wwPDB EM Validation Summary Report (i)

Aug 26, 2024 – 01:39 PM EDT

PDB ID	:	8TW9
EMDB ID	:	EMD-41663
Title	:	Cryo-EM structure of S. cerevisiae PolE-Ctf18-8-1-DNA
Authors	:	Yuan, Z.; Georgescu, R.; O'Donnell, M.; Li, H.
Deposited on	:	2023-08-20
Resolution	:	3.60 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

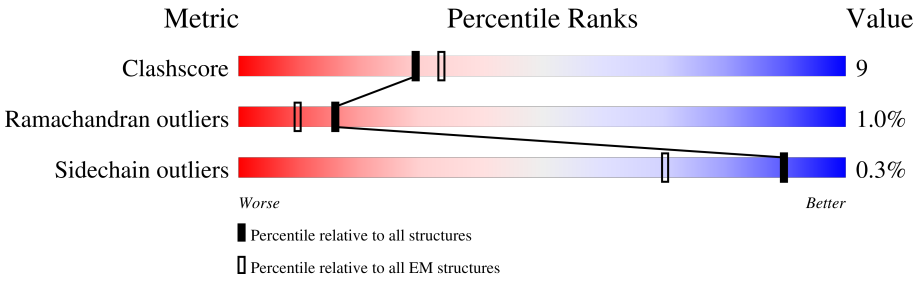
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

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 3.60 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	C	26	73% 27%
2	P	9	11% 67% 22%
3	T	15	7% 33% 60% 7%
4	E	2222	43% 7% 49%
5	D	132	78% 21%
6	B	380	73% 24%

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
7	SF4	E	2301	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13586 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 Chromosome transmission fidelity protein 18.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	C	26	Total	C	N	O	0	0
			206	132	37	37		

- Molecule 2 is a DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	9	Total	C	N	O	P	0	0
			183	88	29	57	9		

- Molecule 3 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	15	Total	C	N	O	P	0	0
			303	147	54	88	14		

- Molecule 4 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	1124	Total	C	N	O	S	0	0
			8919	5681	1507	1690	41		

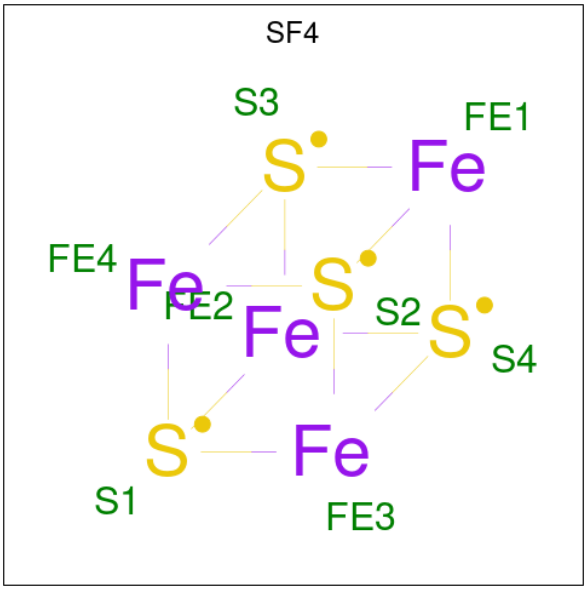
- Molecule 5 is a protein called Chromosome transmission fidelity protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	132	Total	C	N	O	S	0	0
			1014	642	171	194	7		

- Molecule 6 is a protein called Sister chromatid cohesion protein DCC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	374	Total	C	N	O	S	0	0
			2953	1893	489	557	14		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

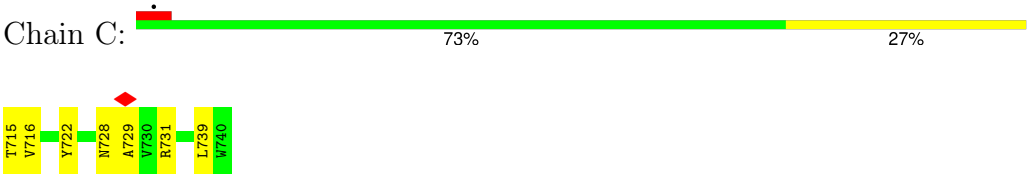


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
7	E	1	8	4	4	0

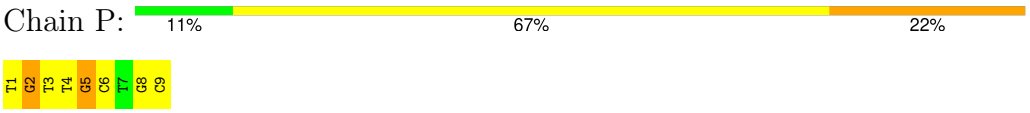
3 Residue-property plots (i)

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.

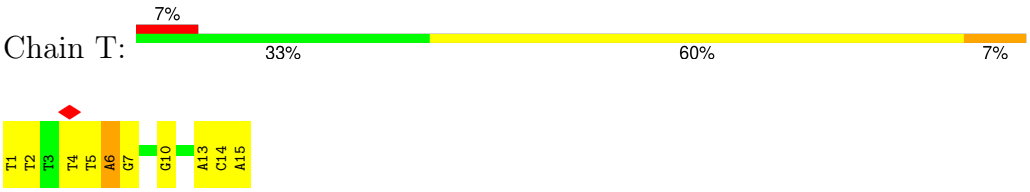
• Molecule 1: Chromosome transmission fidelity protein 18



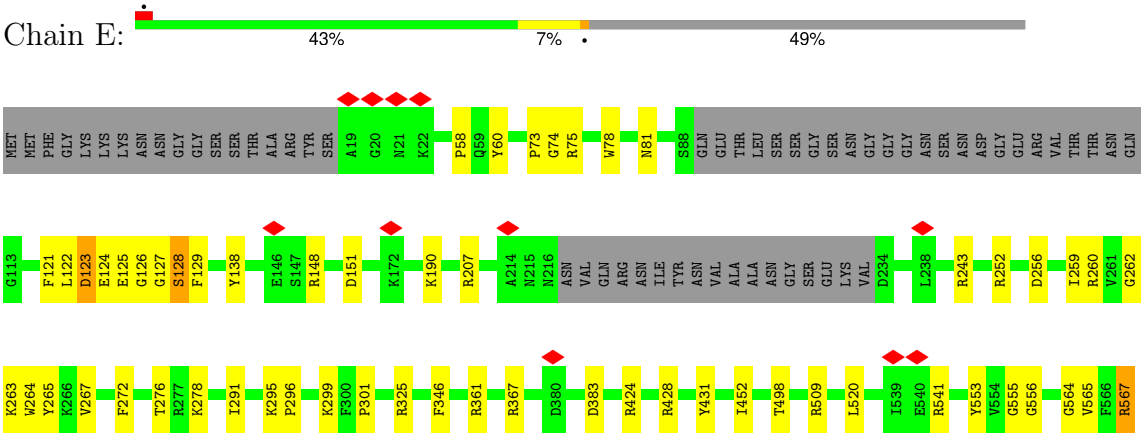
• Molecule 2: Primer DNA

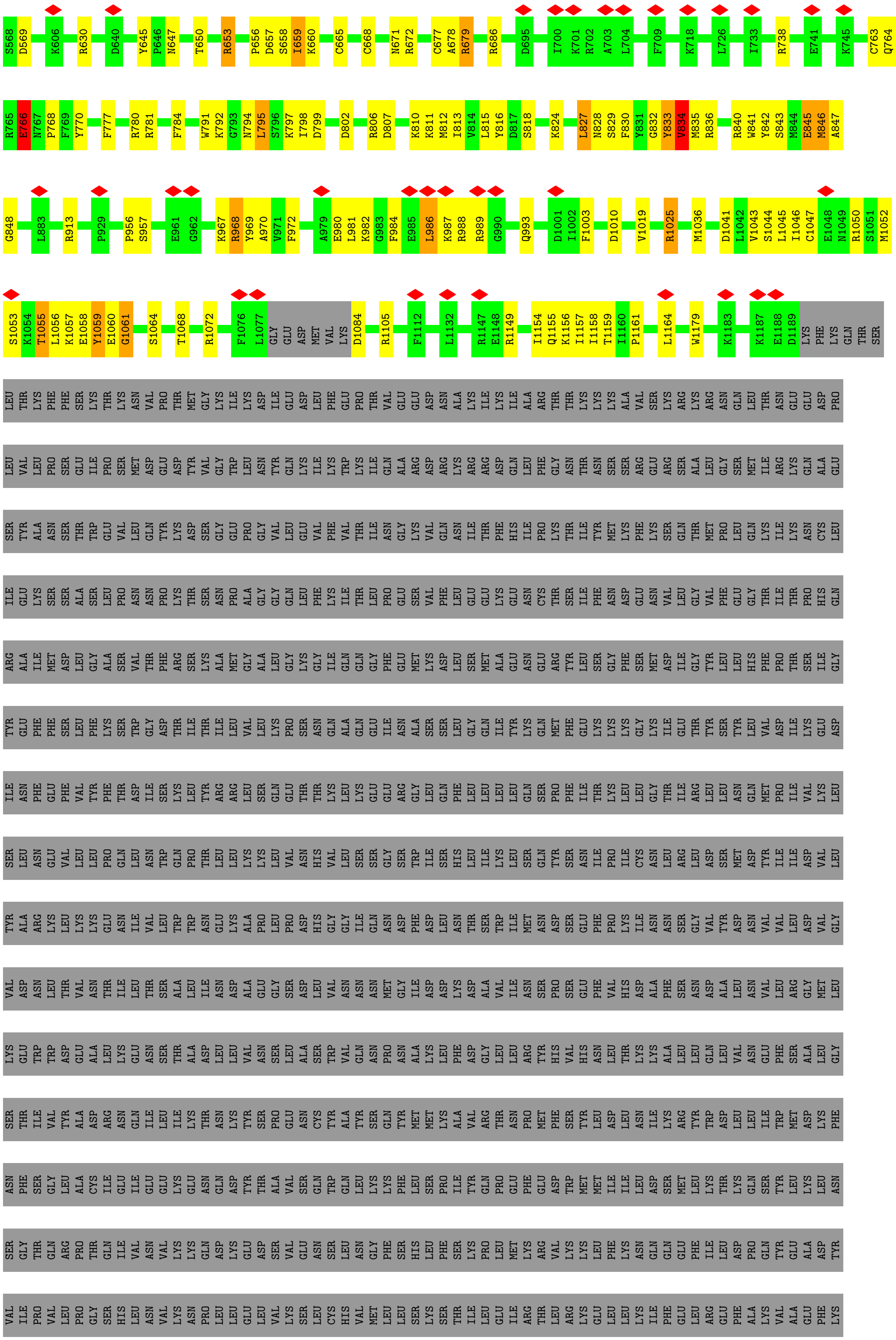


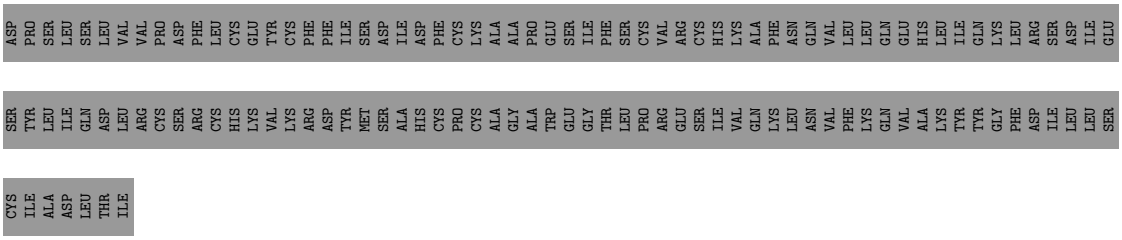
• Molecule 3: Template DNA



• Molecule 4: DNA polymerase epsilon catalytic subunit A

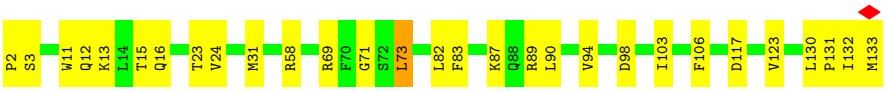



S568 D569 K606 R630 D640 Y645 P646 N647 T650 R653 P656 D657 S658 I659 K660 C665 C668 N671 R672 C677 A678 R679 R686 D695 I700 K701 R702 A703 L704 F709 K718 L726 I733 R738 E741 K745 C763 Q764
R765 E766 N767 P768 F769 Y770 F777 R780 R781 F784 W791 K792 G793 N794 L795 S796 K797 I798 D799 D802 R806 D807 K810 K811 M812 I813 V814 L815 Y816 D817 S818 K824 L827 N828 S829 F830 Y831 G832 Y833 V834 M835 R836 R840 W841 Y842 S843 M844 E845 M846 A847
G848 L883 R913 P929 P956 S957 E961 G962 K967 R968 Y969 A970 V971 F972 A979 E980 L981 K982 G983 F984 E985 L986 K987 R988 R989 G990 Q993 D1001 I1002 F1003 D1010 V1019 R1025 M1036 D1041 L1042 V1043 S1044 L1045 I1046 C1047 E1048 N1049 R1050 S1051 M1052
S1053 K1054 T1055 L1056 K1057 E1058 Y1059 E1060 G1061 S1064 T1068 R1072 F1076 L1077 GLY GLU ASP MET VAL LYS D1084 R1105 F1112 L1132 R1147 E1148 R1149 I1154 Q1155 K1156 I1157 I1158 T1159 I1160 P1161 L1164 W1179 K1183 K1187 E1188 D1189 LYS PHE LYS GLN THR SER
LEU THR LYS PHE PHE SER LYS THR LYS ASN VAL PRO THR MET GLY LYS ILE LYS ASP ILE GLU ASP LEU PHE GLU PRO THR VAL GLU GLU ASP ASN ALA LYS ILE LYS ILE ALA ARG THR THR LYS LYS LYS ALA VAL SER LYS ARG LYS ARG ASN GLN LEU THR ASN GLU GLU ASP PRO
LEU VAL LEU PRO SER GLU ILE PRO SER MET ASP GLU ASP TYR VAL GLY TRP LEU ASN TYR GLN LYS ILE LYS TRP LYS ILE GLN ALA ARG ASP ARG LYS ARG ARG ASP GLN LEU PHE GLY ASN THR ASN SER SER ARG GLU ARG SER ALA LEU GLY SER MET ILE ARG LYS GLN ALA GLU
SER TYR ALA ASN SER THR TRP GLU VAL LEU GLN TYR LYS ASP SER GLY GLU PRO GLY VAL LEU GLU VAL PHE VAL THR ILE ASN GLY LYS VAL GLN ASN ILE THR PHE HIS ILE PRO LYS THR ILE TYR MET LYS PHE LYS SER GLN THR MET PRO LEU GLN LYS ILE LYS ASN CYS LEU
ILE GLU LYS SER SER ALA SER LEU PRO ASN ASN PRO LYS THR SER ASN PRO ALA GLY GLY GLN LEU PHE LYS ILE THR LEU PRO GLU SER VAL PHE LEU GLU GLU LYS GLU ASN CYS THR SER ILE PHE ASN ASP GLU ASN VAL LEU GLY VAL PHE GLU GLY THR ILE THR PRO HIS GLN
ARG ALA ILE MET ASP LEU GLY ALA SER VAL THR PHE ARG SER LYS ALA MET GLY ALA LEU GLY LYS GLY ILE GLN GLN GLY PHE GLU MET LYS ASP LEU SER MET ALA GLU ASN GLU ARG TYR LEU SER GLY PHE SER MET ASP ILE GLY TYR LEU LEU HIS PHE PRO THR SER ILE GLY
TYR GLU PHE PHE SER LEU PHE LYS SER TRP GLY ASP THR ILE THR ILE LEU VAL LEU LYS PRO SER ASN GLN ALA GLN GLU ILE ASN ALA SER SER LEU GLY GLN ILE TYR LYS GLN MET PHE GLU LYS LYS LYS GLY LYS ILE GLU THR TYR SER TYR LEU VAL ASP ILE LYS GLU ASP
ILE ASN PHE GLU PHE VAL TYR PHE THR ASP ILE SER LYS LEU TYR ARG ARG LEU SER GLN GLU THR THR LYS LEU LYS GLU GLU ARG GLY LEU GLN PHE LEU LEU LEU LEU GLN SER PRO PHE ILE THR LYS LEU LEU GLY THR ILE ARG LEU LEU ASN GLN MET PRO ILE VAL LYS LEU
SER LEU ASN GLU VAL LEU LEU PRO GLN LEU ASN TRP GLN PRO THR LEU LEU LYS LYS LEU VAL ASN HIS VAL LEU SER SER GLY SER TRP ILE SER HIS LEU ILE LYS LEU SER GLN TYR SER ASN ILE PRO ILE CYS ASN LEU ARG LEU ASP SER MET ASP TYR ILE ILE ASP VAL LEU
TYR ALA ARG LYS LEU LYS LYS GLU ASN ILE VAL LEU TRP TRP ASN GLU LYS ALA PRO LEU PRO ASP HIS GLY GLY ILE GLN ASN ASP PHE ASP LEU ASN THR SER TRP ILE MET ASN ASP SER GLU PHE PRO LYS ILE ASN ASN SER GLY VAL TYR ASP ASN VAL VAL LEU ASP VAL GLY
VAL ASP ASN LEU THR VAL ASN THR ILE LEU THR SER ALA LEU ILE ASN ASP ALA GLU GLY SER ASP LEU VAL ASN ASN MET GLY ILE ASP ASP LYS ASP ALA VAL ILE ASN SER PRO SER GLU PHE VAL HIS ASP ALA PHE SER ASN ASP ALA LEU ASN VAL LEU ARG GLY MET LEU
LYS GLU TRP TRP ASP GLU ALA LEU LYS GLU ASN SER THR ALA ASP LEU LEU VAL ASN SER LEU ALA SER TRP VAL GLN ASN PRO ASN ALA LYS LEU PHE ASP GLY LEU LEU ARG TYR HIS VAL HIS ASN LEU THR LYS LYS ALA LEU LEU GLN LEU VAL ASN GLU PHE SER ALA LEU GLY
SER THR ILE VAL TYR ALA ASP ARG ASN GLN ILE LEU ILE LYS THR ASN LYS TYR SER PRO GLU ASN CYS TYR ALA TYR SER GLN TYR MET MET LYS ALA VAL ARG THR ASN PRO MET PHE SER TYR LEU ASP LEU ASN ILE LYS ARG TYR TRP ASP LEU LEU ILE TRP MET ASP LYS PHE
ASN PHE SER GLY LEU ALA CYS ILE GLU ILE GLU GLU LYS GLU ASN GLN ASP TYR THR ALA VAL SER GLN TRP GLN LEU LYS LYS PHE LEU SER PRO ILE TYR GLN PRO GLU PHE GLU ASP TRP MET MET ILE ILE LEU ASP SER MET LEU LYS THR LYS GLN SER TYR LEU LYS LEU ASN
SER GLY THR GLN ARG PRO THR GLN ILE VAL ASN VAL LYS LYS GLN ASP LYS GLU ASP SER VAL GLU ASN SER LEU ASN GLY PHE SER HIS LEU PHE SER LYS PRO LEU MET LYS ARG VAL LYS LYS LEU PHE LYS ASN GLN GLN GLU PHE ILE LEU ASP PRO GLN TYR GLU ALA ASP TYR
VAL ILE PRO VAL LEU PRO GLY SER HIS LEU ASN VAL LYS ASN PRO LEU LEU GLU LEU VAL LYS SER LEU CYS HIS VAL MET LEU LEU SER LYS SER THR ILE LEU GLU ILE ARG THR LEU ARG LYS GLU LEU GLU LYS ILE PHE GLU LEU ARG GLU PHE ALA LYS VAL ALA GLU PHE LYS



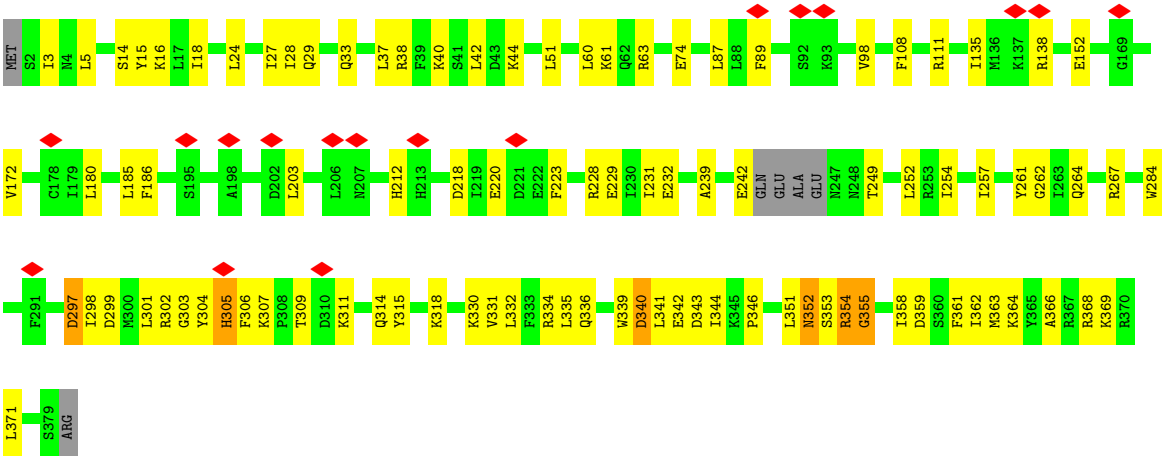
• Molecule 5: Chromosome transmission fidelity protein 8

Chain D:



• Molecule 6: Sister chromatid cohesion protein DCC1

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	385806	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	1.409	Depositor
Minimum map value	-0.591	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.326	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	C	0.42	0/211	0.62	0/289
2	P	1.46	3/203 (1.5%)	1.04	1/311 (0.3%)
3	T	1.41	1/339 (0.3%)	1.00	1/521 (0.2%)
4	E	0.70	1/9121 (0.0%)	0.98	30/12348 (0.2%)
5	D	0.36	0/1030	0.76	1/1387 (0.1%)
6	B	0.51	3/3016 (0.1%)	0.76	8/4083 (0.2%)
All	All	0.69	8/13920 (0.1%)	0.92	41/18939 (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
4	E	0	6
6	B	0	2
All	All	0	8

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	354	ARG	C-N	11.75	1.54	1.33
4	E	766	GLU	C-N	9.57	1.56	1.34
2	P	2	DG	C1'-N9	-8.87	1.34	1.47
2	P	8	DG	C1'-N9	-8.59	1.35	1.47
2	P	5	DG	C1'-N9	-6.77	1.37	1.47

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	325	ARG	NE-CZ-NH1	10.08	125.34	120.30
4	E	913	ARG	NE-CZ-NH1	9.53	125.07	120.30
4	E	672	ARG	NE-CZ-NH2	-9.35	115.62	120.30
4	E	672	ARG	NE-CZ-NH1	9.05	124.83	120.30
4	E	361	ARG	NE-CZ-NH1	9.02	124.81	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	123	ASP	Mainchain
4	E	509	ARG	Sidechain
4	E	567	ARG	Sidechain
4	E	630	ARG	Sidechain
4	E	81	ASN	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	C	206	0	183	8	0
2	P	183	0	102	6	0
3	T	303	0	172	15	0
4	E	8919	0	8572	150	0
5	D	1014	0	1007	29	0
6	B	2953	0	2913	72	0
7	E	8	0	0	6	0
All	All	13586	0	12949	240	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.

The worst 5 of 240 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)
4:E:656:PRO:HB3	4:E:843:SER:HB2	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:5:DT:H4'	4:E:835:MET:CB	2.08	0.83
4:E:60:TYR:CB	4:E:73:PRO:HG3	2.13	0.79
2:P:2:DG:H2'	2:P:3:DT:H71	1.68	0.76
4:E:671:ASN:HB2	7:E:2301:SF4:S3	2.26	0.75

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	24/26 (92%)	22 (92%)	2 (8%)	0	100	100
4	E	1116/2222 (50%)	1051 (94%)	52 (5%)	13 (1%)	11	43
5	D	130/132 (98%)	127 (98%)	3 (2%)	0	100	100
6	B	370/380 (97%)	342 (92%)	25 (7%)	3 (1%)	16	51
All	All	1640/2760 (59%)	1542 (94%)	82 (5%)	16 (1%)	16	46

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	833	TYR
4	E	845	GLU
4	E	846	MET
4	E	987	LYS
4	E	1053	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	20/24 (83%)	20 (100%)	0	100 100
4	E	950/2014 (47%)	946 (100%)	4 (0%)	89 95
5	D	110/119 (92%)	110 (100%)	0	100 100
6	B	326/352 (93%)	326 (100%)	0	100 100
All	All	1406/2509 (56%)	1402 (100%)	4 (0%)	90 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	256	ASP
4	E	795	LEU
4	E	827	LEU
4	E	834	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	828	ASN
4	E	993	GLN
6	B	29	GLN
4	E	997	ASN
4	E	794	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
7	SF4	E	2301	4	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
7	SF4	E	2301	4	-	-	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
7	E	2301	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.

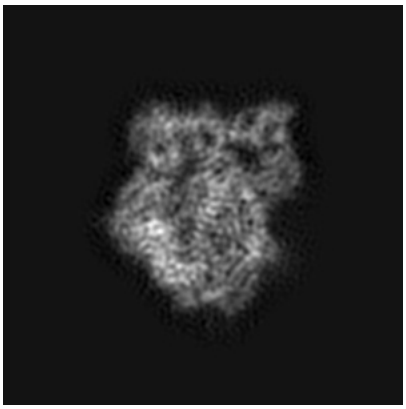
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41663. These allow visual inspection of the internal detail of the map and identification of artifacts.

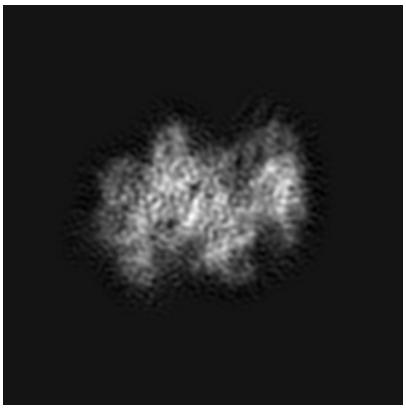
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

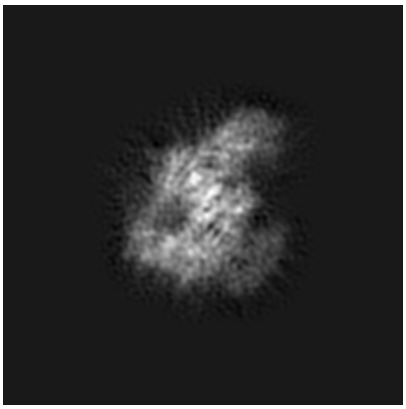
6.1.1 Primary map



X

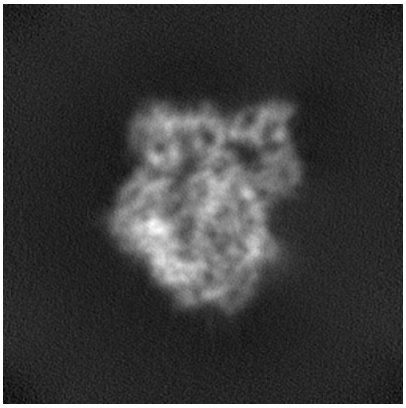


Y

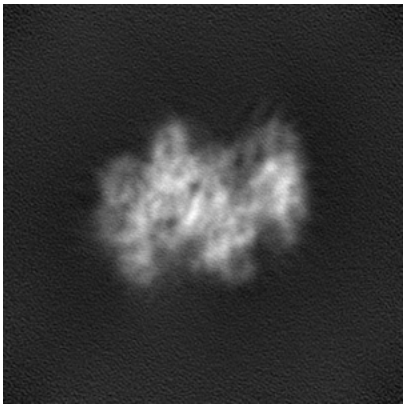


Z

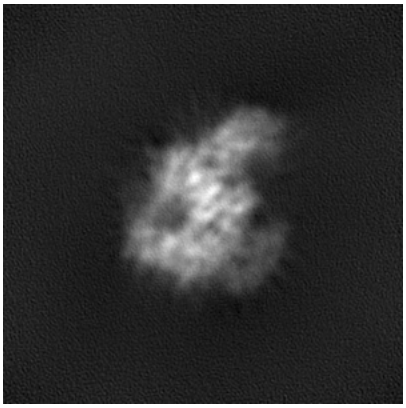
6.1.2 Raw map



X



Y

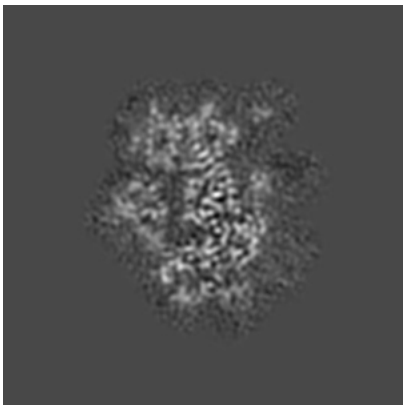


Z

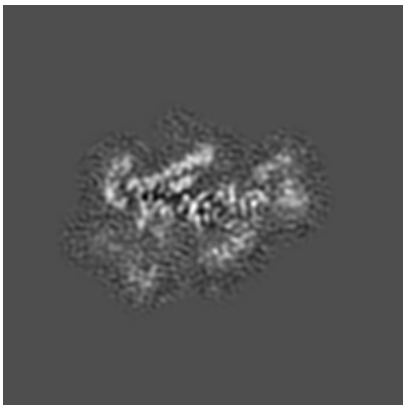
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

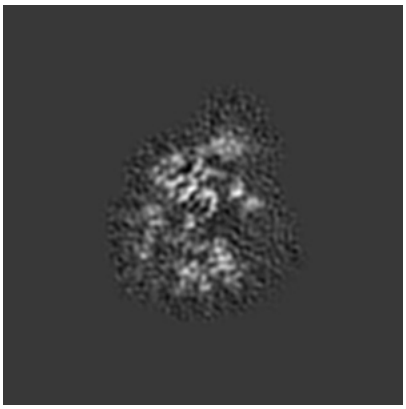
6.2.1 Primary map



X Index: 128

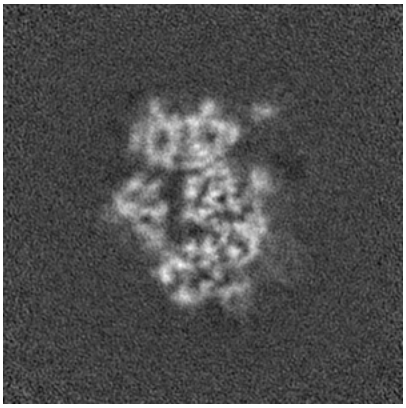


Y Index: 128

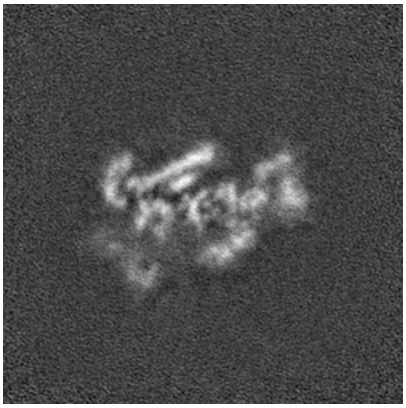


Z Index: 128

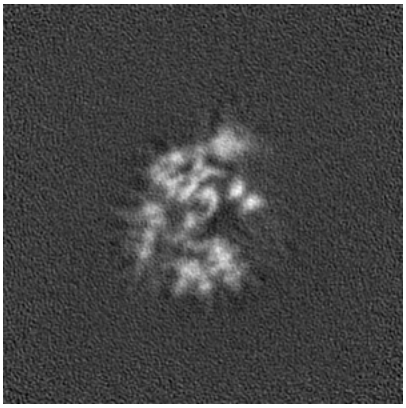
6.2.2 Raw map



X Index: 128



Y Index: 128

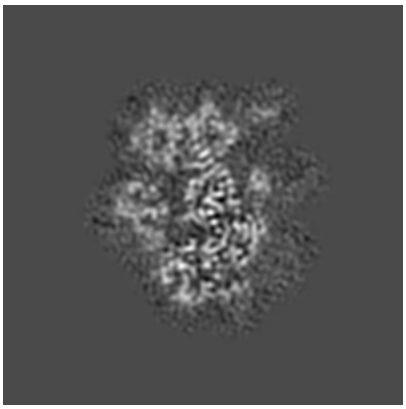


Z Index: 128

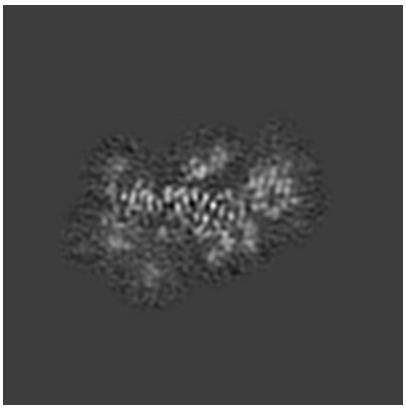
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

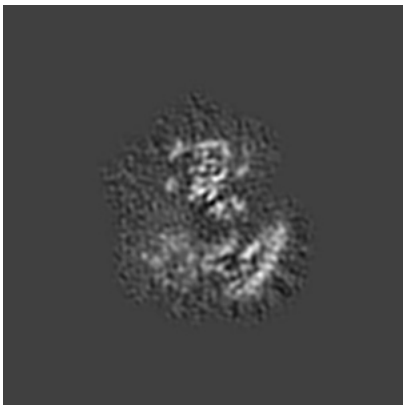
6.3.1 Primary map



X Index: 129

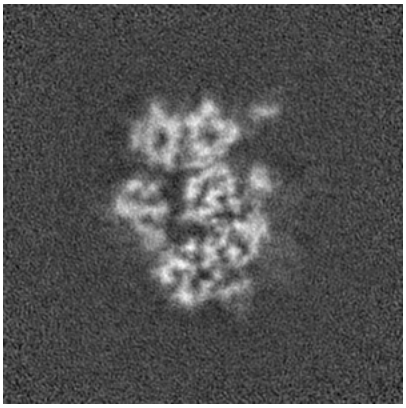


Y Index: 136

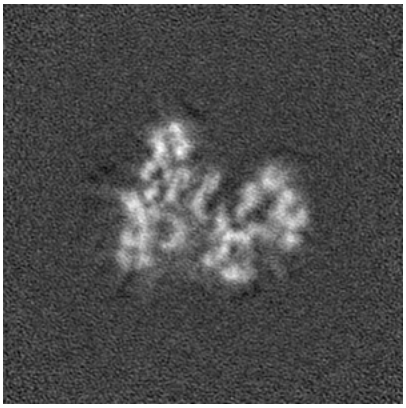


Z Index: 111

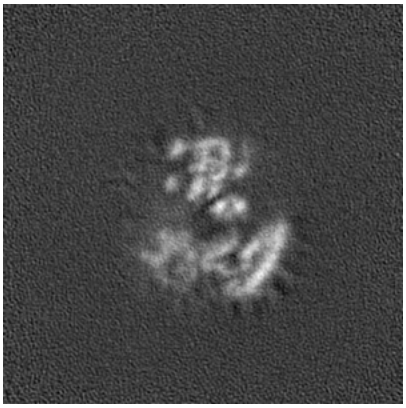
6.3.2 Raw map



X Index: 129



Y Index: 102

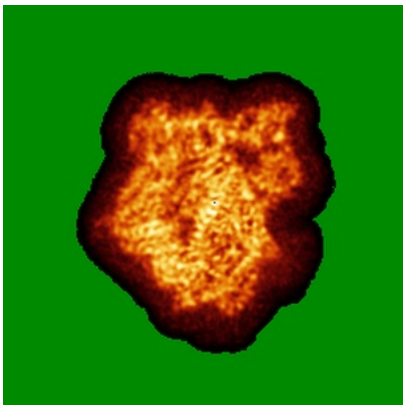


Z Index: 111

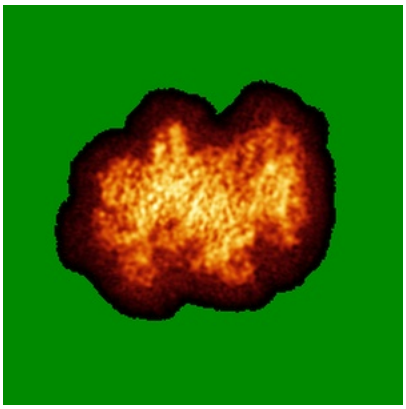
The images above show the largest variance slices of the map in three orthogonal directions.

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

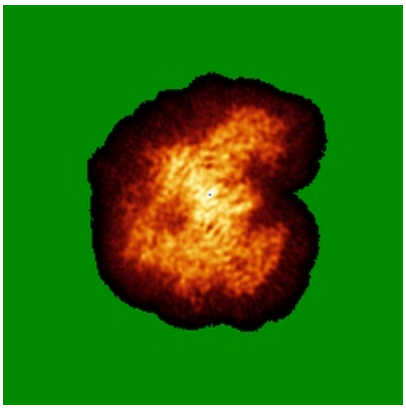
6.4.1 Primary map



X

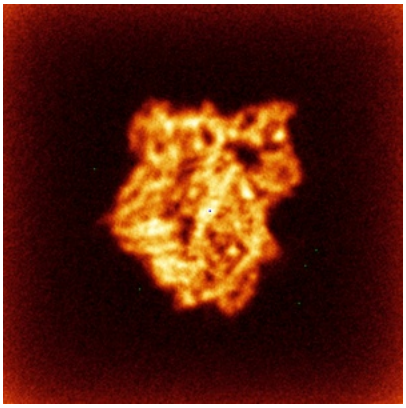


Y

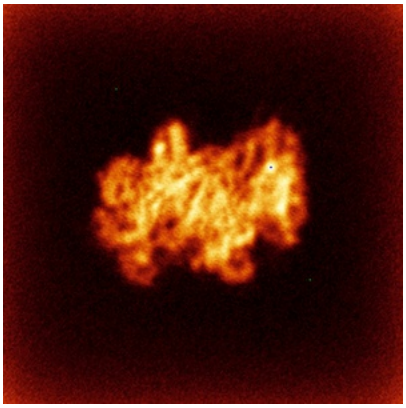


Z

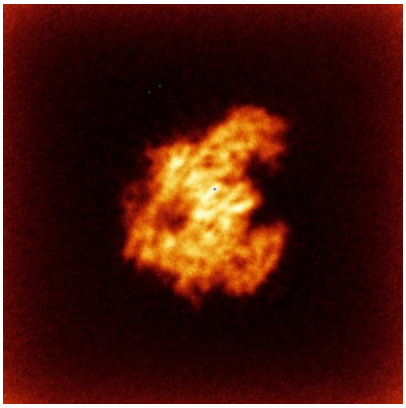
6.4.2 Raw map



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.

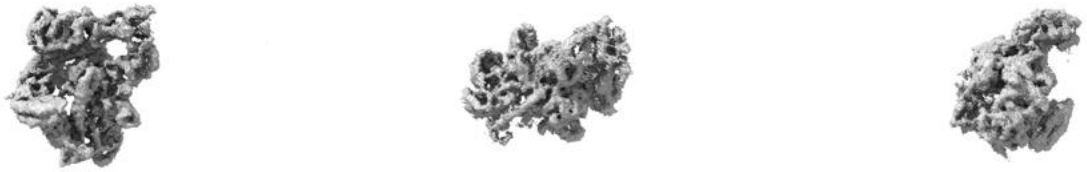
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.326. 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.

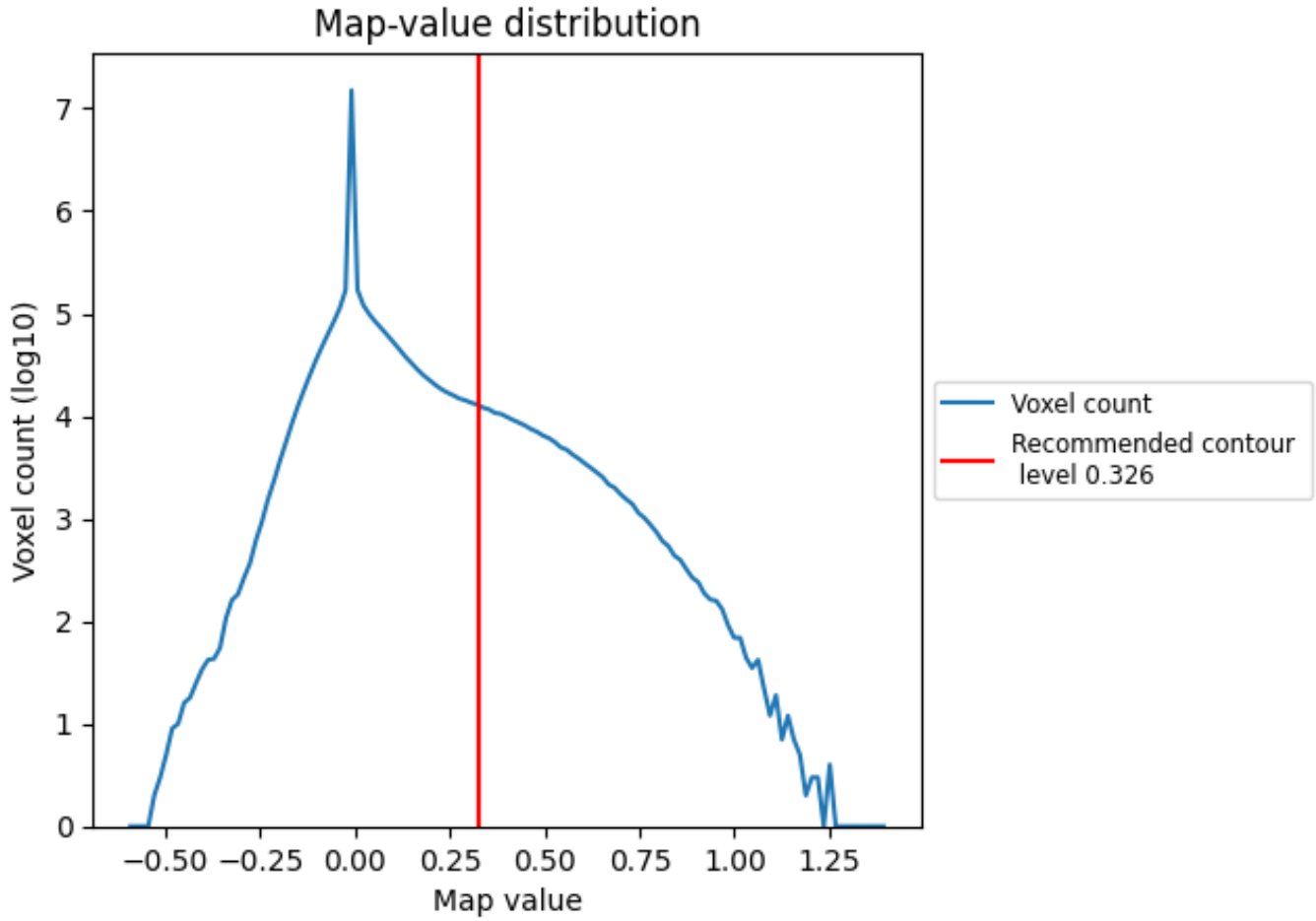
6.6 Mask visualisation (i)

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

7 Map analysis

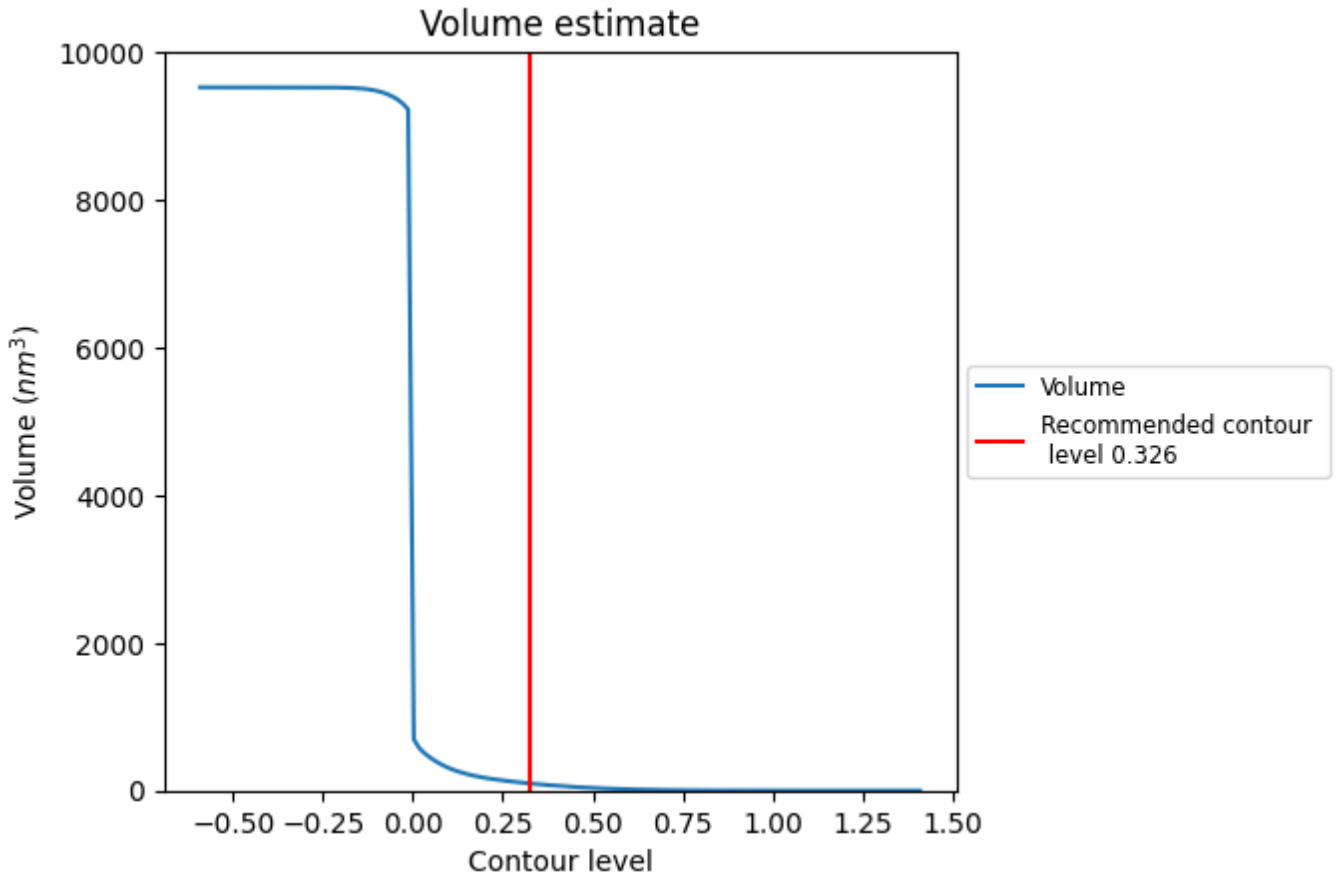
This section contains the results of statistical analysis of the map.

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.

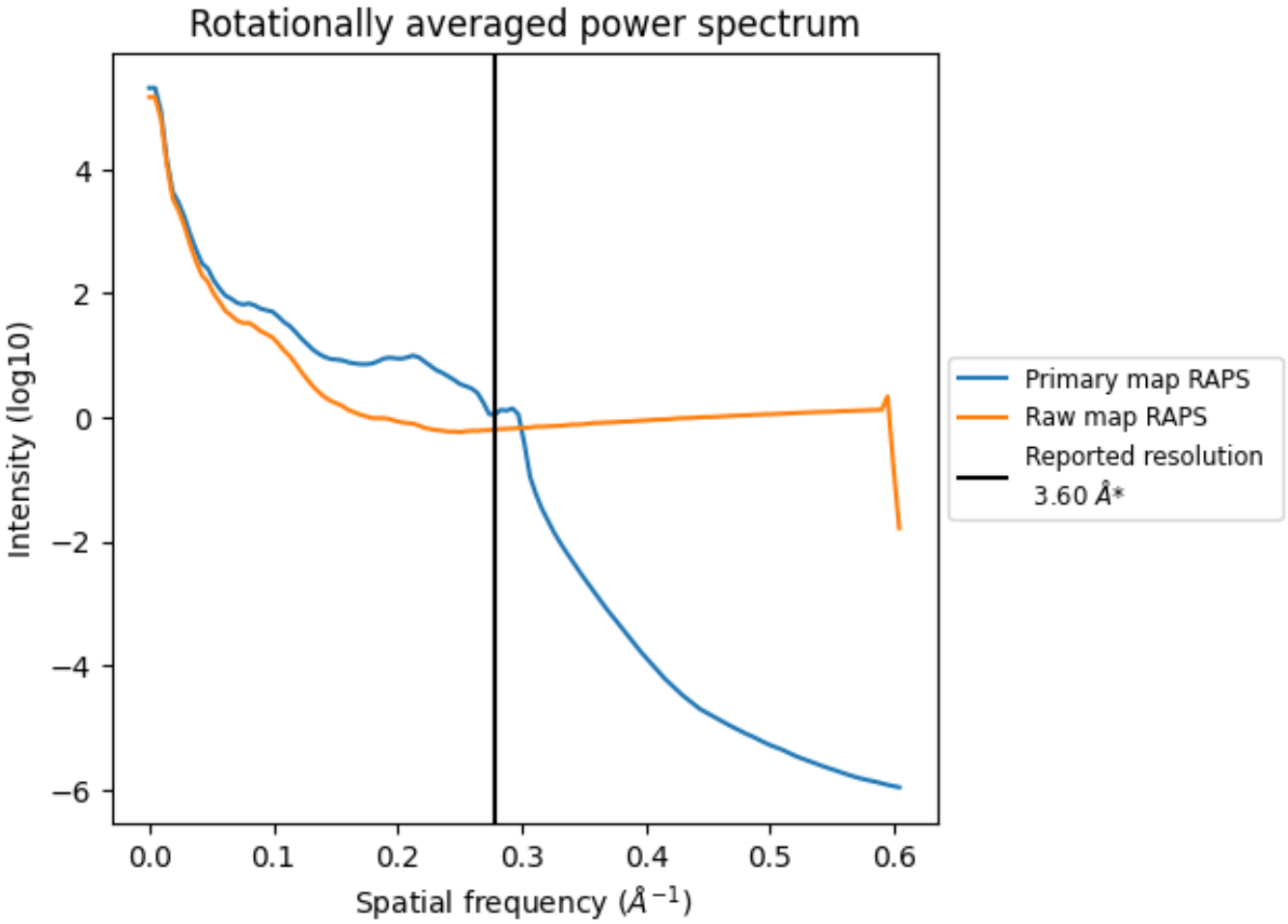
7.2 Volume estimate (i)



The volume at the recommended contour level is 96 nm^3; this corresponds to an approximate mass of 87 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)

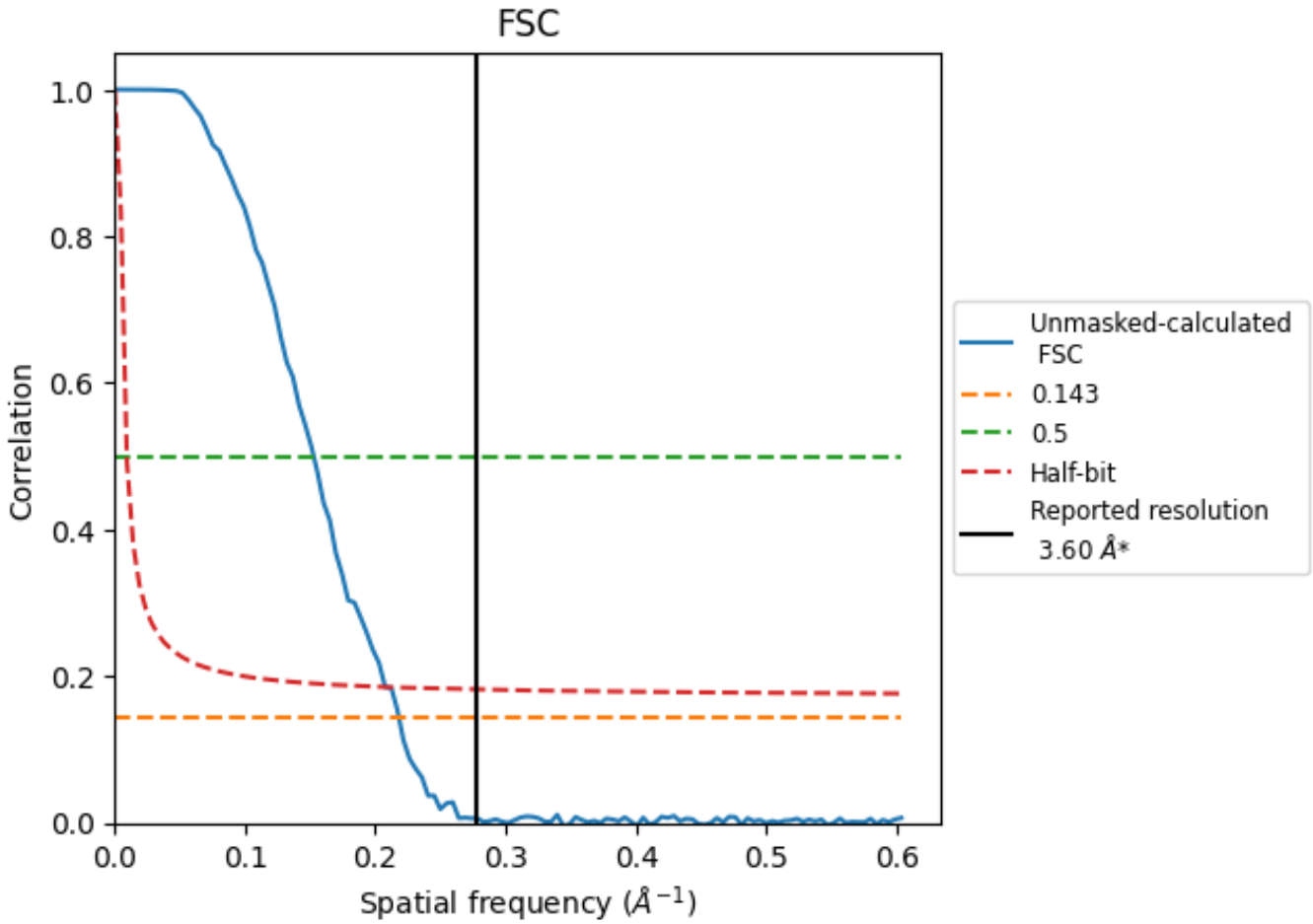


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

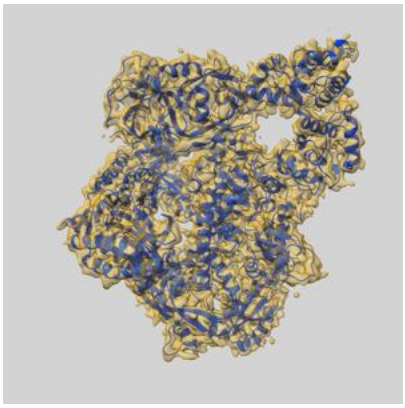
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.58	6.55	4.82

*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 4.58 differs from the reported value 3.6 by more than 10 %

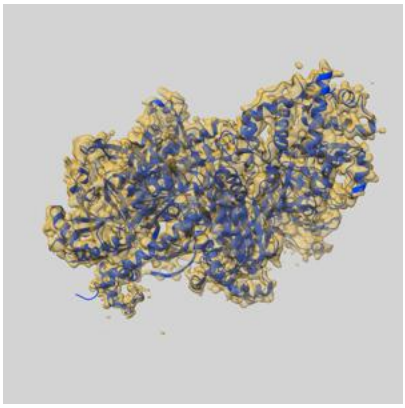
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41663 and PDB model 8TW9. Per-residue inclusion information can be found in section 3 on page 6.

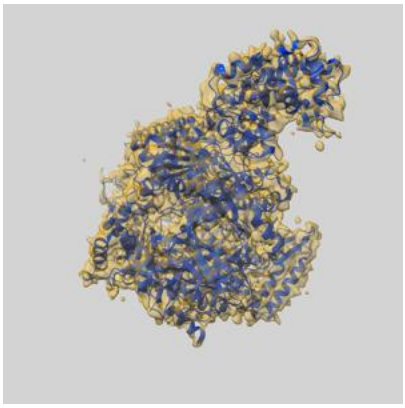
9.1 Map-model overlay



X



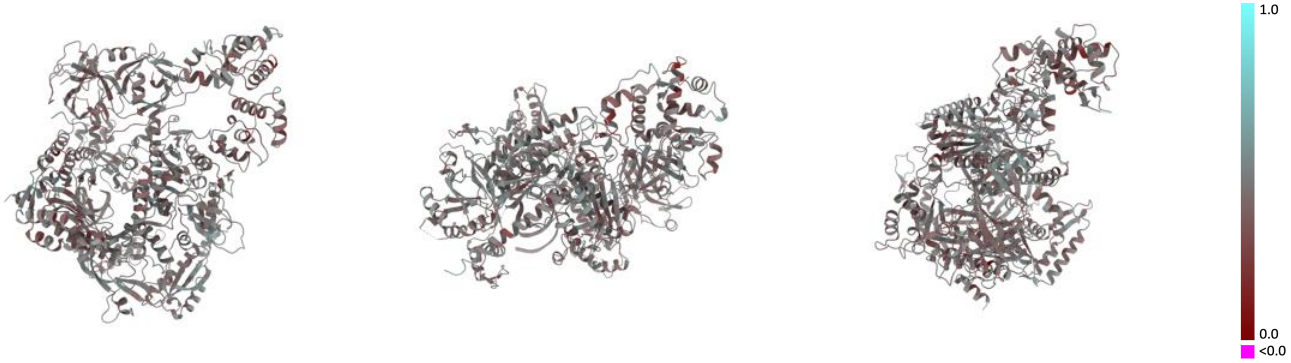
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.326 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.

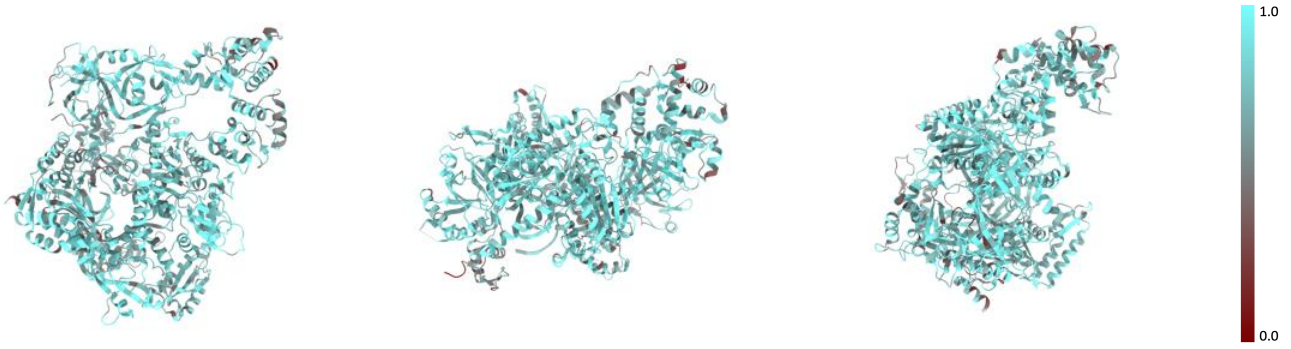
9.2 Q-score mapped to coordinate model (i)



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.

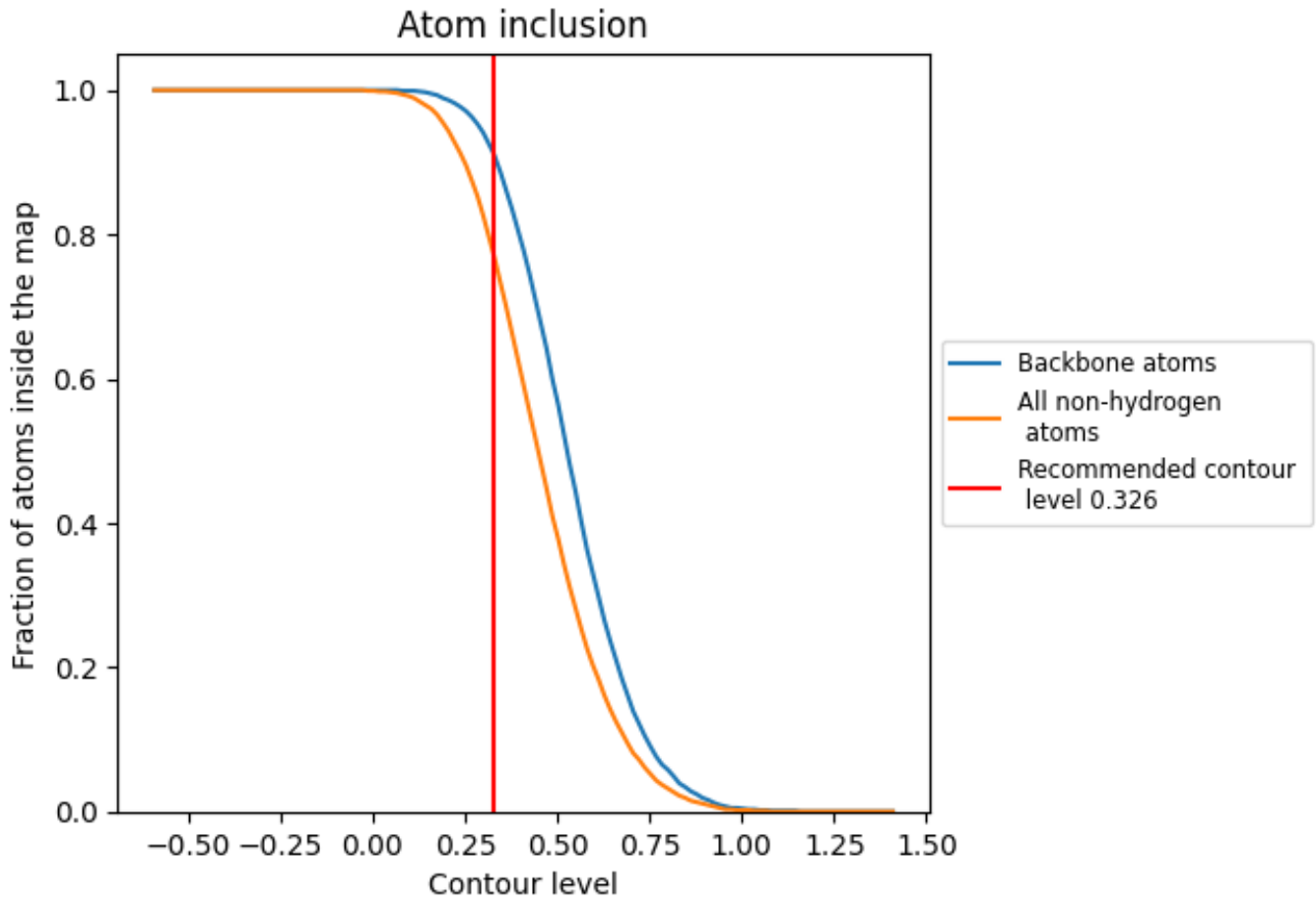
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.326).

9.4 Atom inclusion (i)



At the recommended contour level, 91% 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 (0.326) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7760	0.4380
B	0.7590	0.4310
C	0.7410	0.4140
D	0.7900	0.4270
E	0.7860	0.4430
P	0.7490	0.4260
T	0.6600	0.4240