



Full wwPDB EM Validation Report ⓘ

Sep 29, 2026 – 01:55 pm BST

PDB ID : 9SSC / pdb_00009ssc
EMDB ID : EMD-53144
Title : Cryo-EM structure of essential Mycoplasma pneumoniae lipoprotein Mpn444 homotrimeric assembly
Authors : Manger, S.; Keles, I.
Deposited on : 2025-09-25
Resolution : 5.85 Å(reported)
Based on initial model : 9SRQ

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 Phenix2.2
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) : 2.51

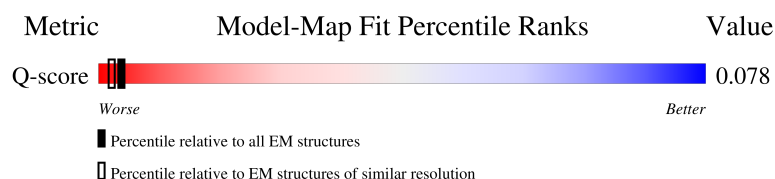
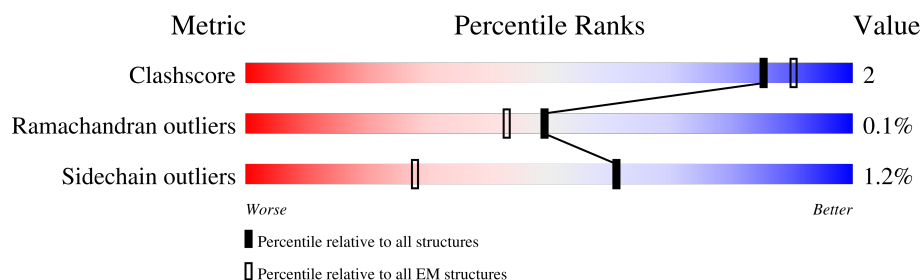
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

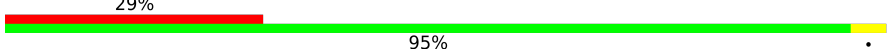
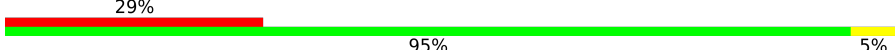
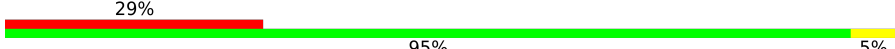
The reported resolution of this entry is 5.85 Å.

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	2937 (4.00 - 5.00)

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	1294	
1	B	1294	
1	C	1294	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 59913 atoms, of which 29673 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.

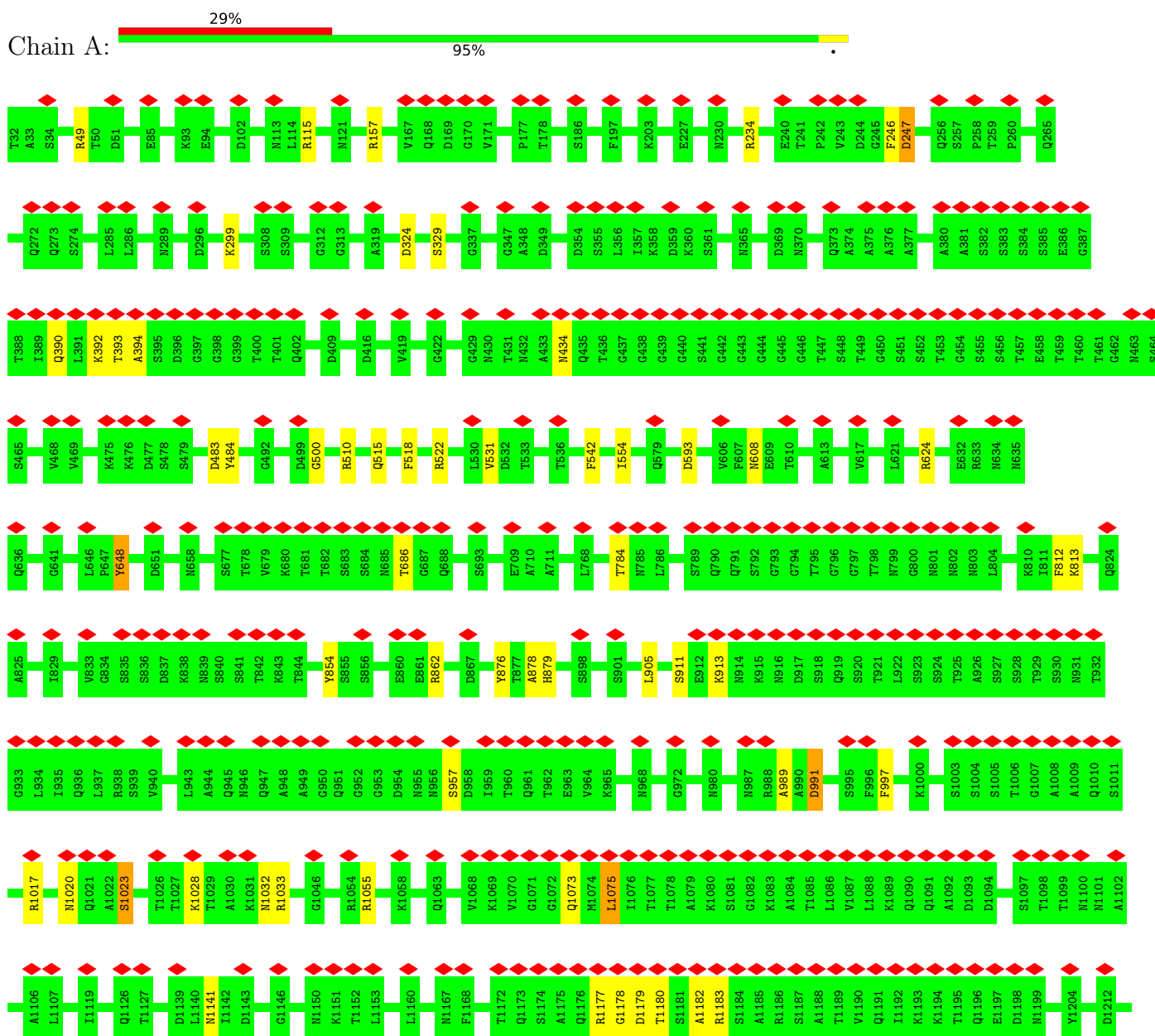
- Molecule 1 is a protein called Uncharacterized lipoprotein MG309 homolog.

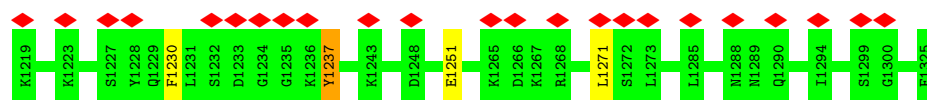
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1294	Total	C	H	N	O	S	0	0
			19971	6291	9891	1719	2064	6		
1	B	1294	Total	C	H	N	O	S	0	0
			19971	6291	9891	1719	2064	6		
1	C	1294	Total	C	H	N	O	S	0	0
			19971	6291	9891	1719	2064	6		

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: Uncharacterized lipoprotein MG309 homolog



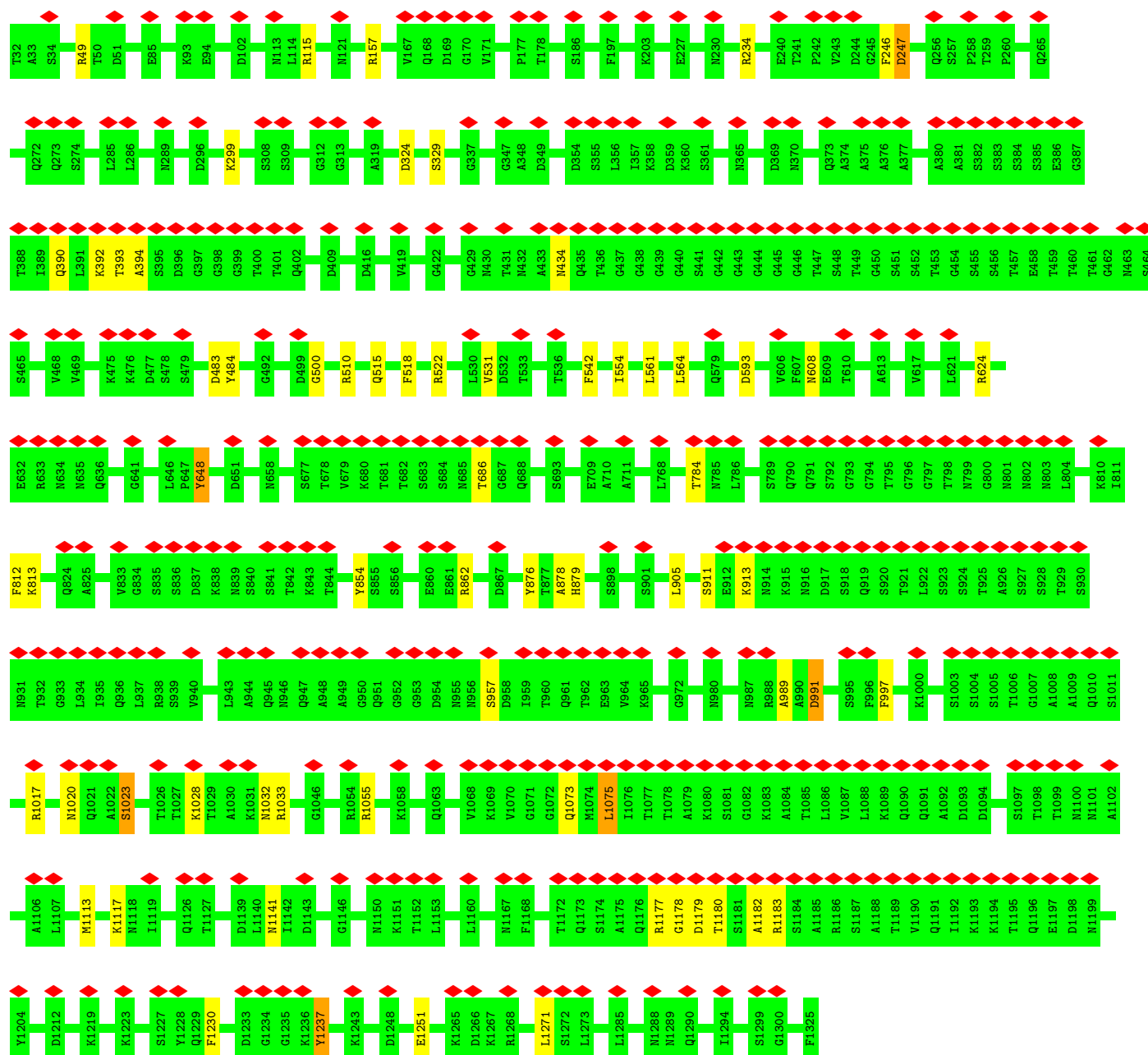


- Molecule 1: Uncharacterized lipoprotein MG309 homolog



- Molecule 1: Uncharacterized lipoprotein MG309 homolog





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	506291	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)	3600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.424	Depositor
Minimum map value	-0.185	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0368	Depositor
Map size (Å)	441.6, 441.6, 441.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92, 0.92, 0.92	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	0.74	0/10238	1.29	29/13819 (0.2%)
1	B	0.74	0/10238	1.29	29/13819 (0.2%)
1	C	0.74	0/10238	1.29	29/13819 (0.2%)
All	All	0.74	0/30714	1.29	87/41457 (0.2%)

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	4
1	B	0	4
1	C	0	4
All	All	0	12

There are no bond length outliers.

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	510	ARG	NE-CZ-NH2	6.91	125.42	119.20
1	A	510	ARG	NE-CZ-NH2	6.90	125.41	119.20
1	C	510	ARG	NE-CZ-NH2	6.89	125.40	119.20
1	B	593	ASP	CA-CB-CG	6.37	118.97	112.60
1	C	593	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	991	ASP	CA-CB-CG	6.33	118.93	112.60
1	C	991	ASP	CA-CB-CG	6.31	118.91	112.60
1	B	991	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	593	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	862	ARG	NE-CZ-NH2	6.26	124.83	119.20
1	B	862	ARG	NE-CZ-NH2	6.24	124.82	119.20
1	C	862	ARG	NE-CZ-NH2	6.22	124.80	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	ARG	NE-CZ-NH2	6.13	124.72	119.20
1	A	522	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	C	522	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	B	624	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	C	624	ARG	NE-CZ-NH2	6.04	124.63	119.20
1	B	522	ARG	NE-CZ-NH2	6.03	124.62	119.20
1	B	115	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	C	115	ARG	NE-CZ-NH2	5.91	124.51	119.20
1	C	997	PHE	CA-CB-CG	5.88	119.68	113.80
1	A	515	GLN	OE1-CD-NE2	-5.86	116.74	122.60
1	A	115	ARG	NE-CZ-NH2	5.86	124.47	119.20
1	C	515	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	A	997	PHE	CA-CB-CG	5.81	119.61	113.80
1	B	515	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	B	997	PHE	CA-CB-CG	5.79	119.59	113.80
1	C	1033	ARG	NE-CZ-NH2	5.72	124.34	119.20
1	C	510	ARG	NE-CZ-NH1	-5.71	115.79	121.50
1	A	510	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	B	1033	ARG	NE-CZ-NH2	5.66	124.30	119.20
1	B	510	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	A	1033	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	B	1032	ASN	N-CA-C	5.66	116.68	107.23
1	A	1032	ASN	N-CA-C	5.65	116.67	107.23
1	B	1230	PHE	CA-CB-CG	5.64	119.44	113.80
1	C	1032	ASN	N-CA-C	5.63	116.64	107.23
1	A	1230	PHE	CA-CB-CG	5.61	119.41	113.80
1	C	1230	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	247	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	1017	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	C	247	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	1017	ARG	NE-CZ-NH2	5.55	124.20	119.20
1	B	247	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	246	PHE	CA-C-N	5.49	128.40	120.38
1	A	246	PHE	C-N-CA	5.49	128.40	120.38
1	A	1017	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	C	246	PHE	CA-C-N	5.45	128.33	120.38
1	C	246	PHE	C-N-CA	5.45	128.33	120.38
1	B	246	PHE	CA-C-N	5.44	128.33	120.38
1	B	246	PHE	C-N-CA	5.44	128.33	120.38
1	A	608	ASN	CA-CB-CG	5.43	118.03	112.60
1	C	434	ASN	CA-CB-CG	5.41	118.01	112.60
1	A	434	ASN	CA-CB-CG	5.41	118.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	608	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	1020	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	542	PHE	CA-CB-CG	-5.36	108.44	113.80
1	B	608	ASN	CA-CB-CG	5.36	117.96	112.60
1	C	542	PHE	CA-CB-CG	-5.33	108.47	113.80
1	B	434	ASN	CA-CB-CG	5.32	117.92	112.60
1	C	1020	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	324	ASP	CA-CB-CG	5.30	117.91	112.60
1	A	542	PHE	CA-CB-CG	-5.30	108.50	113.80
1	B	324	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	957	SER	N-CA-C	-5.27	101.71	109.62
1	A	1020	ASN	CA-CB-CG	5.25	117.86	112.60
1	C	957	SER	N-CA-C	-5.25	101.74	109.62
1	C	299	LYS	CA-C-N	5.25	125.90	120.60
1	C	299	LYS	C-N-CA	5.25	125.90	120.60
1	B	957	SER	N-CA-C	-5.25	101.75	109.62
1	C	324	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	299	LYS	CA-C-N	5.22	125.87	120.60
1	B	299	LYS	C-N-CA	5.22	125.87	120.60
1	A	299	LYS	CA-C-N	5.20	125.85	120.60
1	A	299	LYS	C-N-CA	5.20	125.85	120.60
1	A	49	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	B	1141	ASN	N-CA-C	5.17	118.26	111.28
1	C	1141	ASN	N-CA-C	5.15	118.23	111.28
1	A	1141	ASN	N-CA-C	5.13	118.21	111.28
1	B	49	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	C	49	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	C	879	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	B	1055	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	C	1055	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	B	879	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	A	1055	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	A	879	HIS	CB-CG-CD2	-5.00	124.70	131.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1237	TYR	Sidechain
1	A	157	ARG	Sidechain
1	A	648	TYR	Sidechain
1	A	876	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	1237	TYR	Sidechain
1	B	157	ARG	Sidechain
1	B	648	TYR	Sidechain
1	B	876	TYR	Sidechain
1	C	1237	TYR	Sidechain
1	C	157	ARG	Sidechain
1	C	648	TYR	Sidechain
1	C	876	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	10080	9891	9886	74	0
1	B	10080	9891	9886	76	0
1	C	10080	9891	9886	76	0
All	All	30240	29673	29658	130	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 2.

All (130) 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:A:1180:THR:HA	1:B:392:LYS:HD3	1.32	1.11
1:B:1180:THR:CG2	1:C:394:ALA:HB2	1.80	1.11
1:A:392:LYS:HD3	1:C:1180:THR:HA	1.33	1.10
1:A:394:ALA:HB2	1:C:1180:THR:CG2	1.80	1.10
1:B:1180:THR:HA	1:C:392:LYS:HD3	1.31	1.10
1:A:1180:THR:CG2	1:B:394:ALA:HB2	1.81	1.09
1:A:392:LYS:HE2	1:C:1182:ALA:HB3	1.33	1.09
1:A:1182:ALA:HB3	1:B:392:LYS:HE2	1.31	1.06
1:B:1182:ALA:HB3	1:C:392:LYS:HE2	1.31	1.06
1:B:1178:GLY:HA3	1:C:393:THR:O	1.63	0.99
1:A:392:LYS:NZ	1:C:1183:ARG:HG3	1.78	0.97
1:A:1183:ARG:HG3	1:B:392:LYS:NZ	1.79	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1178:GLY:CA	1:C:393:THR:O	2.12	0.97
1:A:1178:GLY:HA3	1:B:393:THR:O	1.64	0.96
1:A:1178:GLY:CA	1:B:393:THR:O	2.13	0.96
1:A:393:THR:O	1:C:1178:GLY:HA3	1.67	0.95
1:B:1183:ARG:HG3	1:C:392:LYS:NZ	1.80	0.94
1:A:393:THR:O	1:C:1178:GLY:CA	2.16	0.93
1:A:394:ALA:HB2	1:C:1180:THR:HG21	1.49	0.92
1:B:1180:THR:HG21	1:C:394:ALA:HB2	1.50	0.91
1:A:1180:THR:HG21	1:B:394:ALA:HB2	1.51	0.90
1:A:1180:THR:CA	1:B:392:LYS:HD3	2.06	0.86
1:B:1180:THR:CA	1:C:392:LYS:HD3	2.04	0.86
1:A:392:LYS:HD3	1:C:1180:THR:CA	2.05	0.86
1:A:1177:ARG:HH22	1:B:686:THR:CG2	1.92	0.82
1:B:1177:ARG:HH22	1:C:686:THR:CG2	1.93	0.82
1:A:686:THR:CG2	1:C:1177:ARG:HH22	1.94	0.79
1:B:1177:ARG:HH22	1:C:686:THR:HB	1.49	0.78
1:A:392:LYS:NZ	1:C:1183:ARG:CG	2.44	0.78
1:A:686:THR:HB	1:C:1177:ARG:HH22	1.47	0.78
1:A:1177:ARG:HH22	1:B:686:THR:HB	1.49	0.77
1:A:686:THR:CB	1:C:1177:ARG:HH22	1.98	0.77
1:A:1177:ARG:HH22	1:B:686:THR:CB	1.98	0.77
1:B:1177:ARG:HH22	1:C:686:THR:CB	1.98	0.76
1:A:1177:ARG:NH2	1:B:686:THR:CG2	2.51	0.74
1:A:392:LYS:CE	1:C:1183:ARG:HG3	2.18	0.74
1:B:1177:ARG:NH2	1:C:686:THR:CG2	2.51	0.73
1:A:686:THR:CG2	1:C:1177:ARG:NH2	2.52	0.71
1:B:1178:GLY:C	1:C:393:THR:O	2.34	0.71
1:B:1183:ARG:CG	1:C:392:LYS:NZ	2.48	0.70
1:B:1183:ARG:HG3	1:C:392:LYS:CE	2.21	0.70
1:A:390:GLN:HB3	1:C:1183:ARG:HE	1.58	0.69
1:A:1183:ARG:HG3	1:B:392:LYS:CE	2.22	0.69
1:A:1180:THR:CG2	1:B:394:ALA:CB	2.67	0.69
1:A:1178:GLY:C	1:B:393:THR:O	2.36	0.68
1:B:1183:ARG:HE	1:C:390:GLN:HB3	1.58	0.68
1:A:393:THR:O	1:C:1178:GLY:C	2.36	0.68
1:A:1180:THR:HA	1:B:392:LYS:CD	2.19	0.67
1:B:1182:ALA:CB	1:C:392:LYS:HE2	2.19	0.67
1:A:1183:ARG:HE	1:B:390:GLN:HB3	1.59	0.67
1:A:394:ALA:CB	1:C:1180:THR:CG2	2.66	0.67
1:B:1180:THR:HA	1:C:392:LYS:CD	2.17	0.66
1:A:1183:ARG:CG	1:B:392:LYS:NZ	2.47	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LYS:CD	1:C:1180:THR:HA	2.20	0.65
1:A:1182:ALA:CB	1:B:392:LYS:HE2	2.20	0.65
1:B:1180:THR:CG2	1:C:394:ALA:CB	2.67	0.65
1:A:392:LYS:HD2	1:C:1183:ARG:HG3	1.80	0.64
1:A:392:LYS:HE2	1:C:1182:ALA:CB	2.20	0.64
1:C:905:LEU:HD13	1:C:1271:LEU:HD21	1.80	0.64
1:B:905:LEU:HD13	1:B:1271:LEU:HD21	1.80	0.63
1:A:905:LEU:HD13	1:A:1271:LEU:HD21	1.80	0.63
1:B:1179:ASP:O	1:C:392:LYS:HB3	1.98	0.63
1:A:1179:ASP:O	1:B:392:LYS:HB3	1.99	0.62
1:A:392:LYS:CE	1:C:1182:ALA:HB3	2.22	0.61
1:B:1182:ALA:HB3	1:C:392:LYS:CE	2.19	0.61
1:A:394:ALA:CB	1:C:1180:THR:HG21	2.28	0.61
1:A:392:LYS:HB3	1:C:1179:ASP:O	2.01	0.60
1:A:1182:ALA:HB3	1:B:392:LYS:CE	2.20	0.60
1:B:1180:THR:C	1:C:392:LYS:HD3	2.27	0.59
1:B:1183:ARG:HG3	1:C:392:LYS:HD2	1.83	0.59
1:A:392:LYS:HD3	1:C:1180:THR:C	2.28	0.59
1:B:1183:ARG:HE	1:C:390:GLN:CB	2.16	0.59
1:A:392:LYS:CD	1:C:1183:ARG:HG3	2.33	0.59
1:A:1180:THR:HG21	1:B:394:ALA:CB	2.30	0.58
1:A:1183:ARG:HG3	1:B:392:LYS:HD2	1.83	0.58
1:A:390:GLN:CB	1:C:1183:ARG:HE	2.17	0.58
1:A:1183:ARG:HE	1:B:390:GLN:CB	2.17	0.57
1:B:1177:ARG:NH2	1:C:686:THR:HG21	2.20	0.56
1:B:1180:THR:HG21	1:C:394:ALA:CB	2.30	0.56
1:A:1180:THR:C	1:B:392:LYS:HD3	2.30	0.56
1:A:1177:ARG:NH2	1:B:686:THR:HG21	2.19	0.56
1:B:1075:LEU:HD23	1:B:1075:LEU:N	2.21	0.56
1:C:1075:LEU:HD23	1:C:1075:LEU:N	2.21	0.55
1:A:686:THR:HG21	1:C:1177:ARG:NH2	2.21	0.55
1:A:1075:LEU:N	1:A:1075:LEU:HD23	2.21	0.55
1:B:1183:ARG:HG3	1:C:392:LYS:CD	2.37	0.55
1:A:1183:ARG:HG3	1:B:392:LYS:CD	2.37	0.54
1:B:1179:ASP:N	1:C:393:THR:O	2.42	0.52
1:A:1179:ASP:N	1:B:393:THR:O	2.43	0.51
1:A:393:THR:O	1:C:1179:ASP:N	2.43	0.51
1:C:913:LYS:HE2	1:C:1237:TYR:CE2	2.47	0.50
1:A:913:LYS:HE2	1:A:1237:TYR:CE2	2.47	0.49
1:B:913:LYS:HE2	1:B:1237:TYR:CE2	2.47	0.48
1:B:1180:THR:HG23	1:C:394:ALA:HB2	1.84	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:GLY:HA3	1:C:518:PHE:CE2	2.49	0.47
1:A:394:ALA:HB2	1:C:1180:THR:HG23	1.86	0.47
1:A:500:GLY:HA3	1:A:518:PHE:CE2	2.49	0.46
1:B:500:GLY:HA3	1:B:518:PHE:CE2	2.50	0.46
1:B:1073:GLN:HB2	1:B:1075:LEU:HD21	1.98	0.46
1:A:394:ALA:HB2	1:C:1180:THR:HG22	1.88	0.45
1:B:1180:THR:HG22	1:C:394:ALA:HB2	1.88	0.45
1:B:500:GLY:HA3	1:B:518:PHE:CZ	2.52	0.45
1:C:1073:GLN:HB2	1:C:1075:LEU:HD21	1.98	0.45
1:A:500:GLY:HA3	1:A:518:PHE:CZ	2.52	0.45
1:B:1073:GLN:CB	1:B:1075:LEU:HD21	2.47	0.45
1:A:1073:GLN:HB2	1:A:1075:LEU:HD21	1.98	0.44
1:A:1180:THR:HG23	1:B:394:ALA:CB	2.47	0.44
1:C:500:GLY:HA3	1:C:518:PHE:CZ	2.52	0.44
1:C:1073:GLN:CB	1:C:1075:LEU:HD21	2.47	0.44
1:A:1073:GLN:CB	1:A:1075:LEU:HD21	2.47	0.44
1:B:1177:ARG:NH2	1:C:686:THR:HG22	2.32	0.43
1:A:911:SER:HB2	1:A:989:ALA:HB1	2.02	0.42
1:A:812:PHE:CD1	1:A:878:ALA:HB1	2.55	0.42
1:A:1177:ARG:HH22	1:B:686:THR:HG21	1.77	0.42
1:B:812:PHE:CD1	1:B:878:ALA:HB1	2.55	0.42
1:A:813:LYS:HE3	1:A:854:TYR:CE1	2.55	0.42
1:B:813:LYS:HE3	1:B:854:TYR:CE1	2.55	0.42
1:B:1180:THR:O	1:C:392:LYS:NZ	2.53	0.42
1:C:812:PHE:CD1	1:C:878:ALA:HB1	2.55	0.41
1:A:1180:THR:HG23	1:B:394:ALA:HB2	1.86	0.41
1:C:813:LYS:HE3	1:C:854:TYR:CE1	2.55	0.41
1:A:1180:THR:HG22	1:B:394:ALA:HB2	1.87	0.41
1:C:911:SER:HB2	1:C:989:ALA:HB1	2.02	0.41
1:A:390:GLN:CB	1:C:1183:ARG:NE	2.83	0.41
1:B:561:LEU:HA	1:B:564:LEU:HD12	2.03	0.41
1:C:561:LEU:HA	1:C:564:LEU:HD12	2.03	0.41
1:B:911:SER:HB2	1:B:989:ALA:HB1	2.02	0.40
1:A:392:LYS:NZ	1:C:1180:THR:O	2.54	0.40
1:B:1113:MET:SD	1:B:1117:LYS:HE3	2.61	0.40
1:C:1113:MET:SD	1:C:1117:LYS:HE3	2.62	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	1292/1294 (100%)	1208 (94%)	83 (6%)	1 (0%)	48	83
1	B	1292/1294 (100%)	1208 (94%)	83 (6%)	1 (0%)	48	83
1	C	1292/1294 (100%)	1208 (94%)	83 (6%)	1 (0%)	48	83
All	All	3876/3882 (100%)	3624 (94%)	249 (6%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1023	SER
1	B	1023	SER
1	C	1023	SER

5.3.2 Protein sidechains ⓘ

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	1126/1126 (100%)	1112 (99%)	14 (1%)	63	74
1	B	1126/1126 (100%)	1112 (99%)	14 (1%)	63	74
1	C	1126/1126 (100%)	1112 (99%)	14 (1%)	63	74
All	All	3378/3378 (100%)	3336 (99%)	42 (1%)	61	74

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	ARG
1	A	247	ASP
1	A	329	SER
1	A	483	ASP
1	A	484	TYR
1	A	531	VAL
1	A	554	ILE
1	A	648	TYR
1	A	784	THR
1	A	991	ASP
1	A	1023	SER
1	A	1028	LYS
1	A	1075	LEU
1	A	1251	GLU
1	B	234	ARG
1	B	247	ASP
1	B	329	SER
1	B	483	ASP
1	B	484	TYR
1	B	531	VAL
1	B	554	ILE
1	B	648	TYR
1	B	784	THR
1	B	991	ASP
1	B	1023	SER
1	B	1028	LYS
1	B	1075	LEU
1	B	1251	GLU
1	C	234	ARG
1	C	247	ASP
1	C	329	SER
1	C	483	ASP
1	C	484	TYR
1	C	531	VAL
1	C	554	ILE
1	C	648	TYR
1	C	784	THR
1	C	991	ASP
1	C	1023	SER
1	C	1028	LYS
1	C	1075	LEU
1	C	1251	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	110	GLN
1	A	226	ASN
1	A	265	GLN
1	A	370	ASN
1	A	503	HIS
1	A	636	GLN
1	A	685	ASN
1	A	703	ASN
1	A	735	GLN
1	A	755	ASN
1	A	803	ASN
1	A	946	ASN
1	A	980	ASN
1	A	1073	GLN
1	A	1118	ASN
1	A	1121	ASN
1	A	1134	ASN
1	A	1167	ASN
1	A	1201	ASN
1	A	1224	ASN
1	A	1292	GLN
1	B	59	GLN
1	B	110	GLN
1	B	226	ASN
1	B	265	GLN
1	B	370	ASN
1	B	503	HIS
1	B	685	ASN
1	B	703	ASN
1	B	755	ASN
1	B	803	ASN
1	B	980	ASN
1	B	1073	GLN
1	B	1118	ASN
1	B	1121	ASN
1	B	1134	ASN
1	B	1167	ASN
1	B	1201	ASN
1	B	1224	ASN
1	B	1292	GLN
1	C	59	GLN

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Mol	Chain	Res	Type
1	C	110	GLN
1	C	226	ASN
1	C	265	GLN
1	C	295	ASN
1	C	370	ASN
1	C	503	HIS
1	C	636	GLN
1	C	685	ASN
1	C	703	ASN
1	C	755	ASN
1	C	803	ASN
1	C	946	ASN
1	C	980	ASN
1	C	1073	GLN
1	C	1118	ASN
1	C	1121	ASN
1	C	1134	ASN
1	C	1167	ASN
1	C	1201	ASN
1	C	1224	ASN
1	C	1292	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

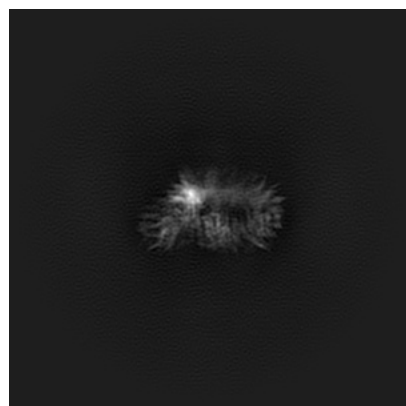
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53144. These allow visual inspection of the internal detail of the map and identification of artifacts.

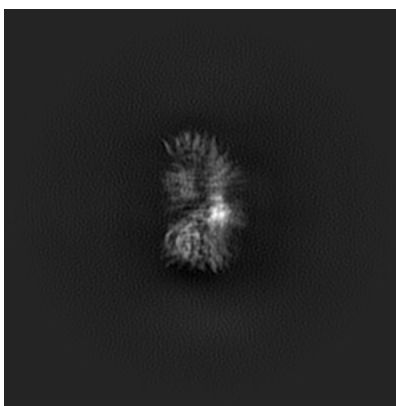
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

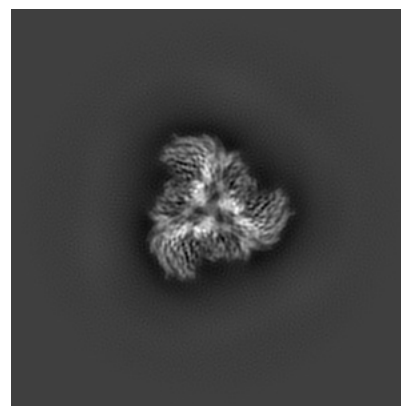
6.1.1 Primary map



X

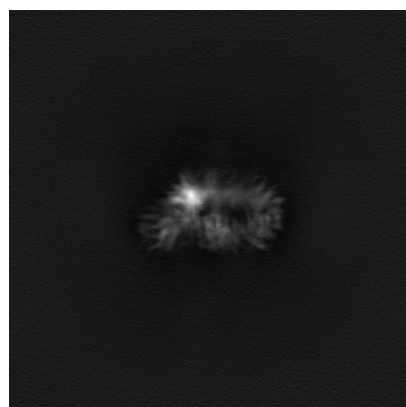


Y

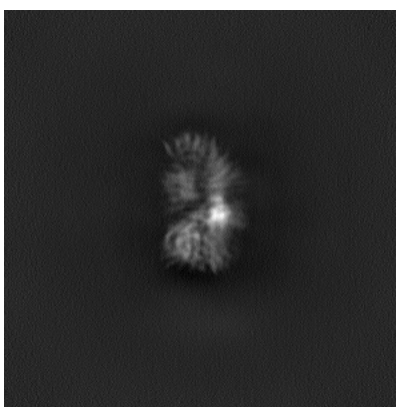


Z

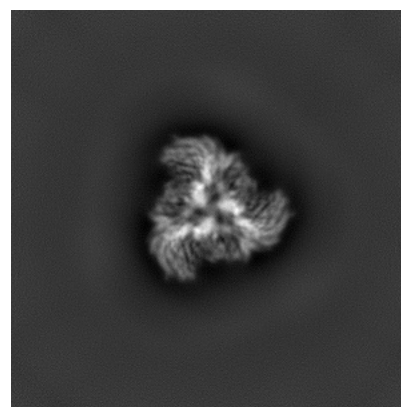
6.1.2 Raw map



X



Y

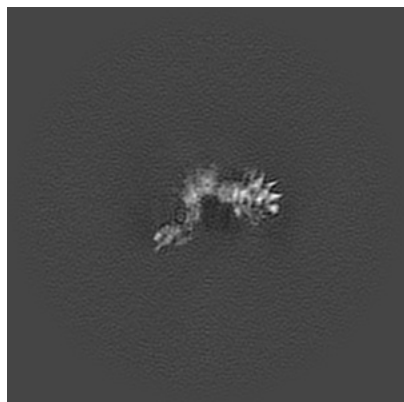


Z

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

6.2 Central slices [i](#)

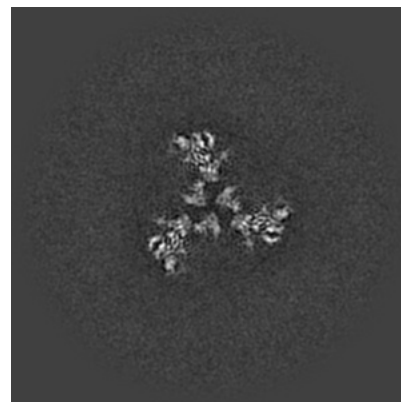
6.2.1 Primary map



X Index: 240

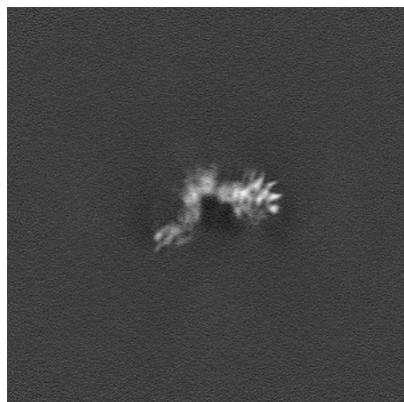


Y Index: 240



Z Index: 240

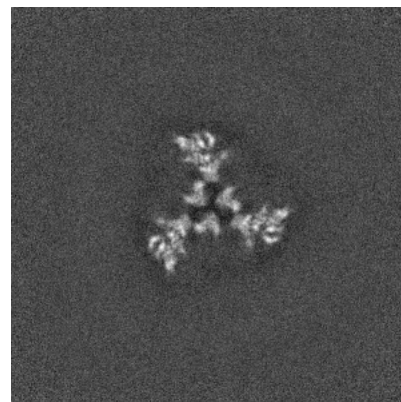
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

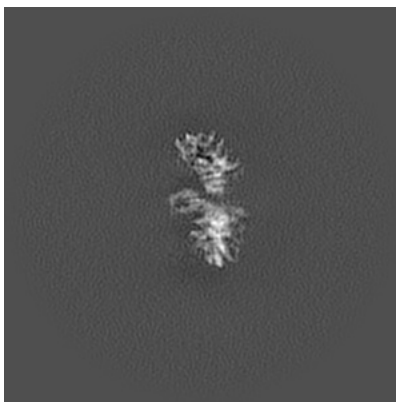
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 232

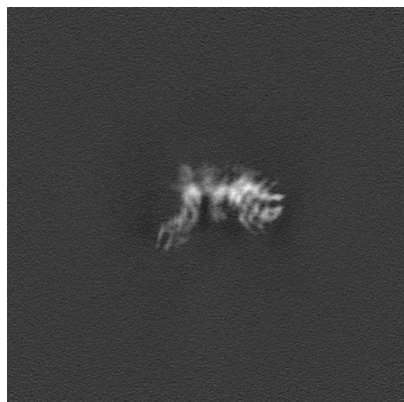


Y Index: 217

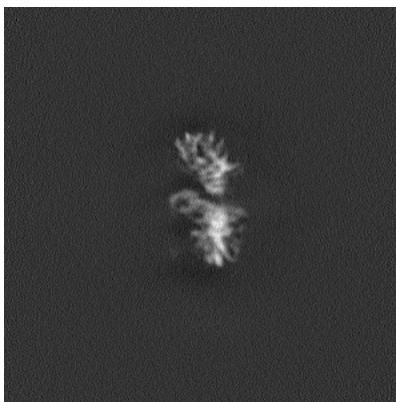


Z Index: 252

6.3.2 Raw map



X Index: 233



Y Index: 218



Z Index: 258

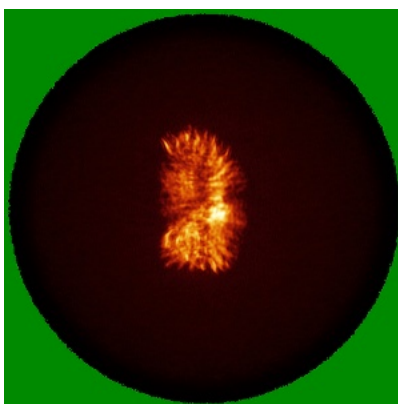
The images above show the largest variance slices of the map in three orthogonal directions.

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

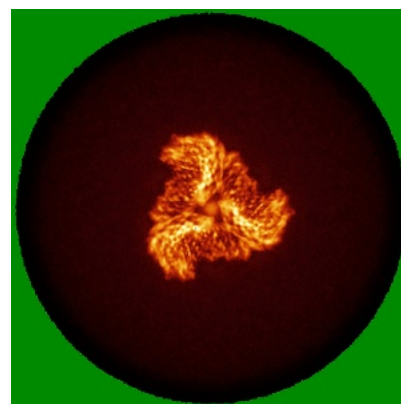
6.4.1 Primary map



X



Y

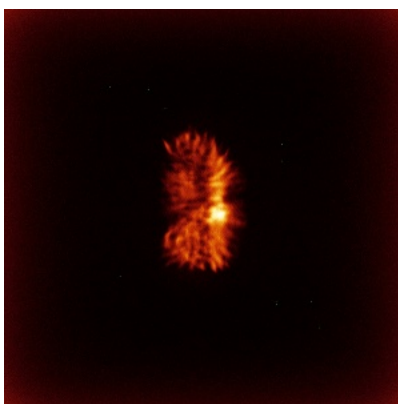


Z

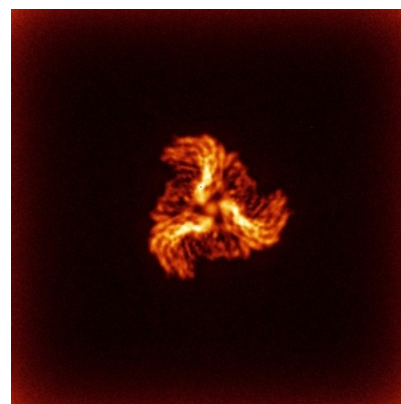
6.4.2 Raw map



X



Y

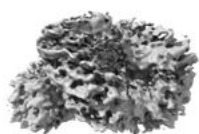


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



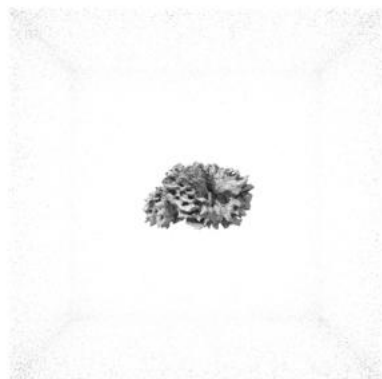
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0368. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

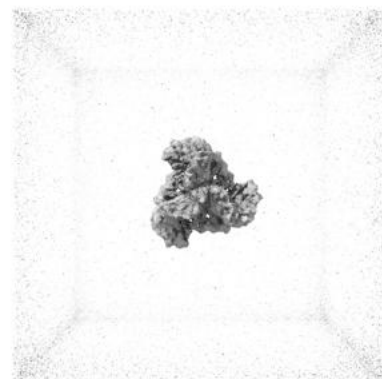
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

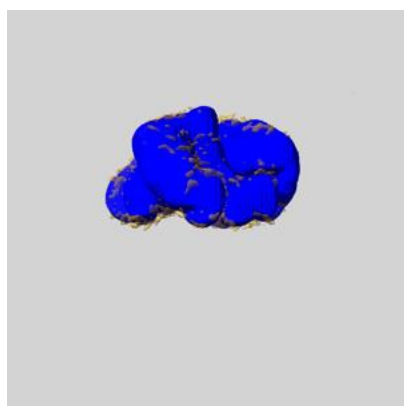
6.6 Mask visualisation [i](#)

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

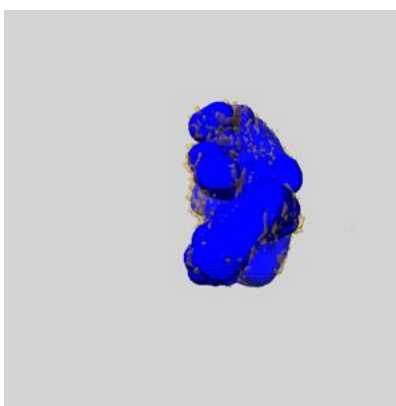
A mask typically either:

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

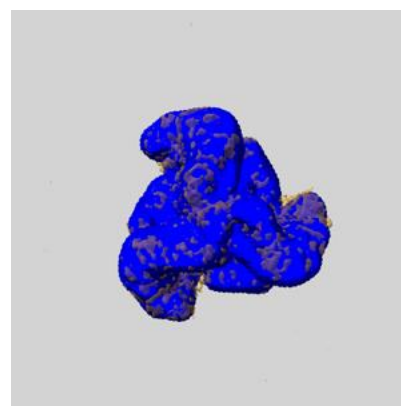
6.6.1 emd_53144_msk_1.map [i](#)



X



Y

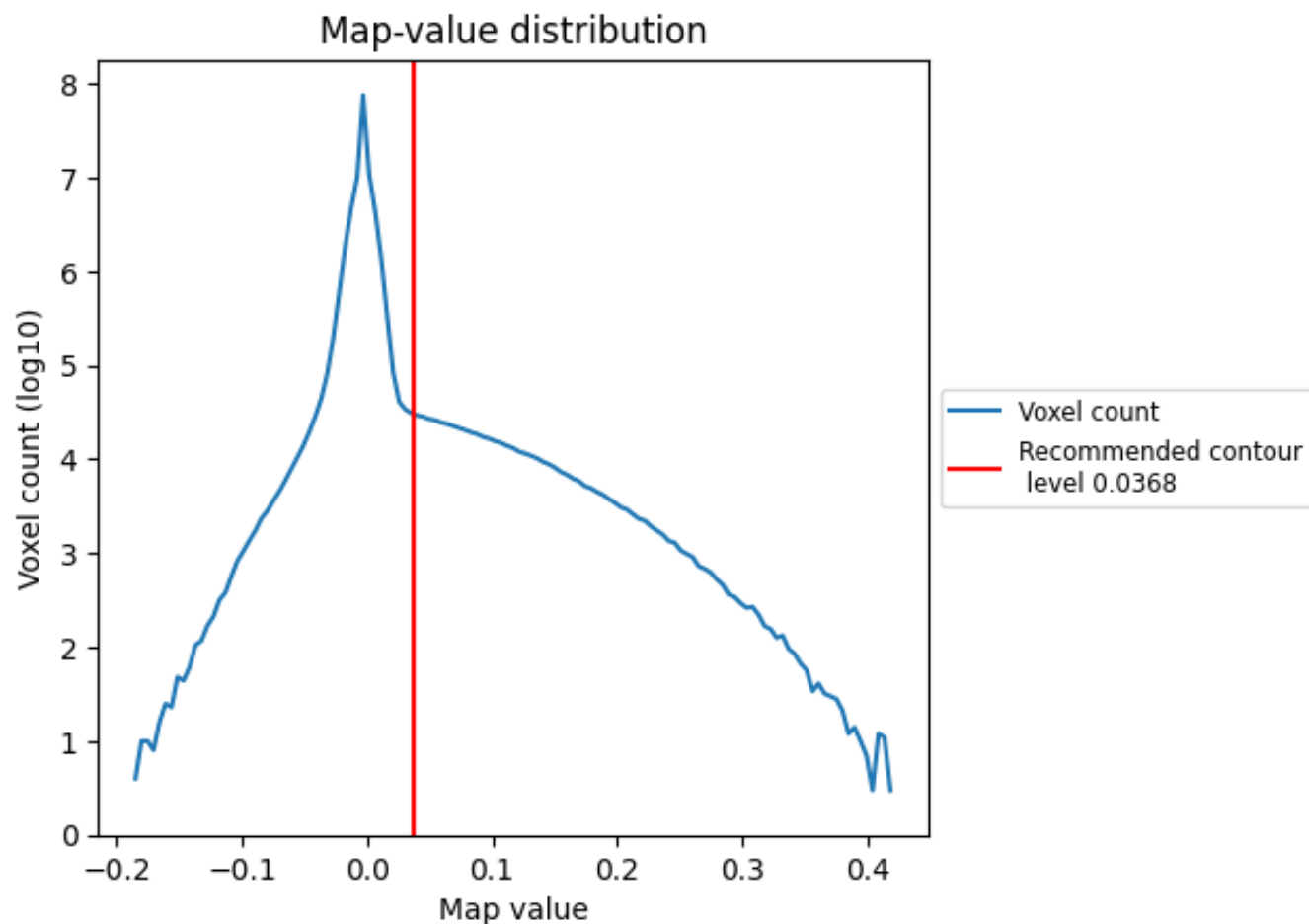


Z

7 Map analysis [i](#)

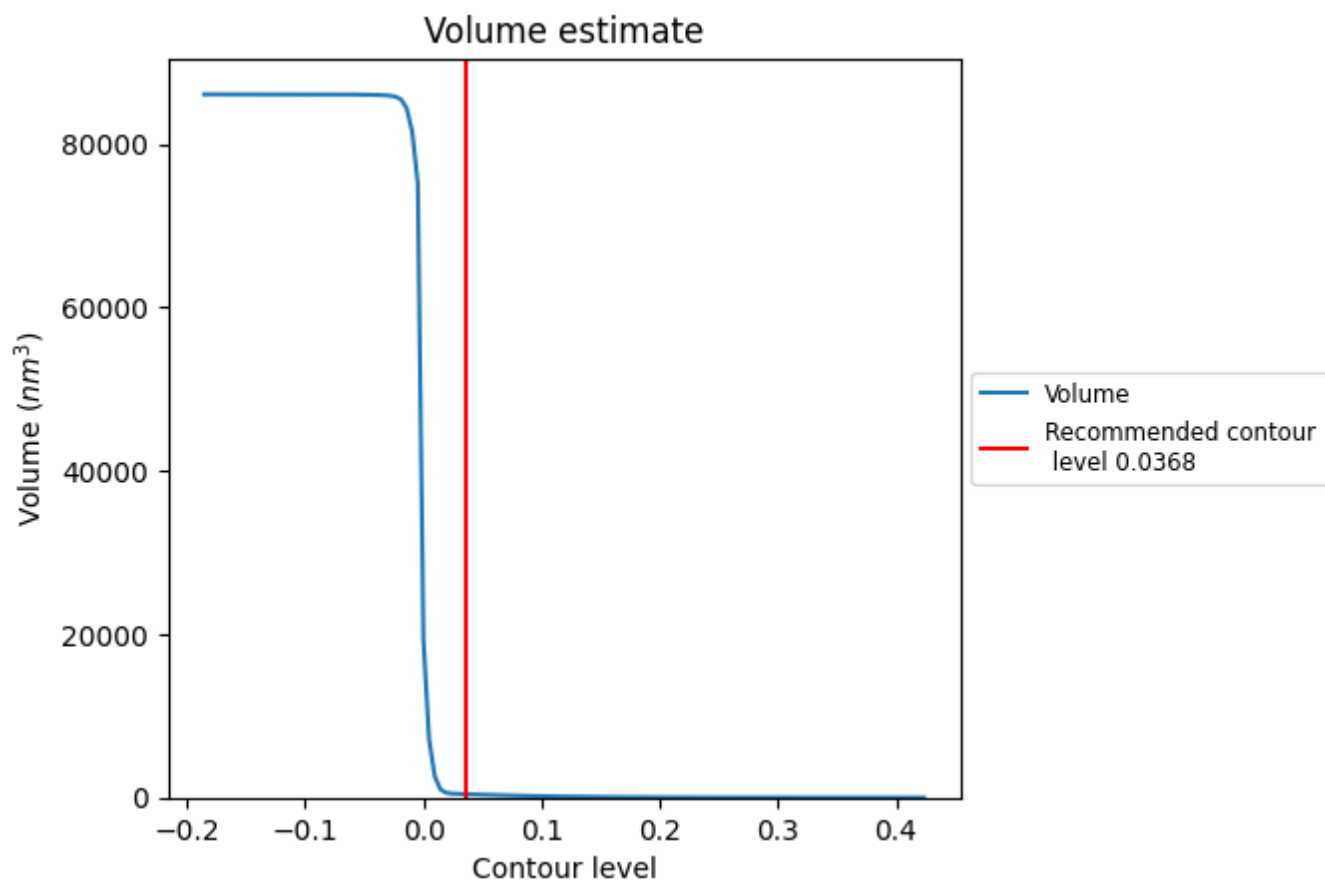
This section contains the results of statistical analysis of the map.

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.

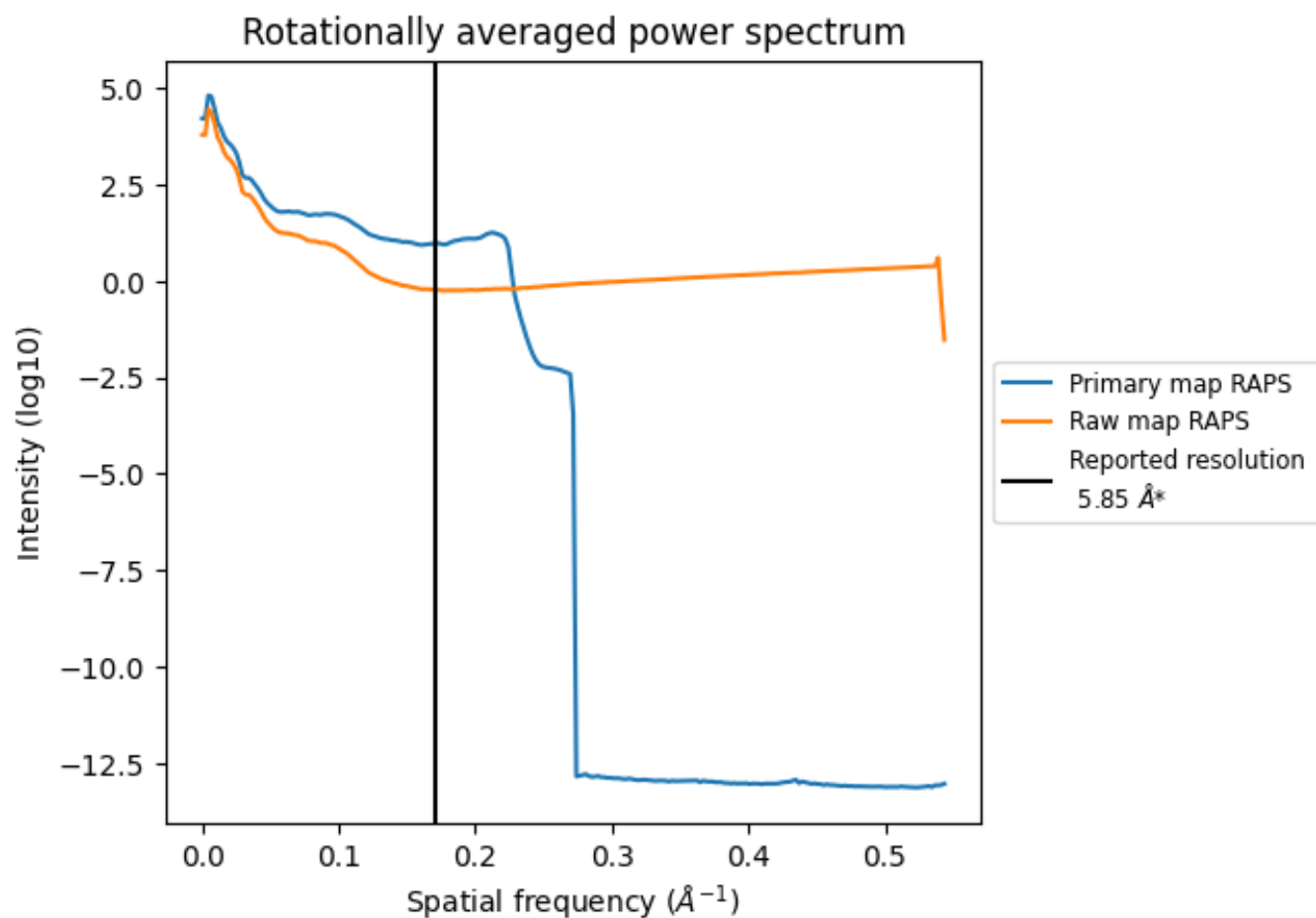
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 411 nm^3 ; this corresponds to an approximate mass of 371 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 ⓘ

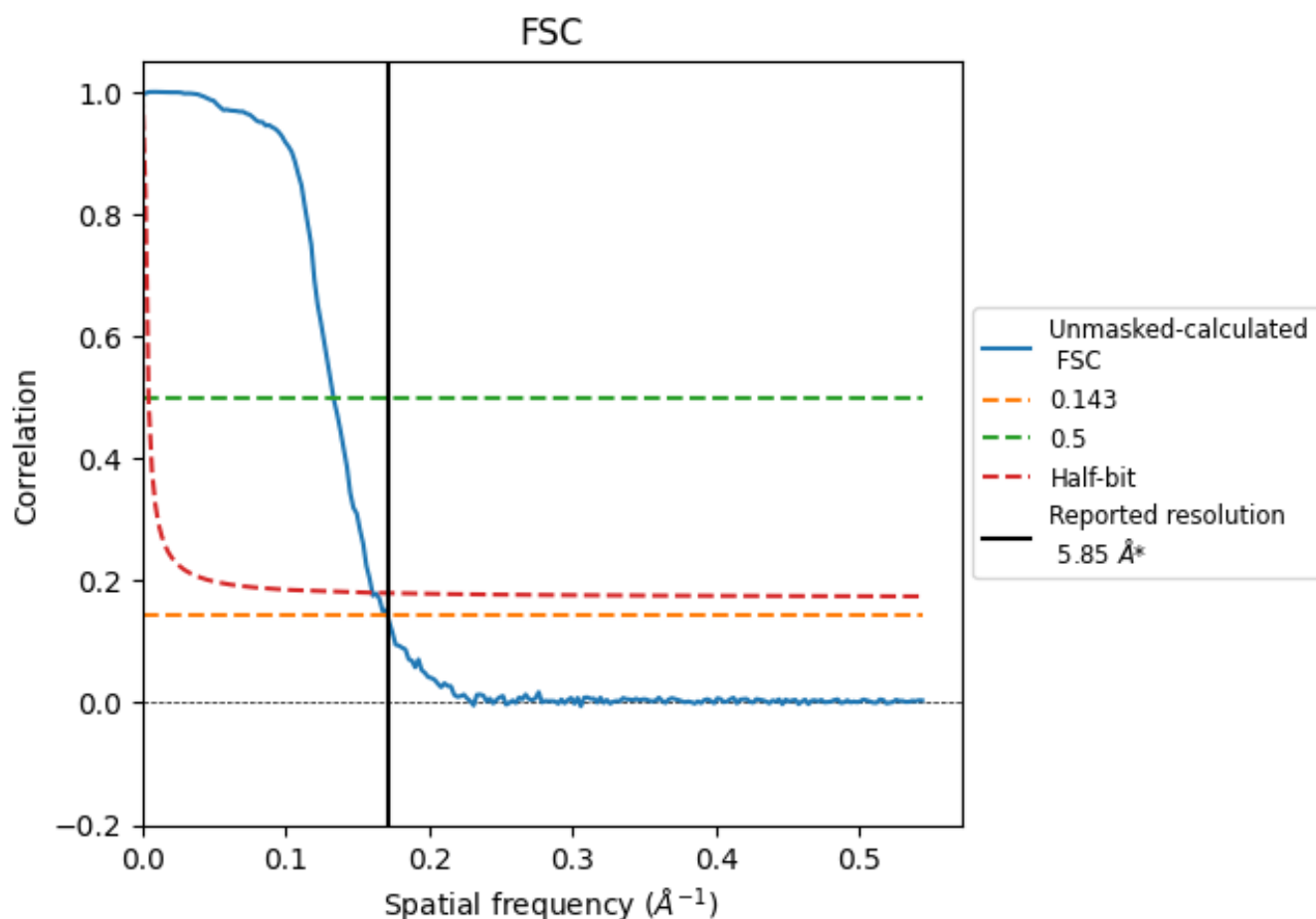


*Reported resolution corresponds to spatial frequency of 0.171 Å⁻¹

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 0.171 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

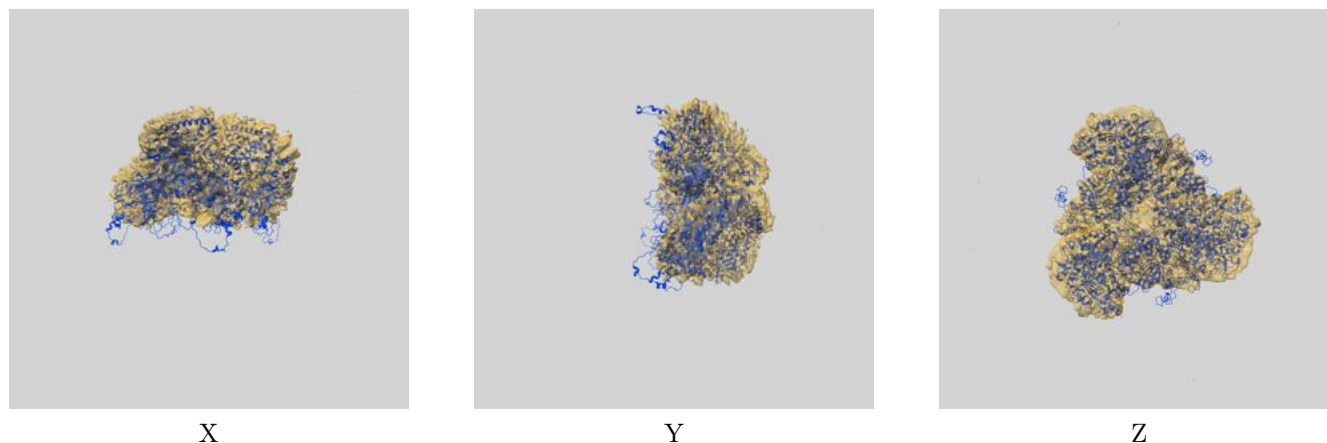
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.85	7.50	6.23

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

9 Map-model fit [i](#)

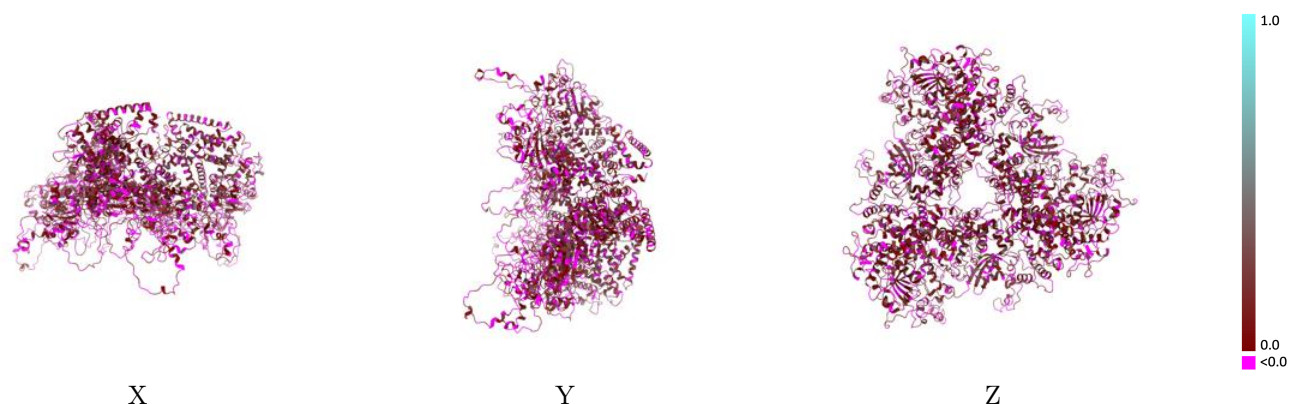
This section contains information regarding the fit between EMDB map EMD-53144 and PDB model 9SSC. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



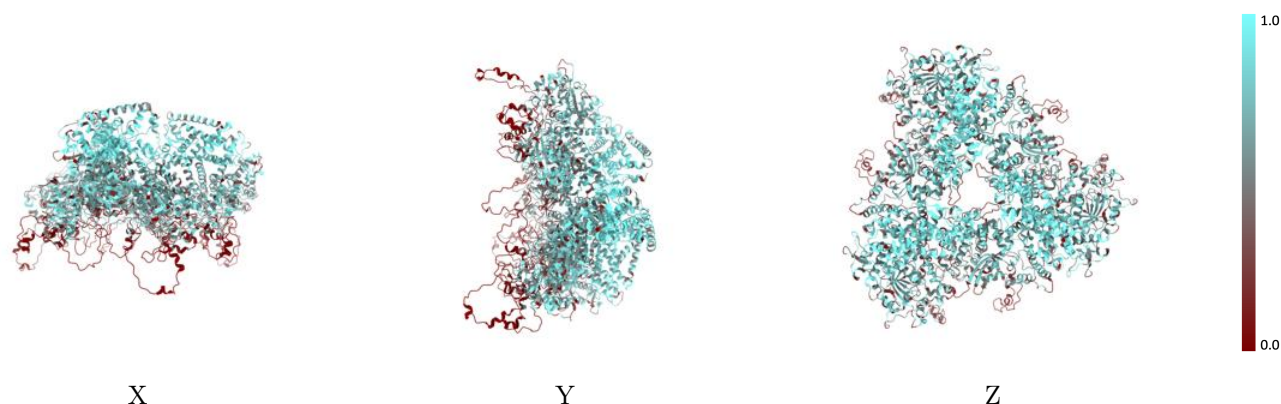
The images above show the 3D surface view of the map at the recommended contour level 0.0368 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



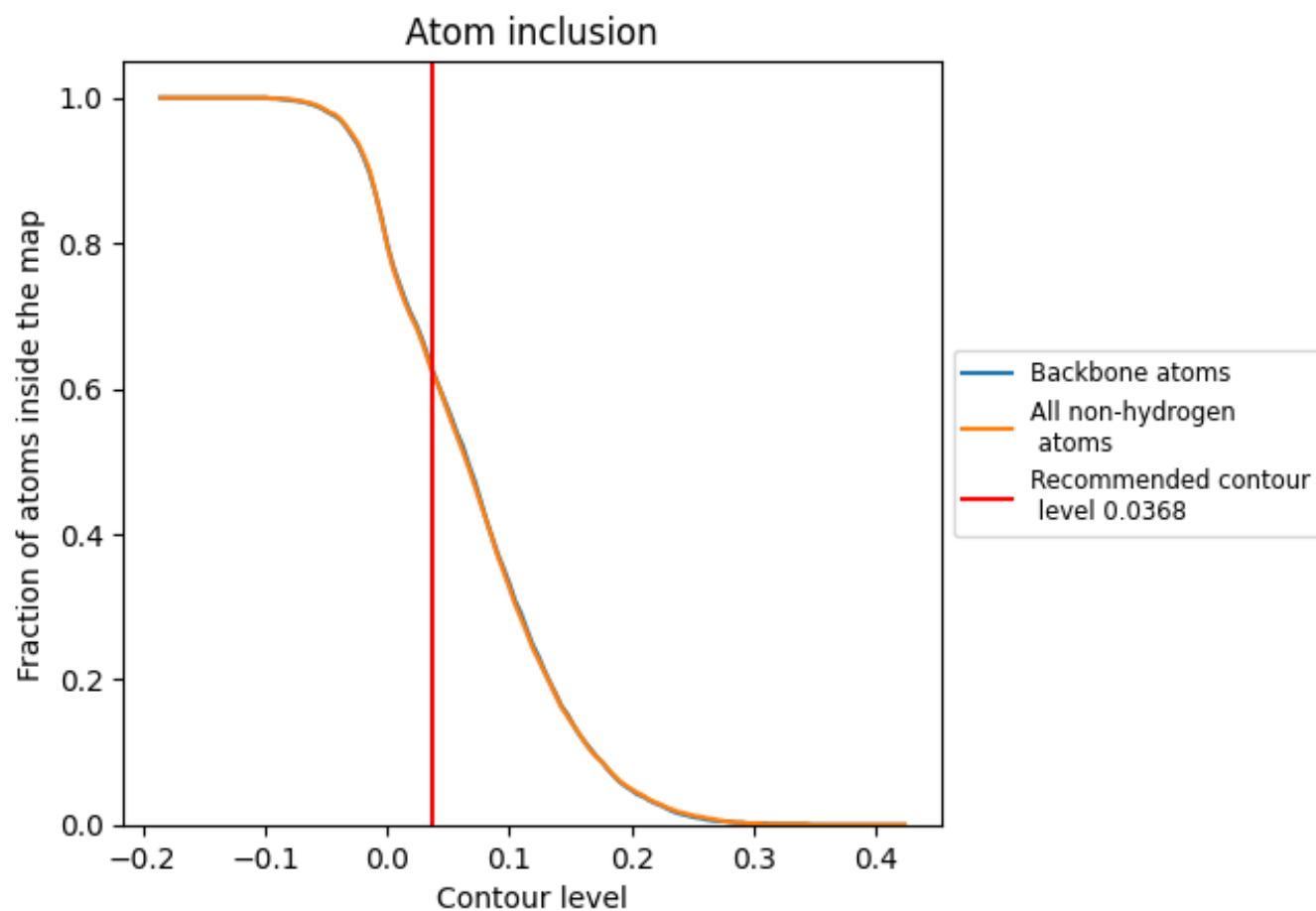
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0368).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 62% 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 (0.0368) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6230	0.0780
A	0.6200	0.0790
B	0.6200	0.0790
C	0.6200	0.0780

