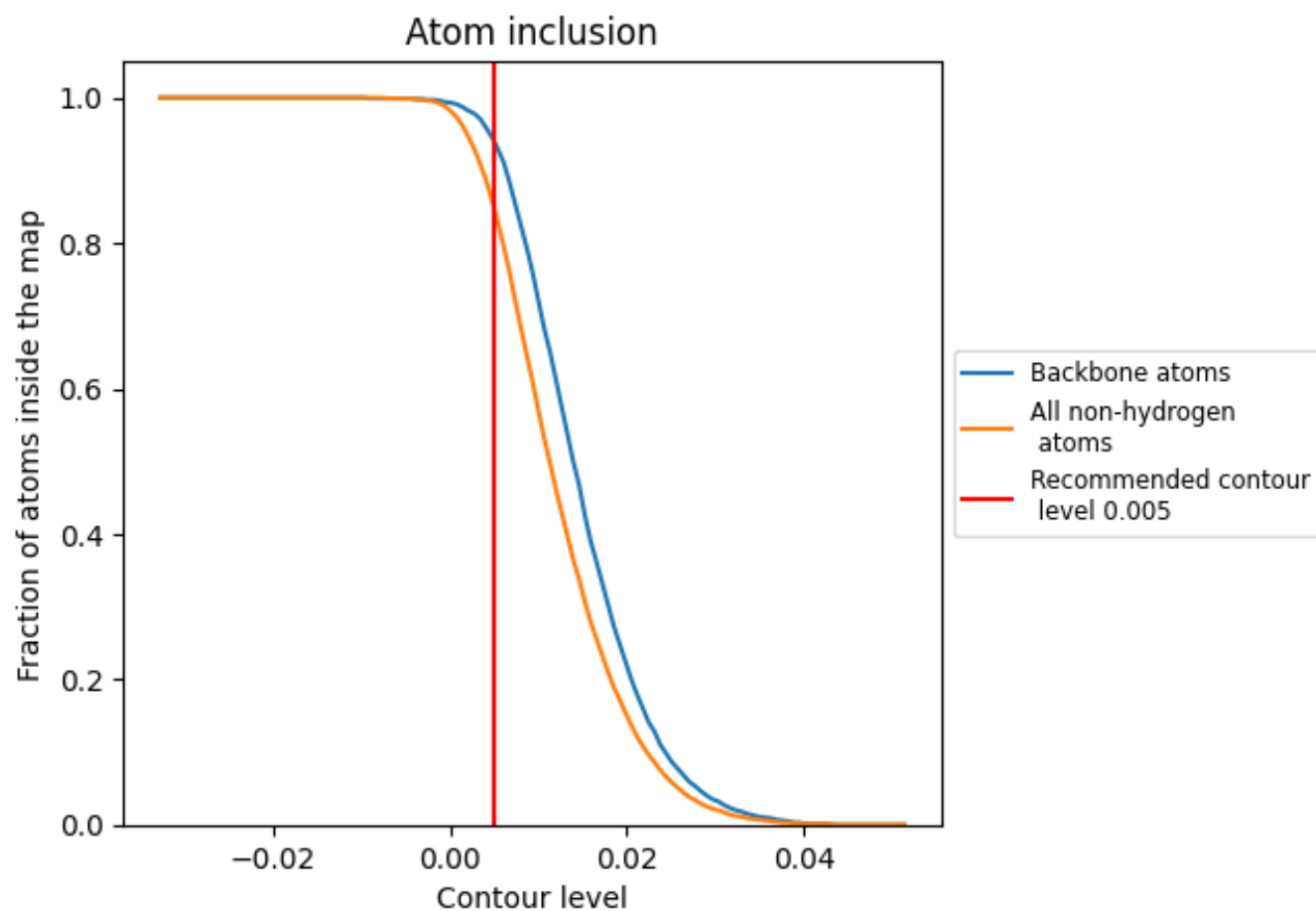
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 85% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8490	0.4080
A	0.8550	0.4140
C	0.7600	0.3350
D	0.8430	0.3970

