



Full wwPDB EM Validation Report ⓘ

Oct 15, 2025 – 01:35 am BST

PDB ID : 9QX1 / pdb_00009qx1
EMDB ID : EMD-53433
Title : Cryo-EM structure of the C. elegans UBR4/KCMF1 complex (C-term dimer interface focused refinement)
Authors : Grabarczyk, D.B.; Clausen, T.
Deposited on : 2025-04-15
Resolution : 2.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

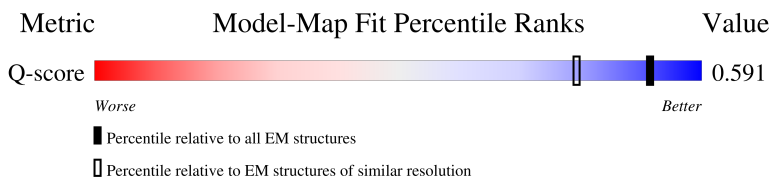
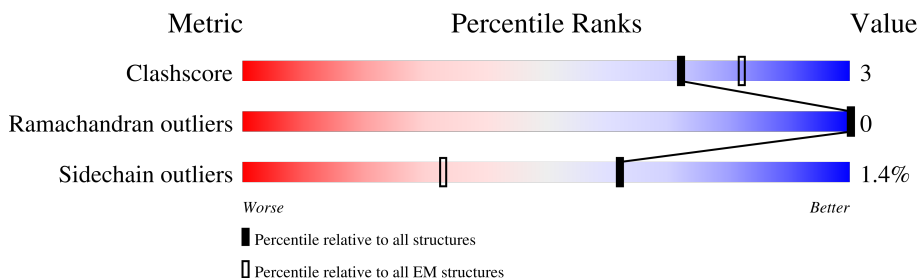
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	8728 (2.10 - 3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4284	
1	B	4284	
2	C	562	
2	D	562	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14940 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 UBR-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	753	Total	C	N	O	S	0	0
			5946	3761	1023	1117	45		
1	B	753	Total	C	N	O	S	0	0
			5946	3761	1023	1117	45		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4212	GLY	-	expression tag	UNP A0A0S4XR36
A	4213	SER	-	expression tag	UNP A0A0S4XR36
A	4214	LEU	-	expression tag	UNP A0A0S4XR36
A	4215	GLU	-	expression tag	UNP A0A0S4XR36
A	4216	VAL	-	expression tag	UNP A0A0S4XR36
A	4217	LEU	-	expression tag	UNP A0A0S4XR36
A	4218	PHE	-	expression tag	UNP A0A0S4XR36
A	4219	GLN	-	expression tag	UNP A0A0S4XR36
A	4220	GLY	-	expression tag	UNP A0A0S4XR36
A	4221	PRO	-	expression tag	UNP A0A0S4XR36
A	4222	ALA	-	expression tag	UNP A0A0S4XR36
A	4223	GLU	-	expression tag	UNP A0A0S4XR36
A	4224	ALA	-	expression tag	UNP A0A0S4XR36
A	4225	ALA	-	expression tag	UNP A0A0S4XR36
A	4226	ALA	-	expression tag	UNP A0A0S4XR36
A	4227	LYS	-	expression tag	UNP A0A0S4XR36
A	4228	GLU	-	expression tag	UNP A0A0S4XR36
A	4229	ALA	-	expression tag	UNP A0A0S4XR36
A	4230	ALA	-	expression tag	UNP A0A0S4XR36
A	4231	ALA	-	expression tag	UNP A0A0S4XR36
A	4232	LYS	-	expression tag	UNP A0A0S4XR36
A	4233	GLU	-	expression tag	UNP A0A0S4XR36
A	4234	ALA	-	expression tag	UNP A0A0S4XR36
A	4235	ALA	-	expression tag	UNP A0A0S4XR36
A	4236	ALA	-	expression tag	UNP A0A0S4XR36
A	4237	LYS	-	expression tag	UNP A0A0S4XR36

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4238	GLU	-	expression tag	UNP A0A0S4XR36
A	4239	ALA	-	expression tag	UNP A0A0S4XR36
A	4240	ALA	-	expression tag	UNP A0A0S4XR36
A	4241	ALA	-	expression tag	UNP A0A0S4XR36
A	4242	LYS	-	expression tag	UNP A0A0S4XR36
A	4243	ALA	-	expression tag	UNP A0A0S4XR36
A	4244	LEU	-	expression tag	UNP A0A0S4XR36
A	4245	GLU	-	expression tag	UNP A0A0S4XR36
A	4246	ALA	-	expression tag	UNP A0A0S4XR36
A	4247	GLU	-	expression tag	UNP A0A0S4XR36
A	4248	ALA	-	expression tag	UNP A0A0S4XR36
A	4249	ALA	-	expression tag	UNP A0A0S4XR36
A	4250	ALA	-	expression tag	UNP A0A0S4XR36
A	4251	LYS	-	expression tag	UNP A0A0S4XR36
A	4252	GLU	-	expression tag	UNP A0A0S4XR36
A	4253	ALA	-	expression tag	UNP A0A0S4XR36
A	4254	ALA	-	expression tag	UNP A0A0S4XR36
A	4255	ALA	-	expression tag	UNP A0A0S4XR36
A	4256	LYS	-	expression tag	UNP A0A0S4XR36
A	4257	GLU	-	expression tag	UNP A0A0S4XR36
A	4258	ALA	-	expression tag	UNP A0A0S4XR36
A	4259	ALA	-	expression tag	UNP A0A0S4XR36
A	4260	ALA	-	expression tag	UNP A0A0S4XR36
A	4261	LYS	-	expression tag	UNP A0A0S4XR36
A	4262	GLU	-	expression tag	UNP A0A0S4XR36
A	4263	ALA	-	expression tag	UNP A0A0S4XR36
A	4264	ALA	-	expression tag	UNP A0A0S4XR36
A	4265	ALA	-	expression tag	UNP A0A0S4XR36
A	4266	LYS	-	expression tag	UNP A0A0S4XR36
A	4267	ALA	-	expression tag	UNP A0A0S4XR36
A	4268	HIS	-	expression tag	UNP A0A0S4XR36
A	4269	HIS	-	expression tag	UNP A0A0S4XR36
A	4270	HIS	-	expression tag	UNP A0A0S4XR36
A	4271	HIS	-	expression tag	UNP A0A0S4XR36
A	4272	HIS	-	expression tag	UNP A0A0S4XR36
A	4273	HIS	-	expression tag	UNP A0A0S4XR36
A	4274	HIS	-	expression tag	UNP A0A0S4XR36
A	4275	HIS	-	expression tag	UNP A0A0S4XR36
A	4276	HIS	-	expression tag	UNP A0A0S4XR36
A	4277	HIS	-	expression tag	UNP A0A0S4XR36
B	4212	GLY	-	expression tag	UNP A0A0S4XR36
B	4213	SER	-	expression tag	UNP A0A0S4XR36

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4214	LEU	-	expression tag	UNP A0A0S4XR36
B	4215	GLU	-	expression tag	UNP A0A0S4XR36
B	4216	VAL	-	expression tag	UNP A0A0S4XR36
B	4217	LEU	-	expression tag	UNP A0A0S4XR36
B	4218	PHE	-	expression tag	UNP A0A0S4XR36
B	4219	GLN	-	expression tag	UNP A0A0S4XR36
B	4220	GLY	-	expression tag	UNP A0A0S4XR36
B	4221	PRO	-	expression tag	UNP A0A0S4XR36
B	4222	ALA	-	expression tag	UNP A0A0S4XR36
B	4223	GLU	-	expression tag	UNP A0A0S4XR36
B	4224	ALA	-	expression tag	UNP A0A0S4XR36
B	4225	ALA	-	expression tag	UNP A0A0S4XR36
B	4226	ALA	-	expression tag	UNP A0A0S4XR36
B	4227	LYS	-	expression tag	UNP A0A0S4XR36
B	4228	GLU	-	expression tag	UNP A0A0S4XR36
B	4229	ALA	-	expression tag	UNP A0A0S4XR36
B	4230	ALA	-	expression tag	UNP A0A0S4XR36
B	4231	ALA	-	expression tag	UNP A0A0S4XR36
B	4232	LYS	-	expression tag	UNP A0A0S4XR36
B	4233	GLU	-	expression tag	UNP A0A0S4XR36
B	4234	ALA	-	expression tag	UNP A0A0S4XR36
B	4235	ALA	-	expression tag	UNP A0A0S4XR36
B	4236	ALA	-	expression tag	UNP A0A0S4XR36
B	4237	LYS	-	expression tag	UNP A0A0S4XR36
B	4238	GLU	-	expression tag	UNP A0A0S4XR36
B	4239	ALA	-	expression tag	UNP A0A0S4XR36
B	4240	ALA	-	expression tag	UNP A0A0S4XR36
B	4241	ALA	-	expression tag	UNP A0A0S4XR36
B	4242	LYS	-	expression tag	UNP A0A0S4XR36
B	4243	ALA	-	expression tag	UNP A0A0S4XR36
B	4244	LEU	-	expression tag	UNP A0A0S4XR36
B	4245	GLU	-	expression tag	UNP A0A0S4XR36
B	4246	ALA	-	expression tag	UNP A0A0S4XR36
B	4247	GLU	-	expression tag	UNP A0A0S4XR36
B	4248	ALA	-	expression tag	UNP A0A0S4XR36
B	4249	ALA	-	expression tag	UNP A0A0S4XR36
B	4250	ALA	-	expression tag	UNP A0A0S4XR36
B	4251	LYS	-	expression tag	UNP A0A0S4XR36
B	4252	GLU	-	expression tag	UNP A0A0S4XR36
B	4253	ALA	-	expression tag	UNP A0A0S4XR36
B	4254	ALA	-	expression tag	UNP A0A0S4XR36
B	4255	ALA	-	expression tag	UNP A0A0S4XR36

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4256	LYS	-	expression tag	UNP A0A0S4XR36
B	4257	GLU	-	expression tag	UNP A0A0S4XR36
B	4258	ALA	-	expression tag	UNP A0A0S4XR36
B	4259	ALA	-	expression tag	UNP A0A0S4XR36
B	4260	ALA	-	expression tag	UNP A0A0S4XR36
B	4261	LYS	-	expression tag	UNP A0A0S4XR36
B	4262	GLU	-	expression tag	UNP A0A0S4XR36
B	4263	ALA	-	expression tag	UNP A0A0S4XR36
B	4264	ALA	-	expression tag	UNP A0A0S4XR36
B	4265	ALA	-	expression tag	UNP A0A0S4XR36
B	4266	LYS	-	expression tag	UNP A0A0S4XR36
B	4267	ALA	-	expression tag	UNP A0A0S4XR36
B	4268	HIS	-	expression tag	UNP A0A0S4XR36
B	4269	HIS	-	expression tag	UNP A0A0S4XR36
B	4270	HIS	-	expression tag	UNP A0A0S4XR36
B	4271	HIS	-	expression tag	UNP A0A0S4XR36
B	4272	HIS	-	expression tag	UNP A0A0S4XR36
B	4273	HIS	-	expression tag	UNP A0A0S4XR36
B	4274	HIS	-	expression tag	UNP A0A0S4XR36
B	4275	HIS	-	expression tag	UNP A0A0S4XR36
B	4276	HIS	-	expression tag	UNP A0A0S4XR36
B	4277	HIS	-	expression tag	UNP A0A0S4XR36

- Molecule 2 is a protein called KCMF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	197	Total	C	N	O	S	0	0
			1523	962	256	298	7		
2	D	197	Total	C	N	O	S	0	0
			1523	962	256	298	7		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP P34664
C	?	-	ALA	deletion	UNP P34664
C	?	-	GLU	deletion	UNP P34664
C	?	-	MET	deletion	UNP P34664
C	?	-	ALA	deletion	UNP P34664
C	?	-	ALA	deletion	UNP P34664
C	?	-	LEU	deletion	UNP P34664
C	?	-	LEU	deletion	UNP P34664

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P34664
C	?	-	ASN	deletion	UNP P34664
C	?	-	MET	deletion	UNP P34664
C	?	-	GLY	deletion	UNP P34664
C	?	-	PRO	deletion	UNP P34664
C	?	-	ASP	deletion	UNP P34664
C	?	-	SER	deletion	UNP P34664
C	?	-	VAL	deletion	UNP P34664
C	?	-	GLU	deletion	UNP P34664
C	?	-	ASP	deletion	UNP P34664
C	?	-	ILE	deletion	UNP P34664
C	?	-	ARG	deletion	UNP P34664
C	?	-	ARG	deletion	UNP P34664
C	?	-	PHE	deletion	UNP P34664
C	?	-	THR	deletion	UNP P34664
C	576	SER	-	expression tag	UNP P34664
C	577	ALA	-	expression tag	UNP P34664
C	578	TRP	-	expression tag	UNP P34664
C	579	SER	-	expression tag	UNP P34664
C	580	HIS	-	expression tag	UNP P34664
C	581	PRO	-	expression tag	UNP P34664
C	582	GLN	-	expression tag	UNP P34664
C	583	PHE	-	expression tag	UNP P34664
C	584	GLU	-	expression tag	UNP P34664
C	585	LYS	-	expression tag	UNP P34664
D	?	-	GLY	deletion	UNP P34664
D	?	-	ALA	deletion	UNP P34664
D	?	-	GLU	deletion	UNP P34664
D	?	-	MET	deletion	UNP P34664
D	?	-	ALA	deletion	UNP P34664
D	?	-	ALA	deletion	UNP P34664
D	?	-	LEU	deletion	UNP P34664
D	?	-	LEU	deletion	UNP P34664
D	?	-	ARG	deletion	UNP P34664
D	?	-	ASN	deletion	UNP P34664
D	?	-	MET	deletion	UNP P34664
D	?	-	GLY	deletion	UNP P34664
D	?	-	PRO	deletion	UNP P34664
D	?	-	ASP	deletion	UNP P34664
D	?	-	SER	deletion	UNP P34664
D	?	-	VAL	deletion	UNP P34664
D	?	-	GLU	deletion	UNP P34664

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASP	deletion	UNP P34664
D	?	-	ILE	deletion	UNP P34664
D	?	-	ARG	deletion	UNP P34664
D	?	-	ARG	deletion	UNP P34664
D	?	-	PHE	deletion	UNP P34664
D	?	-	THR	deletion	UNP P34664
D	576	SER	-	expression tag	UNP P34664
D	577	ALA	-	expression tag	UNP P34664
D	578	TRP	-	expression tag	UNP P34664
D	579	SER	-	expression tag	UNP P34664
D	580	HIS	-	expression tag	UNP P34664
D	581	PRO	-	expression tag	UNP P34664
D	582	GLN	-	expression tag	UNP P34664
D	583	PHE	-	expression tag	UNP P34664
D	584	GLU	-	expression tag	UNP P34664
D	585	LYS	-	expression tag	UNP P34664

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0
3	B	1	Total 1	Zn 1	0









Chain C:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	86845	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.032	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	486.912, 486.912, 486.912	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.268, 1.268, 1.268	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/6039	0.30	0/8174
1	B	0.13	0/6039	0.28	0/8174
2	C	0.12	0/1553	0.26	0/2111
2	D	0.12	0/1553	0.29	0/2111
All	All	0.13	0/15184	0.29	0/20570

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	A	5946	0	6001	37	0
1	B	5946	0	6001	32	0
2	C	1523	0	1496	18	0
2	D	1523	0	1496	20	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	14940	0	14994	95	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 3.

All (95) 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)
2:D:412:LYS:H	2:D:412:LYS:HD2	1.51	0.75
2:C:269:VAL:HB	2:C:397:THR:HG22	1.73	0.69
1:A:3063:GLU:HG2	1:A:3093:VAL:HG22	1.76	0.69
2:D:269:VAL:HB	2:D:397:THR:HG22	1.75	0.68
2:D:273:LEU:HB2	2:D:392:PRO:HG2	1.75	0.68
2:D:492:MET:HE3	2:D:493:PRO:HD2	1.76	0.66
2:C:273:LEU:HB2	2:C:392:PRO:HG2	1.77	0.65
1:B:3063:GLU:HG2	1:B:3093:VAL:HG22	1.80	0.63
1:B:3118:MET:SD	1:B:3190:PRO:HB2	2.41	0.61
1:B:2966:SER:O	1:B:2970:GLN:HG2	2.00	0.61
1:A:2966:SER:O	1:A:2970:GLN:HG2	2.01	0.60
2:C:326:GLU:HA	2:C:329:LYS:HD2	1.82	0.60
1:A:3118:MET:SD	1:A:3190:PRO:HB2	2.41	0.59
2:D:508:PRO:HG2	2:D:510:PHE:HE2	1.68	0.58
1:B:2485:LEU:HD13	1:B:2524:GLN:HB2	1.84	0.58
2:C:278:ILE:HG13	2:C:389:GLY:HA2	1.86	0.57
1:A:3245:CYS:O	1:A:3249:MET:HG3	2.04	0.57
1:A:2451:LYS:HA	1:A:2498:MET:HE1	1.86	0.57
2:D:278:ILE:HG13	2:D:389:GLY:HA2	1.86	0.57
1:B:3245:CYS:O	1:B:3249:MET:HG3	2.06	0.56
1:A:2943:GLU:HG2	2:D:265:ASN:HD22	1.71	0.55
2:D:335:ILE:HD12	2:D:339:ASP:HB3	1.88	0.55
2:C:418:ARG:H	2:C:420:MET:HE3	1.73	0.54
2:C:492:MET:HE3	2:C:493:PRO:HD2	1.89	0.53
1:A:3251:SER:O	1:A:3255:ILE:HG12	2.08	0.53
1:A:3337:HIS:ND1	2:C:480:MET:HE1	2.24	0.53
1:A:2484:VAL:O	1:A:2488:ILE:HG22	2.09	0.52
1:B:2542:LEU:H	1:B:2542:LEU:HD12	1.74	0.52
1:A:2662:MET:HE2	1:A:2676:ILE:O	2.10	0.52
1:A:3000:ASN:HD21	2:D:489:LEU:HD22	1.74	0.52
2:C:267:GLN:HG2	1:B:2942:ILE:HG23	1.92	0.51
2:C:489:LEU:HD22	1:B:3000:ASN:HD21	1.76	0.51
1:A:2485:LEU:HD13	1:A:2524:GLN:HB2	1.93	0.51
2:D:465:LYS:O	2:D:469:GLN:HB3	2.11	0.51
1:B:3200:SER:O	1:B:3206:ARG:HD3	2.12	0.50
1:A:2466:LEU:O	1:A:2470:LYS:HG2	2.12	0.49
2:C:335:ILE:HD12	2:C:339:ASP:HB3	1.94	0.49
1:B:2662:MET:HE2	1:B:2676:ILE:O	2.10	0.49
2:C:265:ASN:HD22	1:B:2943:GLU:HG2	1.78	0.48
1:A:3200:SER:O	1:A:3206:ARG:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3071:PHE:HE1	2:C:422:ARG:NH1	2.12	0.48
2:C:465:LYS:O	2:C:469:GLN:HB3	2.14	0.48
2:D:418:ARG:H	2:D:420:MET:HE3	1.79	0.48
1:A:2874:ILE:HB	1:A:2985:TYR:CD2	2.49	0.47
1:B:2470:LYS:HA	1:B:2470:LYS:HD2	1.49	0.47
1:A:2542:LEU:HD22	1:A:2542:LEU:H	1.79	0.47
2:C:440:ALA:O	2:C:444:ILE:HG13	2.15	0.47
1:B:3268:VAL:HG21	2:D:347:MET:SD	2.55	0.46
1:B:3337:HIS:ND1	2:D:480:MET:HE1	2.30	0.46
2:D:419:LYS:H	2:D:419:LYS:HG2	1.42	0.46
1:A:2946:PRO:HB2	1:A:2947:PHE:HD2	1.80	0.46
1:A:2983:ASN:ND2	2:D:491:ASN:HB2	2.30	0.46
2:D:440:ALA:O	2:D:444:ILE:HG13	2.15	0.46
1:B:2474:GLY:H	1:B:2477:GLN:HB2	1.80	0.46
1:A:2543:SER:HB3	1:A:2588:LEU:HD21	1.98	0.46
1:B:3147:GLU:HA	1:B:3150:LYS:HD2	1.99	0.44
1:B:3193:TRP:CE2	1:B:3194:ILE:HG13	2.52	0.44
1:B:2946:PRO:HA	1:B:2947:PHE:HA	1.61	0.44
1:B:3159:ILE:HD12	1:B:3159:ILE:HA	1.87	0.43
1:A:2531:VAL:O	1:A:2535:ASP:HB2	2.18	0.43
2:C:433:ILE:HG22	2:C:434:MET:HE2	2.01	0.43
1:A:3193:TRP:CE2	1:A:3194:ILE:HG13	2.53	0.43
1:B:3123:GLU:HG2	1:B:3124:ASN:N	2.34	0.43
1:B:3278:ARG:HD2	1:B:3278:ARG:HA	1.89	0.43
1:A:2946:PRO:HA	1:A:2947:PHE:HA	1.66	0.43
1:A:2890:LEU:HD22	1:A:2974:GLN:HG2	2.01	0.43
1:B:3324:LEU:HD22	1:B:3366:ARG:HH21	1.84	0.43
1:B:3206:ARG:HD2	1:B:3244:VAL:O	2.19	0.43
2:D:495:ARG:HA	2:D:495:ARG:HD2	1.92	0.42
1:B:2599:LYS:HD3	1:B:2631:PHE:CE1	2.54	0.42
1:A:3123:GLU:HG2	1:A:3124:ASN:N	2.35	0.42
1:B:3249:MET:HE2	1:B:3305:CYS:HB2	2.01	0.42
1:B:3018:LEU:HD12	1:B:3018:LEU:HA	1.92	0.42
2:C:418:ARG:N	2:C:420:MET:HE3	2.35	0.42
1:A:3249:MET:HE2	1:A:3305:CYS:HB2	2.02	0.42
2:D:508:PRO:HG2	2:D:510:PHE:CE2	2.52	0.41
1:A:3206:ARG:HD2	1:A:3244:VAL:O	2.20	0.41
1:A:3268:VAL:HG21	2:C:347:MET:SD	2.60	0.41
1:A:3276:ILE:HD12	1:A:3276:ILE:HA	1.97	0.41
2:D:329:LYS:O	2:D:333:THR:HG23	2.19	0.41
1:A:3363:LEU:HD23	1:A:3363:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:422:ARG:H	2:C:422:ARG:HG2	1.53	0.41
1:A:2997:LYS:HD2	1:A:2998:PRO:HD2	2.01	0.41
1:B:3188:SER:O	1:B:3189:ASN:C	2.64	0.41
1:A:3278:ARG:HA	1:A:3278:ARG:HD2	1.88	0.41
1:A:2458:LEU:HD23	2:D:510:PHE:CD1	2.56	0.41
1:A:3188:SER:O	1:A:3189:ASN:C	2.63	0.41
1:A:2485:LEU:HD23	1:A:2485:LEU:HA	1.80	0.41
1:B:2543:SER:HB3	1:B:2588:LEU:HD21	2.02	0.41
1:B:3127:LEU:O	1:B:3131:MET:HG2	2.21	0.40
1:A:3049:GLY:HA3	1:A:3089:ILE:HG12	2.03	0.40
1:A:3103:ASP:O	1:A:3106:TRP:HD1	2.04	0.40
1:B:2451:LYS:HE2	1:B:2451:LYS:HB2	1.93	0.40
1:B:3103:ASP:O	1:B:3106:TRP:HD1	2.04	0.40
1:B:3152:LYS:HB2	1:B:3152:LYS:HE2	1.96	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	A	747/4284 (17%)	722 (97%)	25 (3%)	0	100	100
1	B	747/4284 (17%)	727 (97%)	20 (3%)	0	100	100
2	C	189/562 (34%)	182 (96%)	7 (4%)	0	100	100
2	D	189/562 (34%)	181 (96%)	8 (4%)	0	100	100
All	All	1872/9692 (19%)	1812 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	670/3859 (17%)	661 (99%)	9 (1%)	65	84
1	B	670/3859 (17%)	657 (98%)	13 (2%)	52	75
2	C	165/498 (33%)	164 (99%)	1 (1%)	84	94
2	D	165/498 (33%)	164 (99%)	1 (1%)	84	94
All	All	1670/8714 (19%)	1646 (99%)	24 (1%)	62	82

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2472	VAL
1	A	2560	GLU
1	A	2688	THR
1	A	2876	CYS
1	A	2945	LEU
1	A	3141	LYS
1	A	3203	MET
1	A	3336	LEU
1	A	3369	CYS
2	C	412	LYS
1	B	2470	LYS
1	B	2472	VAL
1	B	2494	ILE
1	B	2573	GLN
1	B	2688	THR
1	B	2876	CYS
1	B	2945	LEU
1	B	2974	GLN
1	B	2997	LYS
1	B	3119	ASP
1	B	3301	GLU
1	B	3336	LEU
1	B	3369	CYS
2	D	507	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2506	HIS
1	A	2587	GLN
1	A	2882	GLN
1	A	2928	ASN
1	A	2937	ASN
1	A	3000	ASN
1	A	3017	GLN
1	A	3192	GLN
1	A	3247	GLN
1	A	3297	ASN
1	B	2587	GLN
1	B	2882	GLN
1	B	2965	HIS
1	B	3017	GLN
1	B	3247	GLN
1	B	3261	ASN
1	B	3297	ASN
2	D	450	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

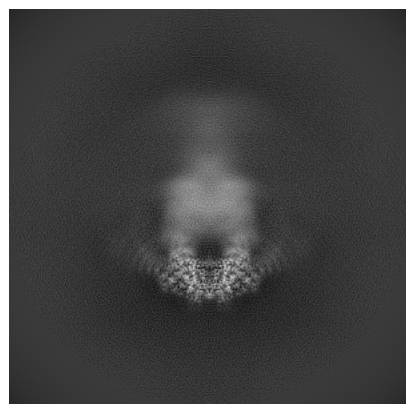
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53433. These allow visual inspection of the internal detail of the map and identification of artifacts.

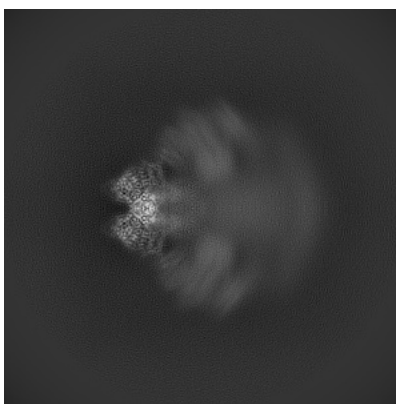
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

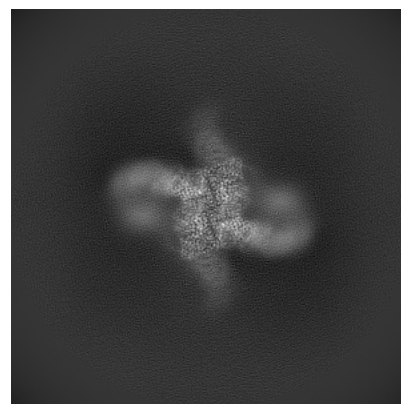
6.1.1 Primary map



X

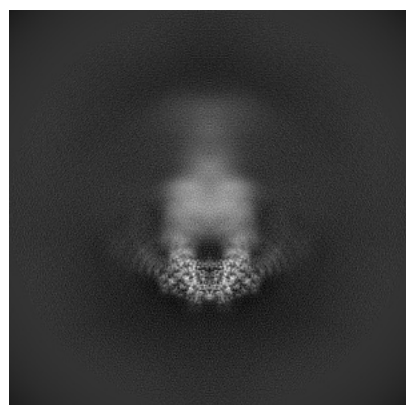


Y

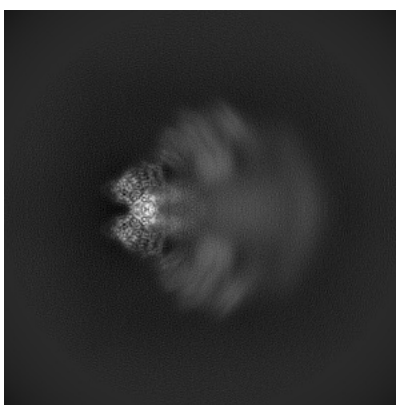


Z

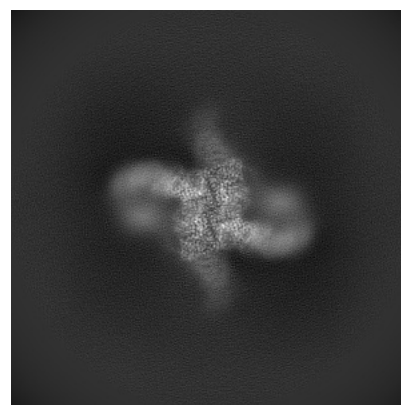
6.1.2 Raw map



X



Y

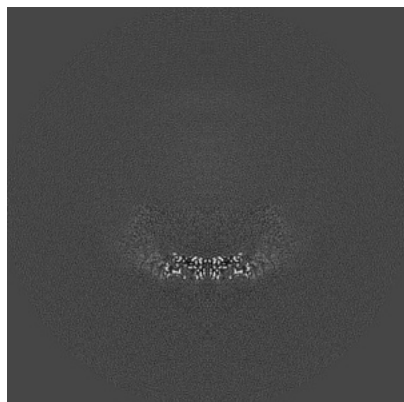


Z

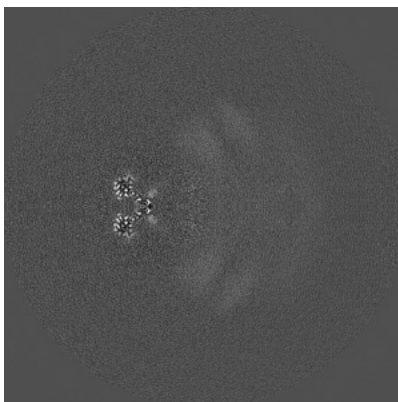
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

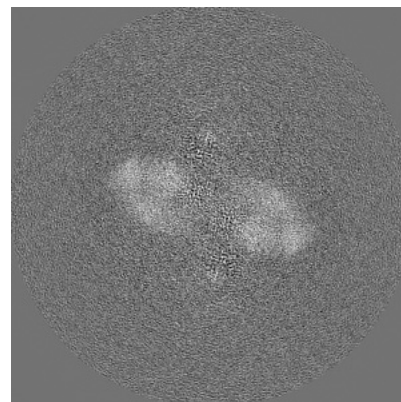
6.2.1 Primary map



X Index: 192

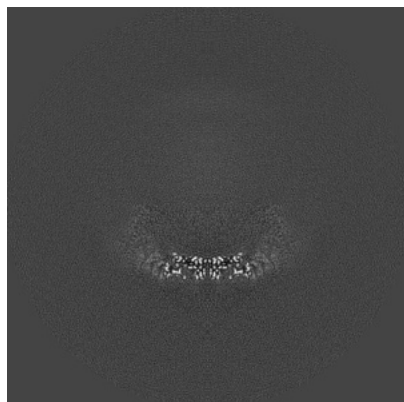


Y Index: 192

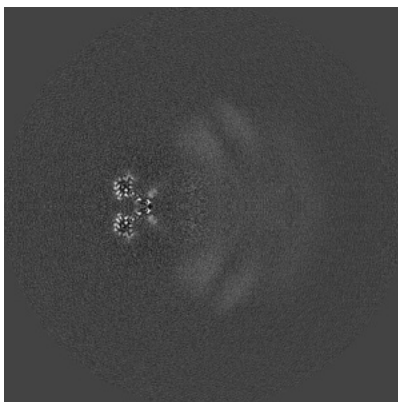


Z Index: 192

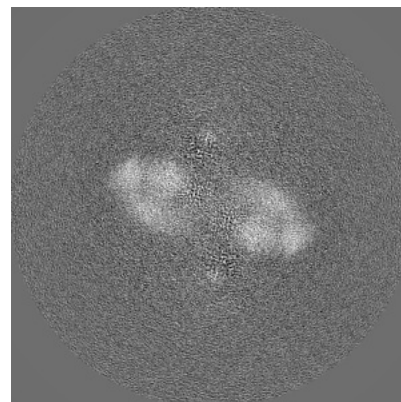
6.2.2 Raw map



X Index: 192



Y Index: 192

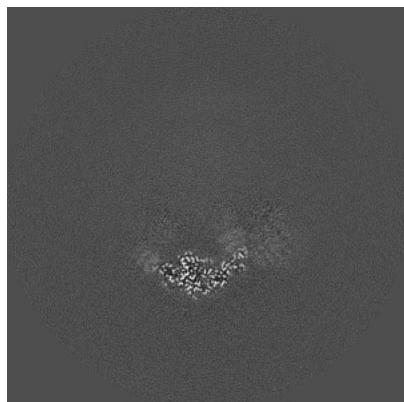


Z Index: 192

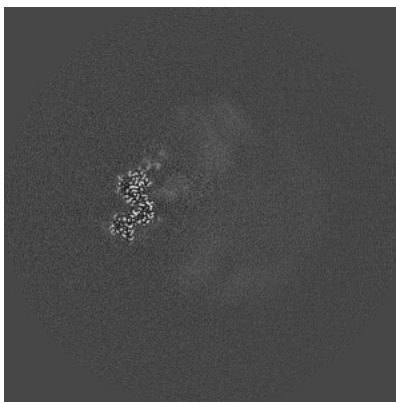
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

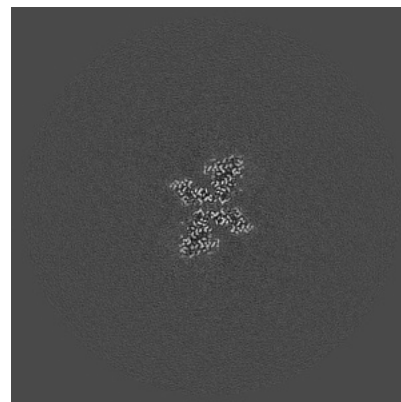
6.3.1 Primary map



X Index: 182

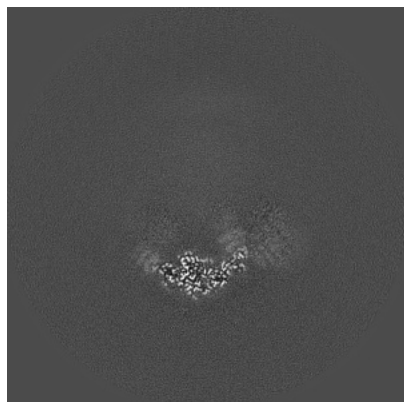


Y Index: 178

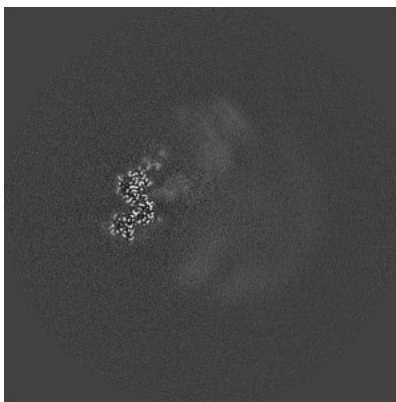


Z Index: 125

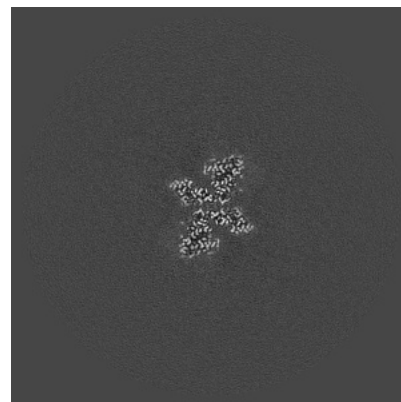
6.3.2 Raw map



X Index: 182



Y Index: 178

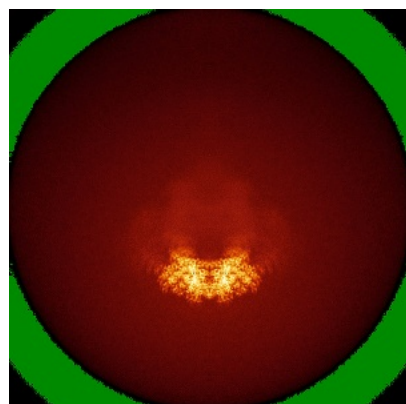


Z Index: 125

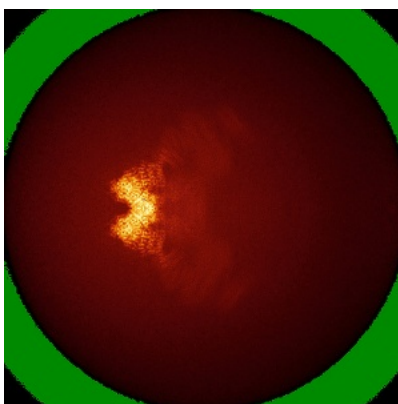
The images above show the largest variance slices of the map in three orthogonal directions.

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

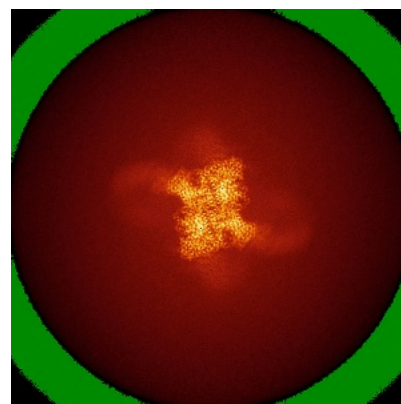
6.4.1 Primary map



X

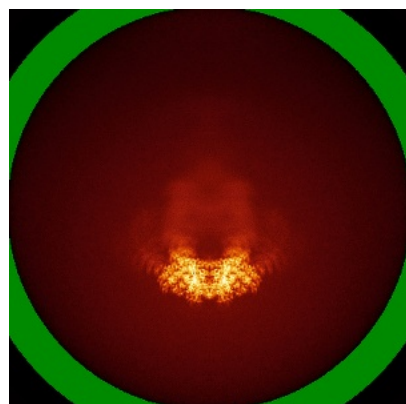


Y

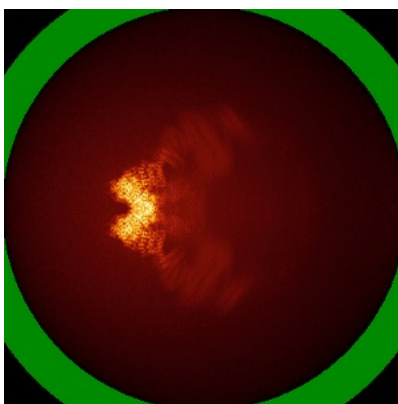


Z

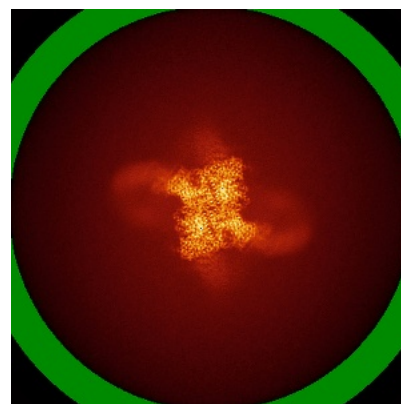
6.4.2 Raw map



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 0.009. 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.

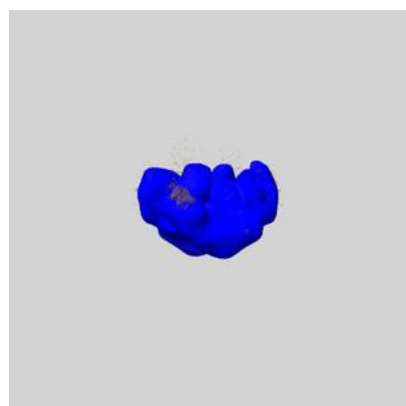
6.6 Mask visualisation [i](#)

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

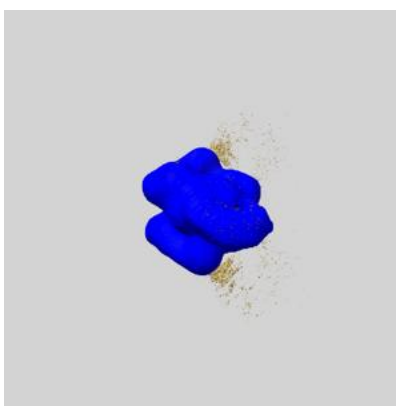
A mask typically either:

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

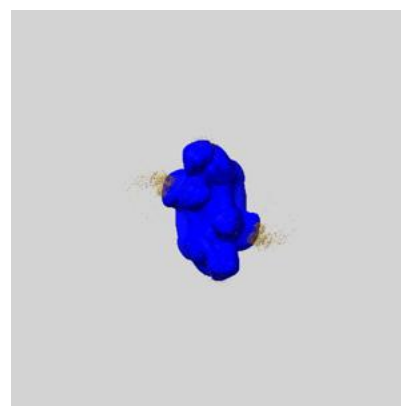
6.6.1 emd_53433_msk_1.map [i](#)



X



Y

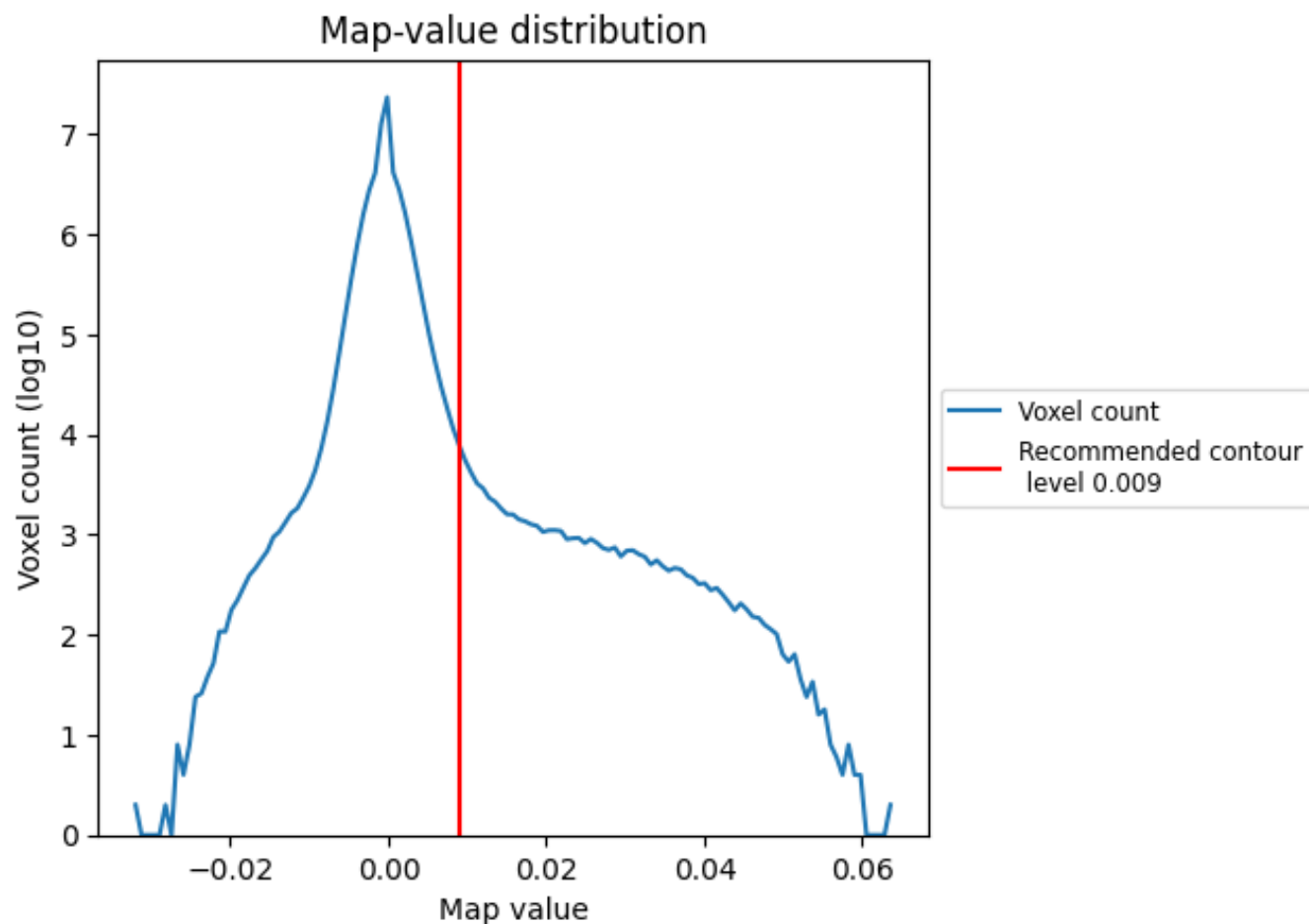


Z

7 Map analysis [i](#)

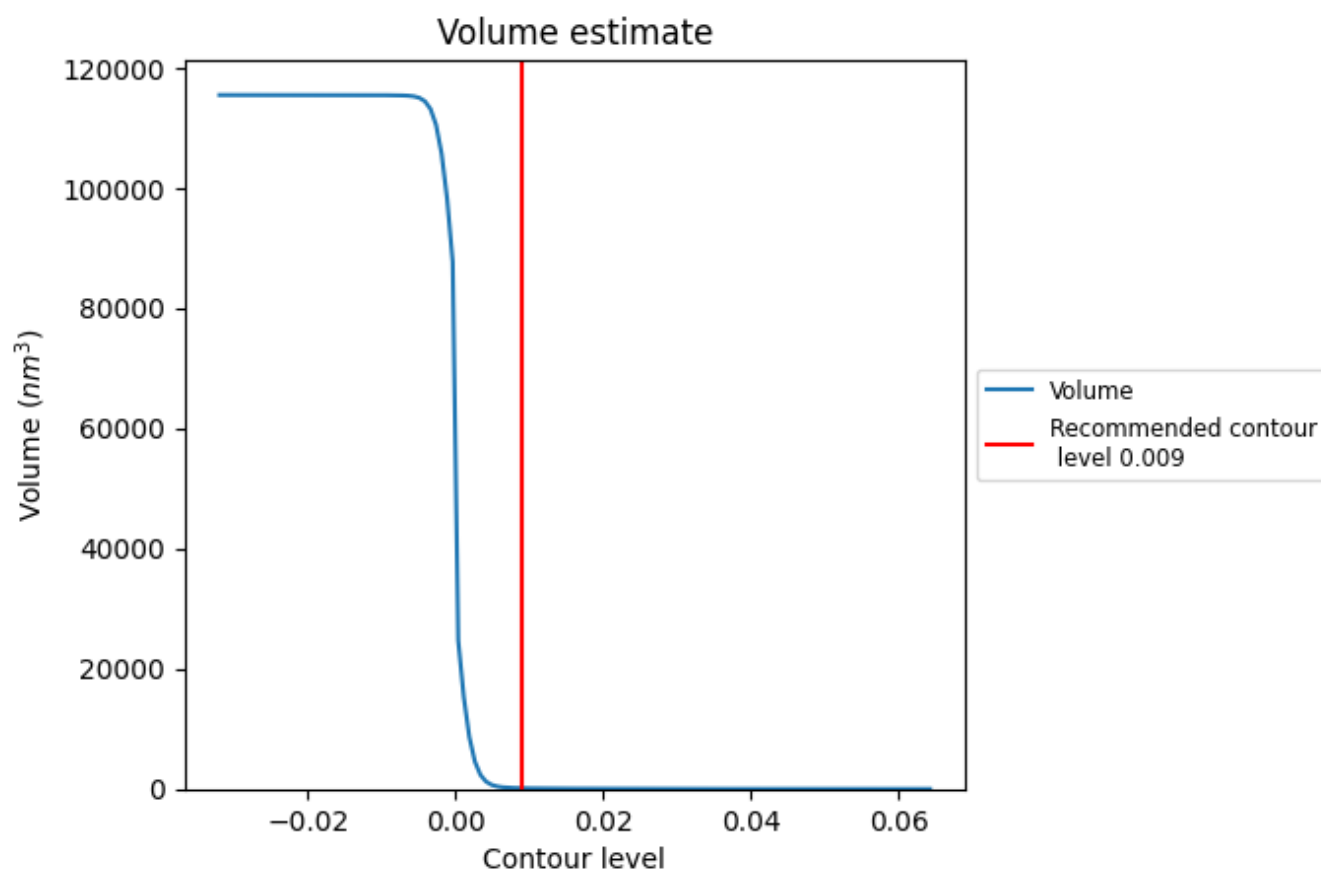
This section contains the results of statistical analysis of the map.

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.

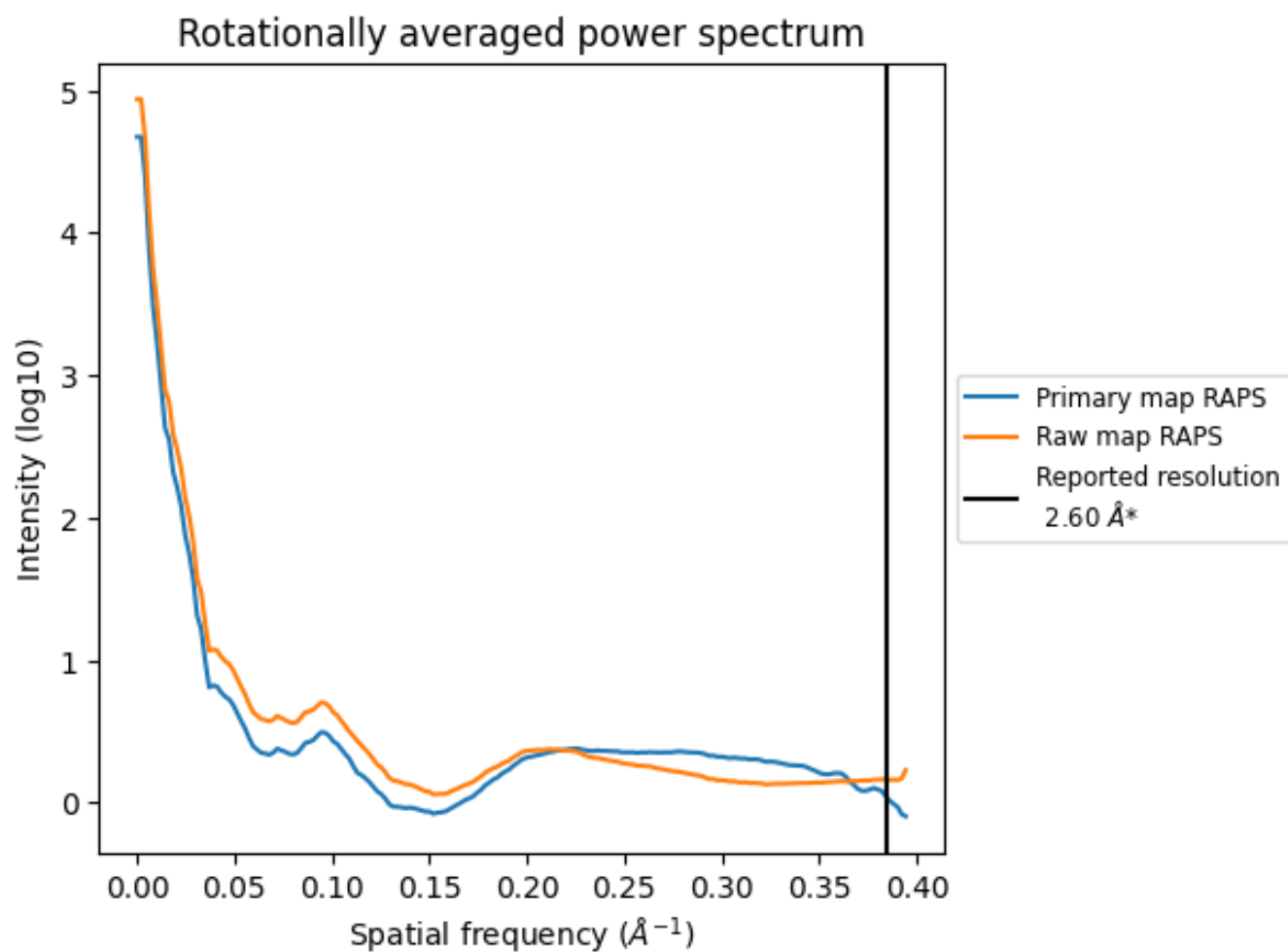
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 124 nm³; this corresponds to an approximate mass of 112 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 ⓘ

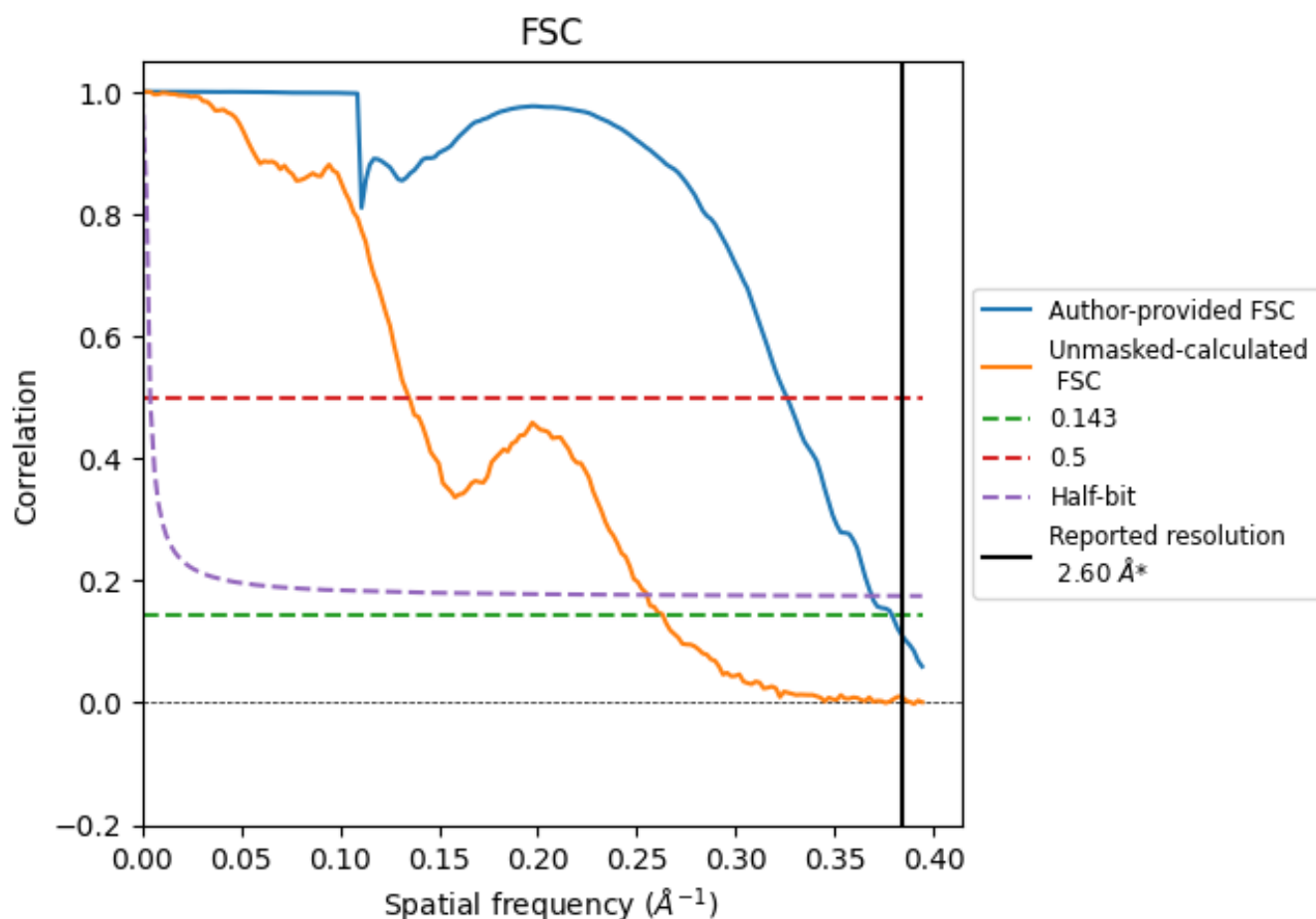


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

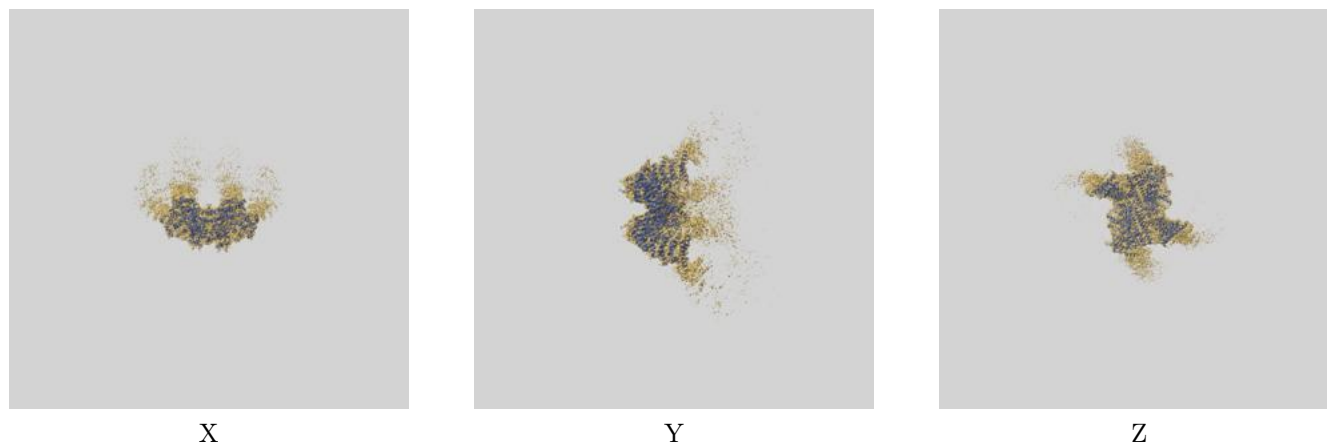
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.64	3.07	2.71
Unmasked-calculated*	3.80	7.42	3.92

*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 3.80 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

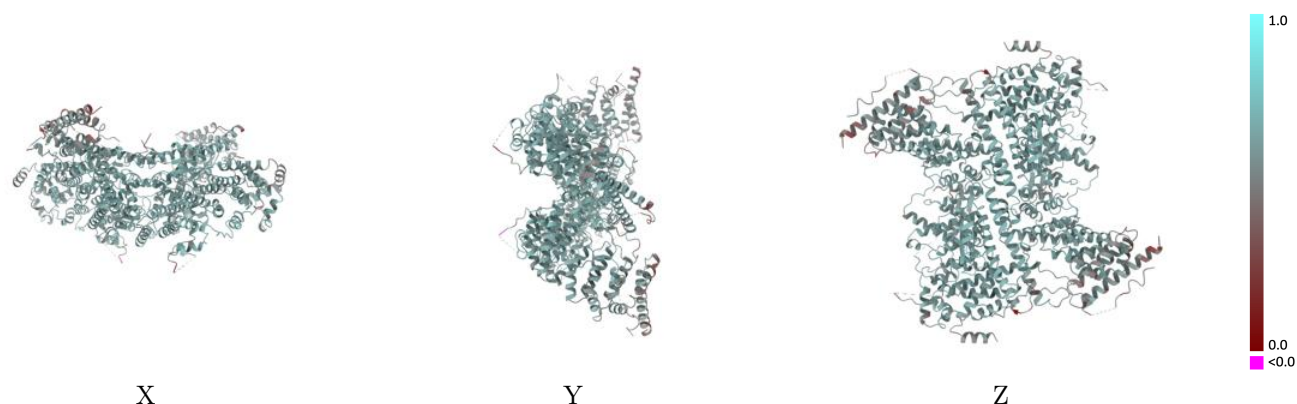
This section contains information regarding the fit between EMDB map EMD-53433 and PDB model 9QX1. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



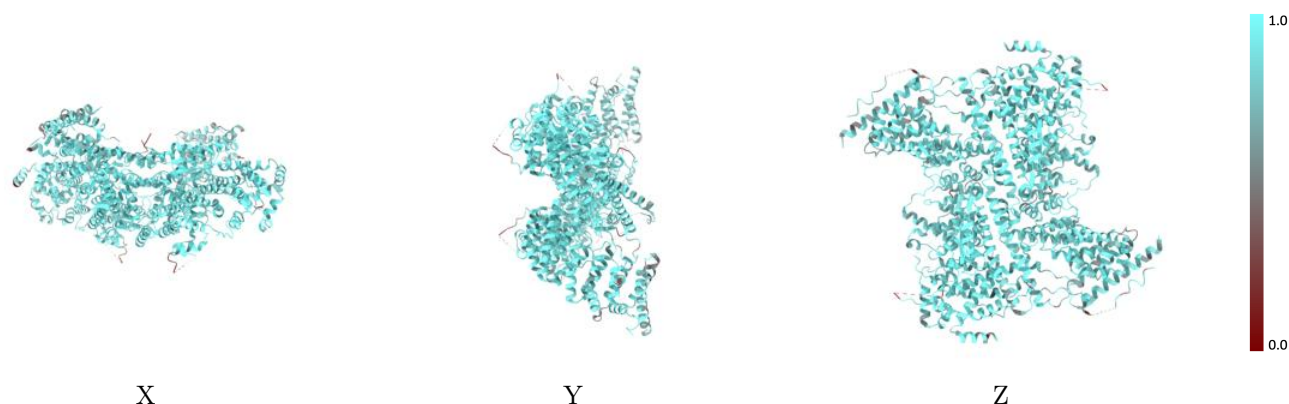
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



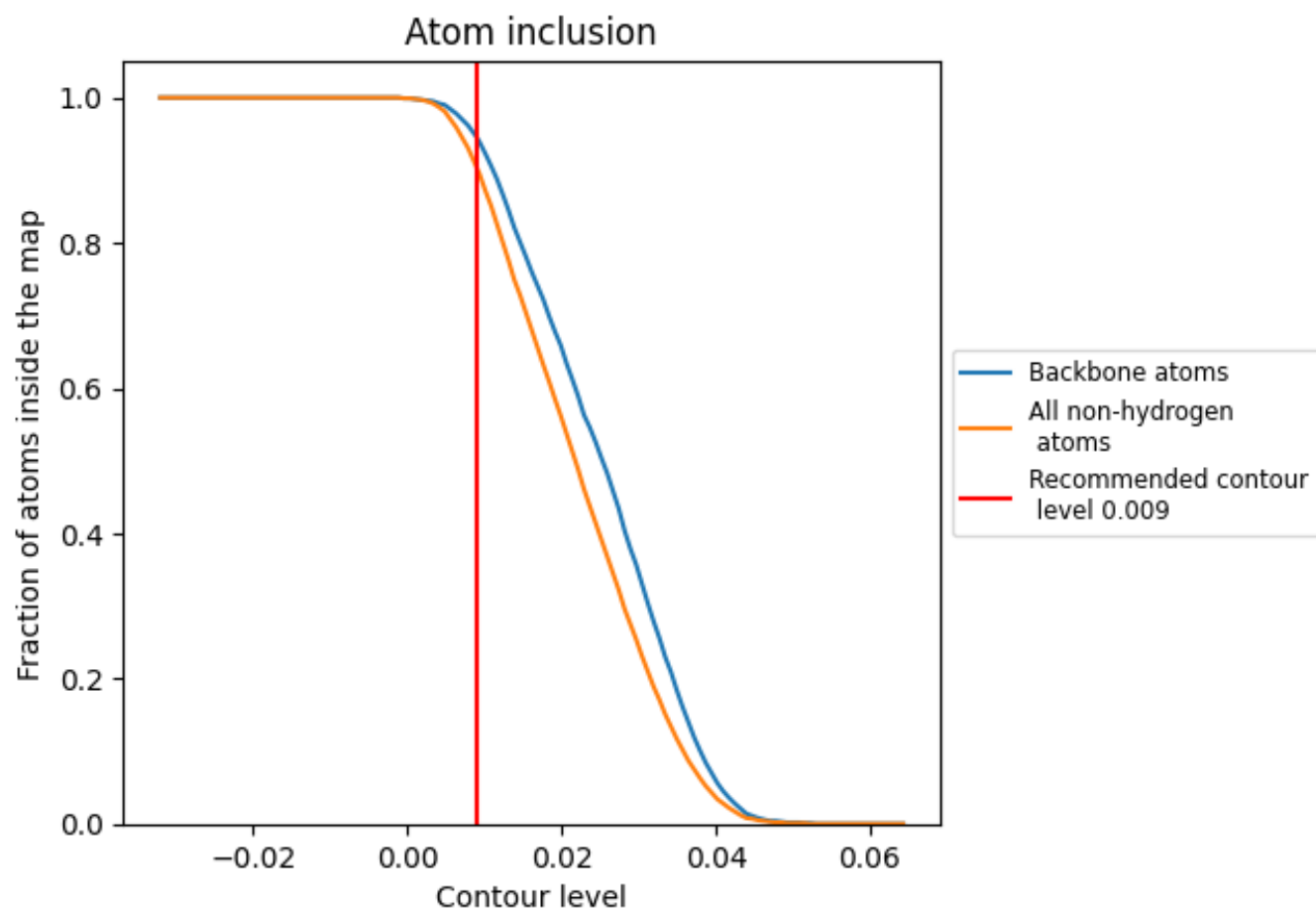
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9050	<div></div> 0.5910
A	<div></div> 0.9080	<div></div> 0.5910
B	<div></div> 0.9100	<div></div> 0.5920
C	<div></div> 0.8910	<div></div> 0.5910
D	<div></div> 0.8820	<div></div> 0.5860

