



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:59 PM UTC

PDB ID : 8R4C / pdb_00008r4c
EMDB ID : EMD-18885
Title : LRR domain of Roco protein from *C. tepidum* bound to the activating Nanobody NbRoco2
Authors : Galicia, C.; Versees, W.
Deposited on : 2023-11-13
Resolution : 3.55 Å (reported)
Based on initial models : ., 6hlu

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.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

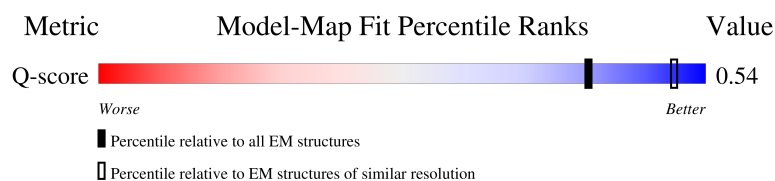
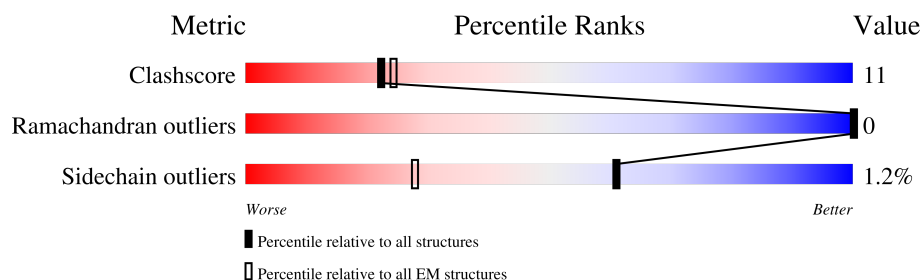
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.55 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	12819 (3.05 - 4.05)

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	130	 68% 22% 11%
2	A	1107	 29% 10% 61%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4027 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 NbRoco2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	116	Total	C	N	O	S	0	0
			843	527	152	160	4		

- Molecule 2 is a protein called Rab family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	437	Total	C	N	O	S	0	0
			3184	2014	517	648	5		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q8KC98
A	-3	ALA	-	expression tag	UNP Q8KC98
A	-2	MET	-	expression tag	UNP Q8KC98
A	-1	GLY	-	expression tag	UNP Q8KC98
A	0	SER	-	expression tag	UNP Q8KC98

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160925	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	8.710	Depositor
Minimum map value	-4.915	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.140	Depositor
Recommended contour level	0.95	Depositor
Map size (Å)	241.59999, 241.59999, 241.59999	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4380952, 1.4380952, 1.4380952	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	0.17	0/857	0.37	0/1165
2	A	0.15	0/3229	0.40	0/4422
All	All	0.15	0/4086	0.39	0/5587

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	843	0	806	19	0
2	A	3184	0	3093	74	0
All	All	4027	0	3899	90	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 11.

All (90) 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:C:34:MET:HE3	1:C:78:VAL:HG13	1.73	0.70
2:A:67:GLU:HG2	2:A:89:MET:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:386:LEU:HD23	2:A:418:PRO:HG2	1.77	0.65
2:A:386:LEU:HD12	2:A:390:ILE:HG21	1.79	0.63
2:A:9:GLN:HA	2:A:12:GLN:HE21	1.64	0.62
2:A:144:ILE:O	2:A:144:ILE:HD12	2.00	0.61
2:A:343:ALA:HA	2:A:366:PRO:HB3	1.83	0.61
1:C:33:VAL:HG22	1:C:52:THR:HG22	1.81	0.61
1:C:66:ARG:NH2	1:C:89:ASP:OD2	2.33	0.61
2:A:410:PHE:HB3	2:A:413:ASN:HD22	1.66	0.59
2:A:93:ASP:OD1	2:A:113:TRP:HB3	2.03	0.59
2:A:21:VAL:HG22	2:A:22:ASP:H	1.68	0.58
2:A:161:ASN:HD22	2:A:163:ILE:HD11	1.68	0.58
2:A:9:GLN:HA	2:A:12:GLN:NE2	2.17	0.58
2:A:52:LEU:HD21	2:A:81:LEU:HG	1.85	0.58
2:A:410:PHE:HB3	2:A:413:ASN:ND2	2.17	0.57
2:A:225:SER:HB3	2:A:247:SER:HB3	1.86	0.57
2:A:258:ALA:HB2	2:A:278:PRO:HB3	1.87	0.57
1:C:32:ASN:OD1	2:A:45:TYR:OH	2.21	0.56
2:A:134:LEU:HB3	2:A:156:LEU:HD12	1.88	0.56
2:A:188:ILE:HG22	2:A:191:LEU:HB2	1.88	0.55
2:A:267:GLN:HA	2:A:289:TRP:HB2	1.88	0.55
2:A:313:SER:O	2:A:315:ASN:ND2	2.39	0.54
2:A:148:ALA:HB2	2:A:168:PRO:HB3	1.91	0.53
1:C:11:LEU:HG	1:C:117:THR:HB	1.90	0.53
2:A:47:CYS:HB2	2:A:73:ASN:HD21	1.74	0.53
2:A:321:ALA:HA	2:A:344:PRO:HB2	1.91	0.52
2:A:161:ASN:HB2	2:A:163:ILE:HG13	1.91	0.52
2:A:312:LEU:N	2:A:333:TRP:O	2.34	0.51
2:A:178:LEU:HD23	2:A:191:LEU:HD21	1.93	0.50
2:A:296:THR:HA	2:A:316:GLN:O	2.13	0.49
2:A:66:SER:HA	2:A:87:LEU:HA	1.94	0.49
2:A:286:SER:O	2:A:308:THR:OG1	2.30	0.49
2:A:166:ILE:HG12	2:A:180:LEU:HD21	1.93	0.48
1:C:22:CYS:HB3	1:C:78:VAL:HG23	1.96	0.48
2:A:305:ASN:HA	2:A:326:LEU:HD23	1.94	0.48
2:A:397:ILE:HG13	2:A:427:LYS:HB2	1.95	0.48
2:A:78:ILE:HD11	2:A:100:ILE:HA	1.95	0.48
2:A:133:GLU:HG2	2:A:155:GLU:HB2	1.96	0.48
2:A:210:ILE:HG22	2:A:213:LEU:HB2	1.96	0.48
2:A:95:ASN:O	2:A:117:ASN:HA	2.14	0.47
2:A:342:ILE:HD11	2:A:364:ILE:HA	1.96	0.47
2:A:299:ALA:HA	2:A:322:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:TRP:NE1	1:C:80:LEU:HB2	2.30	0.47
1:C:93:TYR:O	1:C:113:GLY:HA2	2.15	0.47
2:A:115:PHE:HD2	2:A:135:GLN:HB3	1.80	0.47
2:A:388:GLU:O	2:A:391:THR:HG22	2.15	0.47
2:A:321:ALA:HA	2:A:344:PRO:CB	2.46	0.46
2:A:203:SER:O	2:A:205:ASN:ND2	2.48	0.46
2:A:321:ALA:C	2:A:323:LEU:H	2.22	0.46
2:A:352:SER:O	2:A:374:THR:OG1	2.29	0.46
1:C:32:ASN:O	1:C:52:THR:HA	2.16	0.46
2:A:43:GLY:HA2	2:A:69:SER:HB3	1.98	0.46
1:C:104:LEU:HD21	1:C:106:GLN:HE21	1.80	0.46
2:A:376:PHE:HB3	2:A:408:ILE:HD13	1.97	0.46
1:C:36:TRP:CD1	1:C:80:LEU:HB2	2.51	0.46
1:C:18:LEU:HD12	1:C:19:ARG:H	1.80	0.45
1:C:33:VAL:N	1:C:98:ASP:OD1	2.37	0.45
1:C:10:GLY:HA2	2:A:407:PHE:CZ	2.52	0.45
2:A:74:GLN:N	2:A:95:ASN:OD1	2.50	0.45
1:C:67:PHE:CE1	1:C:82:MET:HB3	2.52	0.45
1:C:48:VAL:HG13	1:C:63:VAL:HG21	1.99	0.45
2:A:251:ILE:N	2:A:271:ASN:OD1	2.46	0.44
2:A:432:GLN:O	2:A:435:GLN:HG3	2.16	0.44
2:A:158:LEU:O	2:A:180:LEU:HD12	2.17	0.44
2:A:417:SER:O	2:A:433:TYR:OH	2.28	0.44
2:A:332:LEU:HG	2:A:334:LEU:HD22	2.00	0.44
2:A:373:LEU:HD12	2:A:373:LEU:HA	1.84	0.44
2:A:428:GLU:O	2:A:432:GLN:HG3	2.18	0.44
2:A:397:ILE:HG23	2:A:408:ILE:HG22	2.00	0.44
2:A:3:ASP:HB3	2:A:6:VAL:HG23	2.01	0.43
2:A:354:LEU:HD12	2:A:373:LEU:HD21	2.00	0.43
2:A:122:ILE:HD11	2:A:144:ILE:HG22	2.01	0.43
2:A:222:LEU:HD23	2:A:244:LEU:HD13	2.01	0.42
2:A:91:TRP:CE2	2:A:111:MET:HE1	2.53	0.42
2:A:85:ASN:OD1	2:A:85:ASN:N	2.52	0.42
2:A:162:ASN:OD1	2:A:184:GLN:NE2	2.53	0.42
2:A:241:LEU:HD12	2:A:241:LEU:H	1.83	0.42
2:A:354:LEU:N	2:A:375:GLY:O	2.50	0.42
1:C:95:CYS:O	1:C:110:TRP:HA	2.20	0.41
2:A:144:ILE:HD13	2:A:169:LEU:HD23	2.02	0.41
2:A:332:LEU:O	2:A:354:LEU:HD23	2.21	0.41
2:A:380:ARG:NH2	2:A:401:ASP:OD2	2.44	0.41
2:A:386:LEU:HD13	2:A:386:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ASN:HB2	2:A:94:ARG:NH1	2.36	0.40
1:C:32:ASN:HB3	1:C:98:ASP:OD2	2.21	0.40
2:A:238:LEU:HD23	2:A:238:LEU:HA	1.92	0.40
2:A:22:ASP:O	2:A:23:LYS:C	2.64	0.40
2:A:178:LEU:HB2	2:A:197:LEU:HD11	2.02	0.40
2:A:68:LEU:HD23	2:A:68:LEU:HA	1.89	0.40

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	114/130 (88%)	109 (96%)	5 (4%)	0	100	100
2	A	435/1107 (39%)	388 (89%)	47 (11%)	0	100	100
All	All	549/1237 (44%)	497 (90%)	52 (10%)	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	82/105 (78%)	80 (98%)	2 (2%)	43	63
2	A	348/999 (35%)	345 (99%)	3 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	430/1104 (39%)	425 (99%)	5 (1%)	61	73

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	46	GLU
1	C	64	LYS
2	A	93	ASP
2	A	388	GLU
2	A	409	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	106	GLN
1	C	109	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 ⓘ

There are no chain breaks in this entry.

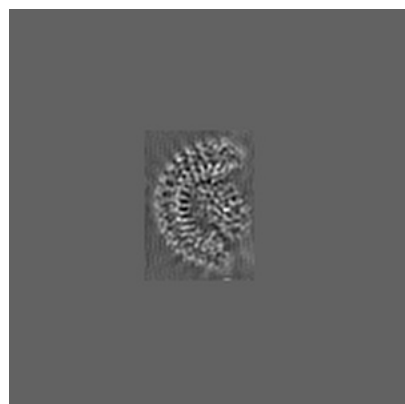
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18885. These allow visual inspection of the internal detail of the map and identification of artifacts.

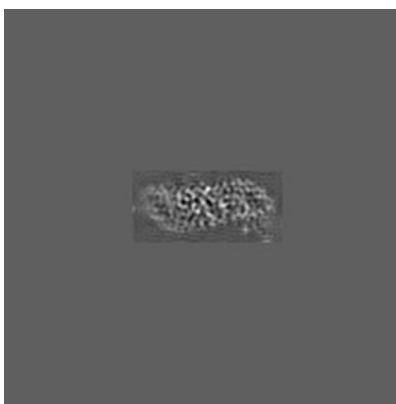
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

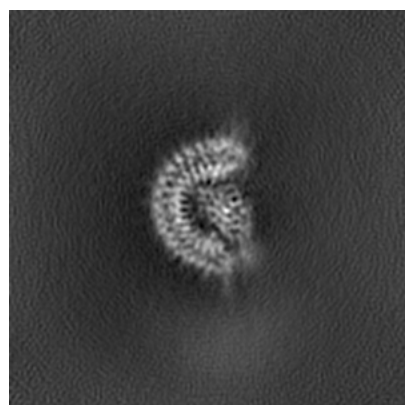


Y

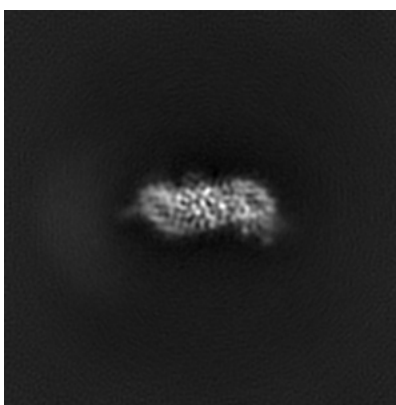


Z

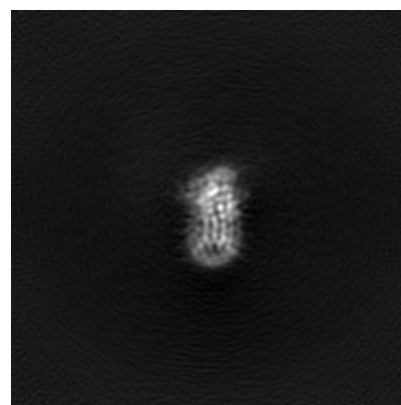
6.1.2 Raw map



X



Y

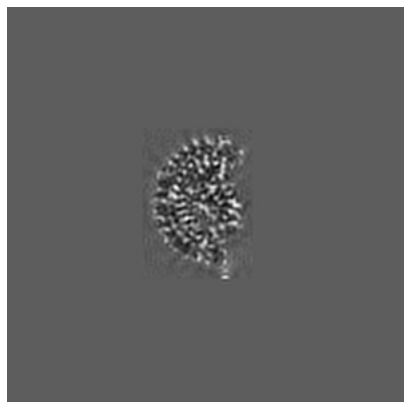


Z

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

6.2 Central slices [i](#)

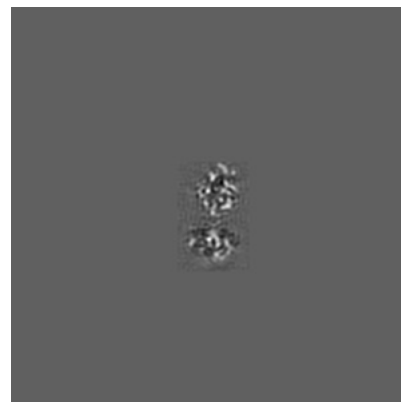
6.2.1 Primary map



X Index: 84

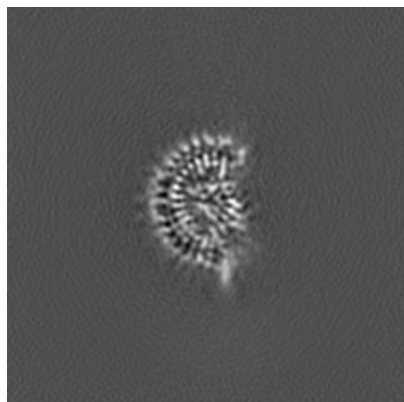


Y Index: 84

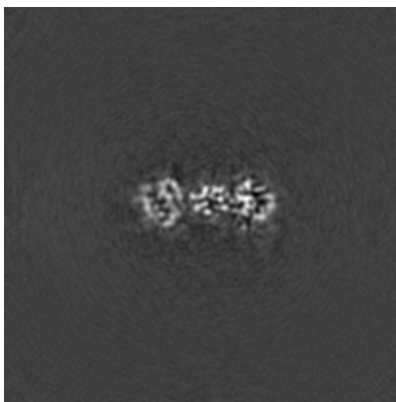


Z Index: 84

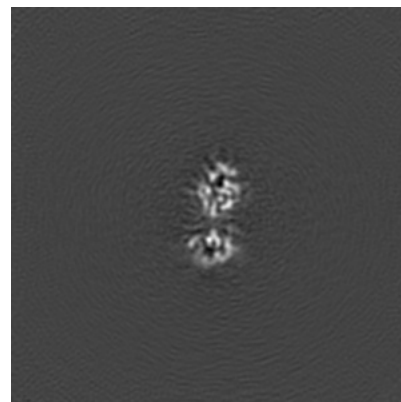
6.2.2 Raw map



X Index: 84



Y Index: 84

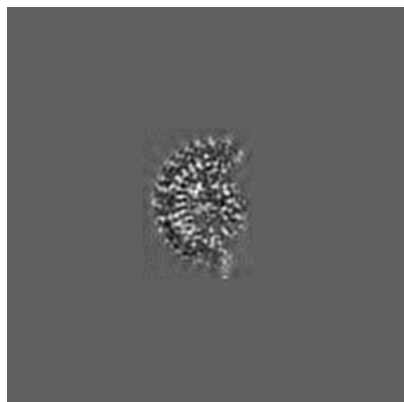


Z Index: 84

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: 85

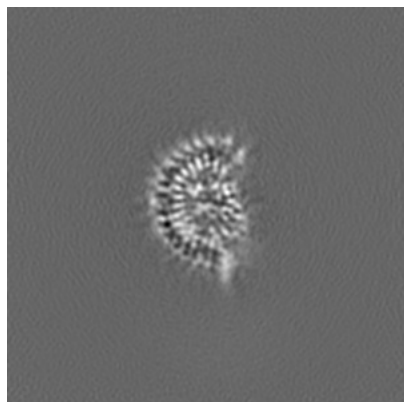


Y Index: 72

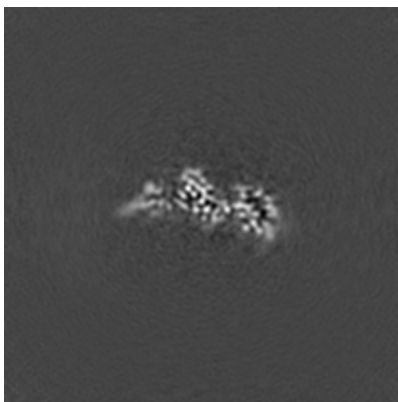


Z Index: 79

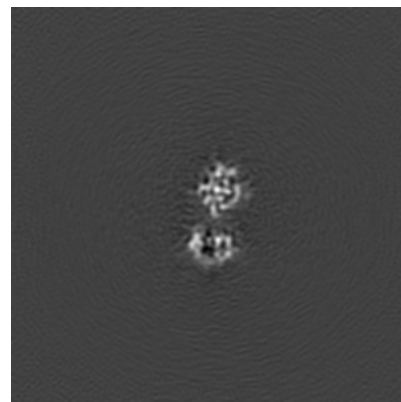
6.3.2 Raw map



X Index: 85



Y Index: 90

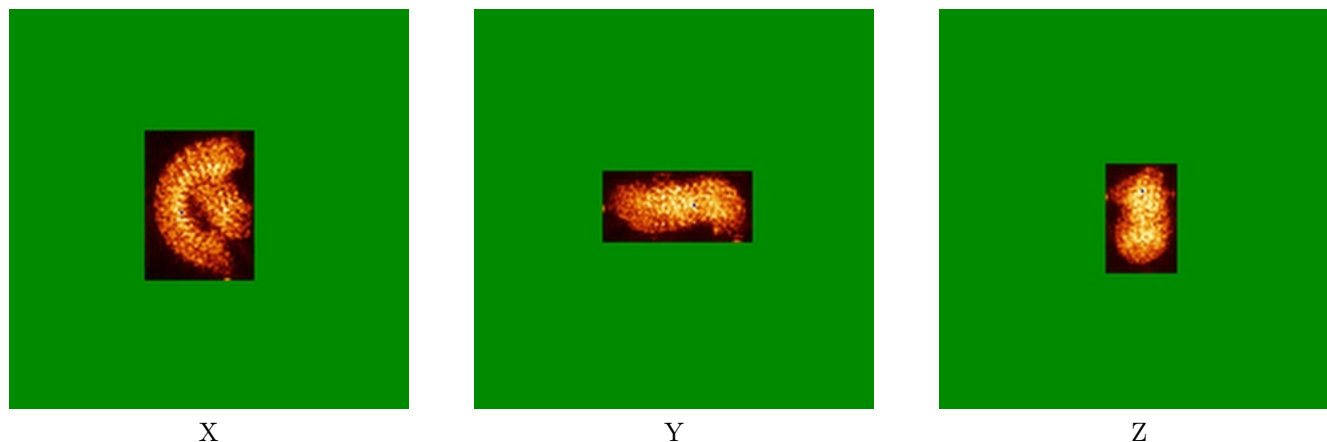


Z Index: 83

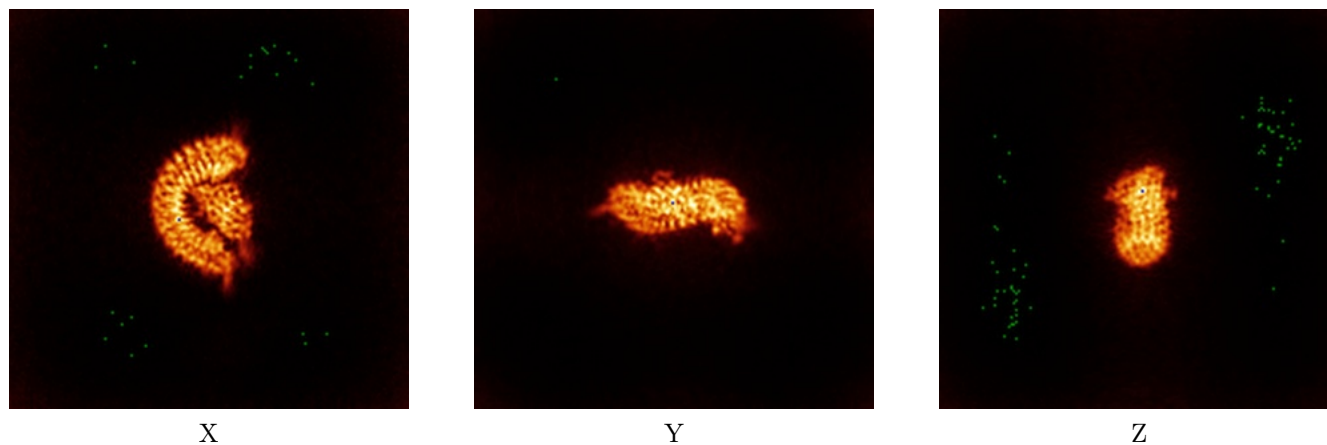
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



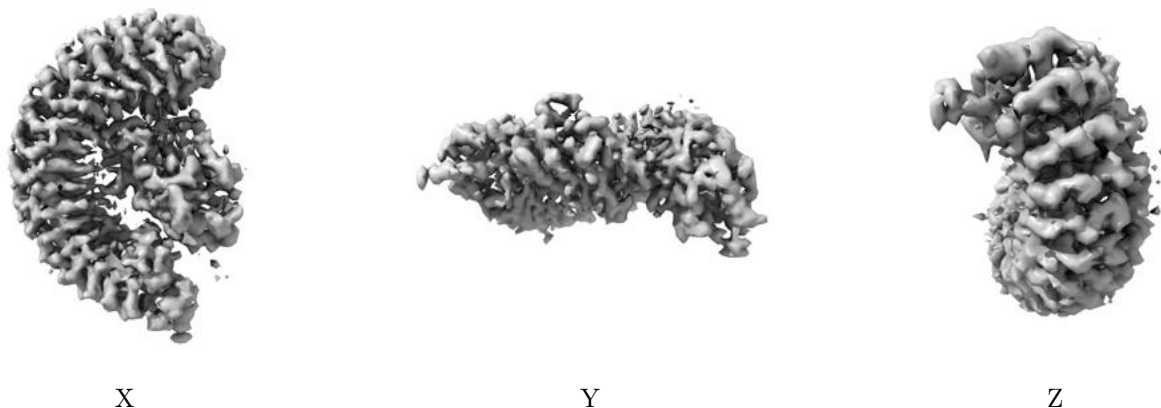
6.4.2 Raw map



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.

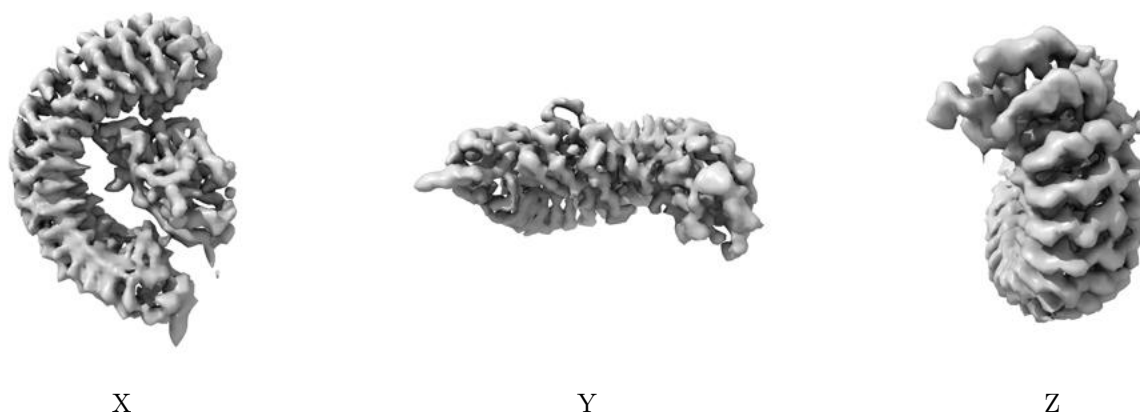
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.95. 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.

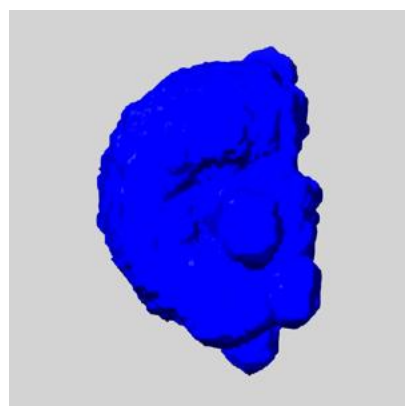
6.6 Mask visualisation [i](#)

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

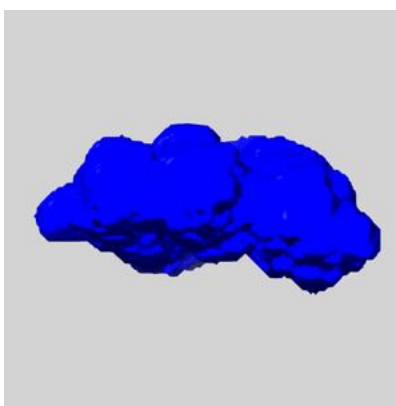
A mask typically either:

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

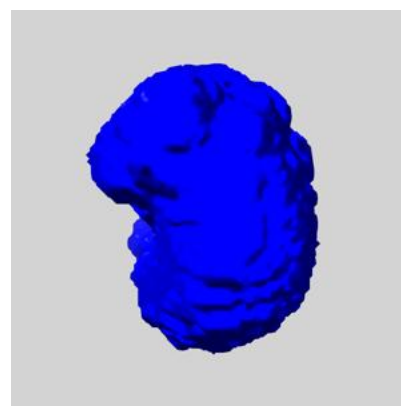
6.6.1 emd_18885_msk_1.map [i](#)



X



Y

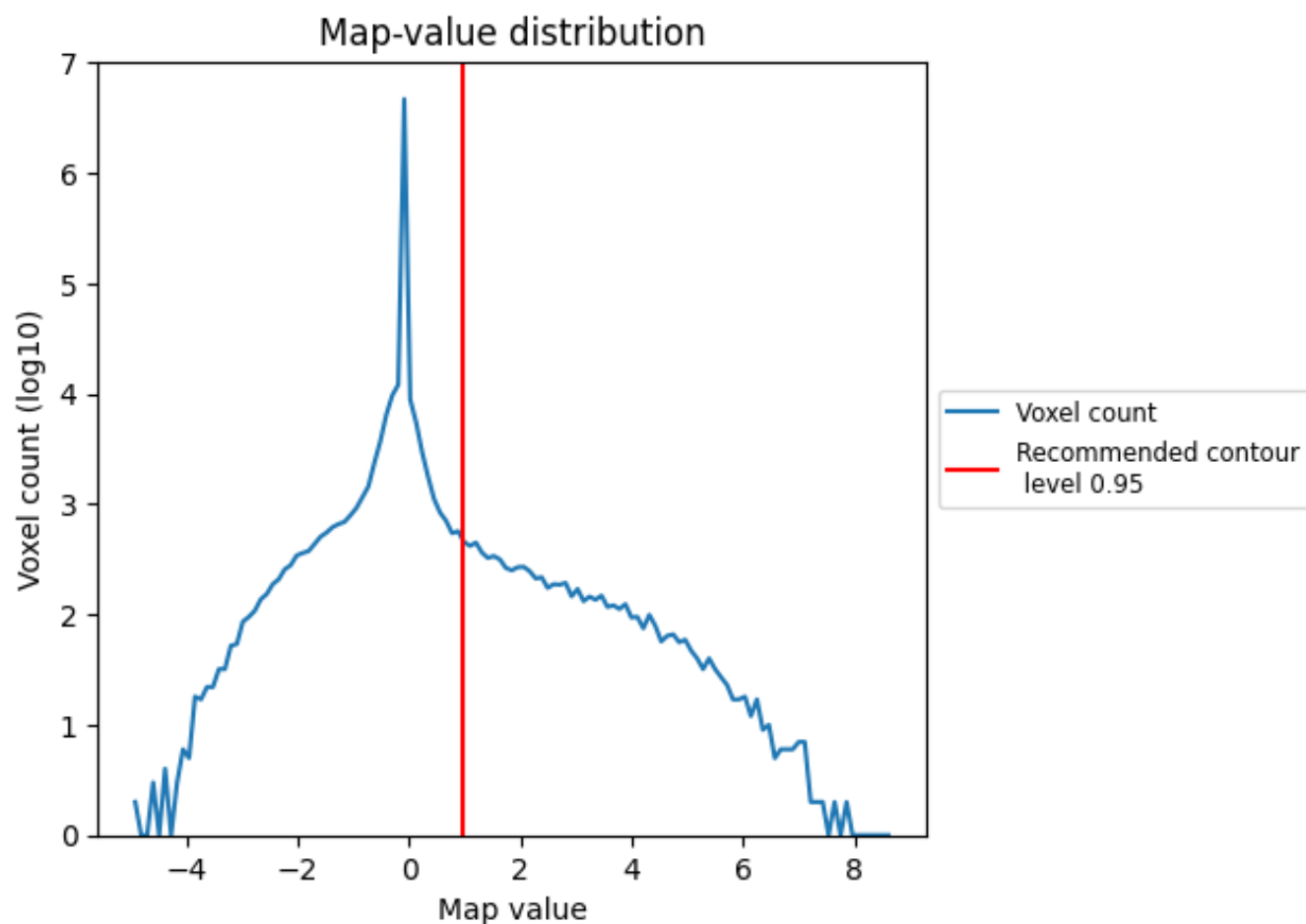


Z

7 Map analysis [i](#)

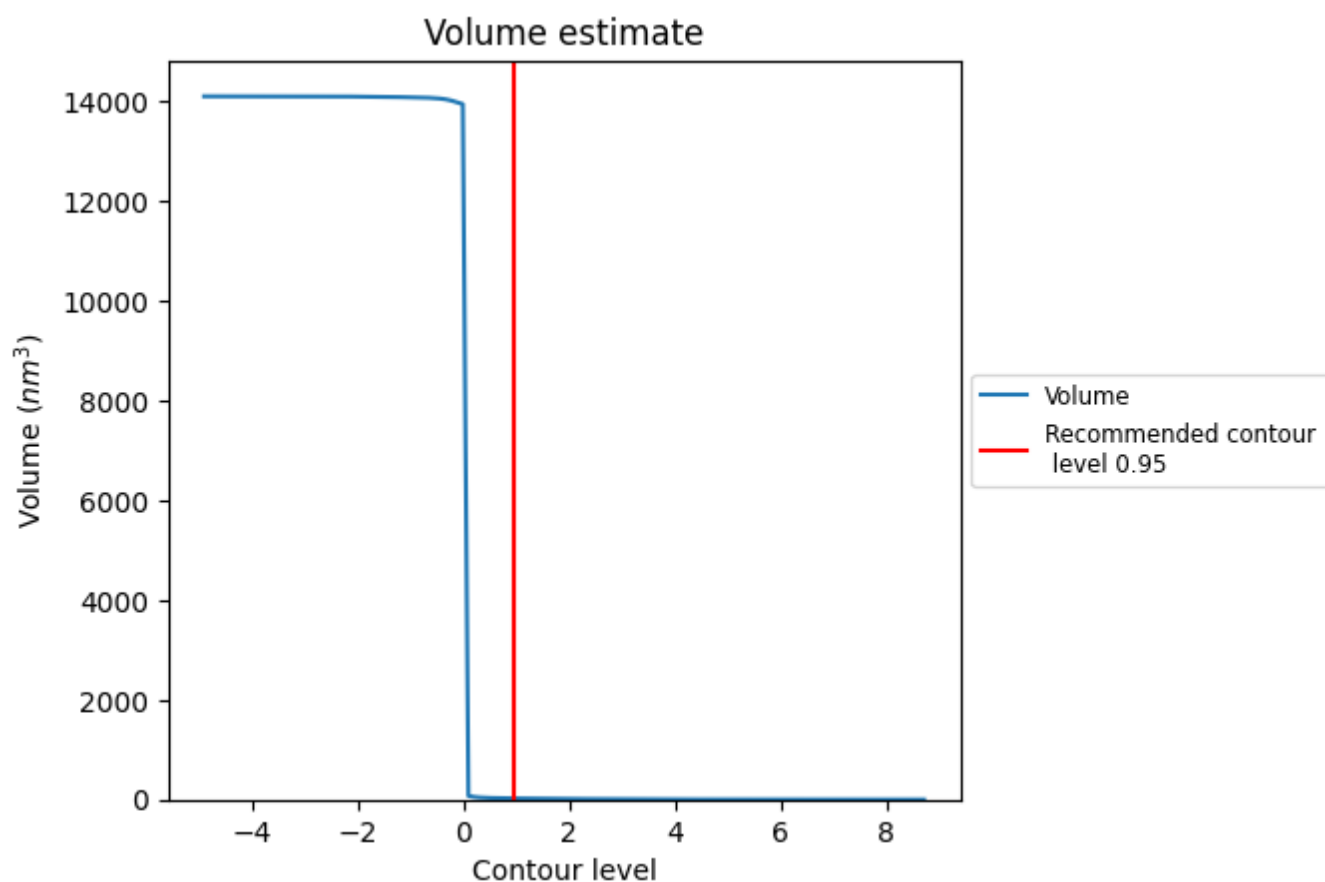
This section contains the results of statistical analysis of the map.

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.

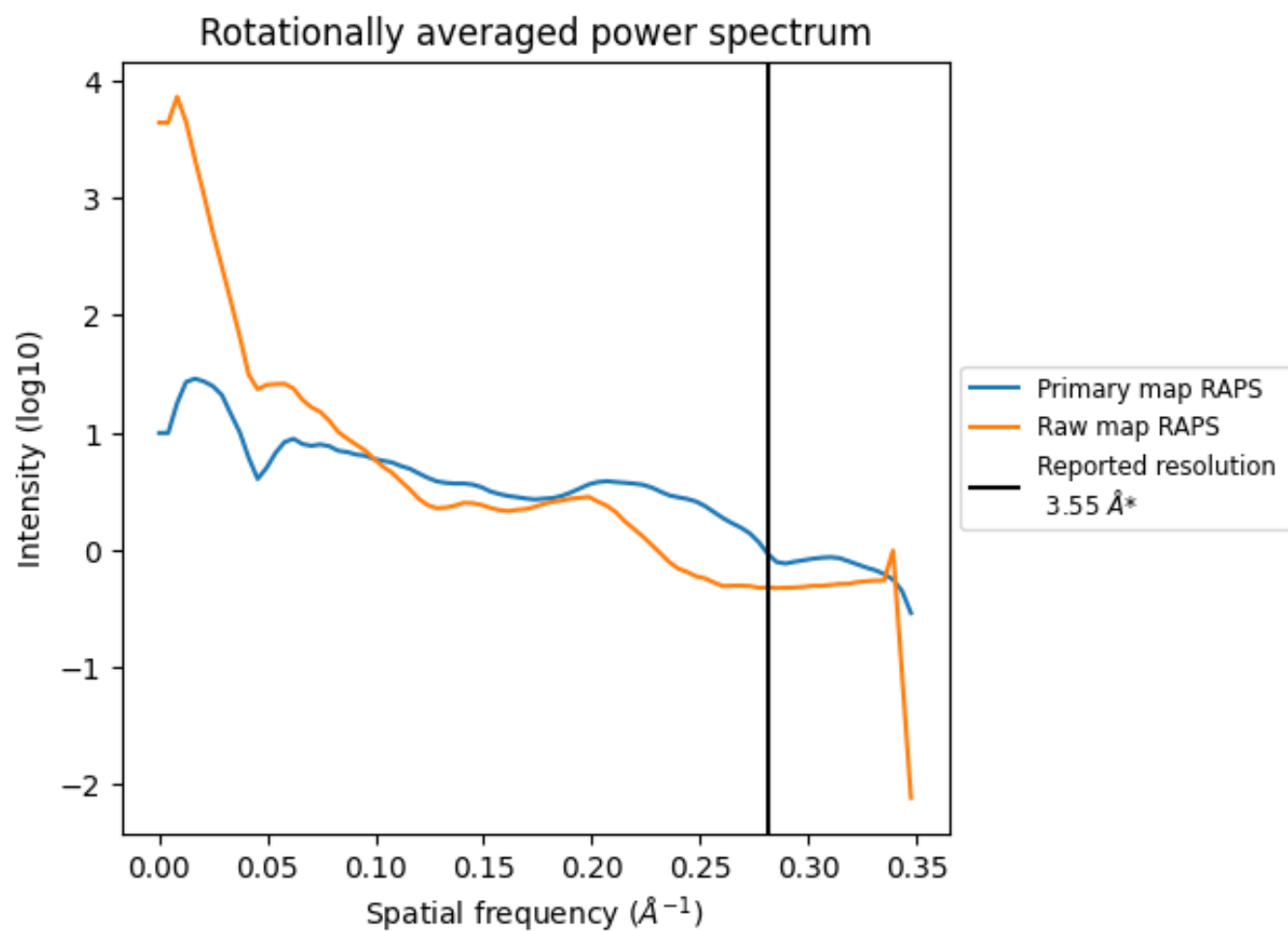
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 23 nm^3 ; this corresponds to an approximate mass of 21 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 ⓘ

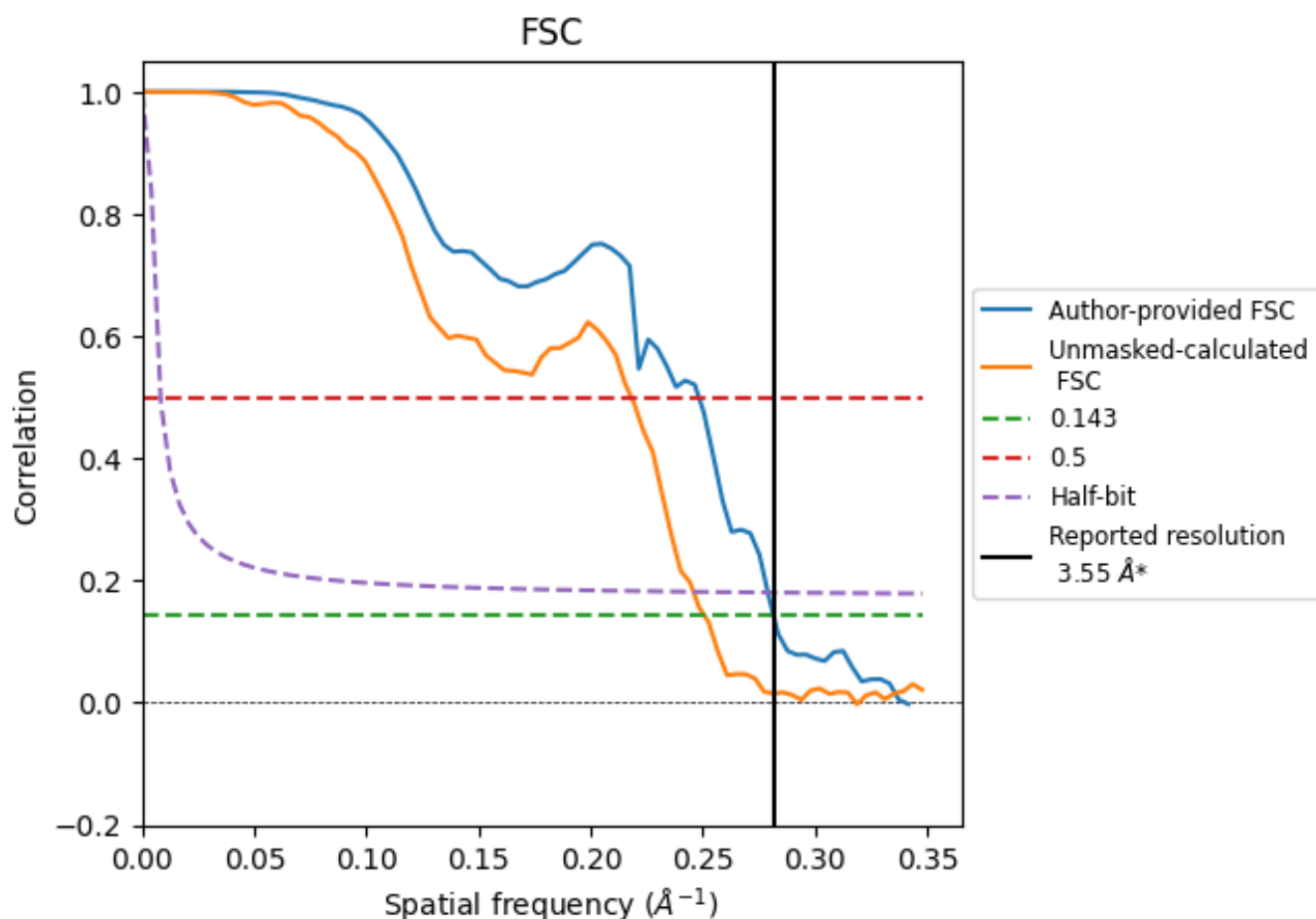


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

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 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

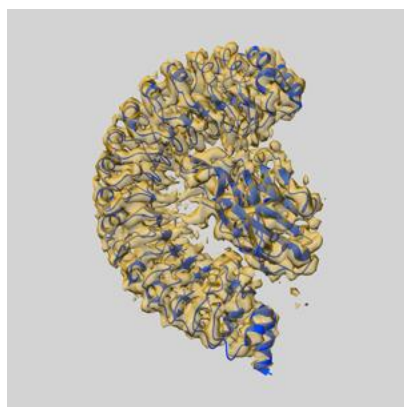
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.55	-	-
Author-provided FSC curve	3.55	4.03	3.59
Unmasked-calculated*	3.99	4.59	4.07

*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 3.99 differs from the reported value 3.55 by more than 10 %

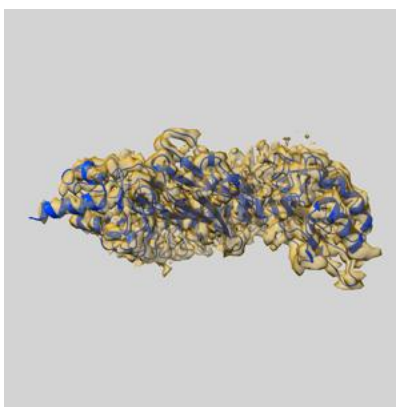
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18885 and PDB model 8R4C. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

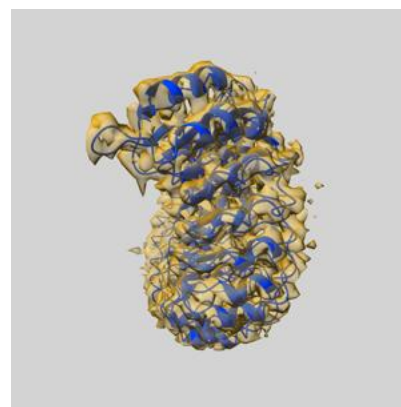
9.1 Map-model overlay [i](#)



X



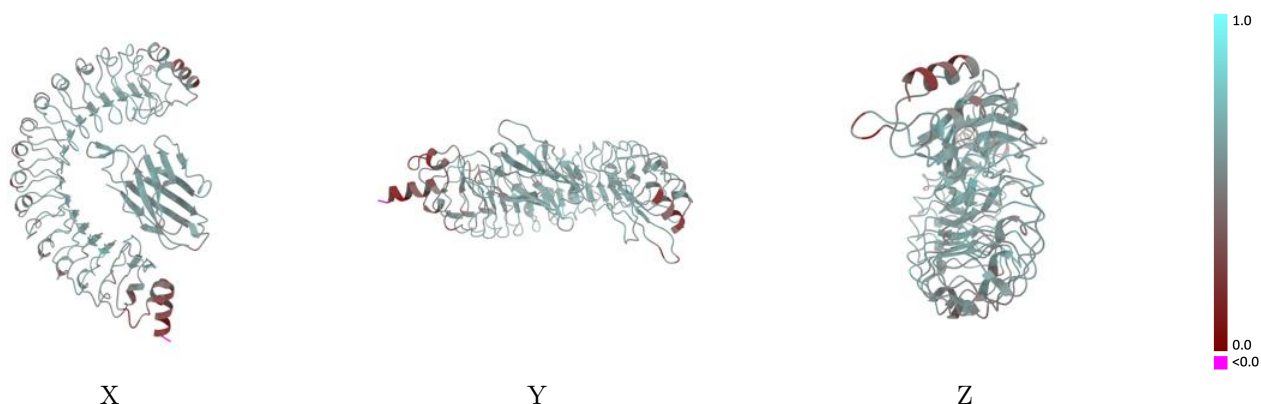
Y



Z

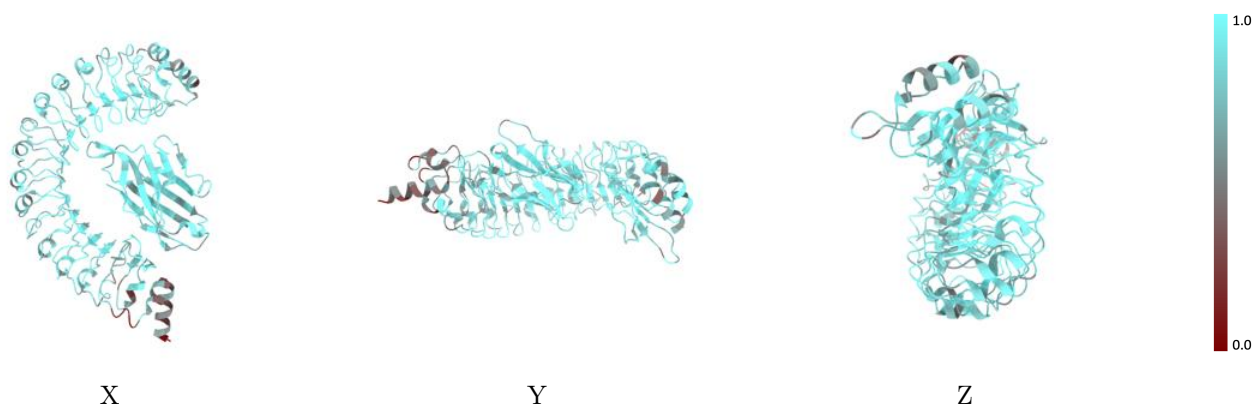
The images above show the 3D surface view of the map at the recommended contour level 0.95 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



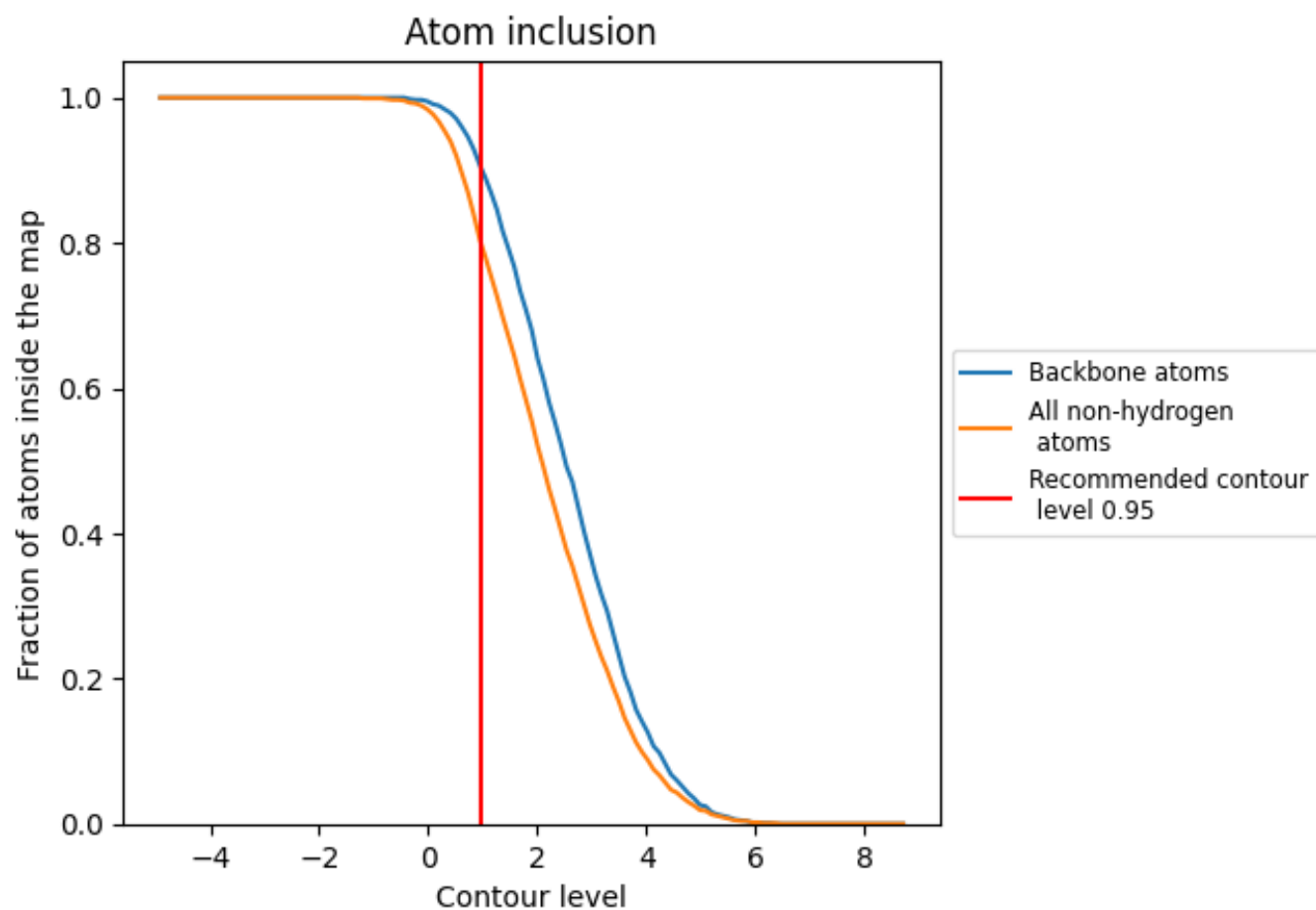
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.95).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 80% 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 (0.95) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.5400
A	0.7890	0.5310
C	0.8570	0.5730

