Full wwPDB EM Validation Report

Aug 5, 2026 – 08:47 AM EDT

PDB ID	:	9B8R / pdb_00009b8r
EMDB ID	:	EMD-44356
Title	:	Cryo-EM structure of S. cerevisiae PolE-core-DNA
Authors	:	Yuan, Z.; Georgescu, R.; O'Donnell, M.; Li, H.
Deposited on	:	2024-03-31
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

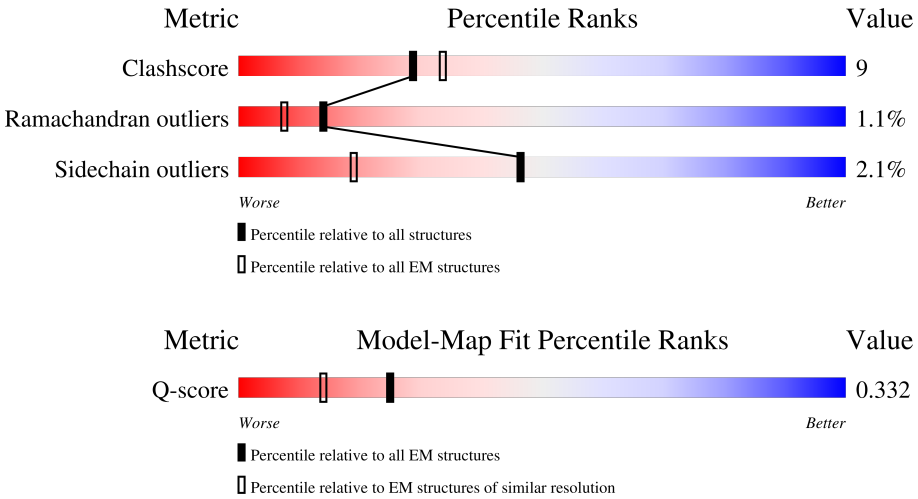
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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 <=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	P	10	20% 20% 70% 10%
2	T	12	17% 58% 42%
3	E	1160	15% 81% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	E	1401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9425 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 DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	10	Total	C	N	O	P	0	0
			202	97	32	63	10		

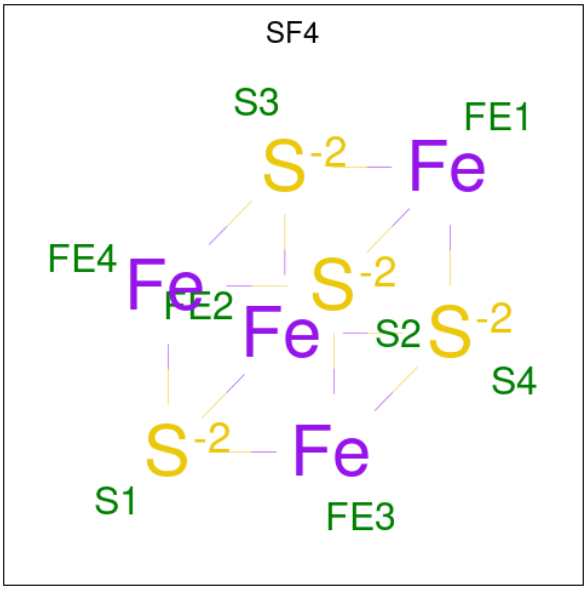
- Molecule 2 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	12	Total	C	N	O	P	0	0
			248	117	51	68	12		

- Molecule 3 is a protein called DNA polymerase epsilon catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1119	Total	C	N	O	S	0	0
			8967	5725	1507	1692	43		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
4	E	1	8	4	4	0

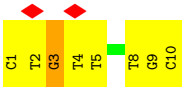
3 Residue-property plots (i)

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: Primer DNA

Chain P:





• Molecule 2: Template DNA

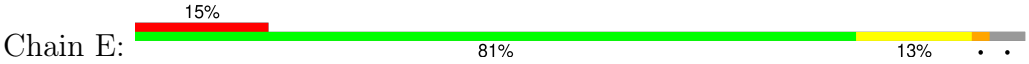
Chain T:

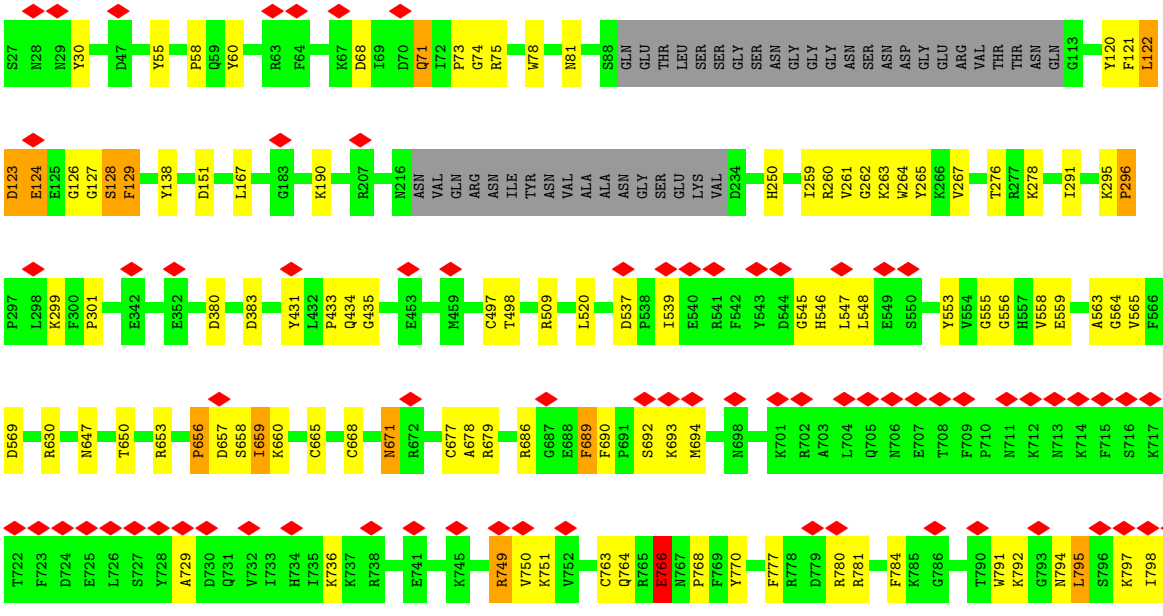


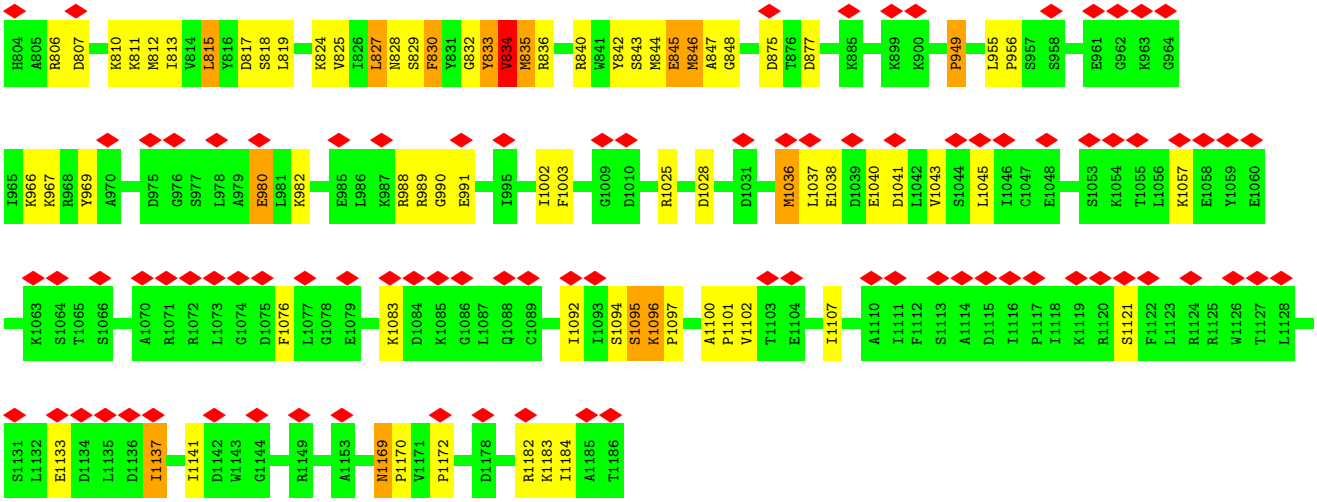


• Molecule 3: DNA polymerase epsilon catalytic subunit

Chain E:






H804 A805 R806 D807 K810 K811 M812 I813 V814 L815 Y816 D817 S818 L819 K824 V825 I826 L827 N828 S829 F830 Y831 G832 Y833 V834 M835 R836 R840 W841 Y842 S843 M844 E845 M846 A847 G848 D875 T876 D877 K885 K899 K900 P949 L955 P956 S957 S958 E961 G962 K963 G964
I965 K966 K967 R968 Y969 A970 D975 G976 S977 L978 A979 E980 L981 K982 E985 L986 K987 R988 R989 G990 E991 I995 I1002 F1003 G1009 D1010 R1025 D1028 D1031 M1036 L1037 E1038 D1039 E1040 D1041 L1042 V1043 S1044 L1045 I1046 C1047 E1048 S1053 K1054 T1055 L1056 K1057 E1058 Y1059 E1060
K1063 S1064 T1065 S1066 A1070 R1071 R1072 L1073 G1074 D1075 F1076 L1077 G1078 E1079 K1083 D1084 K1085 G1086 L1087 Q1088 C1089 I1092 I1093 S1094 S1095 K1096 P1097 A1100 P1101 V1102 T1103 E1104 I1107 A1110 I1111 F1112 S1113 A1114 D1115 I1116 P1117 I1118 K1119 R1120 S1121 F1122 L1123 R1124 R1125 W1126 T1127 L1128
S1131 L1132 E1133 D1134 L1135 D1136 I1137 I1141 D1142 W1143 G1144 R1149 A1153 N1169 P1170 V1171 P1172 D1178 R1182 K1183 I1184 A1185 T1186

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121833	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.989	Depositor
Minimum map value	-0.681	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	211.968, 211.968, 211.968	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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	P	0.69	1/224 (0.4%)	0.88	0/343
2	T	0.71	0/279	0.68	0/428
3	E	0.90	6/9171 (0.1%)	1.25	27/12407 (0.2%)
All	All	0.89	7/9674 (0.1%)	1.23	27/13178 (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
3	E	0	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	949	PRO	C-N	17.84	1.56	1.33
3	E	766	GLU	C-N	10.84	1.55	1.33
3	E	1107	ILE	N-CA	-5.80	1.40	1.46
3	E	1169	ASN	C-N	5.47	1.40	1.34
1	P	3	DG	C1'-N9	-5.40	1.35	1.46
3	E	1170	PRO	N-CD	5.25	1.55	1.47
3	E	1172	PRO	N-CD	5.09	1.54	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	766	GLU	O-C-N	-9.06	111.71	122.95
3	E	122	LEU	N-CA-C	-8.59	100.75	111.75
3	E	656	PRO	N-CA-C	-7.72	103.71	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	151	ASP	CA-CB-CG	7.59	120.19	112.60
3	E	751	LYS	CB-CA-C	-6.99	102.10	112.09
3	E	877	ASP	CA-CB-CG	6.83	119.43	112.60
3	E	120	TYR	CA-C-N	-6.55	113.81	123.11
3	E	120	TYR	C-N-CA	-6.55	113.81	123.11
3	E	949	PRO	CA-C-N	-6.39	111.85	122.21
3	E	949	PRO	C-N-CA	-6.39	111.85	122.21
3	E	380	ASP	CA-CB-CG	6.17	118.77	112.60
3	E	835	MET	N-CA-C	-5.91	104.26	112.30
3	E	1169	ASN	CA-C-N	-5.89	113.74	119.87
3	E	1169	ASN	C-N-CA	-5.89	113.74	119.87
3	E	671	ASN	OD1-CG-ND2	-5.77	116.83	122.60
3	E	124	GLU	N-CA-C	-5.75	102.01	110.52
3	E	296	PRO	N-CA-CB	5.72	106.19	103.22
3	E	830	PHE	N-CA-C	-5.62	102.11	111.37
3	E	71	GLN	N-CA-C	-5.52	105.67	112.90
3	E	129	PHE	CA-C-N	-5.47	112.79	122.74
3	E	129	PHE	C-N-CA	-5.47	112.79	122.74
3	E	834	VAL	CA-C-O	-5.44	113.98	120.78
3	E	817	ASP	O-C-N	5.23	127.67	122.12
3	E	537	ASP	CA-CB-CG	5.15	117.75	112.60
3	E	250	HIS	CB-CG-CD2	-5.12	124.54	131.20
3	E	766	GLU	CA-C-N	5.03	134.06	121.80
3	E	766	GLU	C-N-CA	5.03	134.06	121.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	123	ASP	Mainchain
3	E	509	ARG	Sidechain
3	E	567	ARG	Sidechain
3	E	630	ARG	Sidechain
3	E	749	ARG	Peptide
3	E	766	GLU	Mainchain
3	E	81	ASN	Mainchain
3	E	949	PRO	Mainchain

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	P	202	0	113	17	0
2	T	248	0	134	16	0
3	E	8967	0	8737	157	0
4	E	8	0	0	6	0
All	All	9425	0	8984	171	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 9.

All (171) 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:656:PRO:HB3	3:E:843:SER:HB2	1.46	0.97
3:E:55:TYR:OH	3:E:75:ARG:HG2	1.74	0.86
2:T:5:DG:H4'	3:E:835:MET:CB	2.08	0.83
3:E:60:TYR:CB	3:E:73:PRO:HG3	2.13	0.78
3:E:55:TYR:CZ	3:E:75:ARG:HG2	2.18	0.77
3:E:671:ASN:HB2	4:E:1401:SF4:S3	2.26	0.75
3:E:539:ILE:HG21	3:E:729:ALA:HA	1.67	0.75
3:E:845:GLU:O	3:E:847:ALA:N	2.20	0.74
1:P:8:DT:H5'	3:E:988:ARG:HG2	1.69	0.73
3:E:546:HIS:HA	3:E:692:SER:O	1.88	0.73
1:P:9:DG:N2	2:T:6:DC:H42	1.87	0.73
3:E:74:GLY:O	3:E:75:ARG:HG2	1.89	0.72
3:E:1002:ILE:HD12	3:E:1003:PHE:N	2.05	0.71
3:E:78:TRP:CZ2	3:E:262:GLY:HA2	2.24	0.71
3:E:665:CYS:HA	4:E:1401:SF4:S2	2.30	0.70
3:E:827:LEU:HA	3:E:830:PHE:HD2	1.55	0.70
1:P:8:DT:H2"	1:P:9:DG:H5'	1.75	0.68
3:E:78:TRP:HB2	3:E:264:TRP:CD2	2.29	0.67
3:E:784:PHE:CE2	3:E:819:LEU:HB3	2.28	0.67
3:E:1096:LYS:CB	3:E:1097:PRO:HD3	2.26	0.66
3:E:259:ILE:HA	3:E:265:TYR:CZ	2.31	0.66
3:E:781:ARG:HE	3:E:824:LYS:HB2	1.61	0.66
3:E:260:ARG:N	3:E:265:TYR:OH	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:845:GLU:O	3:E:848:GLY:N	2.29	0.65
3:E:55:TYR:CZ	3:E:75:ARG:CG	2.80	0.65
3:E:78:TRP:HE1	3:E:262:GLY:C	2.05	0.65
3:E:121:PHE:C	3:E:123:ASP:N	2.50	0.64
1:P:3:DG:C8	1:P:4:DT:H72	2.32	0.64
3:E:124:GLU:O	3:E:126:GLY:N	2.30	0.64
3:E:677:CYS:O	3:E:764:GLN:HG2	1.98	0.64
3:E:295:LYS:HB3	3:E:301:PRO:HG3	1.80	0.63
3:E:658:SER:O	3:E:659:ILE:C	2.41	0.62
3:E:656:PRO:HD3	3:E:770:TYR:CE2	2.35	0.61
3:E:829:SER:O	3:E:830:PHE:C	2.44	0.61
3:E:547:LEU:HD21	3:E:736:LYS:HG2	1.83	0.60
1:P:4:DT:H2"	1:P:5:DT:H5'	1.84	0.60
3:E:657:ASP:O	3:E:766:GLU:HG2	2.02	0.59
2:T:7:DA:OP2	3:E:686:ARG:NH1	2.33	0.59
3:E:74:GLY:O	3:E:75:ARG:CG	2.50	0.58
3:E:559:GLU:HA	3:E:966:LYS:HE2	1.86	0.58
3:E:55:TYR:HH	3:E:75:ARG:HG2	1.69	0.58
3:E:262:GLY:C	3:E:498:THR:HG22	2.29	0.58
3:E:749:ARG:HG2	3:E:750:VAL:H	1.68	0.57
3:E:546:HIS:HB2	3:E:689:PHE:HD2	1.70	0.57
3:E:1040:GLU:O	3:E:1043:VAL:HG22	2.05	0.57
2:T:4:DA:H4'	3:E:836:ARG:HA	1.86	0.56
3:E:807:ASP:O	3:E:811:LYS:HG3	2.06	0.56
3:E:548:LEU:HD23	3:E:689:PHE:HB3	1.86	0.56
1:P:10:DC:H5'	3:E:875:ASP:OD2	2.06	0.55
3:E:1043:VAL:HG12	3:E:1137:ILE:CD1	2.36	0.55
1:P:8:DT:OP1	3:E:433:PRO:HB2	2.06	0.55
3:E:558:VAL:HG11	3:E:967:LYS:HE2	1.89	0.55
3:E:546:HIS:HB3	3:E:690:PHE:O	2.06	0.55
3:E:262:GLY:O	3:E:498:THR:HG22	2.07	0.55
3:E:832:GLY:O	3:E:833:TYR:C	2.50	0.55
3:E:827:LEU:HA	3:E:830:PHE:CD2	2.38	0.54
2:T:6:DC:O3'	3:E:555:GLY:N	2.38	0.54
2:T:5:DG:C4'	3:E:835:MET:CB	2.82	0.54
2:T:7:DA:H4'	3:E:556:GLY:O	2.08	0.54
3:E:74:GLY:C	3:E:75:ARG:HG2	2.33	0.54
3:E:545:GLY:O	3:E:694:MET:N	2.42	0.53
3:E:802:ASP:HA	3:E:806:ARG:HE	1.74	0.53
3:E:121:PHE:O	3:E:122:LEU:C	2.51	0.53
3:E:260:ARG:HB2	3:E:263:LYS:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:563:ALA:HB1	3:E:956:PRO:O	2.09	0.53
3:E:296:PRO:HB2	3:E:299:LYS:HD2	1.90	0.53
3:E:799:ASP:OD1	3:E:799:ASP:N	2.38	0.52
3:E:829:SER:O	3:E:832:GLY:N	2.41	0.52
1:P:2:DT:H2"	1:P:3:DG:O5'	2.10	0.52
3:E:78:TRP:HZ2	3:E:262:GLY:HA2	1.73	0.51
3:E:545:GLY:O	3:E:693:LYS:C	2.54	0.51
3:E:658:SER:O	3:E:660:LYS:N	2.43	0.51
3:E:969:TYR:CZ	3:E:982:LYS:HG3	2.46	0.51
3:E:124:GLU:HB3	3:E:264:TRP:HZ3	1.76	0.51
3:E:830:PHE:O	3:E:834:VAL:HG13	2.11	0.51
3:E:291:ILE:HG12	3:E:383:ASP:OD1	2.11	0.51
3:E:546:HIS:CB	3:E:689:PHE:HD2	2.25	0.50
3:E:647:ASN:HA	3:E:650:THR:HG22	1.93	0.50
3:E:78:TRP:CD1	3:E:264:TRP:CD1	2.99	0.50
3:E:567:ARG:HG2	3:E:569:ASP:H	1.75	0.50
3:E:1094:SER:O	3:E:1095:SER:HB2	2.10	0.50
3:E:1137:ILE:HG12	3:E:1141:ILE:HD11	1.93	0.50
3:E:656:PRO:HB3	3:E:843:SER:CB	2.30	0.50
3:E:791:TRP:HB3	3:E:813:ILE:HG12	1.93	0.50
2:T:4:DA:N3	3:E:832:GLY:HA3	2.26	0.50
3:E:276:THR:C	3:E:278:LYS:H	2.19	0.50
3:E:845:GLU:O	3:E:846:MET:C	2.55	0.50
3:E:123:ASP:CB	3:E:129:PHE:CE2	2.95	0.50
3:E:689:PHE:CD1	3:E:689:PHE:N	2.79	0.50
2:T:4:DA:H1'	3:E:833:TYR:N	2.28	0.49
3:E:1137:ILE:HG12	3:E:1141:ILE:CD1	2.43	0.49
2:T:9:DC:C6	2:T:9:DC:H5'	2.48	0.49
3:E:78:TRP:HD1	3:E:264:TRP:CD1	2.31	0.49
3:E:263:LYS:HE3	3:E:498:THR:O	2.13	0.49
3:E:78:TRP:NE1	3:E:262:GLY:C	2.71	0.48
3:E:435:GLY:N	3:E:989:ARG:HB2	2.28	0.48
3:E:770:TYR:OH	3:E:834:VAL:HG12	2.13	0.48
3:E:564:GLY:N	3:E:955:LEU:O	2.35	0.48
3:E:777:PHE:HA	3:E:780:ARG:HG2	1.96	0.48
1:P:9:DG:H22	2:T:6:DC:H42	1.62	0.47
3:E:1037:LEU:HD21	3:E:1045:LEU:HD12	1.96	0.47
3:E:1094:SER:O	3:E:1095:SER:CB	2.63	0.47
3:E:832:GLY:O	3:E:834:VAL:N	2.47	0.47
1:P:8:DT:H2"	1:P:9:DG:C5'	2.44	0.47
3:E:784:PHE:CD2	3:E:819:LEU:HB3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:840:ARG:C	3:E:842:TYR:N	2.72	0.47
3:E:845:GLU:C	3:E:847:ALA:N	2.72	0.47
3:E:815:LEU:O	3:E:818:SER:OG	2.28	0.46
3:E:990:GLY:O	3:E:991:GLU:HB2	2.14	0.46
3:E:129:PHE:CD1	3:E:129:PHE:O	2.69	0.46
3:E:980:GLU:HG2	3:E:982:LYS:HE2	1.97	0.46
2:T:7:DA:P	3:E:555:GLY:H	2.39	0.46
3:E:74:GLY:O	3:E:75:ARG:CD	2.64	0.46
3:E:78:TRP:HB2	3:E:264:TRP:CE3	2.51	0.46
3:E:668:CYS:HB3	4:E:1401:SF4:S3	2.56	0.46
3:E:763:CYS:SG	4:E:1401:SF4:S1	3.14	0.46
3:E:78:TRP:HB2	3:E:264:TRP:CE2	2.51	0.46
1:P:10:DC:H2'	1:P:10:DC:O2	2.15	0.45
2:T:6:DC:H5'	3:E:553:TYR:CE2	2.51	0.45
3:E:564:GLY:O	3:E:955:LEU:N	2.25	0.45
3:E:792:LYS:HA	3:E:795:LEU:HD23	1.98	0.45
3:E:671:ASN:N	4:E:1401:SF4:S3	2.90	0.45
1:P:1:DC:H2'	1:P:2:DT:C6	2.52	0.45
3:E:1182:ARG:O	3:E:1183:LYS:C	2.57	0.45
2:T:5:DG:H5'	3:E:835:MET:O	2.16	0.45
3:E:78:TRP:HA	3:E:264:TRP:HA	1.97	0.45
3:E:546:HIS:ND1	3:E:692:SER:O	2.49	0.45
3:E:563:ALA:CB	3:E:956:PRO:O	2.65	0.45
3:E:678:ALA:HB2	4:E:1401:SF4:S4	2.57	0.45
3:E:123:ASP:CB	3:E:129:PHE:HE2	2.30	0.44
3:E:138:TYR:CG	3:E:190:LYS:HE3	2.52	0.44
3:E:520:LEU:CD1	3:E:833:TYR:CE2	3.00	0.44
3:E:1096:LYS:CB	3:E:1097:PRO:CD	2.94	0.44
3:E:431:TYR:O	3:E:431:TYR:CG	2.70	0.44
3:E:812:MET:HG3	3:E:815:LEU:HD23	1.99	0.44
3:E:276:THR:C	3:E:278:LYS:N	2.75	0.43
2:T:6:DC:H5'	3:E:553:TYR:CZ	2.53	0.43
3:E:1043:VAL:HG12	3:E:1137:ILE:HD12	2.00	0.43
1:P:1:DC:H3'	1:P:2:DT:H71	2.00	0.43
3:E:267:VAL:HG13	3:E:267:VAL:O	2.19	0.43
3:E:810:LYS:HA	3:E:813:ILE:HD12	2.00	0.43
3:E:833:TYR:O	3:E:836:ARG:N	2.39	0.43
3:E:794:ASN:HA	3:E:797:LYS:HG2	2.01	0.43
3:E:812:MET:HA	3:E:815:LEU:HB3	1.99	0.43
1:P:10:DC:N4	2:T:5:DG:H22	2.17	0.43
3:E:434:GLN:O	3:E:989:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:833:TYR:O	3:E:835:MET:N	2.53	0.42
3:E:1100:ALA:HB1	3:E:1101:PRO:CD	2.50	0.42
3:E:834:VAL:O	3:E:834:VAL:HG23	2.20	0.42
3:E:843:SER:O	3:E:844:MET:C	2.62	0.42
3:E:679:ARG:HB3	3:E:764:GLN:NE2	2.35	0.42
3:E:58:PRO:HD2	3:E:74:GLY:HA2	2.01	0.42
3:E:127:GLY:O	3:E:128:SER:CB	2.67	0.41
3:E:565:VAL:HG13	3:E:565:VAL:O	2.19	0.41
3:E:68:ASP:HB3	3:E:71:GLN:CD	2.45	0.41
1:P:4:DT:H2"	1:P:5:DT:C5'	2.47	0.41
3:E:824:LYS:HG2	3:E:828:ASN:HD21	1.85	0.41
3:E:74:GLY:O	3:E:75:ARG:HD2	2.20	0.41
1:P:3:DG:C2'	1:P:4:DT:H72	2.50	0.41
3:E:259:ILE:HA	3:E:265:TYR:CE1	2.56	0.41
3:E:547:LEU:HD23	3:E:690:PHE:CD2	2.56	0.41
3:E:842:TYR:CD2	3:E:843:SER:N	2.89	0.41
3:E:657:ASP:OD2	3:E:657:ASP:C	2.64	0.41
1:P:10:DC:OP2	3:E:982:LYS:HB3	2.21	0.40
3:E:520:LEU:HD12	3:E:833:TYR:CE2	2.56	0.40
3:E:653:ARG:NH2	3:E:768:PRO:HB3	2.37	0.40
3:E:261:VAL:O	3:E:497:CYS:C	2.65	0.40
3:E:784:PHE:HE2	3:E:819:LEU:HB3	1.80	0.40
3:E:840:ARG:C	3:E:842:TYR:H	2.30	0.40
3:E:261:VAL:HB	3:E:497:CYS:HB3	2.04	0.40
3:E:1028:ASP:HB3	3:E:1036:MET:HE1	2.03	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
3	E	1113/1160 (96%)	1053 (95%)	48 (4%)	12 (1%)	11 43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	833	TYR
3	E	845	GLU
3	E	846	MET
3	E	1095	SER
3	E	1096	LYS
3	E	659	ILE
3	E	1102	VAL
3	E	128	SER
3	E	834	VAL
3	E	798	ILE
3	E	1169	ASN
3	E	1137	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	E	972/1044 (93%)	952 (98%)	20 (2%)	47 66

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	30	TYR
3	E	167	LEU
3	E	689	PHE
3	E	795	LEU
3	E	815	LEU
3	E	825	VAL
3	E	827	LEU
3	E	834	VAL
3	E	980	GLU
3	E	1025	ARG
3	E	1036	MET
3	E	1038	GLU
3	E	1041	ASP

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Mol	Chain	Res	Type
3	E	1057	LYS
3	E	1076	PHE
3	E	1083	LYS
3	E	1092	ILE
3	E	1121	SER
3	E	1133	GLU
3	E	1184	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	36	GLN
3	E	185	GLN
3	E	197	ASN
3	E	523	GLN
3	E	526	GLN
3	E	572	ASN
3	E	631	ASN
3	E	828	ASN
3	E	924	GLN
3	E	973	ASN
3	E	993	GLN
3	E	997	ASN

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

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SF4	E	1401	3	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	E	1401	3	-	-	0/6/5/5

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.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1401	SF4	6	0

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.

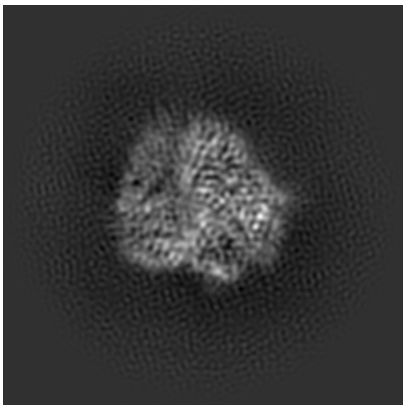
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44356. These allow visual inspection of the internal detail of the map and identification of artifacts.

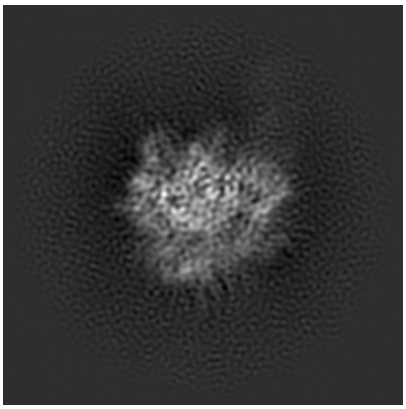
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

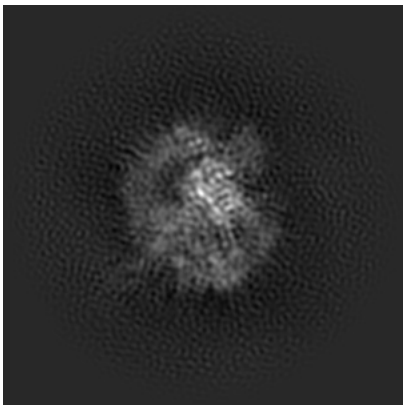
6.1.1 Primary map



X

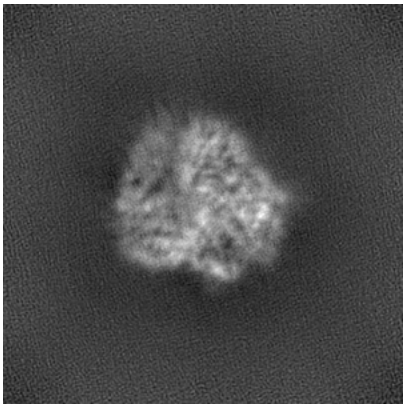


Y

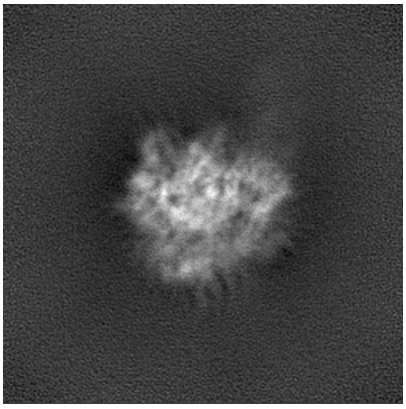


Z

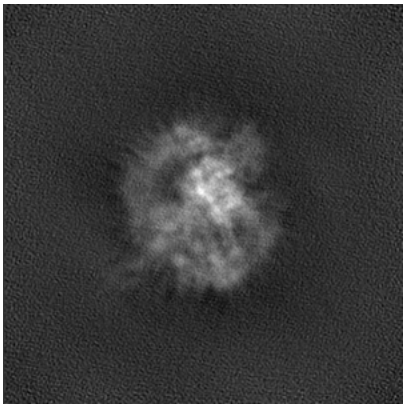
6.1.2 Raw map



X



Y

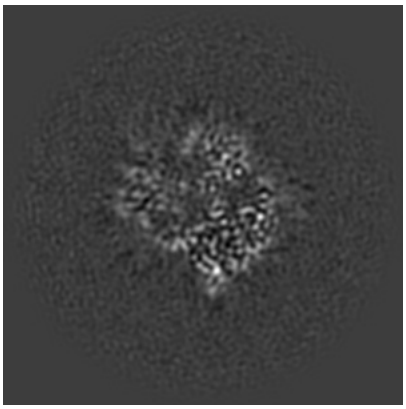


Z

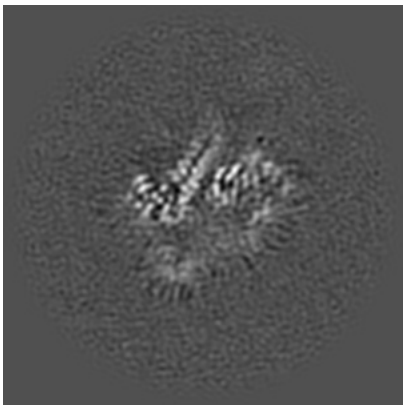
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

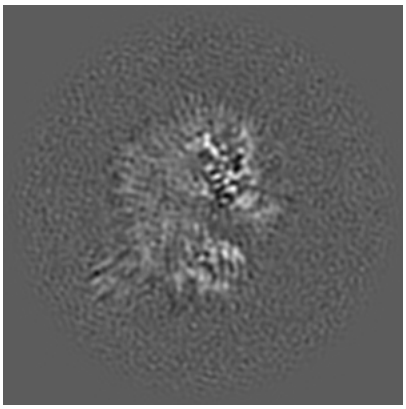
6.2.1 Primary map



X Index: 128

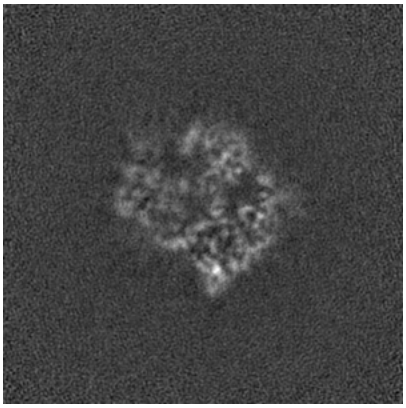


Y Index: 128

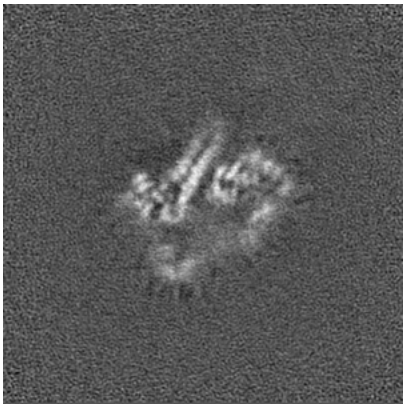


Z Index: 128

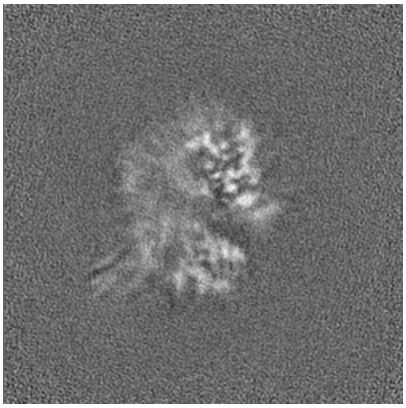
6.2.2 Raw map



X Index: 128



Y Index: 128

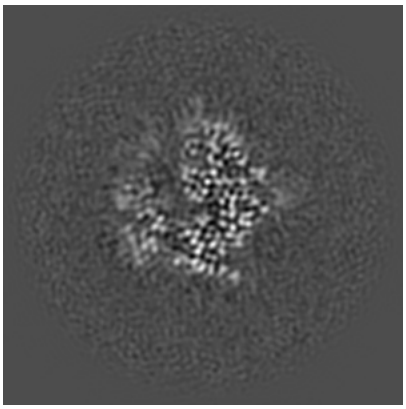


Z Index: 128

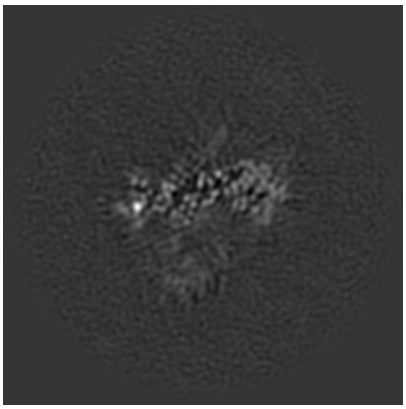
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

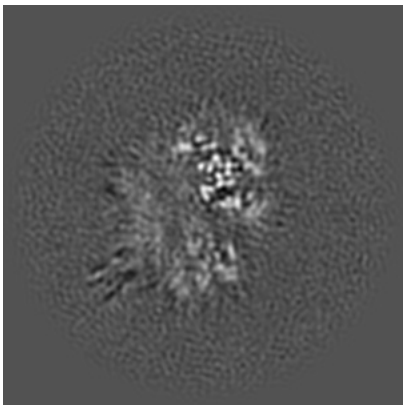
6.3.1 Primary map



X Index: 137

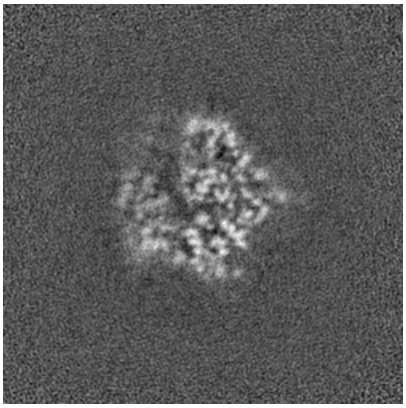


Y Index: 136

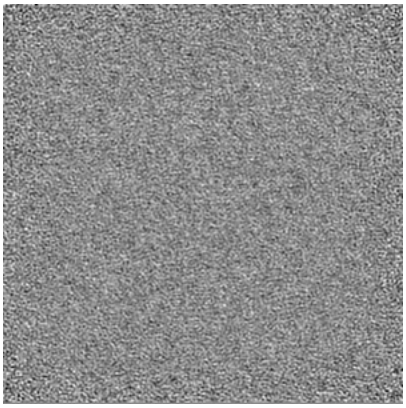


Z Index: 122

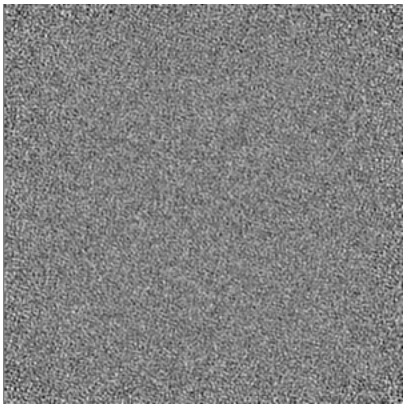
6.3.2 Raw map



X Index: 135



Y Index: 0

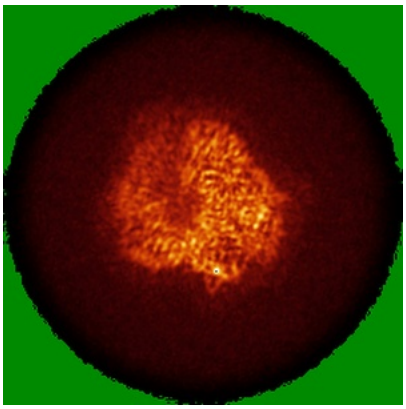


Z Index: 0

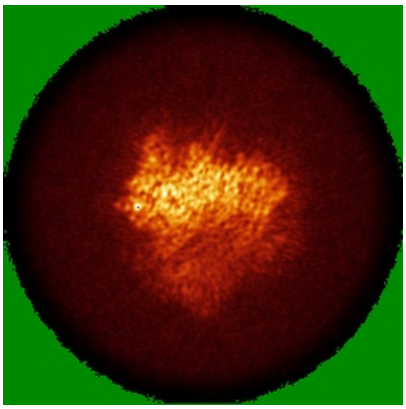
The images above show the largest variance slices of the map in three orthogonal directions.

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

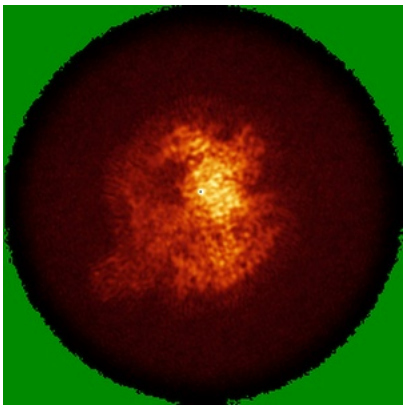
6.4.1 Primary map



X

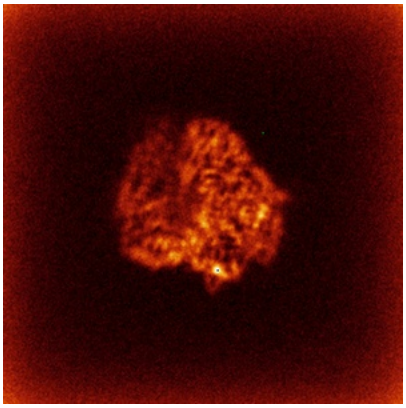


Y

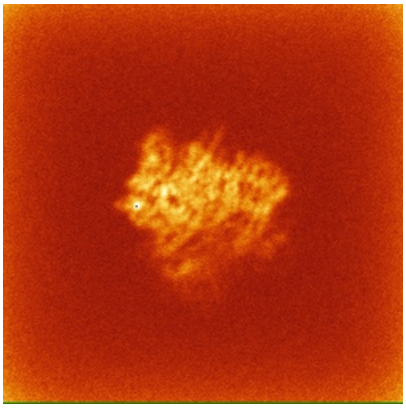


Z

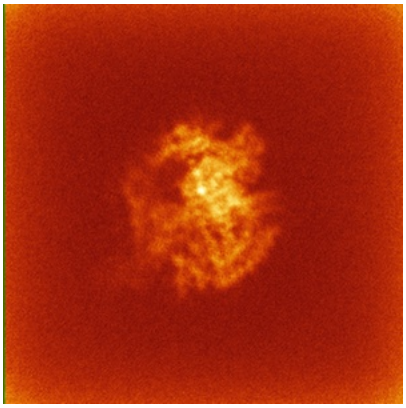
6.4.2 Raw map



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 0.2. 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.

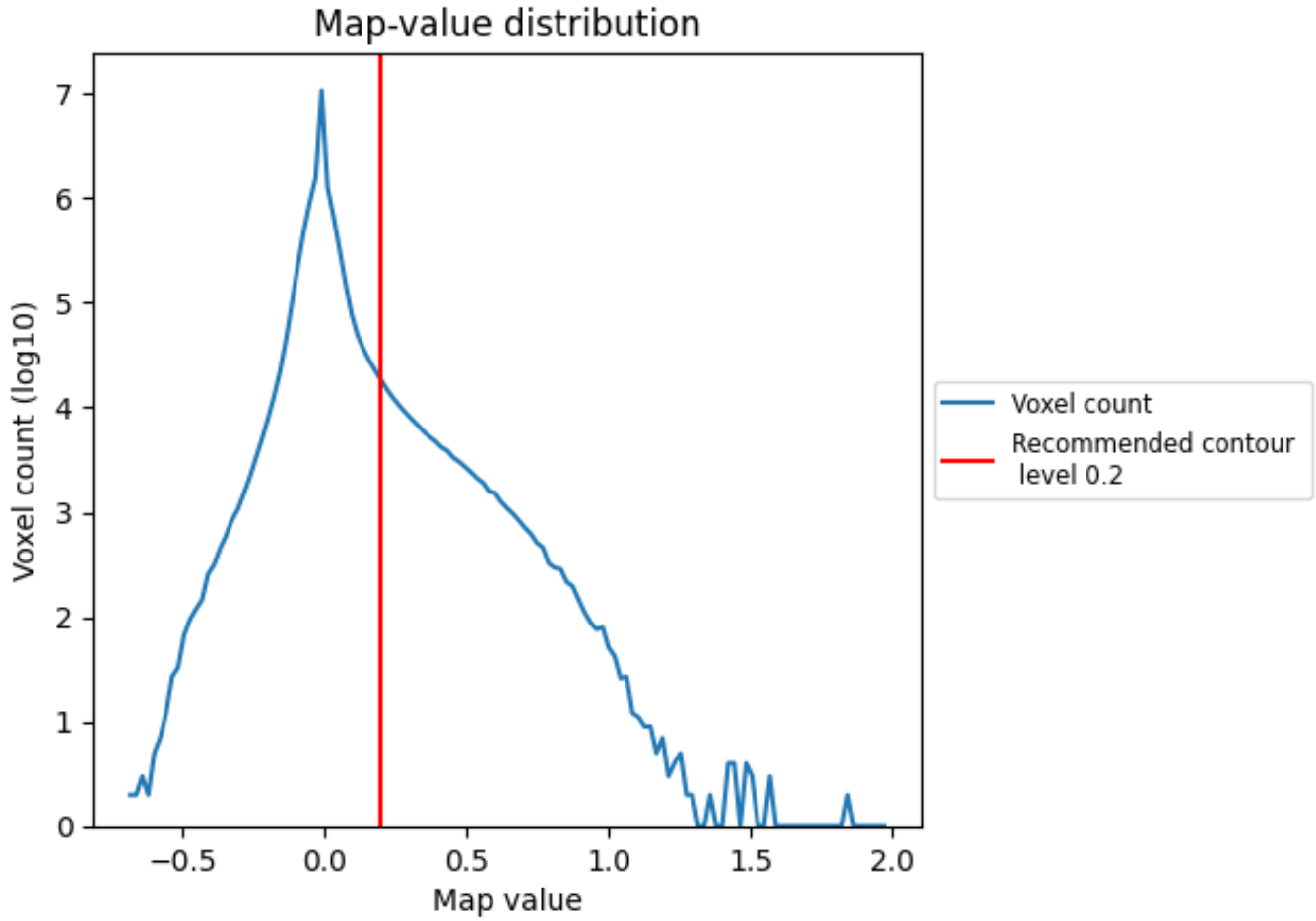
6.6 Mask visualisation (i)

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

7 Map analysis

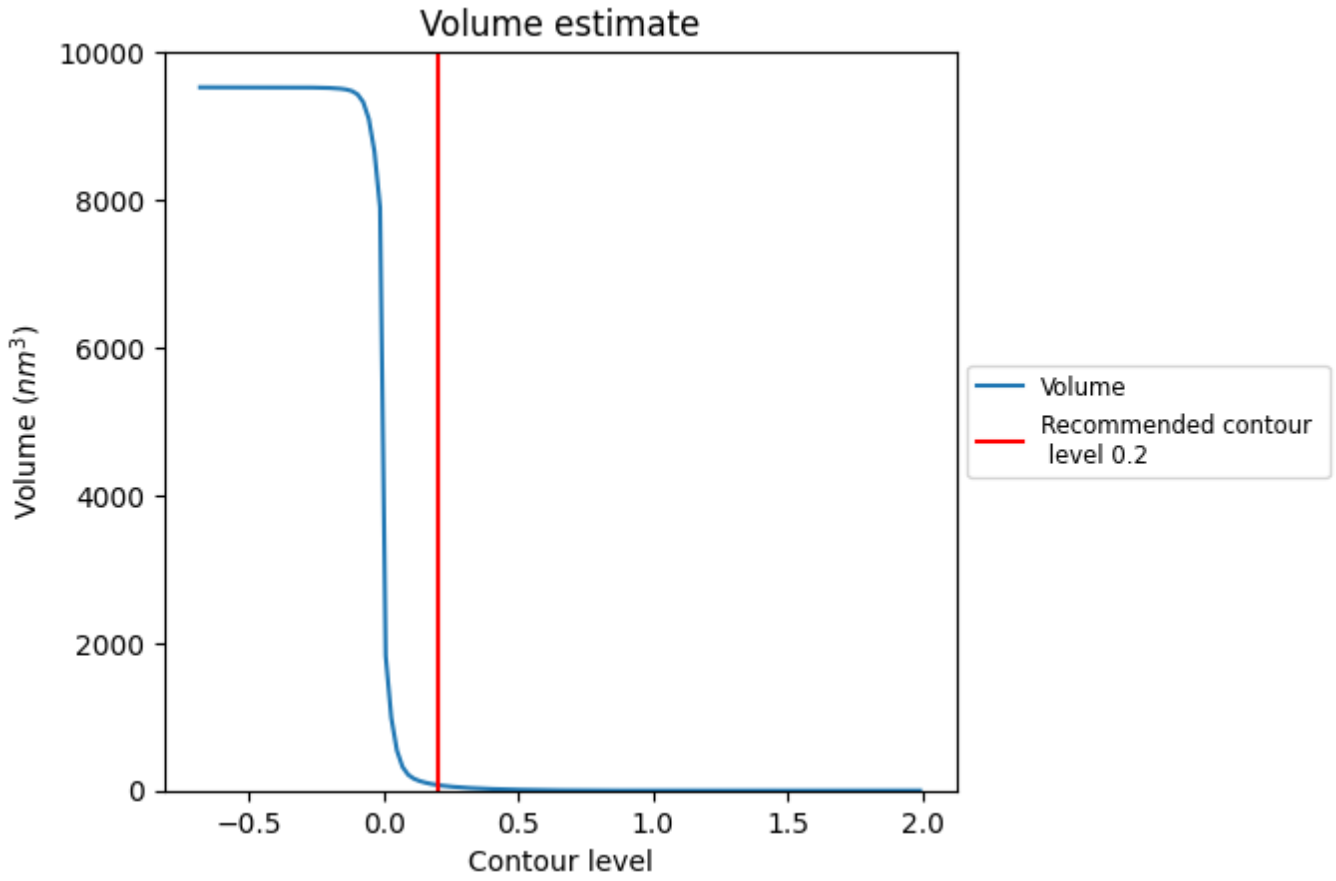
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

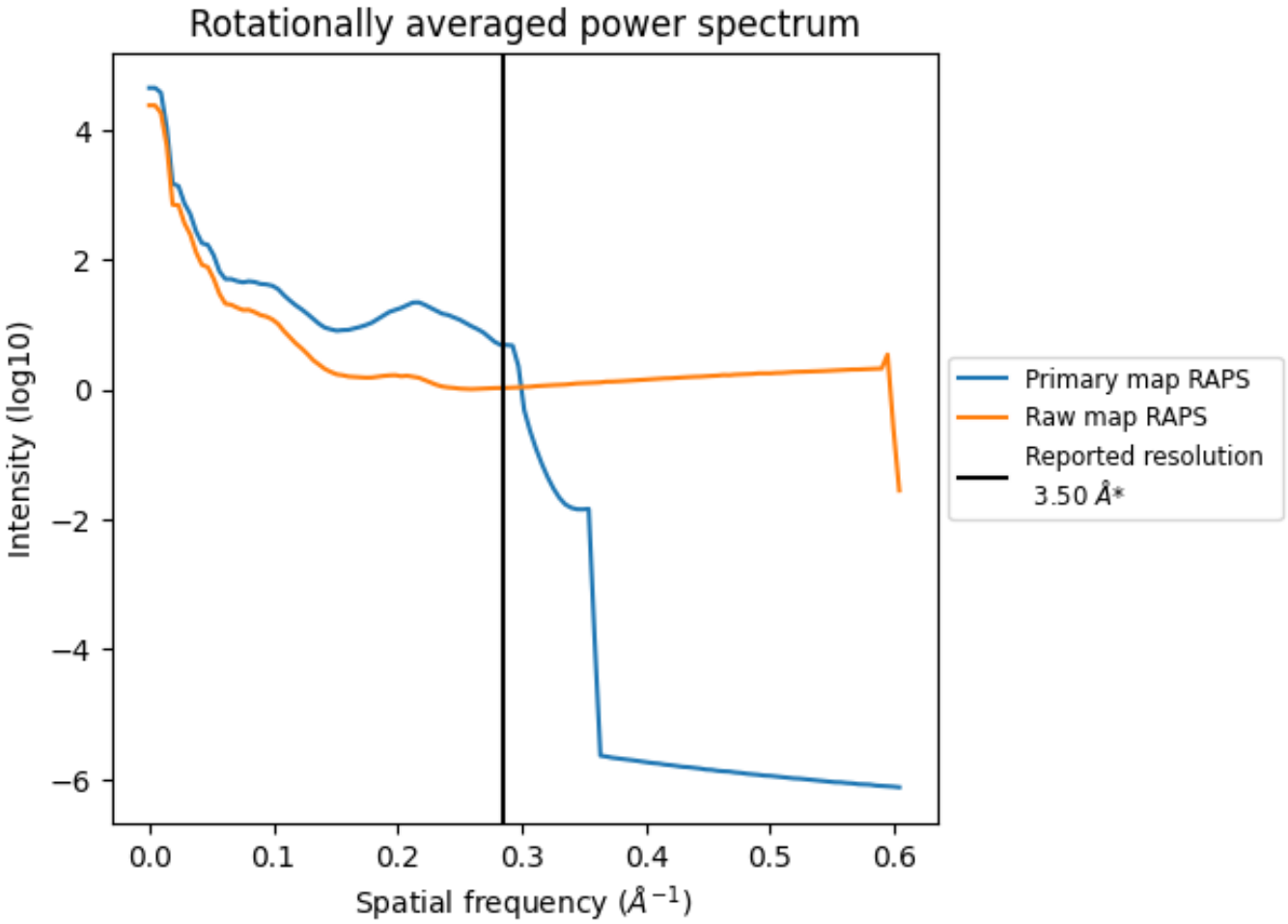
7.2 Volume estimate



The volume at the recommended contour level is 75 nm^3; this corresponds to an approximate mass of 68 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 (i)

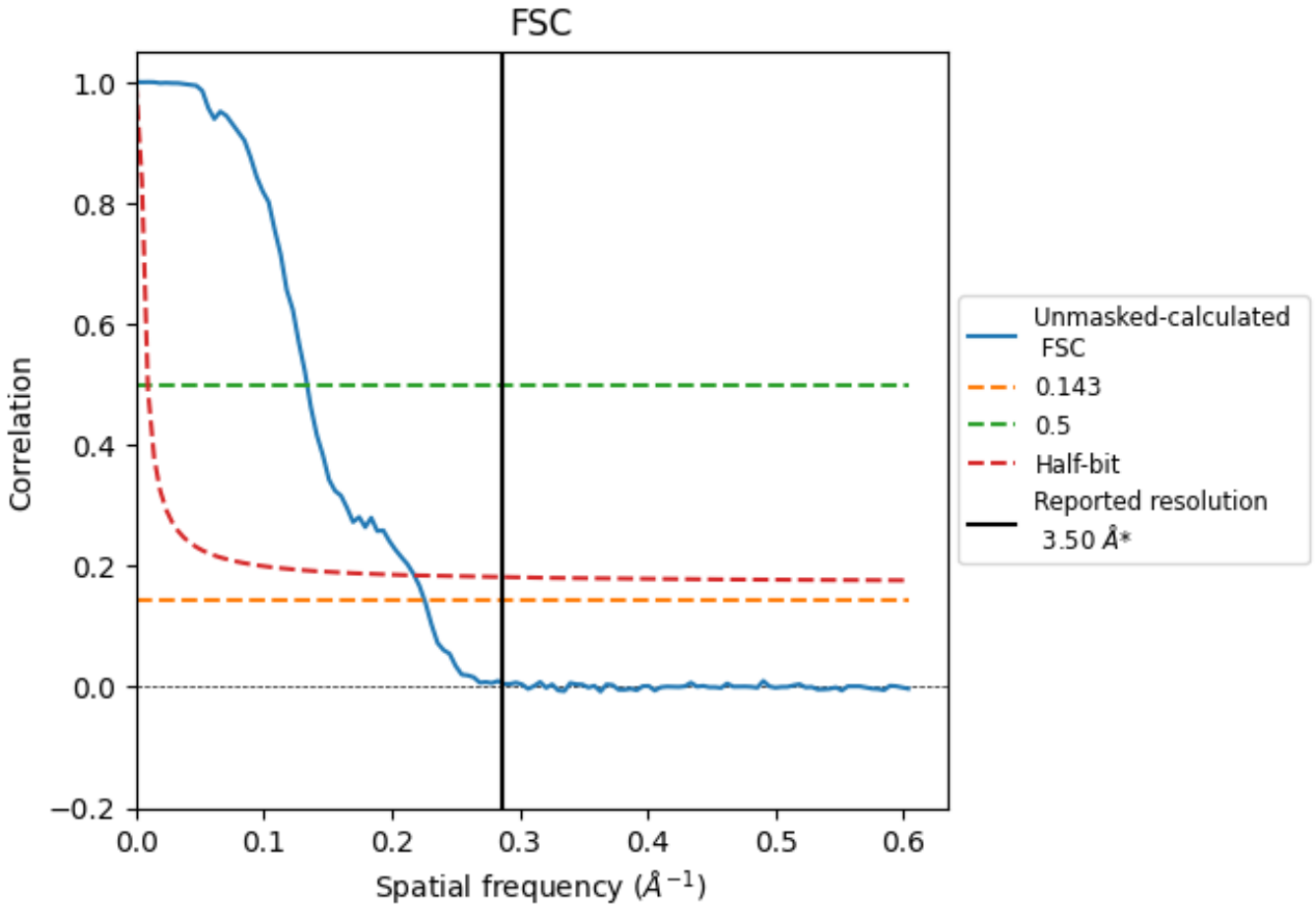


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

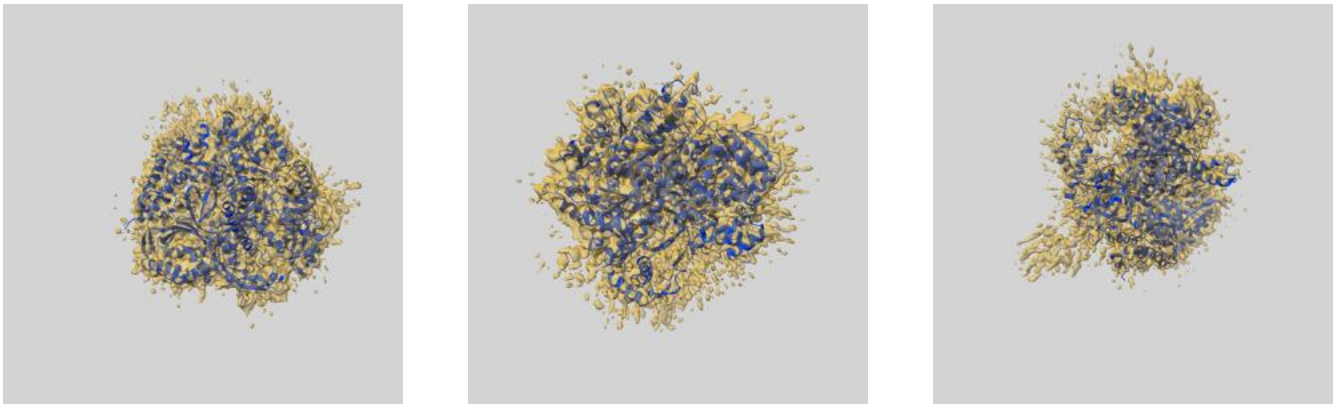
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.43	7.47	4.60

*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 4.43 differs from the reported value 3.5 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44356 and PDB model 9B8R. Per-residue inclusion information can be found in section 3 on page 6.

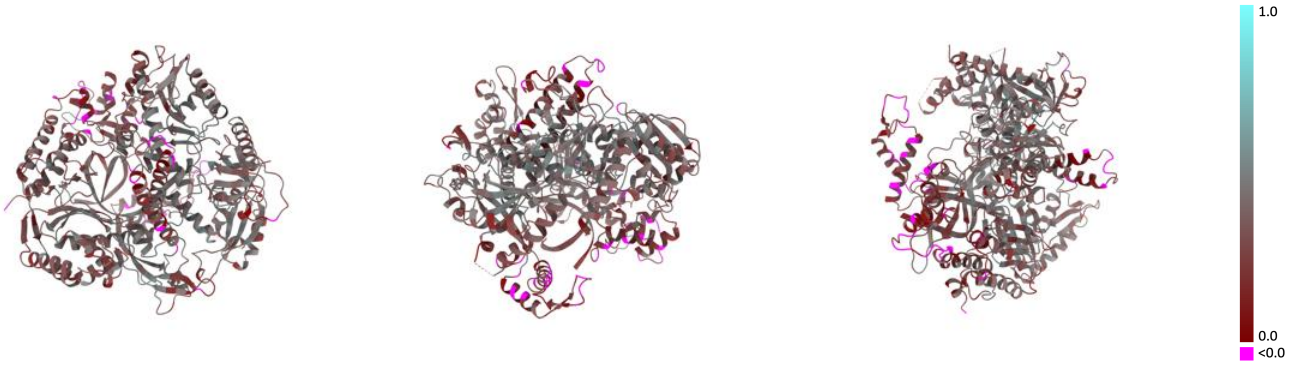
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

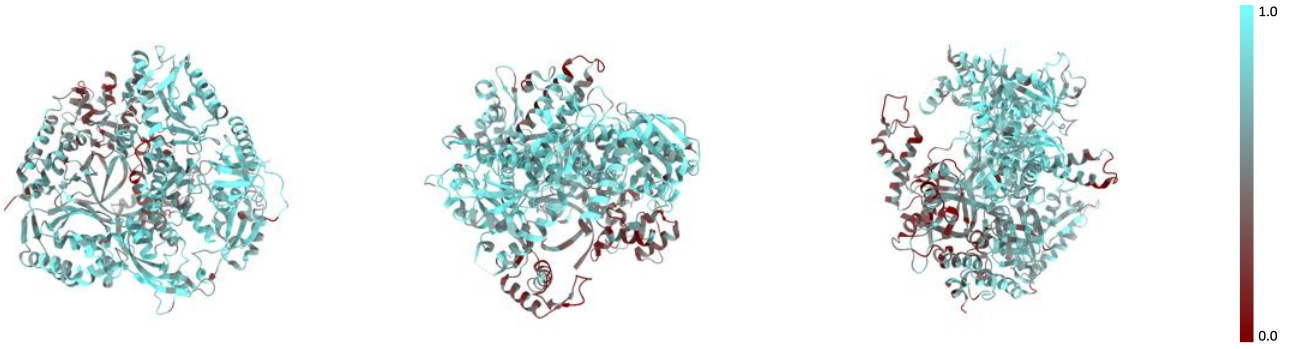
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

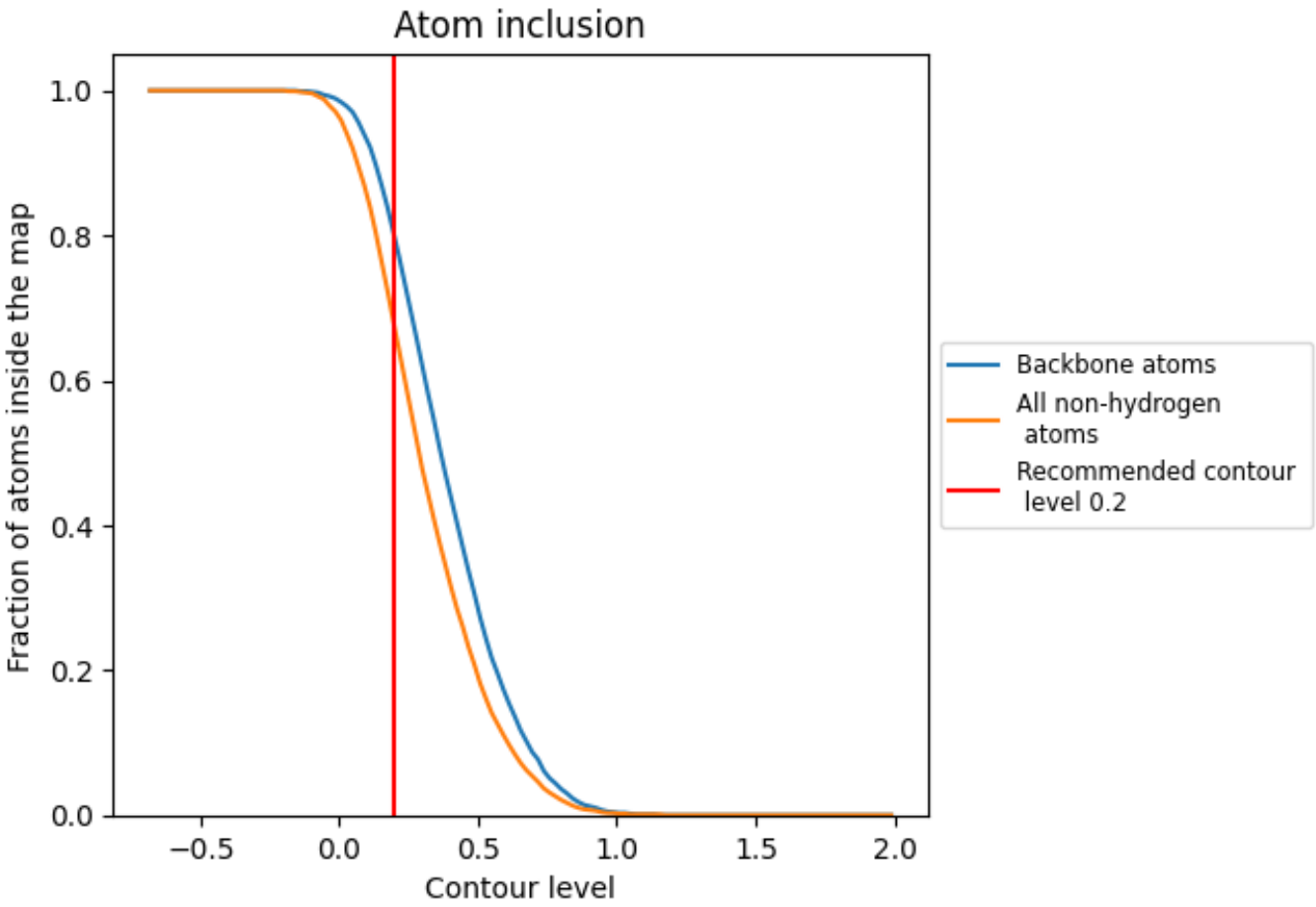
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 67% 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 (0.2) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.6720	0.3320
E	0.6780	0.3300
P	0.5640	0.3620
T	0.5520	0.3480