



Full wwPDB EM Validation Report ⓘ

Aug 25, 2025 – 11:14 AM EDT

PDB ID : 9MN4 / pdb_00009mn4
EMDB ID : EMD-48412
Title : Structure of the human mitochondrial initially transcribing complex, IC3
Authors : Herbine, K.H.; Nayak, A.R.; Temiakov, D.
Deposited on : 2024-12-20
Resolution : 3.05 Å (reported)
Based on initial model : 6ERP

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.dev126
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

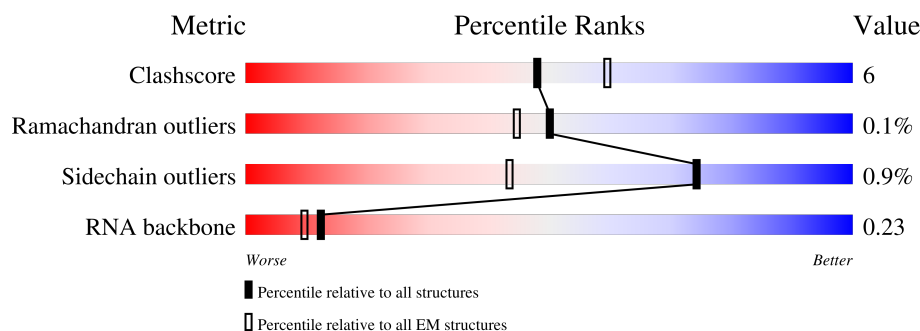
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	246	<div> <div>50%</div> <div>70%</div> <div>9%</div> <div>22%</div> </div>
2	B	396	<div> <div>66%</div> <div>16%</div> <div>18%</div> </div>
3	E	1230	<div> <div>73%</div> <div>13%</div> <div>14%</div> </div>
4	N	60	<div> <div>20%</div> <div>63%</div> <div>20%</div> <div>17%</div> </div>
5	R	3	<div> <div>100%</div> </div>
6	T	60	<div> <div>23%</div> <div>55%</div> <div>25%</div> <div>17%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14835 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 Transcription factor A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	192	Total	C	N	O	S	0	0
			1615	1019	291	300	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	SER	CYS	conflict	UNP Q00059

- Molecule 2 is a protein called Dimethyladenosine transferase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	324	Total	C	N	O	S	0	0
			2632	1699	453	465	15		

- Molecule 3 is a protein called DNA-directed RNA polymerase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1062	Total	C	N	O	S	0	0
			8480	5391	1532	1503	54		

- Molecule 4 is a DNA chain called Non-Template Strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	50	Total	C	N	O	P	0	0
			1035	492	198	296	49		

- Molecule 5 is a RNA chain called RNA (RNA3mt).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	3	Total	C	N	O	P	0	0
			68	30	15	20	3		

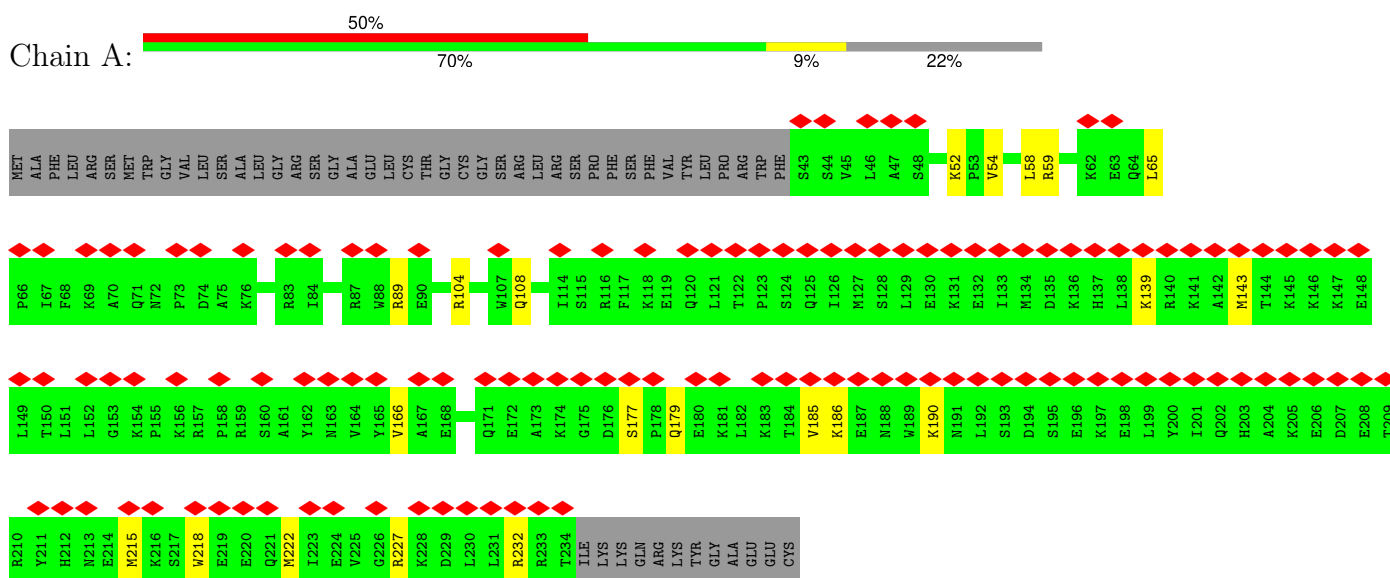
- Molecule 6 is a DNA chain called Template Strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	50	Total	C	N	O	P	0	0
			1005	481	179	296	49		

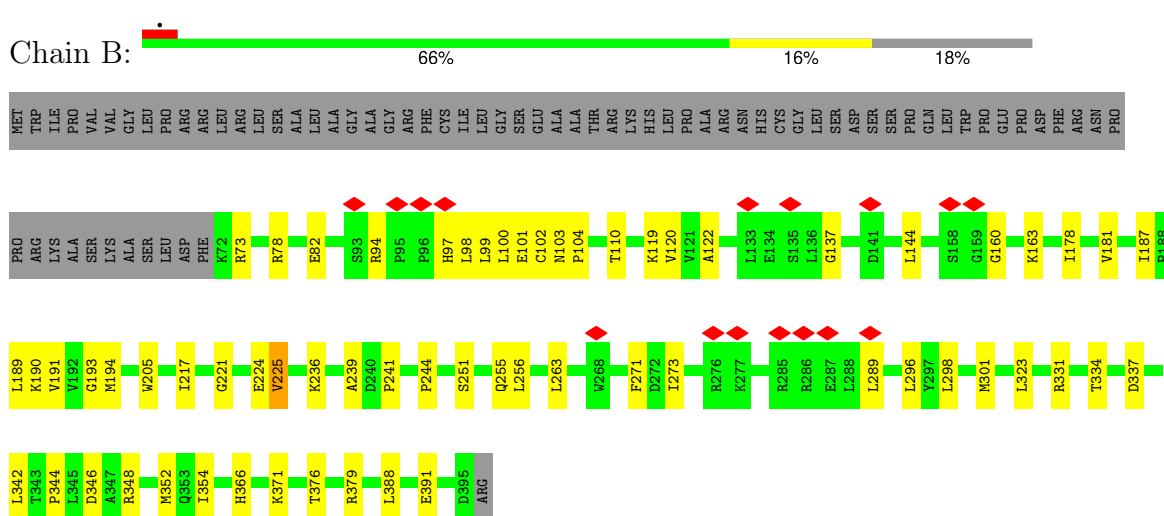
3 Residue-property plots

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: Transcription factor A, mitochondrial



- Molecule 2: Dimethyladenosine transferase 2, mitochondrial



- Molecule 3: DNA-directed RNA polymerase, mitochondrial

Chain E:  73% 13% 14%

MET SER ALA LEU VAL TRP GLY ARG GLY ALA ARG LEU LYS ALA ARG VAL LEU LYS ALA ARG VAL SER ARG PRO CYS GLY ARG VAL PRO GLY LYS VAL THR ALA GLY VAL CYS VAL CYS PRO ARG SER ARG SER SER ALA SER PRO LYS VAL GLN GLN MET GLY ALA LYS ASP ARG ASP ARG LYS ASP TRP TRP HIS GLY VAL

GLU LEU LEU VAL LEU GLN ALA ARG VAL ARG GLN GLN ALA ARG VAL SER VAL SER GLU VAL VAL VAL ASN ARG VAL ASP VAL VAL ALA ARG LEU PRO GLU CYS GLY SER GLY ASP GLY SER LEU GLN SER SER GLN PRO ARG LYS VAL VAL MET GLY LYS ASP ASP THR THR VAL PRO CYS GLY VAL

ARG W122 A123 K124 I125 L126 E127 K128 D129 K130 R131 M135 R139 A142 K143 L144 Q145 M146 F147 F148 Q149 S150 G151 E152 F153 K154 A155 Q161 R165 L166 L167 S168 K169 Q170 M171 A172 G173 C174 L175 E176 D177 C178 T179 R180 Q181 A181 PRO GLU S186 P186 W187 E188 E189 A192

L195 Q196 E197 ALA PRO GLY LYS LEU SER LEU LEU ASP VAL GLU GLN ALA PRO PRO GLY SER GLN HIS SER GLN ALA Q218 F230 K231 L241 L246 V247 Q254 T260 M263 Y264 M265 A266 V267 M268 L284 Y299 A302 L303 Q304 C305 M306 G307 R308 Q311 D312

T315 I316 E317 R318 M323 L328 L364 K388 L396 F400 Q403 V412 S424 V427 K428 H429 T433 E442 A448 T452 L456 V460 S466 V480 L483 T498 R502 S505 R511 V514 Q515 R516 Q527

H528 H529 Y530 L534 S539 P559 A561 L562 R563 E564 Q572 K577 L583 R598 L606 Y610 Q617 L621 Q629 K633 E636 P637 T638 V646 P647 M648 P651 V655 L665 L670 L684 L696 V709 N710 V713 L714

A738 PRO GLN PRO PRO ALA HIS LEU PRO HIS SER SER ALA ALA PRO PRO ALA ARG ARG LYS ALA LEU ARG ARG GLU LEU A763 H764 C765 Q766 R770 L785 R790 F794 W795 D801 F802 R803 Y807 F813 R814 H815 L816 G817 S818 D819 A823 L824 L825 E826 K842

G850 K853 R854 E855 P856 K859 R860 L861 D870 E871 L872 L879 T880 G881 R882 C898 V901 R906 N926 A933 R936 S957 V963 R967 D970 A971 K975 A978 L981 I985 T993 T996 G1005 G1006 Q1009 I1010

F1020 V1025 L1032 V1033 E1066 R1069 S1062 R1083 S1086 Q1090 I1091 Q1096 S1097 N1103 R1108 R1113 K1114 Q1115 N1122 S1148 V1149 H1150 D1151 C1152 M1163 R1168 Q1181 L1199 E1200 L1204 G1215 Y1227 F1228 F1229 S1230

• Molecule 4: Non-Template Strand DNA

Chain N:  20% 63% 20% 17%

DG DA DA DA DA DT DA DA DT DG T1 G2 T3 T4 A5 G6 T7 T8 G9 G10 G11 G12 G13 G14 T15 G16 G20 T21 T22 A23 G36 C37 C38 A41 A42 A46 C50

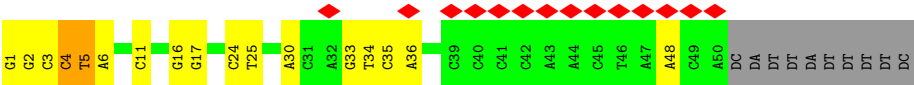
• Molecule 5: RNA (RNA3mt)

Chain R:  100%

There are no outlier residues recorded for this chain.

• Molecule 6: Template Strand DNA

Chain T:  23% 55% 25% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	109470	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 ($e^-/\text{\AA}^2$)	47.69	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.198	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	288.384, 288.384, 288.384	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.751, 0.751, 0.751	Depositor

5 Model quality

5.1 Standard geometry

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	0.12	0/1646	0.26	0/2202
2	B	0.21	0/2697	0.50	0/3646
3	E	0.22	0/8675	0.50	4/11752 (0.0%)
4	N	0.26	0/1164	0.47	0/1798
5	R	0.59	0/76	0.93	0/117
6	T	0.42	2/1124 (0.2%)	0.75	5/1728 (0.3%)
All	All	0.24	2/15382 (0.0%)	0.51	9/21243 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	3	DC	O3'-P	-8.01	1.49	1.61
6	T	5	DT	O3'-P	-5.01	1.53	1.61

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	3	DC	P-O3'-C3'	-12.92	100.82	120.20
6	T	4	DC	O3'-P-O5'	11.27	120.91	104.00
6	T	3	DC	C4'-C3'-O3'	-7.60	98.60	110.00
3	E	819	ASP	N-CA-C	-7.19	105.12	114.04
6	T	3	DC	OP1-P-O3'	-6.97	87.10	108.00
3	E	816	LEU	N-CA-C	-6.00	103.33	111.55
3	E	1113	ARG	N-CA-C	-5.71	106.35	113.55
3	E	1163	MET	CB-CG-SD	5.15	128.16	112.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	11	DC	O3'-P-O5'	-5.09	96.37	104.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	1148	SER	Peptide
3	E	178	CYS	Peptide

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	1615	0	1655	13	0
2	B	2632	0	2682	39	0
3	E	8480	0	8590	97	0
4	N	1035	0	564	11	0
5	R	68	0	34	0	0
6	T	1005	0	563	19	0
All	All	14835	0	14088	165	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 6.

All (165) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:629:GLN:O	3:E:633:LYS:HB2	1.73	0.86
6:T:5:DT:H2''	6:T:6:DA:C8	2.19	0.78
1:A:222:MET:HB3	1:A:227:ARG:HB2	1.68	0.75
3:E:617:GLN:HG2	4:N:36:DG:H21	1.54	0.70
3:E:870:ASP:OD1	3:E:882:ARG:NH2	2.25	0.69
3:E:1096:GLN:HE21	6:T:16:DG:H5'	1.59	0.67
3:E:403:GLN:NE2	3:E:648:MET:SD	2.69	0.66
3:E:967:ARG:HE	3:E:981:LEU:HB3	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:516:ARG:HH22	3:E:564:GLU:H	1.46	0.61
3:E:161:GLN:HE21	3:E:247:VAL:HG13	1.65	0.60
2:B:160:GLY:O	2:B:163:LYS:NZ	2.34	0.60
3:E:856:PRO:HG2	3:E:859:LYS:HG3	1.83	0.60
3:E:303:LEU:HD11	3:E:323:MET:HE1	1.84	0.60
3:E:1083:ARG:HD3	3:E:1108:ARG:HG3	1.84	0.60
3:E:563:ARG:NH1	3:E:665:LEU:O	2.36	0.59
3:E:303:LEU:HD22	3:E:317:GLU:HG2	1.83	0.59
3:E:304:GLN:HE21	3:E:308:ARG:HH22	1.50	0.58
3:E:396:LEU:HD13	3:E:534:LEU:HD11	1.84	0.58
3:E:1149:VAL:HB	3:E:1152:CYS:HB3	1.86	0.58
3:E:872:LEU:HD22	3:E:906:ARG:HH21	1.68	0.58
6:T:5:DT:C2	6:T:6:DA:C2	2.93	0.57
3:E:516:ARG:HH12	3:E:564:GLU:HB2	1.70	0.57
3:E:879:LEU:HG	3:E:880:THR:HG23	1.85	0.57
2:B:137:GLY:HA3	2:B:144:LEU:HD23	1.87	0.56
3:E:818:SER:OG	3:E:819:ASP:N	2.34	0.56
3:E:1103:ASN:OD1	3:E:1108:ARG:NH2	2.38	0.56
3:E:606:LEU:HD22	3:E:621:LEU:HB3	1.89	0.55
3:E:1010:ILE:HD11	3:E:1033:VAL:HB	1.88	0.55
2:B:104:PRO:HG3	2:B:122:ALA:HB1	1.88	0.55
3:E:396:LEU:HB3	3:E:534:LEU:HD21	1.88	0.55
3:E:505:SER:OG	3:E:572:GLN:O	2.23	0.54
2:B:101:GLU:OE2	2:B:103:ASN:N	2.33	0.54
3:E:967:ARG:HH22	3:E:1032:LEU:HA	1.72	0.54
3:E:315:THR:HB	3:E:318:ARG:HB2	1.90	0.54
1:A:54:VAL:O	1:A:59:ARG:NH2	2.40	0.54
2:B:100:LEU:HD11	2:B:189:LEU:HD23	1.90	0.54
3:E:498:THR:HG22	3:E:502:ARG:HE	1.73	0.54
2:B:271:PHE:HE2	2:B:296:LEU:HD22	1.73	0.53
2:B:94:ARG:NH2	2:B:187:ILE:O	2.39	0.53
3:E:606:LEU:HD13	3:E:621:LEU:HD23	1.91	0.53
2:B:263:LEU:HB2	2:B:298:LEU:HD22	1.90	0.53
2:B:241:PRO:HD3	2:B:366:HIS:HA	1.91	0.53
4:N:20:DG:H3'	4:N:21:DT:H72	1.91	0.53
2:B:241:PRO:HG3	2:B:366:HIS:CD2	2.43	0.52
3:E:188:GLU:OE2	3:E:311:GLN:NE2	2.43	0.52
3:E:936:ARG:HB2	3:E:1215:GLY:H	1.75	0.52
1:A:232:ARG:NH1	6:T:48:DA:OP1	2.41	0.52
3:E:1062:SER:OG	3:E:1115:GLN:OE1	2.26	0.52
3:E:710:ASN:ND2	3:E:826:GLU:OE1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:530:TYR:OH	3:E:651:PRO:O	2.26	0.52
6:T:5:DT:C4	6:T:6:DA:N1	2.78	0.51
3:E:610:TYR:OH	6:T:17:DG:OP1	2.28	0.51
3:E:971:ALA:HB1	3:E:978:ALA:HB2	1.93	0.51
2:B:391:GLU:OE2	3:E:766:GLN:NE2	2.44	0.51
3:E:709:VAL:HG11	3:E:790:ARG:HA	1.92	0.51
6:T:35:DC:H2"	6:T:36:DA:C8	2.46	0.50
1:A:177:SER:OG	1:A:179:GLN:OE1	2.29	0.50
2:B:323:LEU:HD12	2:B:342:LEU:HD13	1.93	0.50
3:E:388:LYS:HD3	3:E:539:SER:HA	1.94	0.50
3:E:1181:GLN:N	3:E:1181:GLN:OE1	2.44	0.50
1:A:104:ARG:O	1:A:108:GLN:NE2	2.44	0.50
3:E:1090:GLN:NE2	3:E:1097:SER:OG	2.44	0.50
3:E:933:ALA:O	3:E:936:ARG:NH1	2.44	0.49
1:A:89:ARG:NH1	4:N:21:DT:OP1	2.46	0.49
2:B:98:LEU:HD23	2:B:119:LYS:H	1.78	0.49
2:B:102:CYS:HB2	2:B:193:GLY:HA3	1.94	0.49
3:E:655:TRP:HB3	3:E:696:LEU:HD22	1.95	0.49
2:B:344:PRO:HD3	2:B:388:LEU:HD23	1.95	0.49
6:T:5:DT:N3	6:T:6:DA:C2	2.81	0.49
2:B:256:LEU:HG	2:B:371:LYS:HE2	1.95	0.48
3:E:1168:ARG:NH2	3:E:1228:PHE:O	2.46	0.48
1:A:186:LYS:HE2	1:A:190:LYS:HE3	1.95	0.48
3:E:577:LYS:NZ	3:E:1091:ILE:O	2.47	0.48
3:E:646:VAL:HG13	3:E:785:LEU:HD11	1.96	0.48
4:N:22:DT:H2"	4:N:23:DA:C8	2.48	0.48
3:E:1086:SER:HB2	3:E:1108:ARG:HD3	1.93	0.48
3:E:1200:GLU:HG2	3:E:1204:LEU:HD12	1.96	0.47
3:E:975:MET:SD	3:E:975:MET:N	2.87	0.47
2:B:239:ALA:O	2:B:255:GLN:NE2	2.43	0.47
6:T:5:DT:C5	6:T:6:DA:C6	3.03	0.47
1:A:166:VAL:HA	1:A:185:VAL:HG11	1.96	0.47
2:B:73:ARG:NH2	2:B:194:MET:SD	2.87	0.47
3:E:713:VAL:HG11	3:E:823:ALA:HB1	1.96	0.47
3:E:801:ASP:HB3	3:E:807:TYR:HE1	1.79	0.47
2:B:193:GLY:C	2:B:194:MET:HE2	2.40	0.47
2:B:97:HIS:HB3	2:B:189:LEU:HG	1.97	0.47
3:E:299:TYR:HB3	3:E:323:MET:HE2	1.97	0.47
3:E:854:ARG:HH12	3:E:957:SER:HB2	1.81	0.46
2:B:348:ARG:O	2:B:352:MET:HG3	2.14	0.46
2:B:163:LYS:HB3	4:N:41:DA:H62	1.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:714:LEU:HB3	3:E:824:LEU:HD22	1.98	0.46
2:B:273:ILE:HD13	2:B:289:LEU:HD12	1.97	0.46
2:B:190:LYS:NZ	2:B:224:GLU:OE1	2.39	0.46
3:E:260:THR:H	3:E:263:MET:HE3	1.81	0.46
3:E:713:VAL:HG11	3:E:823:ALA:O	2.16	0.45
1:A:218:TRP:CD1	1:A:222:MET:HE3	2.51	0.45
2:B:100:LEU:HB2	2:B:191:VAL:HG22	1.98	0.45
2:B:178:ILE:HG12	2:B:189:LEU:HD11	1.98	0.45
2:B:244:PRO:O	2:B:331:ARG:NH2	2.39	0.45
6:T:1:DG:H2''	6:T:2:DG:C8	2.51	0.45
2:B:354:ILE:HG22	2:B:376:THR:HG21	1.98	0.45
3:E:1006:GLY:O	3:E:1010:ILE:HG12	2.15	0.45
2:B:346:ASP:OD1	2:B:346:ASP:N	2.46	0.45
2:B:334:THR:HG23	2:B:337:ASP:H	1.82	0.45
4:N:9:DG:H2''	4:N:10:DG:H5''	1.99	0.45
3:E:265:ASN:HA	3:E:268:MET:HE3	1.99	0.44
3:E:442:GLU:HG2	3:E:480:VAL:HG11	1.98	0.44
3:E:516:ARG:NH2	3:E:564:GLU:H	2.15	0.44
6:T:5:DT:C6	6:T:6:DA:C6	3.06	0.44
3:E:246:LEU:HD22	3:E:267:VAL:HG11	1.98	0.44
3:E:850:GLY:O	3:E:853:LYS:NZ	2.45	0.44
3:E:898:CYS:HA	3:E:901:VAL:HG22	1.98	0.44
2:B:376:THR:HG22	2:B:379:ARG:HH12	1.83	0.44
3:E:412:VAL:HG21	3:E:646:VAL:HG21	1.99	0.44
3:E:302:ALA:O	3:E:306:MET:HG3	2.18	0.44
3:E:400:PHE:HE1	3:E:527:GLN:HG2	1.83	0.43
3:E:670:LEU:HD23	3:E:684:LEU:HD23	1.99	0.43
3:E:963:VAL:HG23	3:E:985:ILE:HD12	1.99	0.43
3:E:1020:PHE:HE2	3:E:1025:VAL:HG22	1.81	0.43
1:A:52:LYS:HB3	6:T:30:DA:H5''	2.00	0.43
2:B:98:LEU:HG	2:B:99:LEU:HD23	1.99	0.43
3:E:967:ARG:HH21	3:E:981:LEU:HG	1.83	0.43
1:A:139:LYS:O	1:A:143:MET:HG3	2.18	0.43
2:B:225:VAL:HG23	2:B:301:MET:HB2	2.00	0.43
3:E:230:PHE:CD2	3:E:263:MET:HG2	2.53	0.43
3:E:284:LEU:HD23	3:E:284:LEU:HA	1.83	0.43
3:E:1227:TYR:HA	3:E:1230:SER:HB2	2.00	0.43
2:B:110:THR:HA	2:B:120:VAL:HG21	2.00	0.43
3:E:424:SER:H	3:E:427:VAL:HB	1.84	0.42
3:E:803:ARG:NH1	3:E:1122:ASN:OD1	2.42	0.42
1:A:65:LEU:HD21	6:T:33:DG:H5'	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:TRP:NE1	4:N:38:DC:OP2	2.45	0.42
3:E:125:ILE:HA	3:E:128:LYS:HE2	2.02	0.42
3:E:231:LYS:HE3	3:E:231:LYS:HB3	1.87	0.42
3:E:429:HIS:O	3:E:433:THR:OG1	2.33	0.42
3:E:926:ASN:HD22	3:E:1151:ASP:HB3	1.84	0.42
3:E:176:GLU:O	3:E:180:ARG:HB2	2.20	0.41
3:E:241:LEU:HD23	3:E:460:VAL:HG11	2.02	0.41
3:E:254:GLN:NE2	6:T:25:DT:OP1	2.35	0.41
2:B:205:TRP:HE1	4:N:38:DC:P	2.42	0.41
3:E:323:MET:HG2	3:E:328:LEU:HB2	2.01	0.41
4:N:46:DA:N1	6:T:6:DA:H2	2.16	0.41
3:E:815:HIS:HB3	3:E:825:LEU:HD22	2.02	0.41
3:E:816:LEU:HG	3:E:1149:VAL:HG13	2.02	0.41
3:E:1005:GLY:O	3:E:1009:GLN:HG3	2.20	0.41
3:E:131:ARG:O	3:E:135:MET:HG3	2.20	0.41
3:E:794:PHE:C	3:E:795:TRP:HD1	2.29	0.41
3:E:511:ARG:HA	3:E:514:VAL:HG22	2.03	0.41
2:B:78:ARG:NH1	2:B:82:GLU:OE1	2.53	0.41
3:E:448:ALA:O	3:E:452:THR:OG1	2.30	0.41
1:A:58:LEU:HD12	6:T:30:DA:H2'	2.03	0.41
3:E:529:HIS:CE1	3:E:559:PRO:HD3	2.56	0.41
3:E:993:THR:HA	3:E:996:THR:HG22	2.03	0.41
3:E:1056:GLU:OE2	3:E:1059:ARG:NH1	2.54	0.41
4:N:41:DA:H2''	4:N:42:DA:C8	2.56	0.41
3:E:175:LEU:O	3:E:179:THR:OG1	2.17	0.40
3:E:483:LEU:HB3	3:E:583:LEU:HD12	2.03	0.40
3:E:842:LYS:HE3	3:E:861:LEU:HD11	2.03	0.40
2:B:181:VAL:HG23	2:B:221:GLY:HA3	2.03	0.40
3:E:456:LEU:HB3	3:E:466:SER:OG	2.21	0.40
4:N:37:DC:H4'	4:N:38:DC:H5'	2.02	0.40
6:T:4:DC:H6	6:T:4:DC:H2'	1.74	0.40
6:T:24:DC:H2''	6:T:25:DT:C5	2.57	0.40
6:T:33:DG:H2'	6:T:34:DT:H71	2.04	0.40
2:B:236:LYS:O	2:B:251:SER:OG	2.30	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	190/246 (77%)	190 (100%)	0	0	100	100
2	B	322/396 (81%)	296 (92%)	26 (8%)	0	100	100
3	E	1054/1230 (86%)	1016 (96%)	37 (4%)	1 (0%)	48	77
All	All	1566/1872 (84%)	1502 (96%)	63 (4%)	1 (0%)	50	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	818	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	178/222 (80%)	177 (99%)	1 (1%)	84	90
2	B	290/349 (83%)	288 (99%)	2 (1%)	81	89
3	E	924/1057 (87%)	915 (99%)	9 (1%)	73	85
All	All	1392/1628 (86%)	1380 (99%)	12 (1%)	74	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	MET
2	B	217	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	225	VAL
3	E	364	LEU
3	E	460	VAL
3	E	646	VAL
3	E	714	LEU
3	E	813	PHE
3	E	819	ASP
3	E	826	GLU
3	E	1114	LYS
3	E	1163	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	203	HIS
1	A	212	HIS
2	B	294	GLN
2	B	366	HIS
3	E	161	GLN
3	E	196	GLN
3	E	222	GLN
3	E	249	HIS
3	E	304	GLN
3	E	311	GLN
3	E	512	HIS
3	E	528	ASN
3	E	680	HIS
3	E	764	HIS
3	E	788	HIS
3	E	921	GLN
3	E	926	ASN
3	E	930	HIS
3	E	972	GLN
3	E	1035	GLN
3	E	1080	GLN
3	E	1090	GLN
3	E	1164	ASN
3	E	1170	GLN
3	E	1209	GLN
3	E	1221	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	R	2/3 (66%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

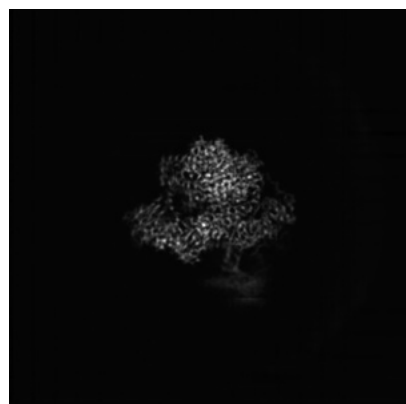
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48412. These allow visual inspection of the internal detail of the map and identification of artifacts.

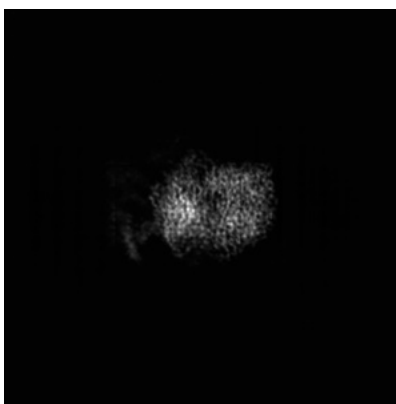
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

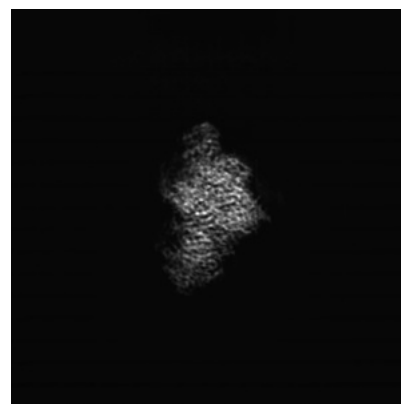
6.1.1 Primary map



X

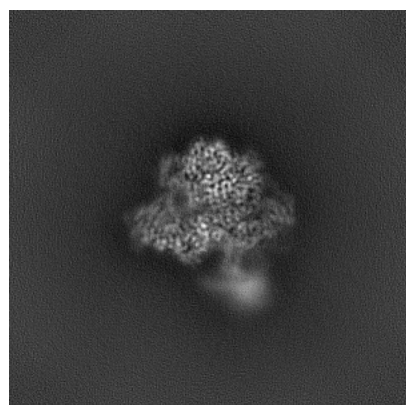


Y

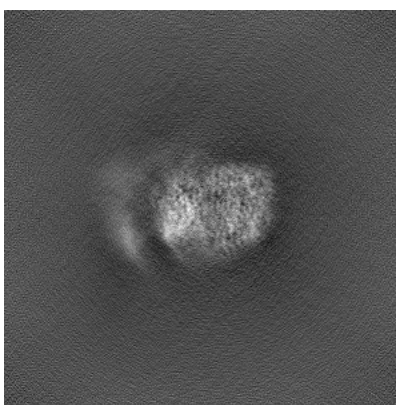


Z

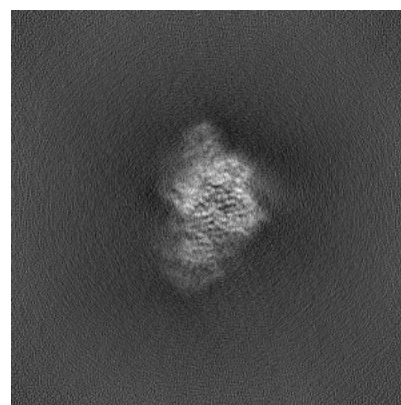
6.1.2 Raw map



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

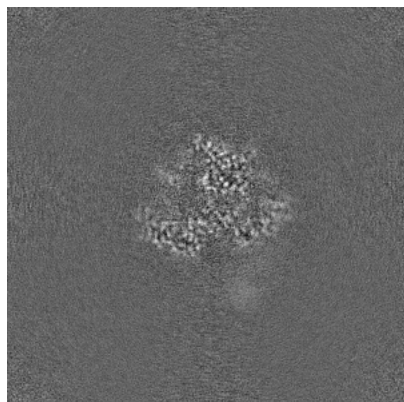


Y Index: 192

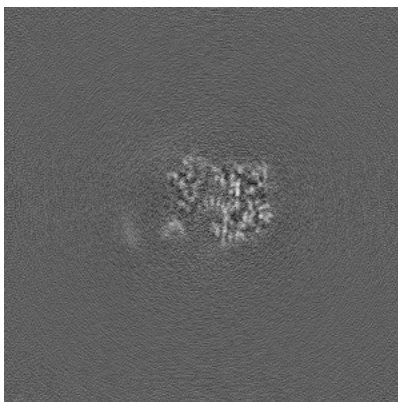


Z Index: 192

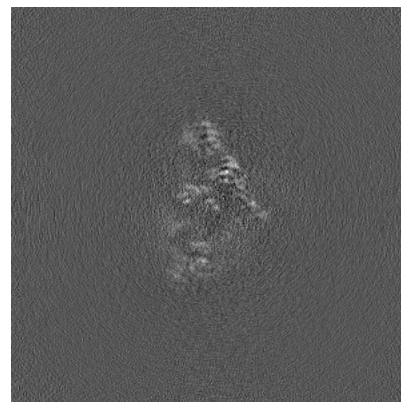
6.2.2 Raw map



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: 190

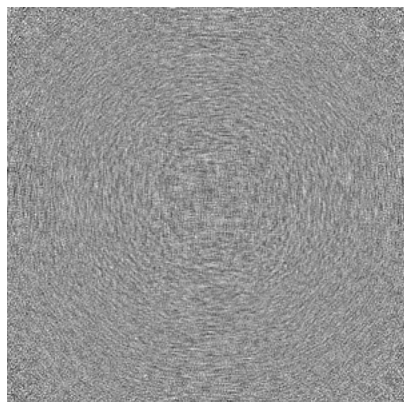


Y Index: 188

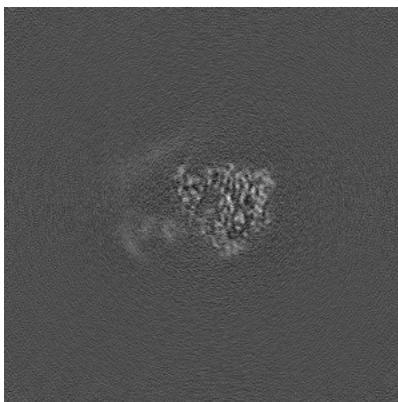


Z Index: 171

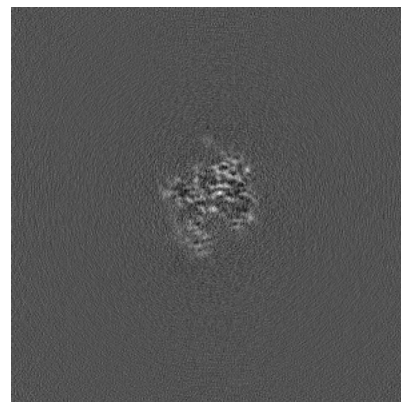
6.3.2 Raw map



X Index: 0



Y Index: 205

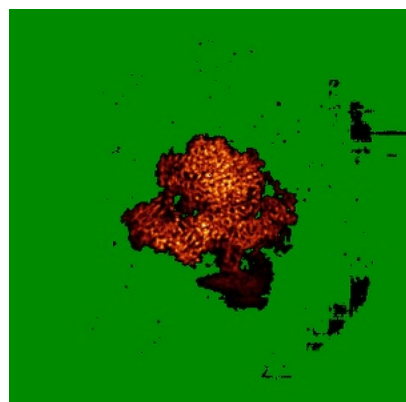


Z Index: 215

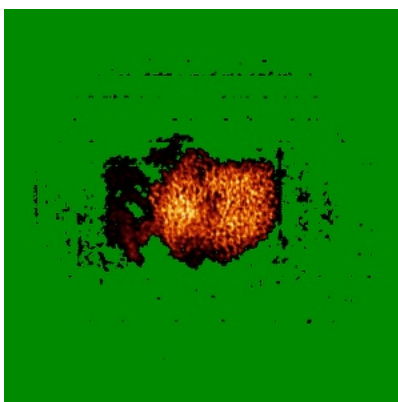
The images above show the largest variance slices of the map in three orthogonal directions.

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

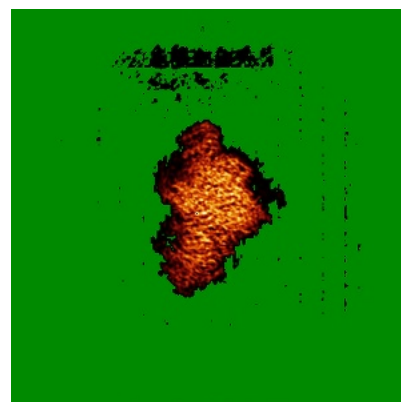
6.4.1 Primary map



X

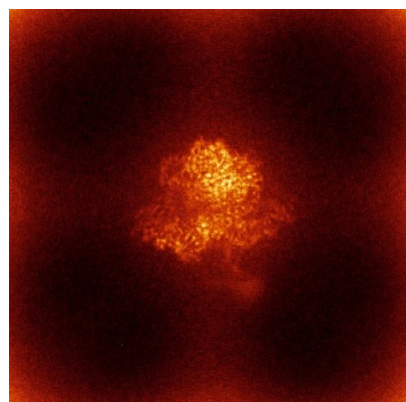


Y

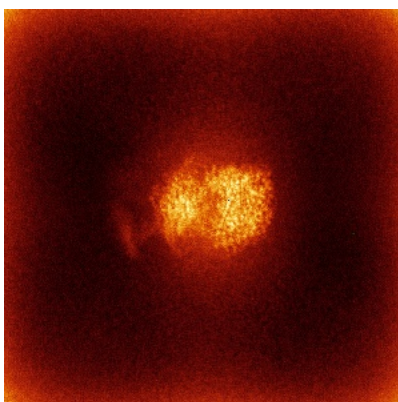


Z

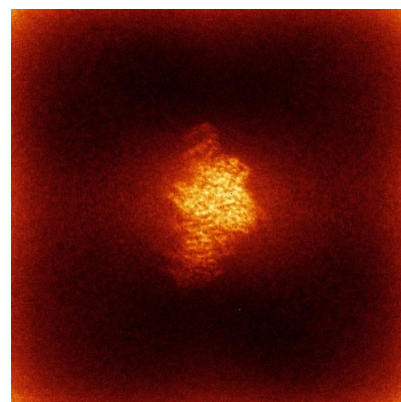
6.4.2 Raw map



X



Y

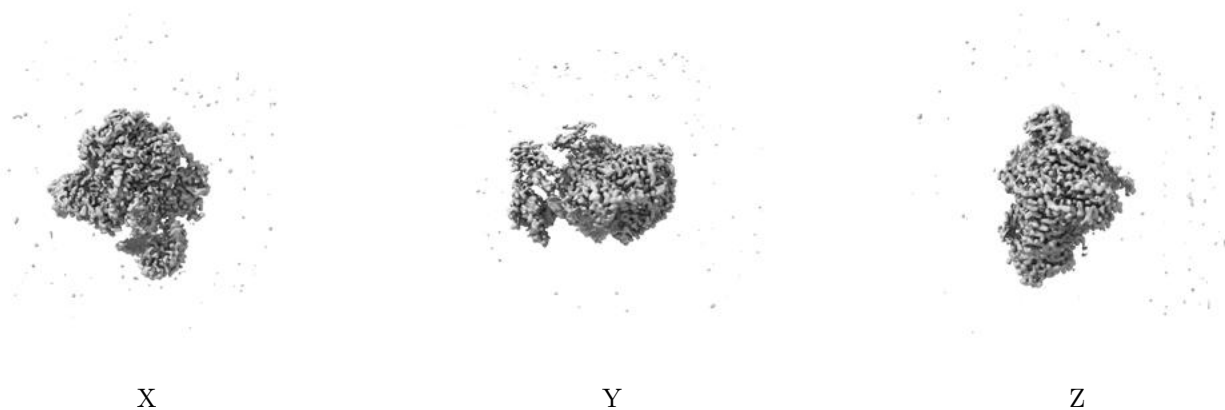


Z

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.

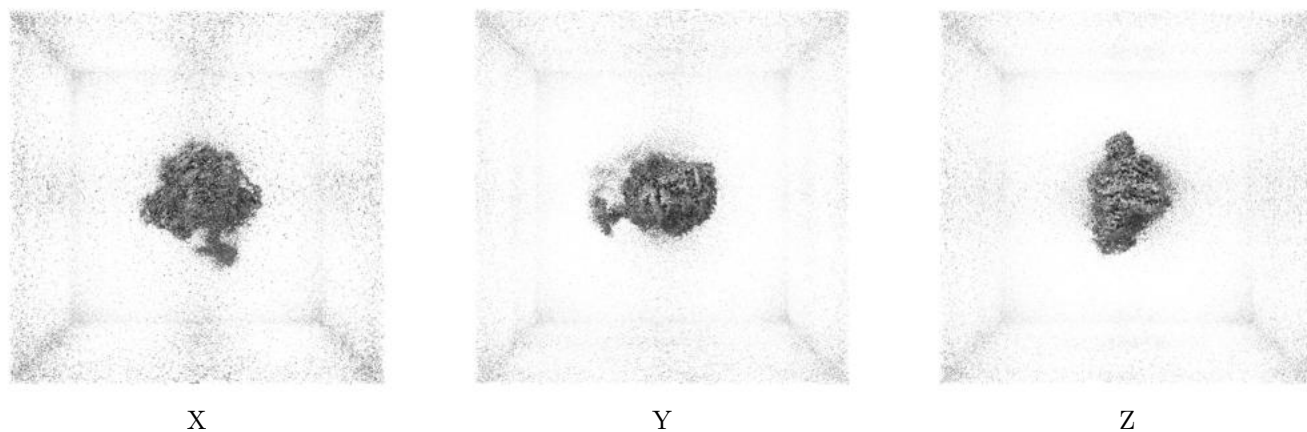
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

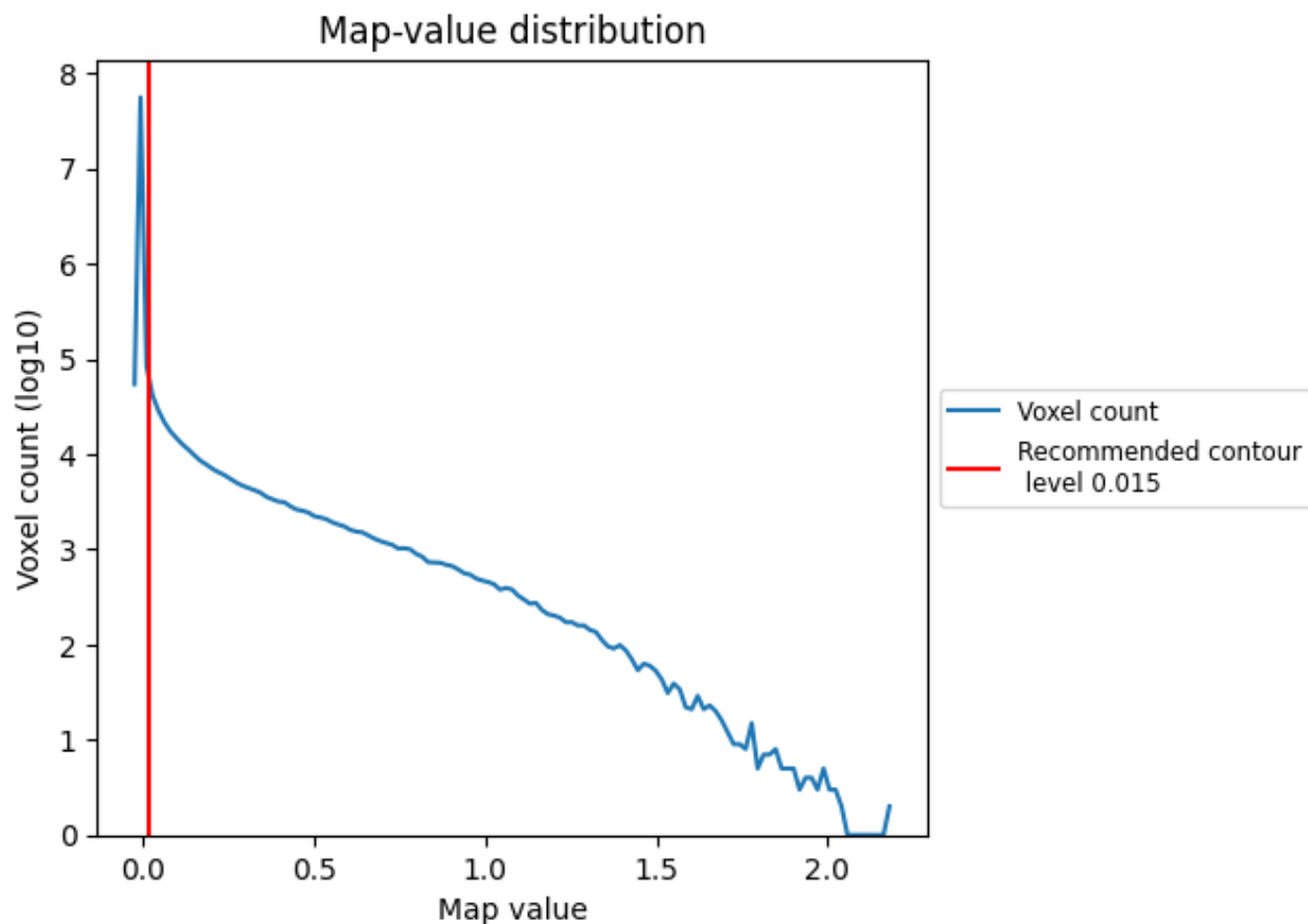
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

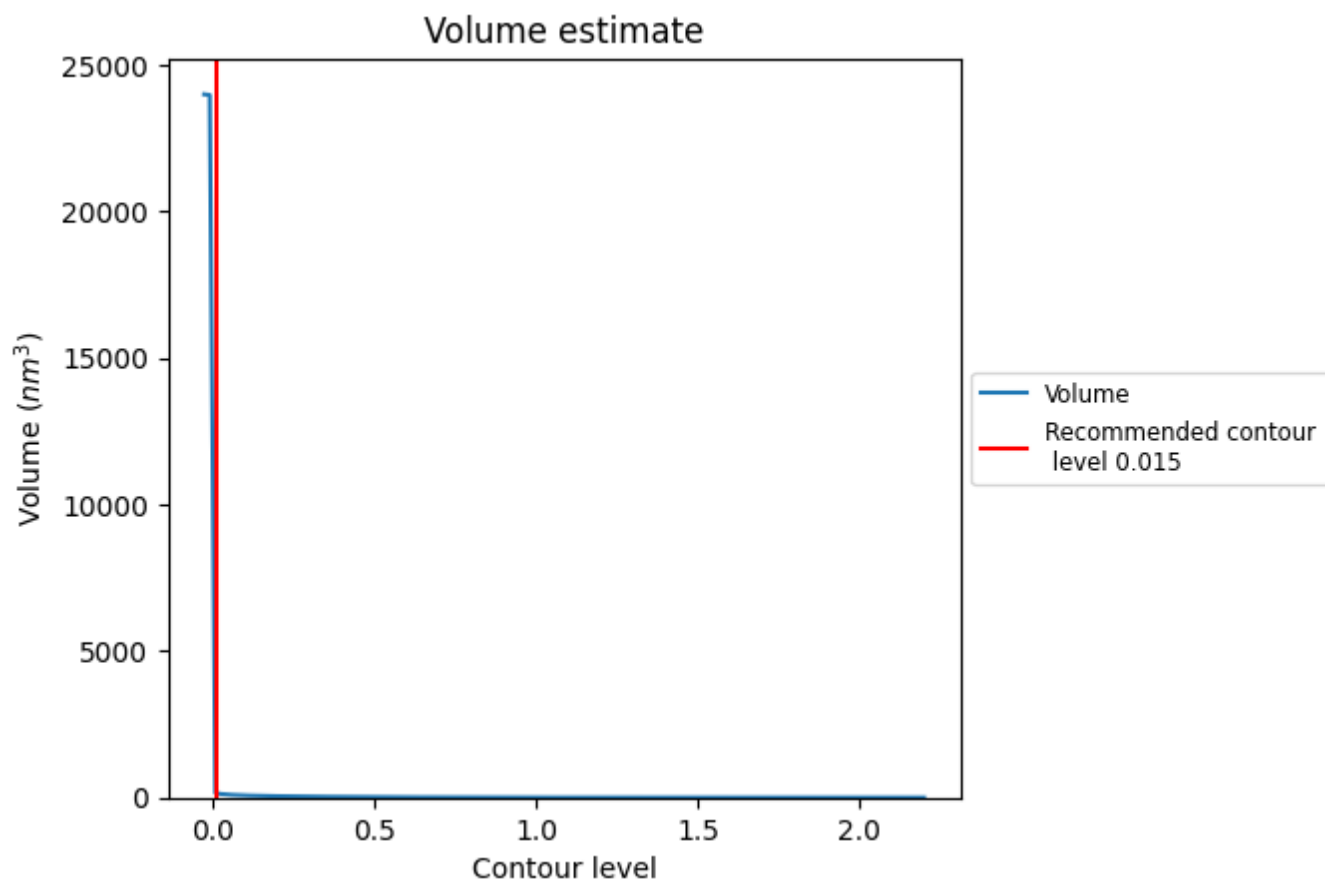
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

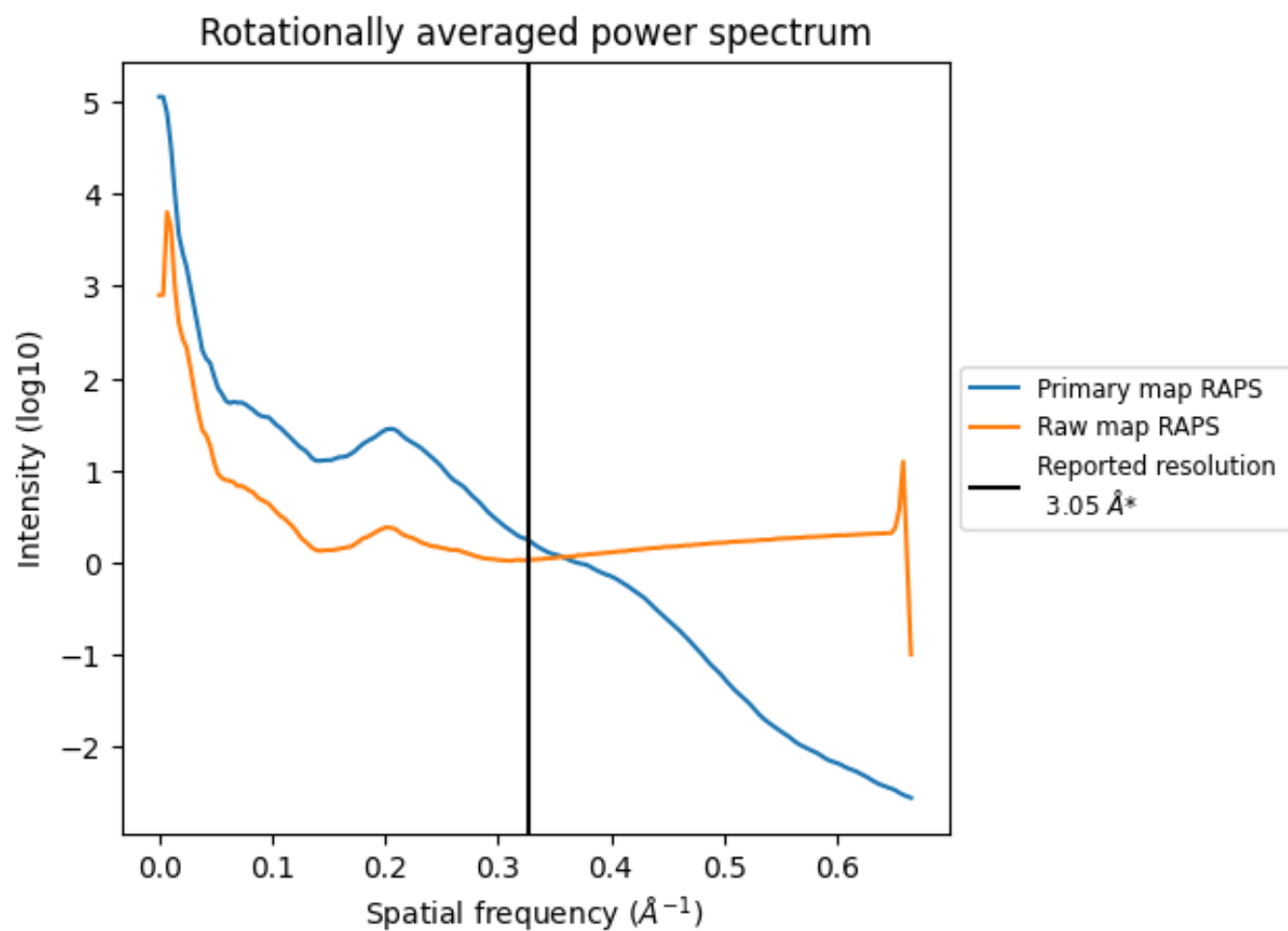
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147 nm³; this corresponds to an approximate mass of 133 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 ⓘ

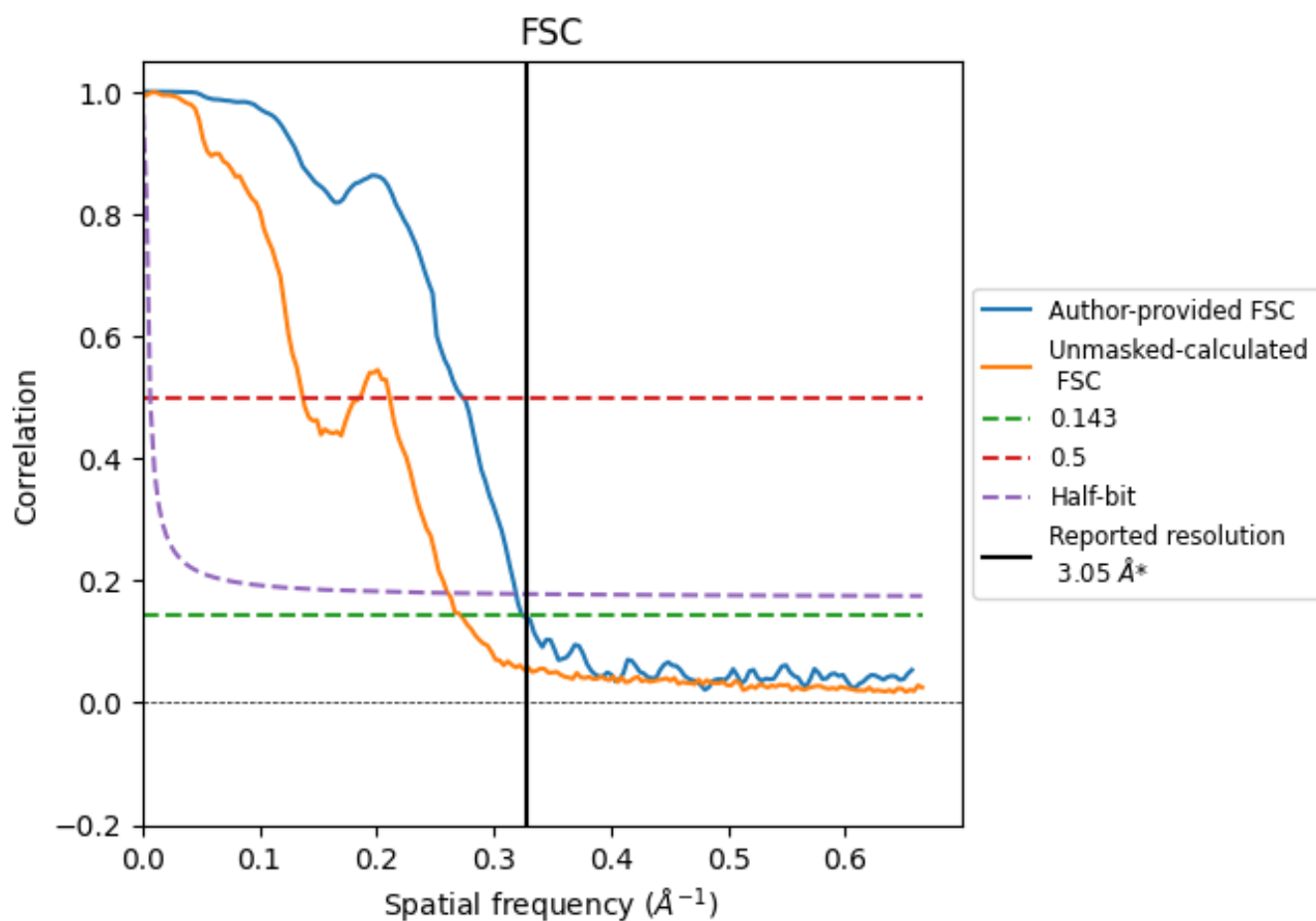


*Reported resolution corresponds to spatial frequency of 0.328 Å⁻¹

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 0.328 \AA^{-1}

8.2 Resolution estimates [i](#)

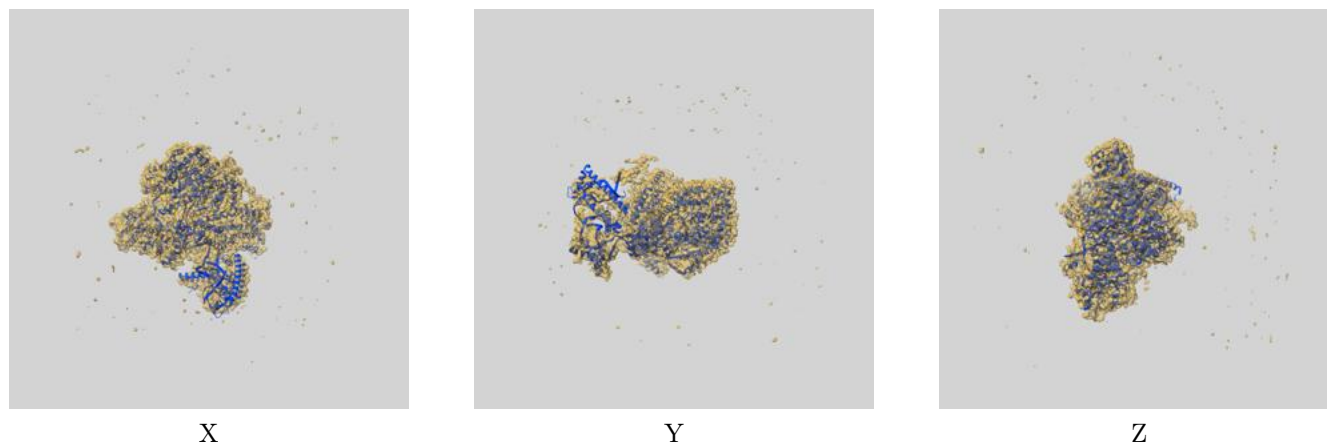
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	3.08	3.66	3.13
Unmasked-calculated*	3.68	7.29	3.83

*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 3.68 differs from the reported value 3.05 by more than 10 %

9 Map-model fit [i](#)

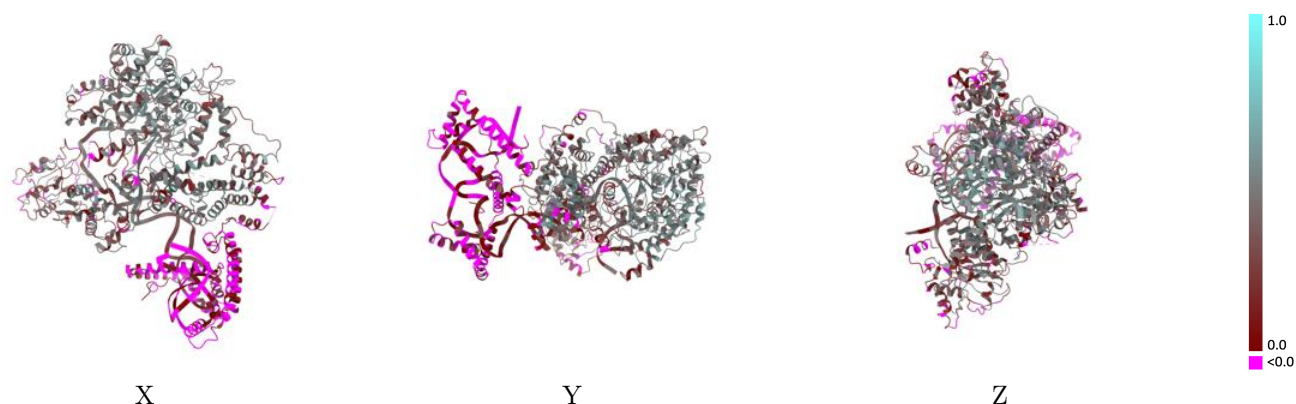
This section contains information regarding the fit between EMDB map EMD-48412 and PDB model 9MN4. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



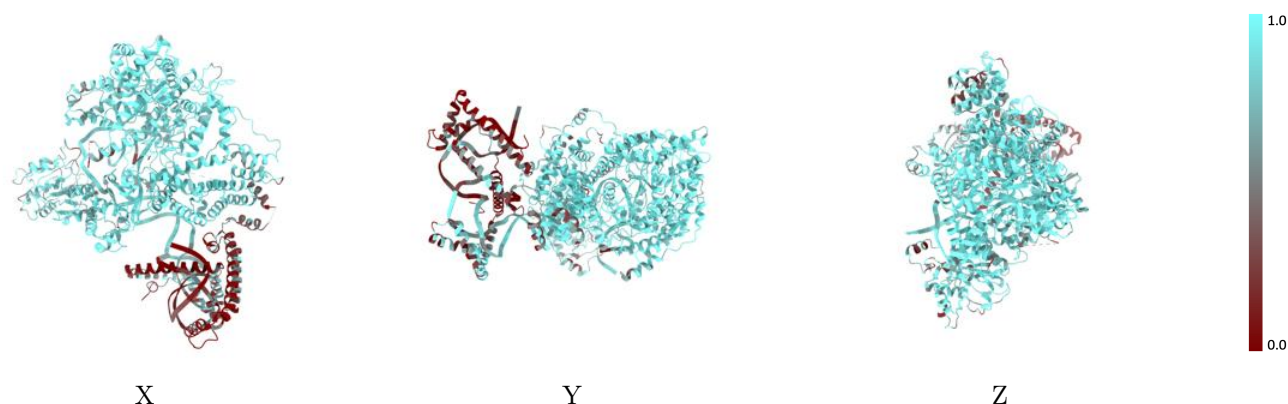
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



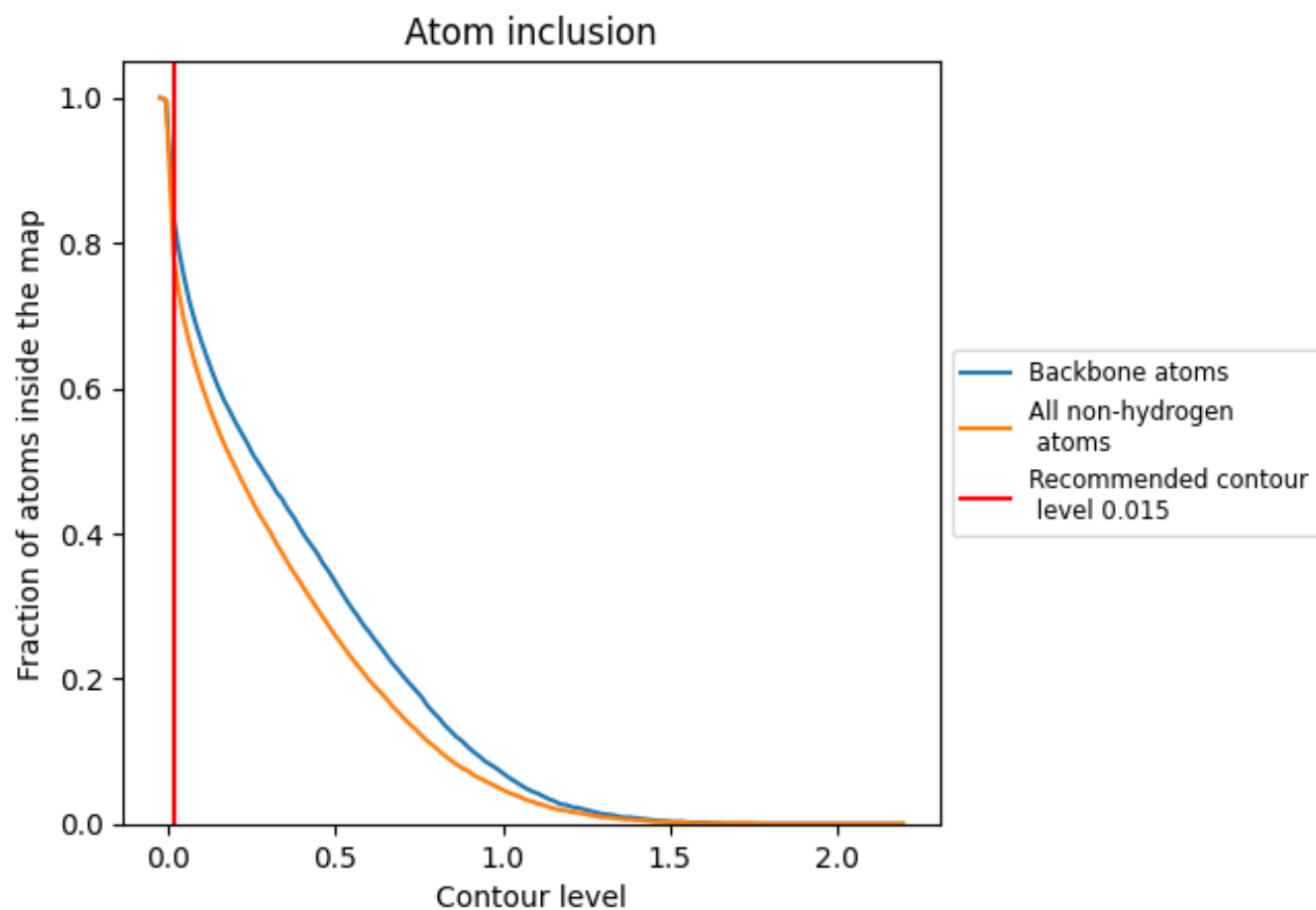
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7820	<div></div> 0.3130
A	<div></div> 0.3320	<div></div> -0.0130
B	<div></div> 0.8410	<div></div> 0.3180
E	<div></div> 0.8800	<div></div> 0.4040
N	<div></div> 0.6470	<div></div> 0.1610
R	<div></div> 0.9120	<div></div> 0.5140
T	<div></div> 0.6550	<div></div> 0.1980

