



Full wwPDB EM Validation Report ⓘ

Jun 27, 2026 – 09:57 AM EDT

PDB ID : 9BF3 / pdb_00009bf3
EMDB ID : EMD-44489
Title : Cryo-EM Structure of GCN2 HRSL Domain
Authors : Solorio-Kirpichyan, K.M.; Golovenko, D.; Xiao, F.; Yan, N.; Korostelev, A.A.; Korennykh, A.V.
Deposited on : 2024-04-16
Resolution : 3.18 Å(reported)

This is a Full wwPDB EM Validation 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.dev133
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 EMD 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) : 2.50

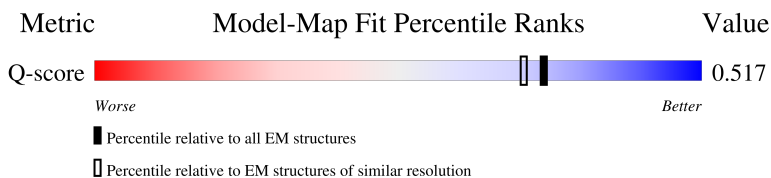
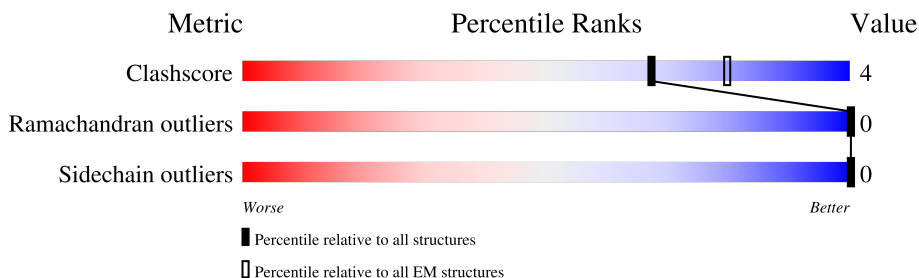
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 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	14470 (2.68 - 3.68)

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	1673	 26% 71%
1	B	1673	 26% 71%

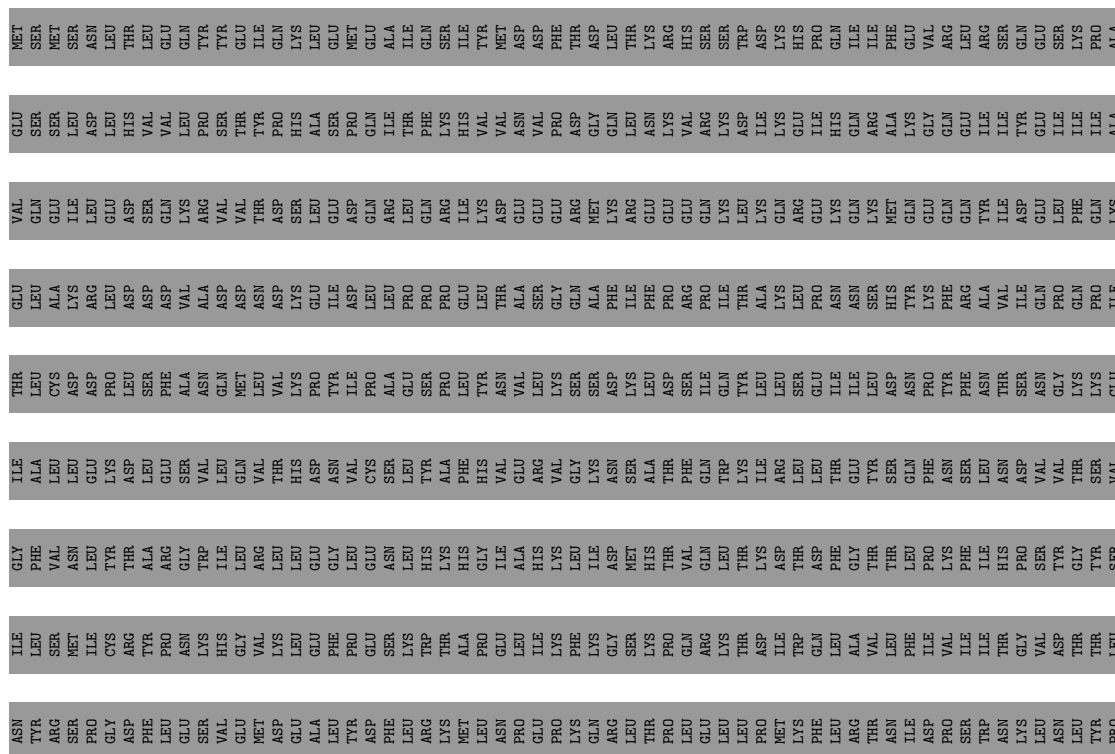
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7796 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 non-specific serine/threonine protein kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	486	Total	C	N	O	S	0	0
			3898	2492	652	741	13		
1	B	486	Total	C	N	O	S	0	0
			3898	2492	652	741	13		



ARG	THR	SER	VAL	LYS	LYS	ARG	D1271	L1032	GLU	ALA	SER	GLN	ARG	THR	LYS	GLU	THR	ASP	THR	ASP
	LEU	ALA	ILE	ARG	R1475			D1035	LYS	LEU	THR	GLY	ASN	THR	LEU	ILE	GLU	THR	THR	GLU
	GLN	TYR	ILE	ILE	V1481		E1279	I1036	LEU	VAL	ILE	ILE	ILE	ALA	VAL	ALA	VAL	ALA	ILE	ILE
	PRO	ASN	PRO	PRO	K1482		Y1291		PRO	ALA	THR	THR	THR	GLU	GLU	GLY	GLY	GLY	GLY	LEU
	ASP	ASN	ASN	ASN	D1489		R1299		LYS	SER	GLU	ARG	ARG	GLY	ASP	ASN	ASN	ASN	ASN	LEU
	GLU	PRO	ALA	ALA	M1492		Y1339		ILE	ILE	LYS	LYS	LYS	TYR	TYR	TYR	TYR	TYR	TYR	LYS
	LEU	THR	ARG	ARG	L1499		R1348		ILE	HIS	SER	SER	SER	GLU	GLY	GLY	GLY	GLY	GLY	VAL
	LYS	ALA	ALA	LYS	S1506		P1349		ARG	GLY	LEU	LEU	LEU	ASP	ASP	ASP	ASP	ASP	ASP	ALA
	VAL	PHE	GLY	LYS	K1507		G1350		LEU	ASN	LEU	LEU	LEU	TYR	TYR	TYR	TYR	TYR	TYR	SER
	GLY	GLY	PRO	PRO			G1351		ASP	ASN	ASP	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	VAL
	LYS	SER	SER	LYS	ASP		G1352		HIS	GLY	ASP	ASP	ASP	LEU	LEU	LEU	LEU	LEU	LEU	SER
	ALA	ALA	LYS	LYS	THR		K1353		PRO	VAL	THR	THR	THR	ASP	ASP	ASP	ASP	ASP	ASP	GLN
	ASN	ASN	LYS	LYS	ASN		N1138		LYS	VAL	LYS	LYS	LYS	ASP	ASP	ASP	ASP	ASP	ASP	VAL
	SER	SER	ASP	ASP	ASP		L1354		THR	ASP	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	GLY	ALA
	ALA	ALA	TRP	TRP	MET		M1355		PRO	MET	ASP	ASP	ASP	TYR	TYR	TYR	TYR	TYR	TYR	ASP
	ARG	VAL	VAL	VAL	ASN		H1356		ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LEU
	SER	PHE	GLU	GLU	LYS		I1357		ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR
	ALA	ALA	GLU	GLU	GLU		L1365		SER	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ASP
	THR	THR	SER	SER	ASP		G1382		ALA	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ASP
	ALA	ILE	ALA	ALA	PHE		G1383		LEU	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	THR
	ASN	ASN	ASN	ASN	ASN		ARG		LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ALA
	ASN	ASN	SER	SER	GLU		THR		ASN	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	THR
	LEU	LEU	LYS	LYS	ASP		LYS		GLN	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	TYR	ASP
	SER	GLN	GLN	GLN	ASP		THR		ASN	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	GLY
	LYS	LEU	LEU	LEU	ILE		LYS		LYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ASP
	ALA	ALA	ALA	ALA	ASN		GLY		ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LEU
	LYS	SER	SER	SER	TRP		GLY		GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ARG
	LEU	LEU	LEU	LEU	ASP		LEU		GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	SER
	ALA	GLY	GLY	GLY	ASN		LEU		ASN	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	PHE
	LYS	THR	THR	THR	GLU		THR		ASP	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	THR
	THR	GLY	GLY	GLY	ASP		T1419		LYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ALA
	GLY	ASP	ASP	ASP	THR		I1420		THR	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER
	LYS	LYS	LYS	LYS	ASN		I1422		ASP	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	LEU
	THR	THR	THR	THR	ASN		V1456		LEU	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	THR
	VAL	VAL	VAL	VAL	LEU		Q1465		SER	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR
	VAL	VAL	VAL	VAL	SER		M1466		THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA
	ASP	ASP	ASP	ASP	ASN		Y1467		GLY	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	THR
	LEU	LEU	LEU	LEU	GLY		SER		PRO	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ASP
	PRO	PRO	PRO	PRO	PRO		ILE		GLN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	PHE
	ILE	ILE	ILE	ILE	ILE		ASN													LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	215101	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.453	Depositor
Minimum map value	-0.170	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.111	Depositor
Map size ($\text{\AA}$)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	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	0.09	0/3979	0.24	1/5380 (0.0%)
1	B	0.09	0/3979	0.24	1/5380 (0.0%)
All	All	0.09	0/7958	0.24	2/10760 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1349	PRO	CA-N-CD	-5.43	104.39	112.00
1	B	1349	PRO	CA-N-CD	-5.40	104.43	112.00

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	3898	0	3882	28	0
1	B	3898	0	3882	31	0
All	All	7796	0	7764	59	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.

All (59) 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:1234:ASP:O	1:B:1238:GLN:HB2	1.86	0.76
1:A:1234:ASP:O	1:A:1238:GLN:HB2	1.86	0.76
1:A:1184:THR:HG23	1:A:1186:THR:H	1.62	0.64
1:B:1184:THR:HG23	1:B:1186:THR:H	1.62	0.63
1:B:1013:PRO:HA	1:B:1018:GLN:HE22	1.64	0.62
1:A:1153:ASP:OD2	1:A:1339:TYR:OH	2.17	0.62
1:A:1232:LYS:HG3	1:A:1246:LEU:HD23	1.82	0.62
1:A:1013:PRO:HA	1:A:1018:GLN:HE22	1.64	0.61
1:B:1153:ASP:OD2	1:B:1339:TYR:OH	2.17	0.61
1:B:1232:LYS:HG3	1:B:1246:LEU:HD23	1.82	0.61
1:B:1032:LEU:O	1:B:1036:ILE:HD12	2.02	0.60
1:A:1177:VAL:HG11	1:A:1188:VAL:HG11	1.85	0.59
1:A:1032:LEU:O	1:A:1036:ILE:HD12	2.01	0.59
1:B:1203:ASP:OD1	1:B:1212:ARG:NH2	2.32	0.58
1:A:1203:ASP:OD1	1:A:1212:ARG:NH2	2.32	0.58
1:B:1177:VAL:HG11	1:B:1188:VAL:HG11	1.85	0.58
1:A:1176:ILE:HG21	1:A:1365:LEU:HD11	1.88	0.55
1:B:1176:ILE:HG21	1:B:1365:LEU:HD11	1.88	0.54
1:A:1262:LYS:NZ	1:A:1279:GLU:OE1	2.41	0.53
1:A:1032:LEU:HG	1:A:1036:ILE:HD11	1.90	0.53
1:B:1032:LEU:HG	1:B:1036:ILE:HD11	1.90	0.53
1:A:1262:LYS:NZ	1:A:1266:GLU:OE2	2.42	0.52
1:A:1013:PRO:HA	1:A:1018:GLN:NE2	2.25	0.52
1:B:1262:LYS:NZ	1:B:1266:GLU:OE2	2.42	0.51
1:A:1124:LYS:NZ	1:A:1168:GLU:OE2	2.34	0.50
1:B:1262:LYS:NZ	1:B:1279:GLU:OE1	2.41	0.50
1:B:1013:PRO:HA	1:B:1018:GLN:NE2	2.25	0.50
1:B:1193:ASN:OD1	1:B:1194:HIS:N	2.45	0.50
1:A:1193:ASN:OD1	1:A:1194:HIS:N	2.45	0.49
1:A:1008:LYS:O	1:A:1011:SER:OG	2.31	0.48
1:B:1124:LYS:NZ	1:B:1168:GLU:OE2	2.34	0.47
1:A:1347:ALA:O	1:A:1350:SER:OG	2.31	0.47
1:A:1177:VAL:HG12	1:A:1299:ARG:HH21	1.79	0.47
1:B:1177:VAL:HG12	1:B:1299:ARG:HH21	1.79	0.46
1:B:1036:ILE:HD12	1:B:1036:ILE:H	1.81	0.45
1:A:1036:ILE:HD12	1:A:1036:ILE:H	1.81	0.45
1:A:1027:SER:O	1:A:1027:SER:OG	2.30	0.45
1:A:1164:VAL:HG22	1:A:1291:TYR:CZ	2.53	0.44
1:A:1408:LEU:HG	1:A:1456:VAL:HG11	2.00	0.44
1:B:1164:VAL:HG22	1:B:1291:TYR:CZ	2.53	0.43
1:A:1357:ILE:HD13	1:A:1357:ILE:HA	1.88	0.43
1:B:1499:LEU:HD12	1:B:1499:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1408:LEU:HG	1:B:1456:VAL:HG11	2.00	0.43
1:B:1008:LYS:O	1:B:1011:SER:OG	2.31	0.43
1:B:1357:ILE:HD13	1:B:1357:ILE:HA	1.88	0.43
1:B:1256:SER:HB3	1:B:1260:THR:HB	2.01	0.43
1:B:1070:ILE:HD13	1:B:1070:ILE:HA	1.84	0.43
1:A:1032:LEU:O	1:A:1035:ASP:N	2.53	0.42
1:B:1032:LEU:O	1:B:1035:ASP:N	2.52	0.42
1:B:1482:LYS:NZ	1:B:1489:ASP:OD2	2.38	0.42
1:A:1256:SER:HB3	1:A:1260:THR:HB	2.01	0.41
1:A:1482:LYS:NZ	1:A:1489:ASP:OD2	2.38	0.41
1:B:1056:MET:HE3	1:B:1056:MET:HB3	1.88	0.41
1:B:1408:LEU:HD23	1:B:1408:LEU:HA	1.81	0.41
1:A:1293:LYS:HB3	1:A:1294:PRO:HD3	2.03	0.41
1:A:1055:GLN:HG3	1:A:1402:PRO:HA	2.03	0.40
1:B:1422:ILE:HD13	1:B:1422:ILE:HA	1.95	0.40
1:B:1419:THR:OG1	1:B:1420:ILE:N	2.54	0.40
1:B:1481:VAL:HB	1:B:1492:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	480/1673 (29%)	470 (98%)	10 (2%)	0	100	100
1	B	480/1673 (29%)	470 (98%)	10 (2%)	0	100	100
All	All	960/3346 (29%)	940 (98%)	20 (2%)	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	441/1519 (29%)	441 (100%)	0	100	100
1	B	441/1519 (29%)	441 (100%)	0	100	100
All	All	882/3038 (29%)	882 (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. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1104	GLN
1	A	1358	GLN
1	B	1104	GLN
1	B	1118	ASN
1	B	1358	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.

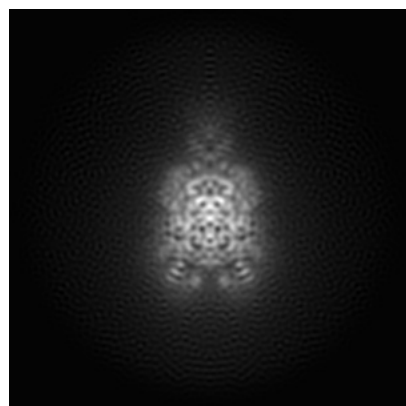
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44489. These allow visual inspection of the internal detail of the map and identification of artifacts.

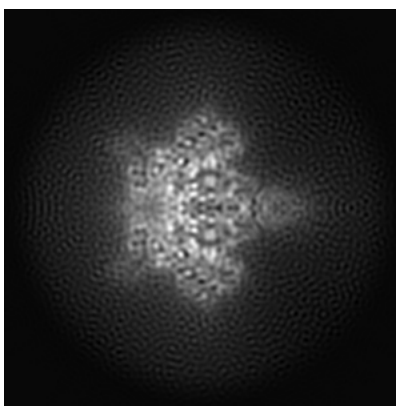
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

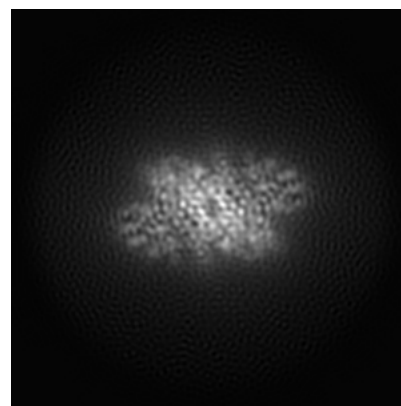
6.1.1 Primary map



X

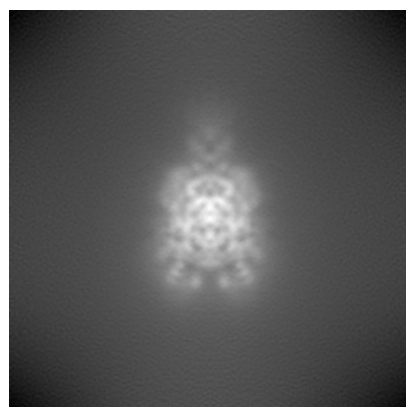


Y

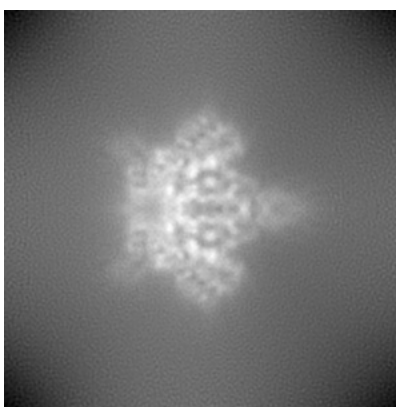


Z

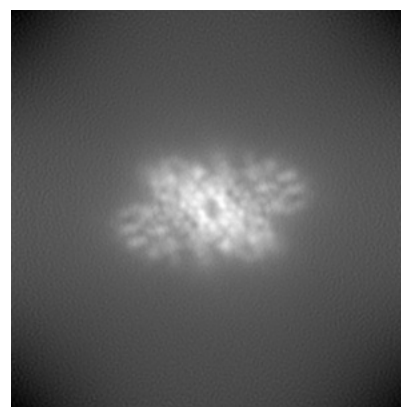
6.1.2 Raw map



X



Y

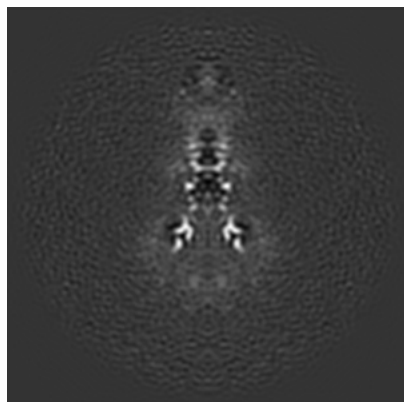


Z

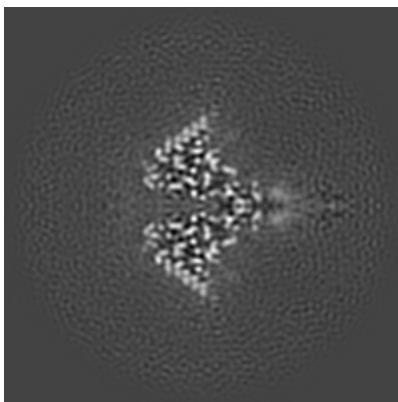
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

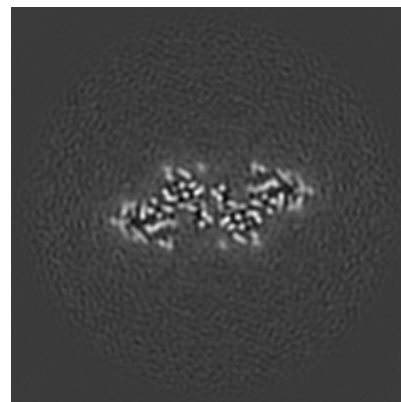
6.2.1 Primary map



X Index: 100

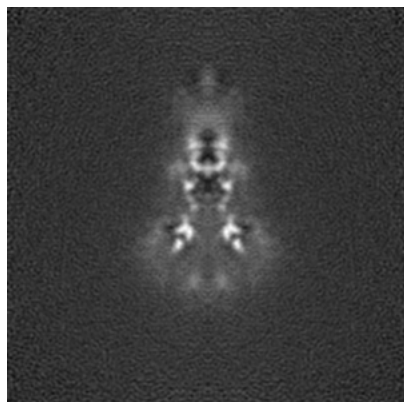


Y Index: 100

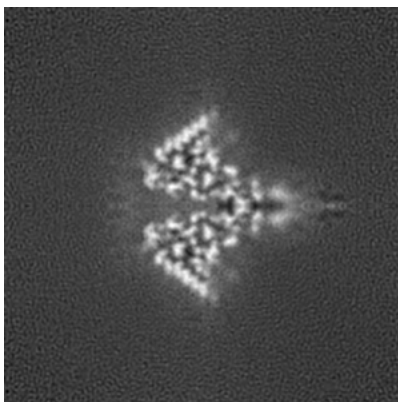


Z Index: 100

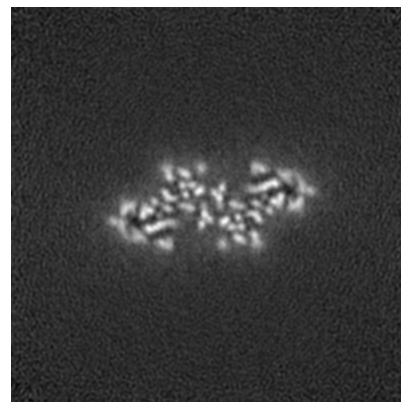
6.2.2 Raw map



X Index: 100



Y Index: 100

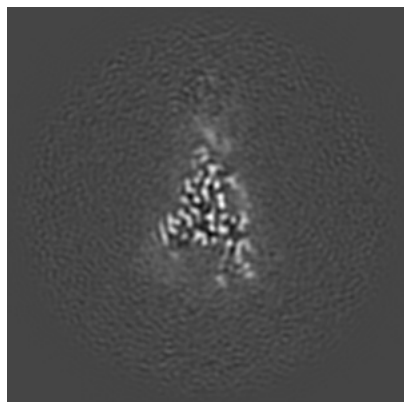


Z Index: 100

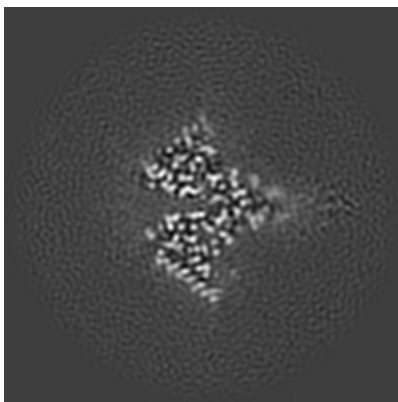
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

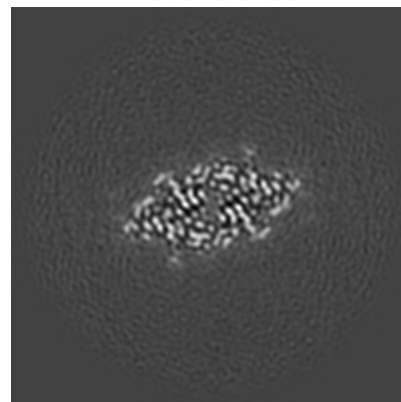
6.3.1 Primary map



X Index: 93

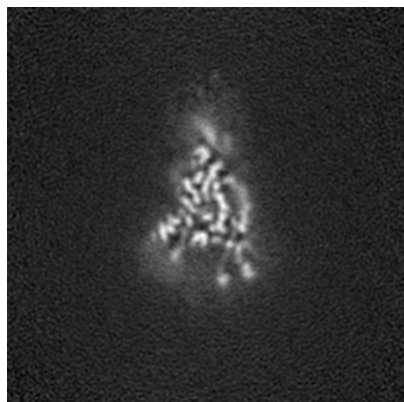


Y Index: 98

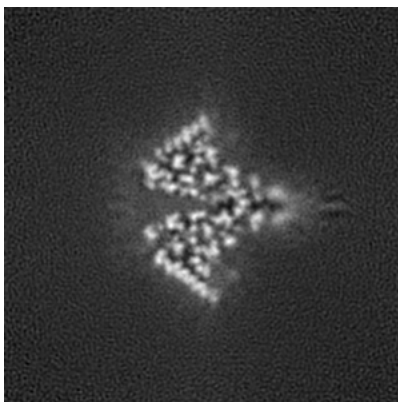


Z Index: 92

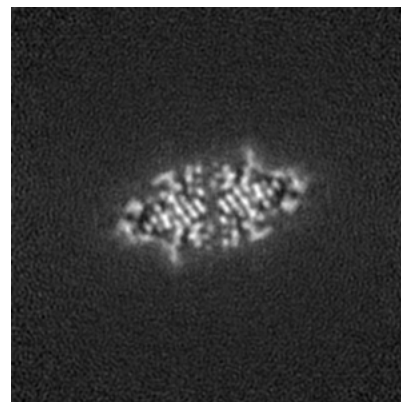
6.3.2 Raw map



X Index: 94



Y Index: 99

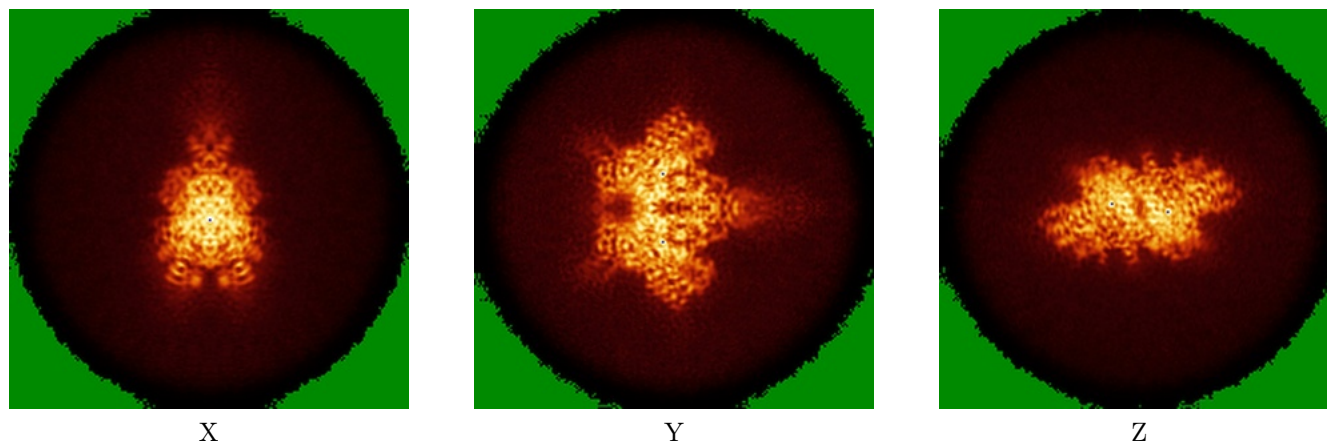


Z Index: 94

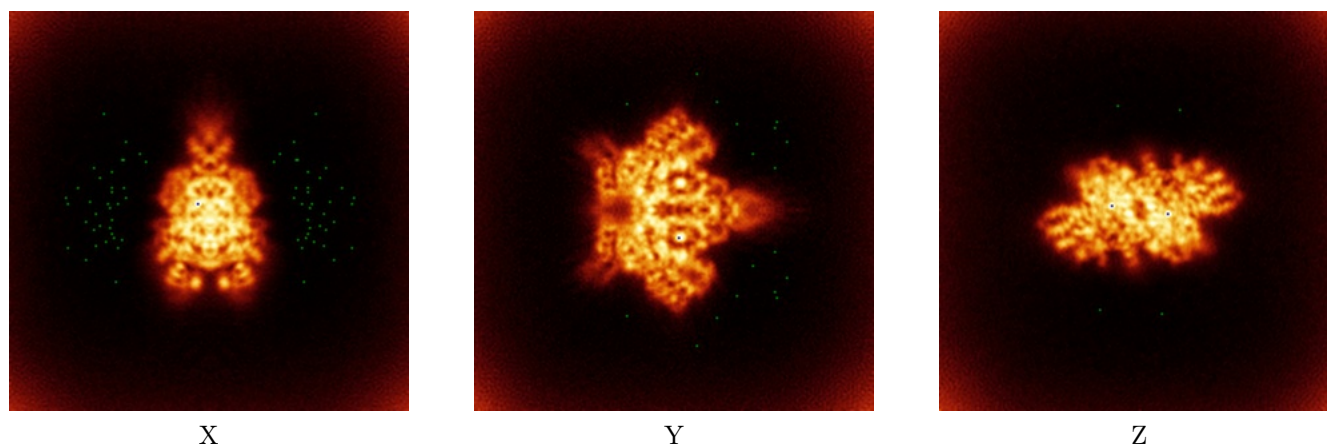
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



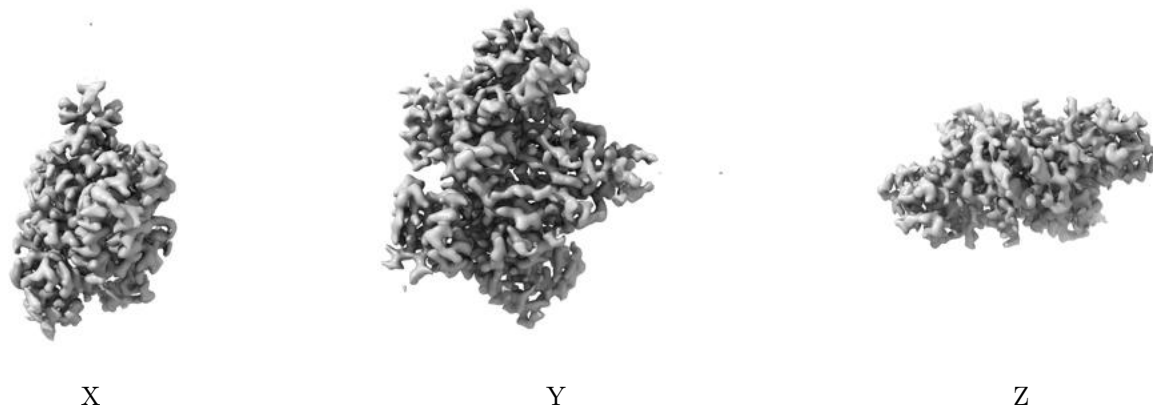
6.4.2 Raw map



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.

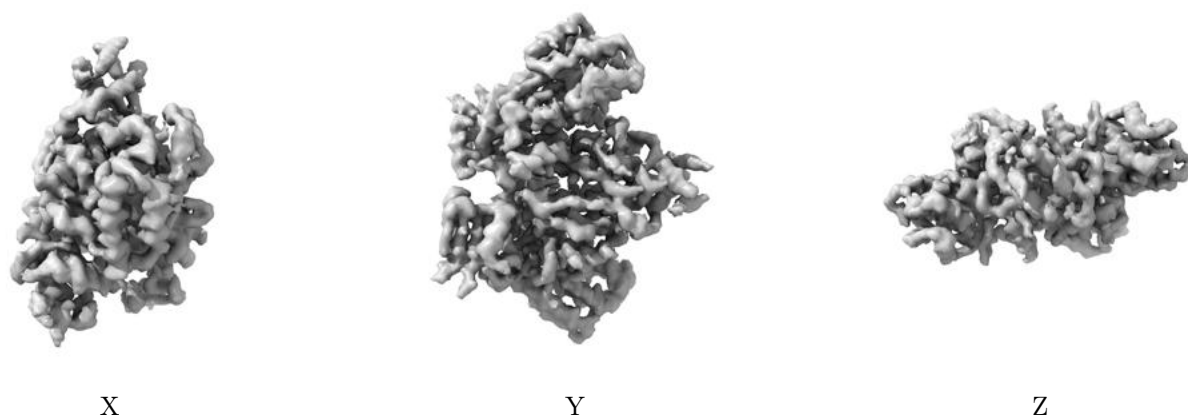
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.111. 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.

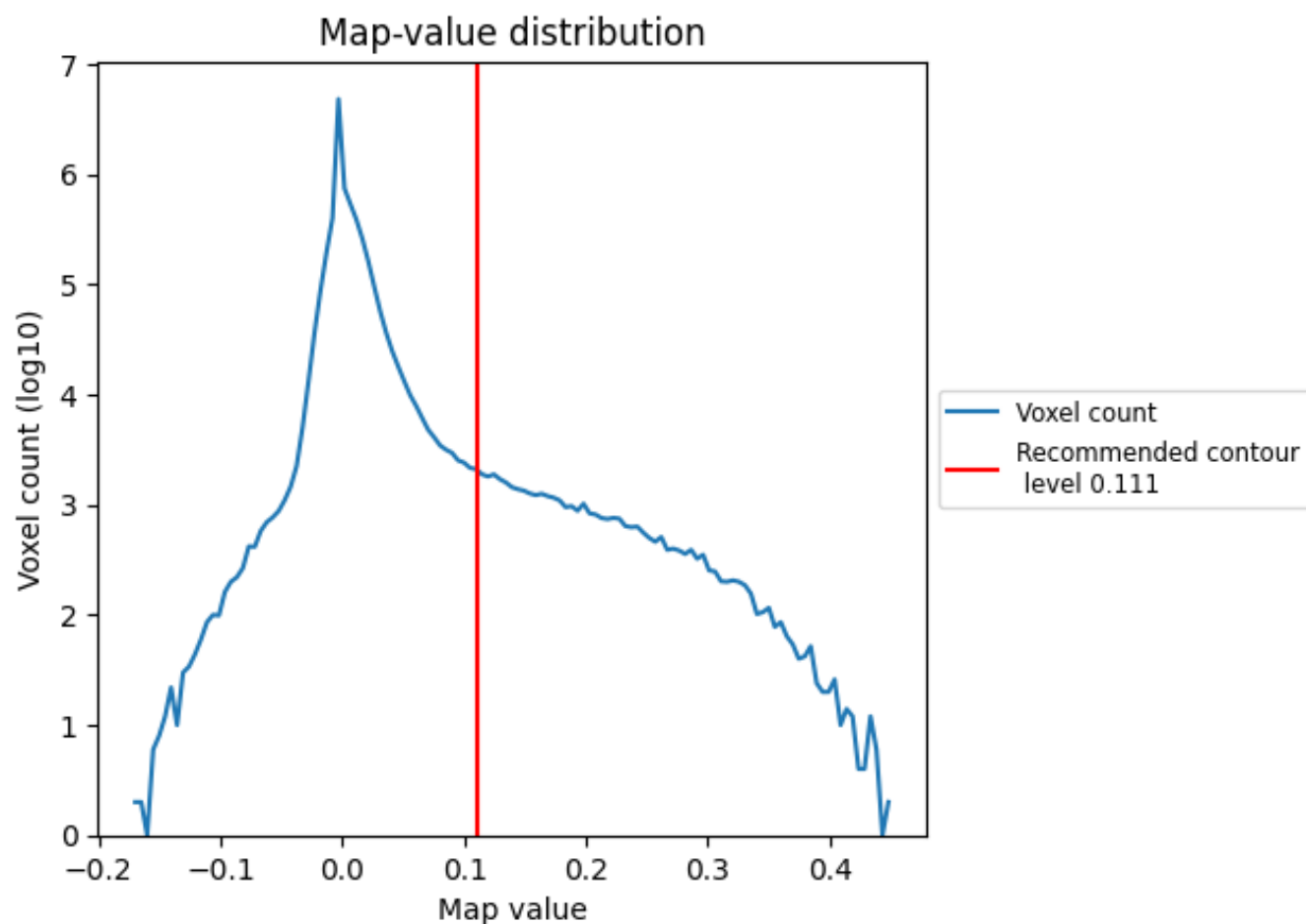
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

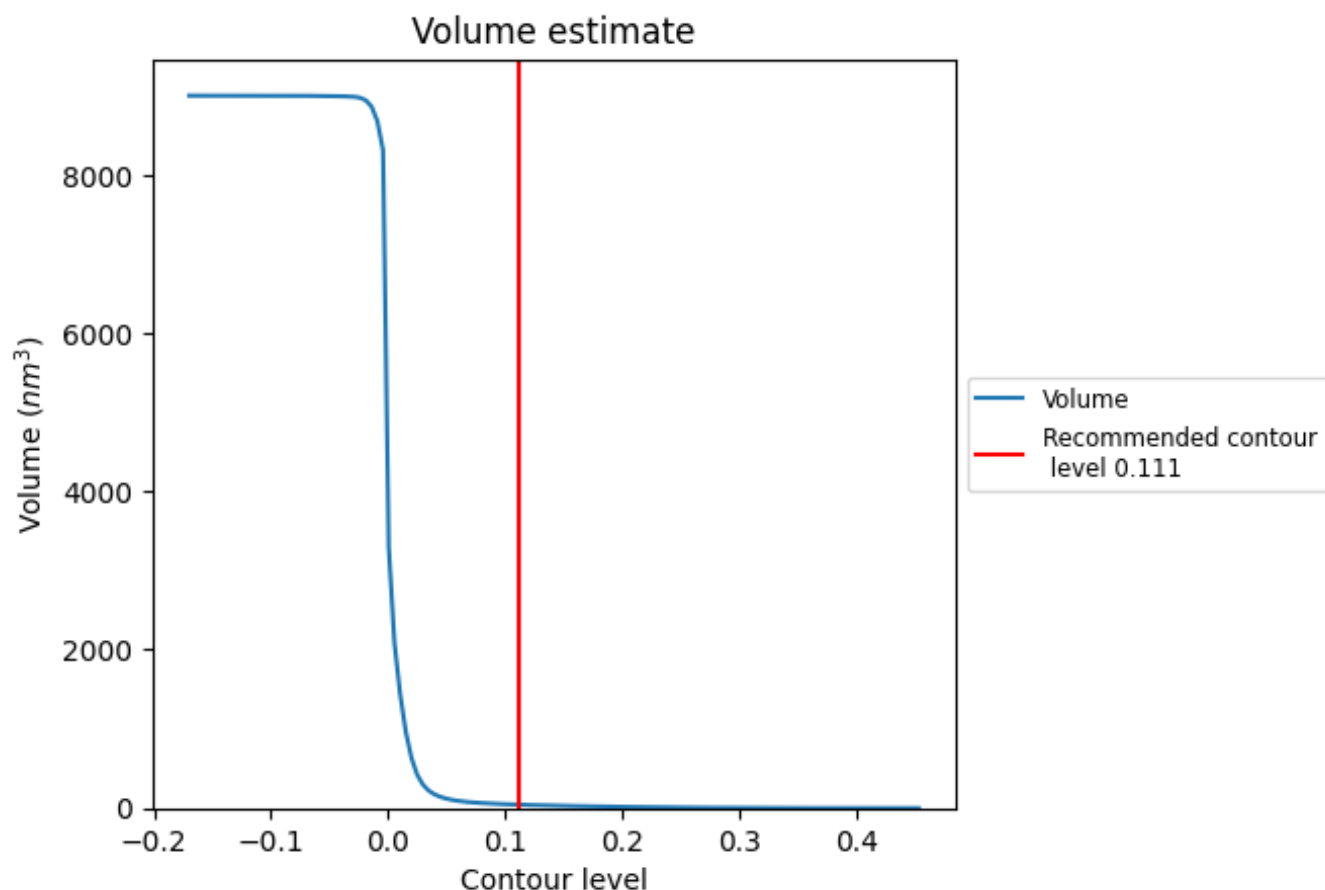
This section contains the results of statistical analysis of the map.

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.

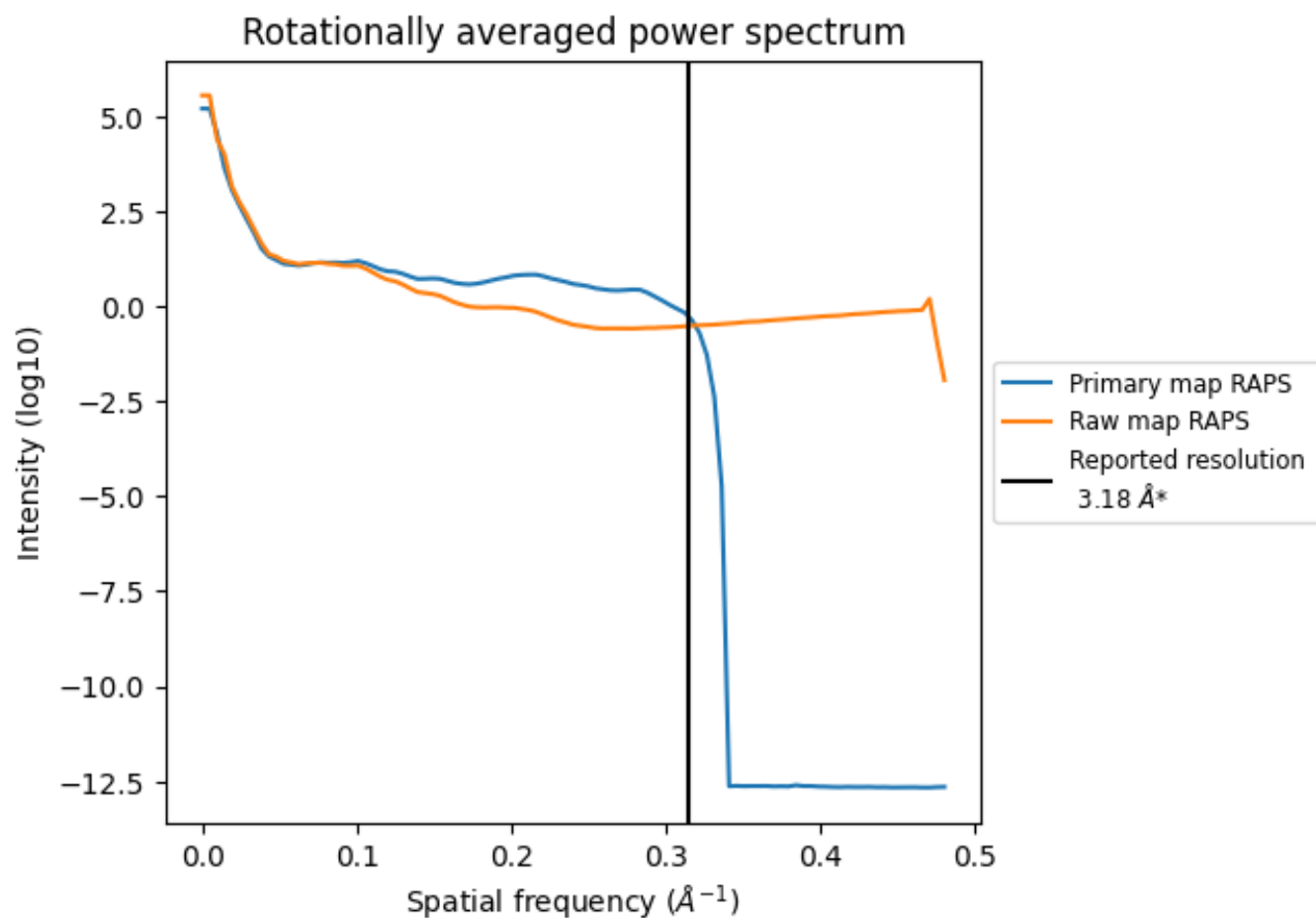
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 44 nm³; this corresponds to an approximate mass of 40 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 ⓘ

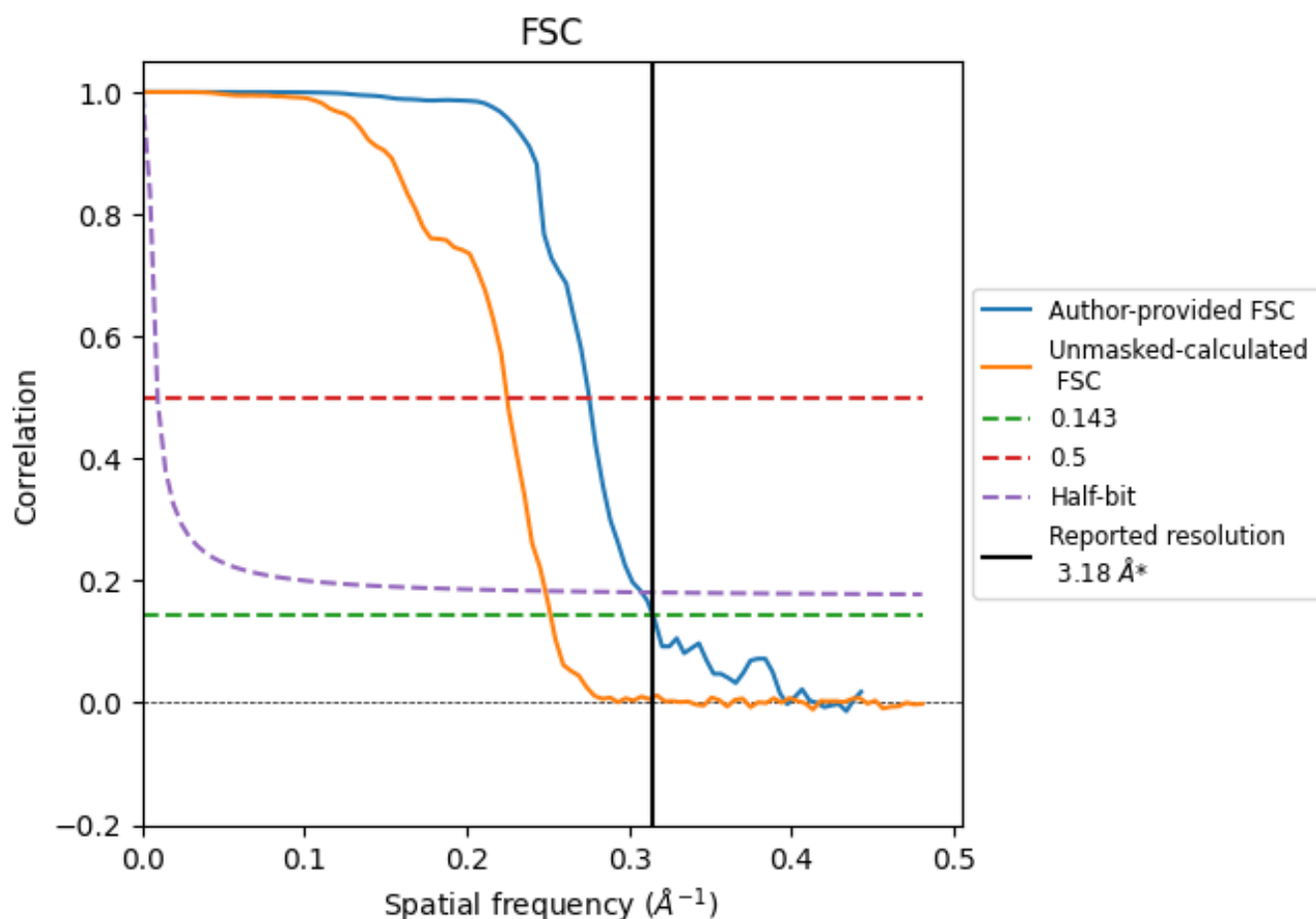


*Reported resolution corresponds to spatial frequency of 0.314 Å⁻¹

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 $0.314 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

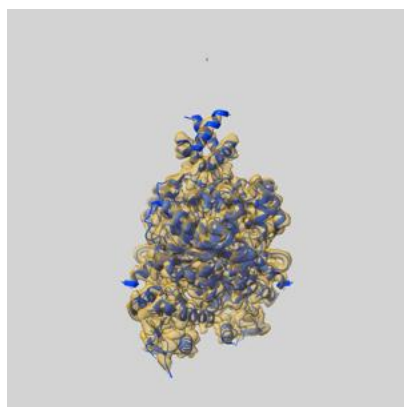
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.18	3.63	3.25
Unmasked-calculated*	3.97	4.45	4.02

*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 3.97 differs from the reported value 3.18 by more than 10 %

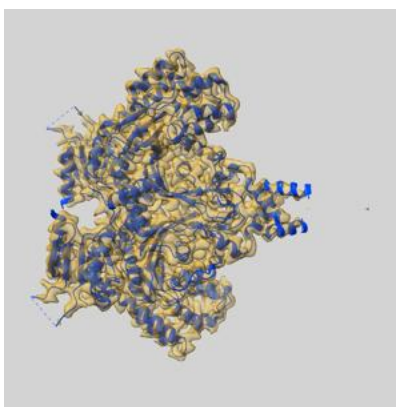
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44489 and PDB model 9BF3. Per-residue inclusion information can be found in section [3](#) on page [4](#).

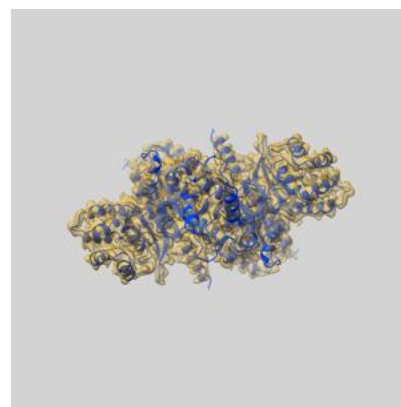
9.1 Map-model overlay [i](#)



X



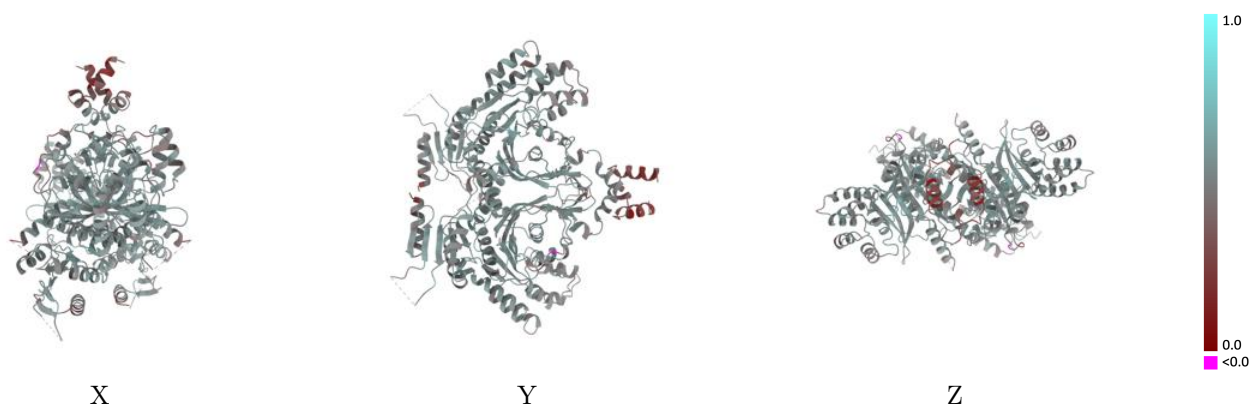
Y



Z

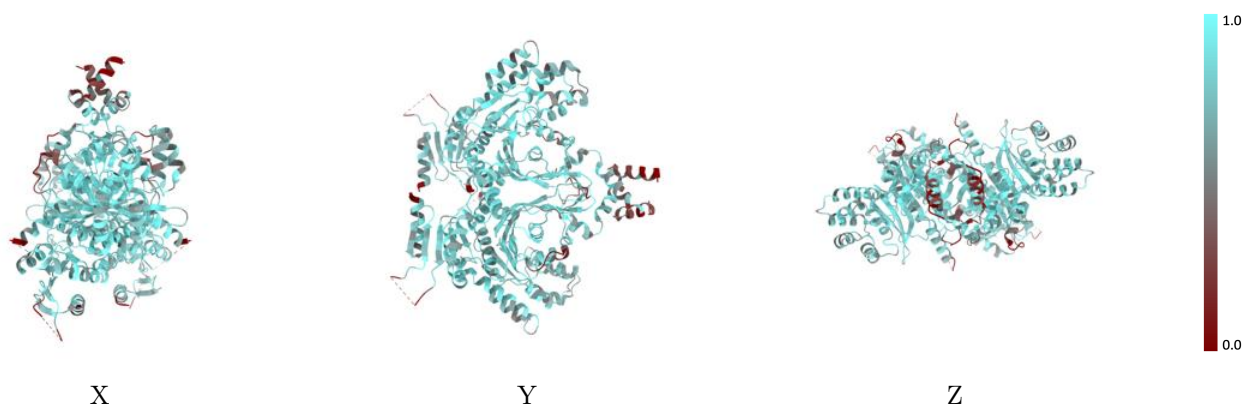
The images above show the 3D surface view of the map at the recommended contour level 0.111 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



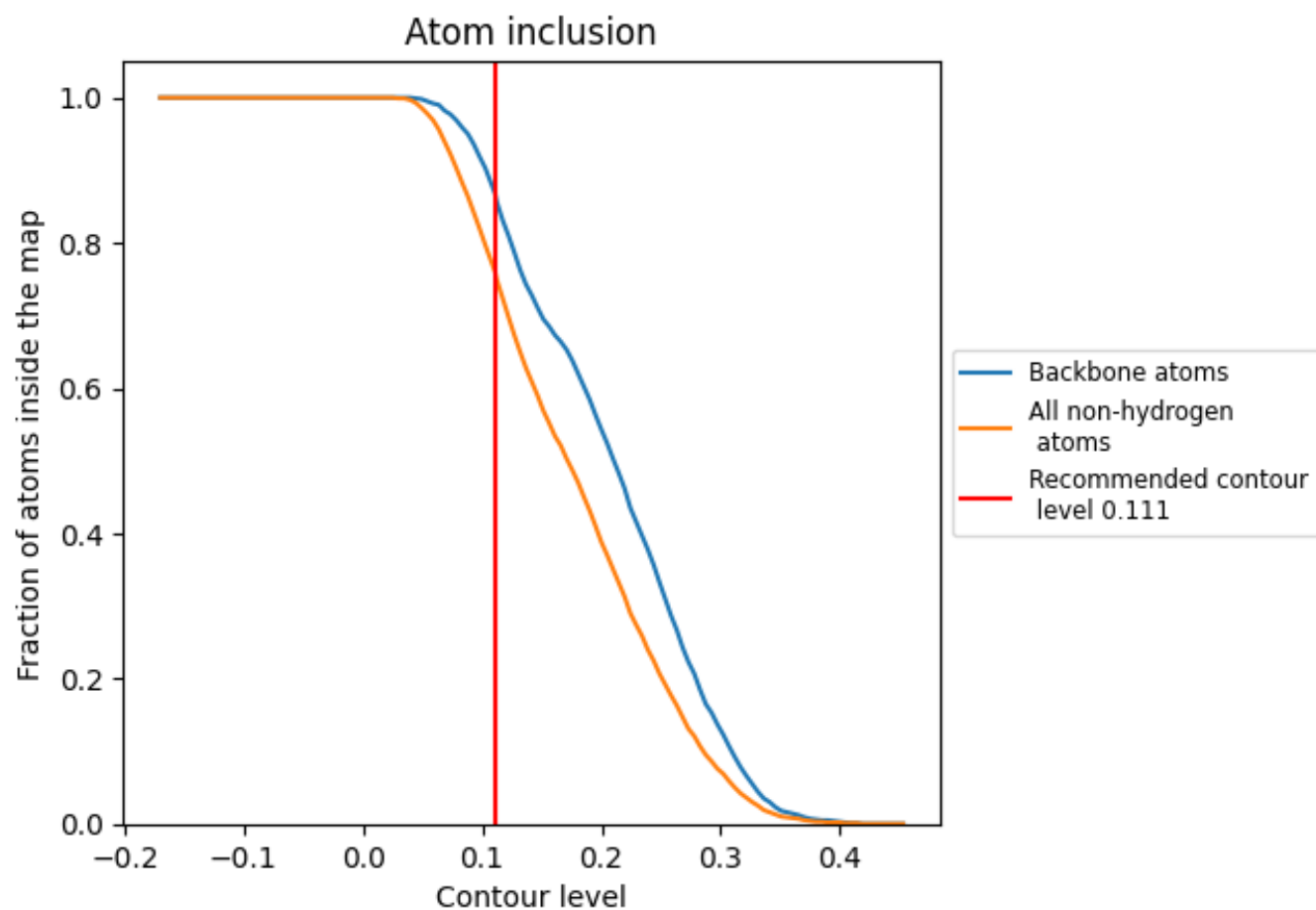
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.111).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 76% 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 (0.111) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7590	0.5170
A	0.7590	0.5170
B	0.7590	0.5160

