wwPDB EM Validation Summary Report (i)

Aug 4, 2026 – 02:35 PM EDT

PDB ID	:	8TW9 / pdb_00008tw9
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 (1)) were used in the production of this report:

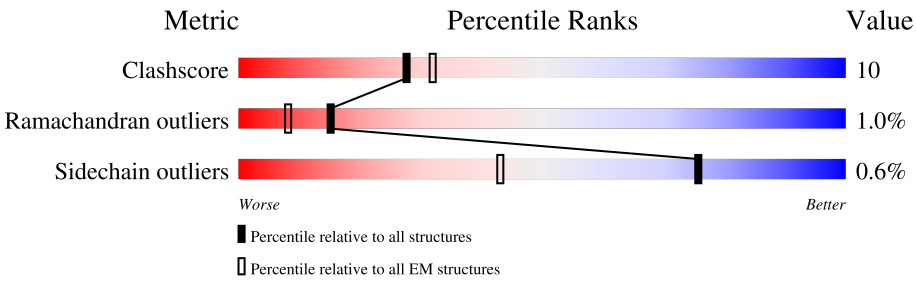
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13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

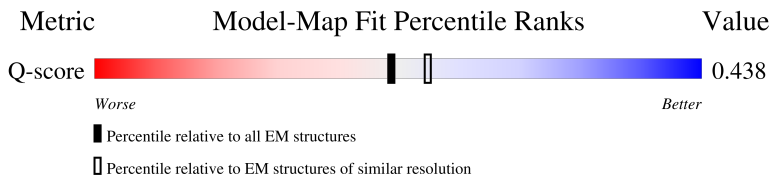
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	22% 67% 11%
3	T	15	7% 40% 60%
4	E	2222	• 43% 7% • 49%

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Mol	Chain	Length	Quality of chain
5	D	132	77% 22%
6	B	380	72% 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
			Total	C	N	O		
1	C	26	206	132	37	37	0	0

- Molecule 2 is a DNA chain called Primer DNA.

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

- Molecule 3 is a DNA chain called Template DNA.

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

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

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

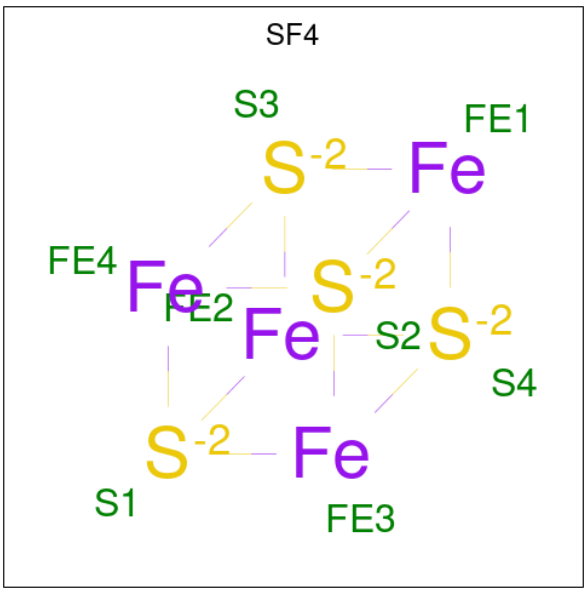
- Molecule 5 is a protein called Chromosome transmission fidelity protein 8.

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

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

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

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



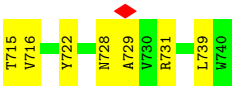
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
7	E	1	8	4	4	0

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

Chain C:

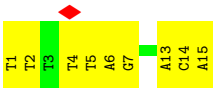


- Molecule 2: Primer DNA

Chain P:

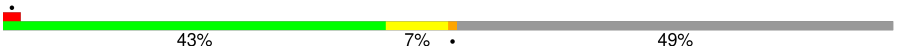
- Molecule 3: Template DNA

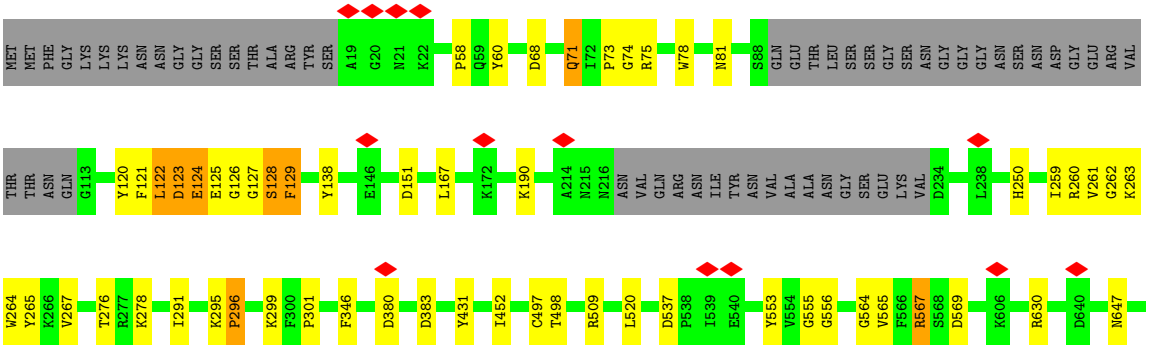
Chain T:

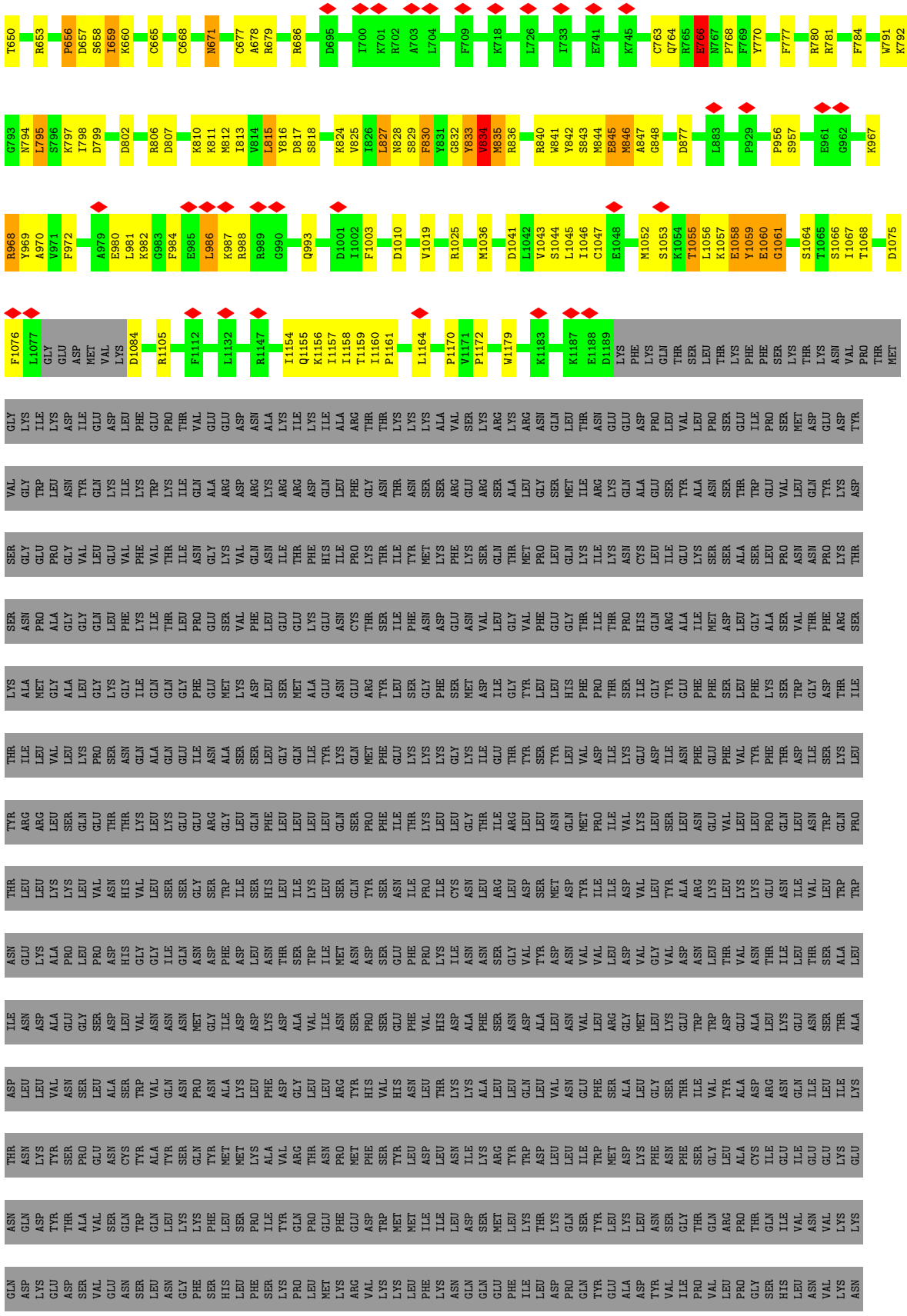


- Molecule 4: DNA polymerase epsilon catalytic subunit A

Chain E:






T650 R653 P656 D657 S658 I659 K660 C665 C668 N671 C677 A678 R679 R686 D695 I700 K701 R702 A703 L704 F709 K718 L726 I733 E741 K745 C763 Q764 R765 E766 M767 P768 F769 Y770 F777 R780 R781 F784 W791 K792
G793 N794 L795 S796 K797 I798 D799 D802 R806 D807 K810 K811 M812 I813 W814 L815 Y816 D817 S818 K824 V825 I826 L827 N828 S829 F830 Y831 G832 Y833 V834 M835 R836 R840 W841 Y842 S843 M844 E845 M846 A847 G848 D877 L883 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 M1052 S1053 K1054 T1055 L1056 K1057 E1058 Y1059 E1060 G1061 S1064 T1065 S1066 I1067 T1068 D1075
F1076 L1077 GLY GLU ASP MET VAL LYS D1084 R1105 F1112 L1132 R1147 I1154 Q1155 K1156 I1157 I1158 T1159 I1160 P1161 L1164 P1170 V1171 P1172 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 GLU ASP LEU PHE GLU PRO THR VAL GLU GLU ASP ASN ALA LYS ILE LYS ILE ALA ARG THR THR 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 GLU 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 LYS 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 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 LEU 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 GLU GLY TYR LEU LEU HIS PHE PRO THR SER ILE GLY TYR GLU PHE PHE SER LEU GLY TYR 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 MET PHE GLU LYS LYS LYS GLY LYS ILE GLU THR TYR SER TYR LEU VAL 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 ASP SER MET ASP TYR ILE ILE ASP VAL LEU TYR ALA ARG LYS LEU LYS LYS SER GLU GLU ILE ASN 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 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 ILE ASN ILE
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 VAL LEU ARG GLY MET LEU LYS GLU TRP TRP ASP GLU ALA ASP LYS LEU ASN GLU ASN
ASP LEU LEU VAL ASN SER LEU ALA SER TRP VAL GLN ASN PRO ASN ALA LYS LEU PHE ASP LYS LEU LEU ARG TYR HIS VAL HIS ASN LEU THR LYS LYS ALA LEU LEU LEU GLN LEU VAL ASN GLU VAL LEU SER PHE SER ALA LEU ASN GLN ILE LEU VAL TYR ALA ASP ARG ASN GLN ILE
THR ASN LYS TYR SER PRO TYR ALA TYR SER GLN TYR TRP ALA LYS LYS ARG TYR TRP ASP LEU THR LYS LYS LEU ASN ILE ASP ALA PHE SER ASN ASP ASP LEU LEU LEU LEU ASP LEU LEU ILE TRP MET ASP SER PHE ASN PHE SER GLY LEU VAL TYR ALA ASP VAL LYS GLU ILE GLU ILE GLU GLU ILE LYS
ASN GLN ASP TYR THR ALA VAL SER GLN TRP LEU LYS LYS PHE ASP PRO GLU PRO ASN ILE ILE ASP PHE PHE GLU ASP TYR LEU ASP SER GLN SER TYR LEU LYS LEU LEU ASP SER MET MET LYS ARG VAL ALA ASP TRP TRP GLU ALA ASP LYS LYS ASN GLN GLN GLU PHE ILE LEU ASP PRO GLN GLN TYR GLU ALA ASP TYR VAL ILE PRO VAL LEU PRO VAL THR GLN SER HIS LEU ASN VAL LYS
GLN ASP LYS GLU ASP SER GLN ASN SER GLN LEU LEU ASN GLY SER HIS LEU PHE SER LYS PRO LEU MET LYS ARG VAL LYS LYS PHE LYS ASN GLN PHE LYS ILE LEU ASP PRO GLN GLN TYR GLU ASP PHE PHE ILE LEU ASN VAL LYS LYS

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 LEU LYS ILE PHE GLU LEU ARG GLU PHE ALA LYS VAL ALA GLU PHE LYS ASP PRO SER LEU SER LEU VAL VAL PRO ASP PHE LEU CYS GLU

TYR CYS PHE PHE ILE SER ASP ILE ASP PHE CYS LYS ALA ALA PRO GLU SER ILE PHE SER CYS VAL ARG CYS HIS LYS ALA PHE ASN GLN VAL LEU LEU GLN GLU HIS LEU ILE GLN LYS LEU ARG SER ASP ILE GLU SER TYR LEU ILE GLN ASP LEU ARG CYS SER ARG CYS HIS LYS

VAL LYS ARG ASP TYR MET SER ALA HIS CYS PRO CYS ALA GLY ALA TRP GLU GLY THR LEU PRO ARG GLU SER ILE VAL GLN LYS LEU ASN VAL PHE LYS GLN VAL ALA LYS TYR TYR GLY PHE ASP ILE LEU LEU SER CYS ILE ALA ASP LEU THR ILE

- Molecule 5: Chromosome transmission fidelity protein 8

Chain D:

P2 S3 W11 Q12 K13 L14 T15 Q16 T23 V24 M31 R58 L67 I68 R69 F70 G71 S72 L73 L82 F83 K87 Q88 R89 L90 V94 D98 I103 F106 D117 V123 L130 P131 I132 M133

- Molecule 6: Sister chromatid cohesion protein DCC1

Chain B:

MET S2 I3 N4 L5 S14 Y15 K16 L17 I18 L24 I27 I28 Q29 Q33 R38 F39 K40 K44 L51 L60 K61 Q62 R63 M72 R73 E74 L87 L88 F89 S92 K93 V98 F108 R111 I135 M136 K137 R138 E152 G169 V172

C178 I179 L180 L185 F186 S195 A196 M197 A198 D202 L203 L206 N207 H212 H213 D218 I219 E220 D221 E222 F223 R228 E229 I230 I231 E232 A239 E242 GLN GLU ALA GLU N247 N248 T249 L252 R253 I254 I257 Y261 G262 I263 Q264 R267 W284

F291 F292 D297 I298 D299 M300 L301 R302 G303 Y304 H305 F306 K307 P308 T309 D310 K311 Q314 Y315 K318 K330 V331 L332 F333 R334 L335 Q336 W339 D340 L341 E342 D343 I344 K345 P346 L351 N352 S353 R354 G355 M356 K357 I358 D359 S360 F361 I362 M363 K364 Y365 A366 R367 R368

K369 T375 S379 ARG

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 (i)

5.1 Standard geometry (i)

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	0.35	0/211	0.79	0/289
2	P	0.88	2/203 (1.0%)	0.73	0/311
3	T	0.73	0/339	0.66	0/521
4	E	0.82	1/9121 (0.0%)	1.29	29/12348 (0.2%)
5	D	0.33	0/1030	0.85	0/1387
6	B	0.56	3/3016 (0.1%)	0.93	13/4083 (0.3%)
All	All	0.74	6/13920 (0.0%)	1.16	42/18939 (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 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	354	ARG	C-N	14.18	1.54	1.33
4	E	766	GLU	C-N	10.87	1.56	1.33
6	B	297	ASP	C-O	7.92	1.32	1.23
6	B	355	GLY	C-N	-7.54	1.21	1.33
2	P	2	DG	C1'-N9	-5.81	1.34	1.46

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	766	GLU	O-C-N	-9.10	111.66	122.95
4	E	1060	GLU	N-CA-C	-8.71	100.61	111.75
4	E	122	LEU	N-CA-C	-8.60	100.75	111.75
6	B	355	GLY	CA-C-N	-8.13	108.23	123.27
6	B	355	GLY	C-N-CA	-8.13	108.23	123.27

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	159	0
5	D	1014	0	1007	30	0
6	B	2953	0	2913	80	0
7	E	8	0	0	6	0
All	All	13586	0	12949	257	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 10.

The worst 5 of 257 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%)	10	41
5	D	130/132 (98%)	127 (98%)	3 (2%)	0	100	100
6	B	370/380 (97%)	342 (92%)	25 (7%)	3 (1%)	16	49
All	All	1640/2760 (59%)	1542 (94%)	82 (5%)	16 (1%)	15	45

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%)	944 (99%)	6 (1%)	78	79
5	D	110/119 (92%)	108 (98%)	2 (2%)	51	68
6	B	326/352 (93%)	325 (100%)	1 (0%)	86	83
All	All	1406/2509 (56%)	1397 (99%)	9 (1%)	76	79

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	73	LEU
6	B	28	ILE
4	E	825	VAL
4	E	827	LEU
4	E	834	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	54	HIS
6	B	34	ASN
4	E	924	GLN
6	B	33	GLN
4	E	828	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.

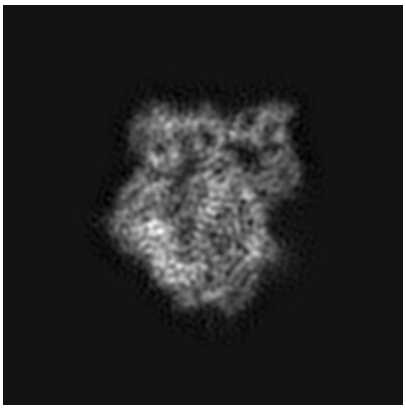
6 Map visualisation (i)

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.

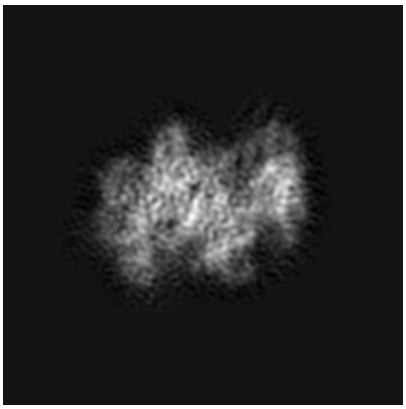
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

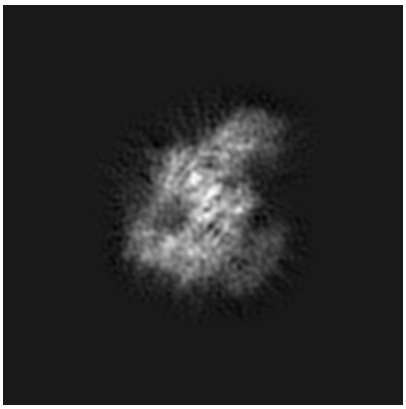
6.1.1 Primary map



X

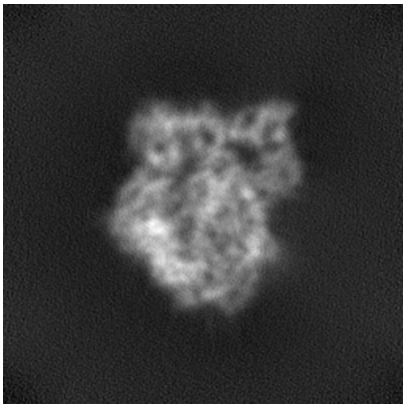


Y

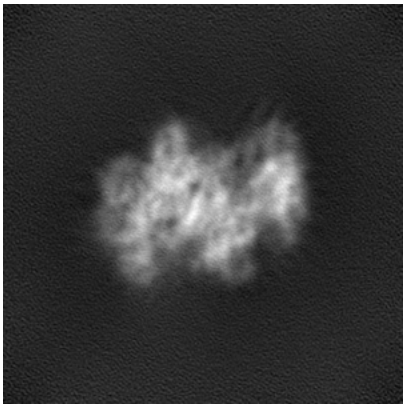


Z

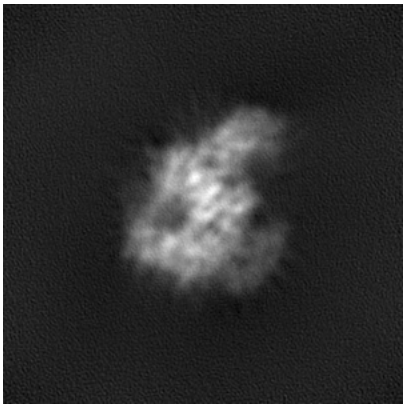
6.1.2 Raw map



X



Y

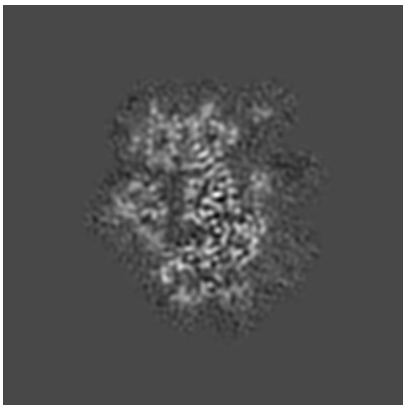


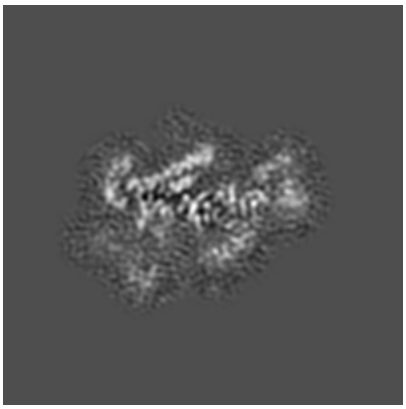
Z

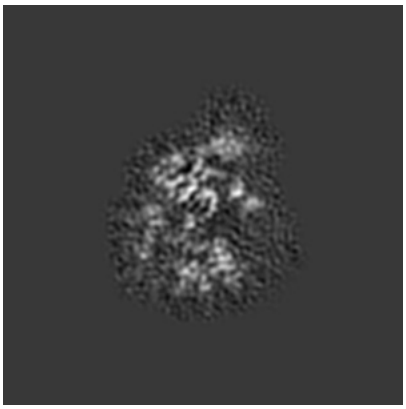
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

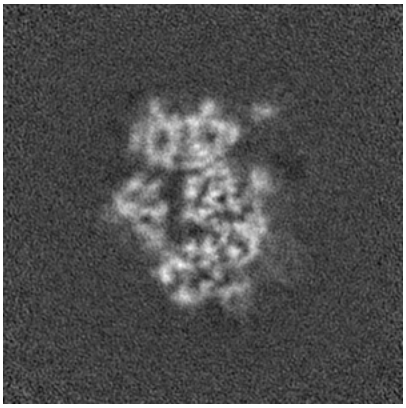
6.2.1 Primary map

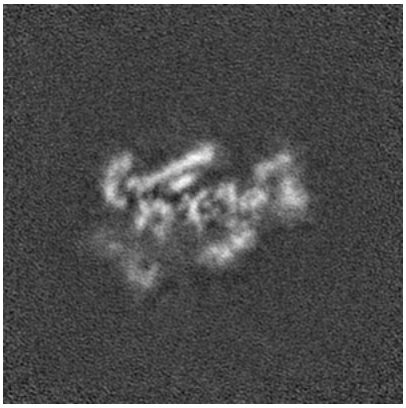

X Index: 128

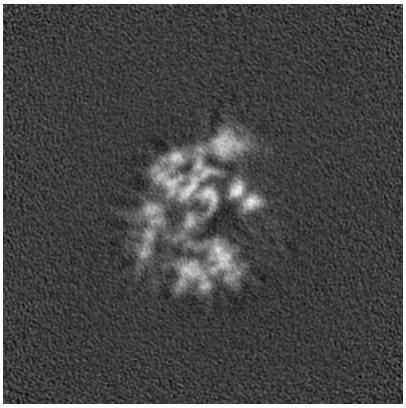

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

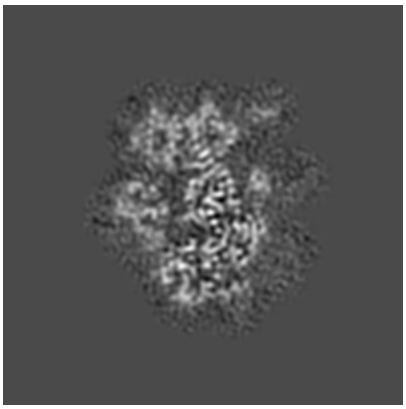

Y Index: 128


Z Index: 128

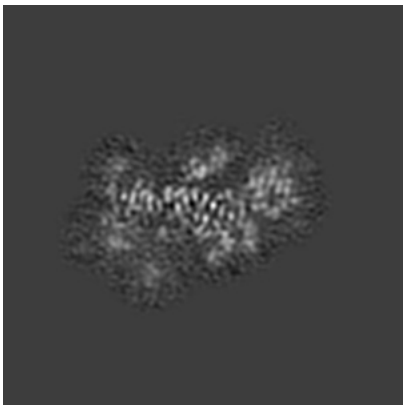
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

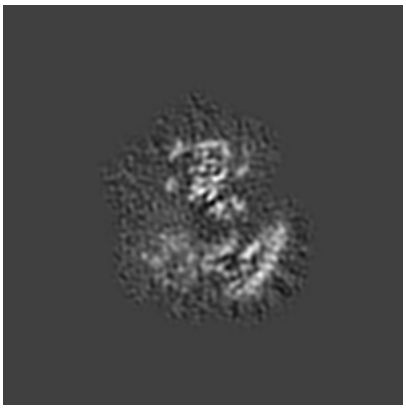
6.3.1 Primary map



X Index: 129

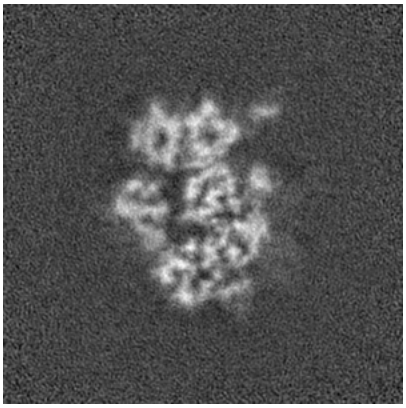


Y Index: 136

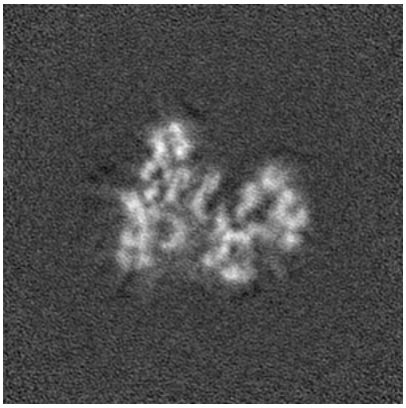


Z Index: 111

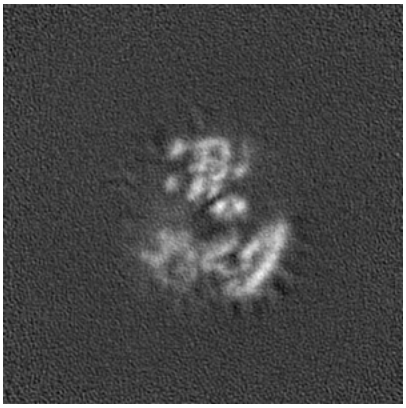
6.3.2 Raw map



X Index: 129



Y Index: 102

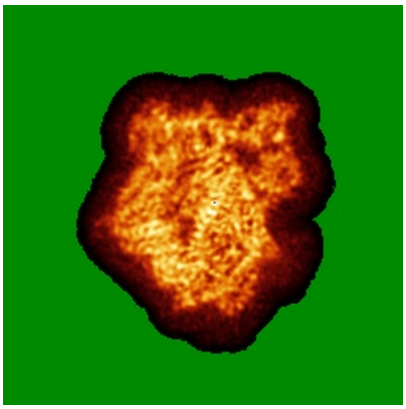


Z Index: 111

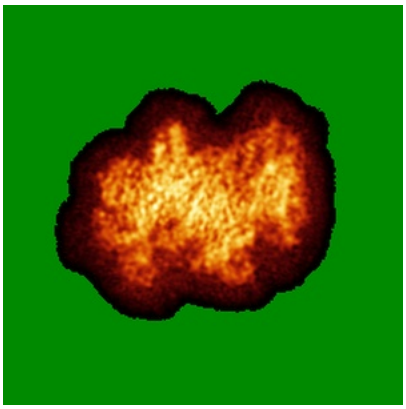
The images above show the largest variance slices of the map in three orthogonal directions.

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

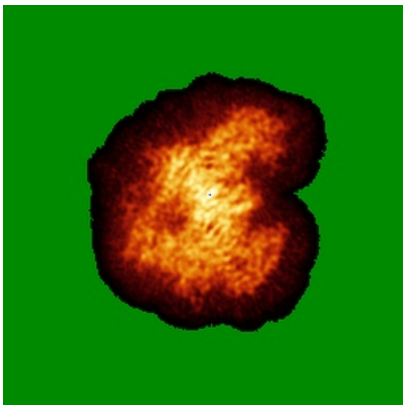
6.4.1 Primary map



X

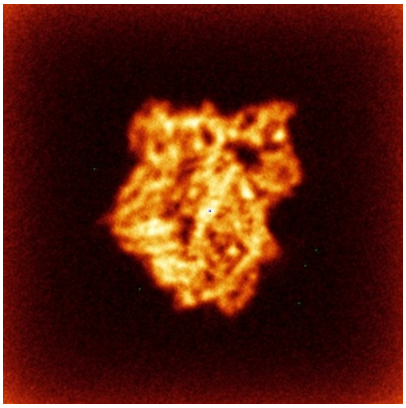


Y

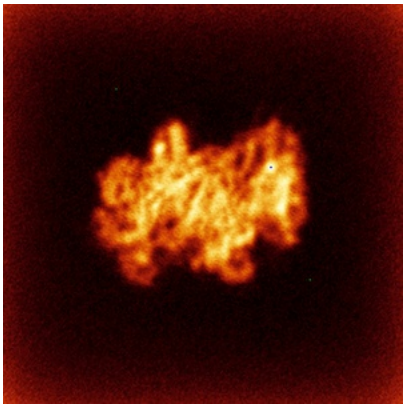


Z

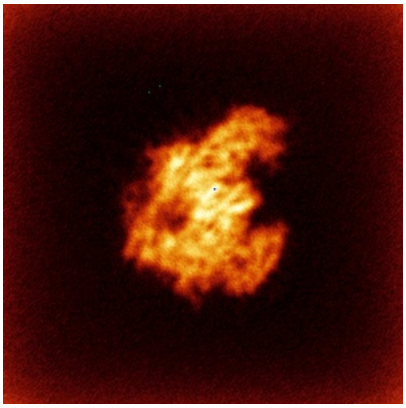
6.4.2 Raw map



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.

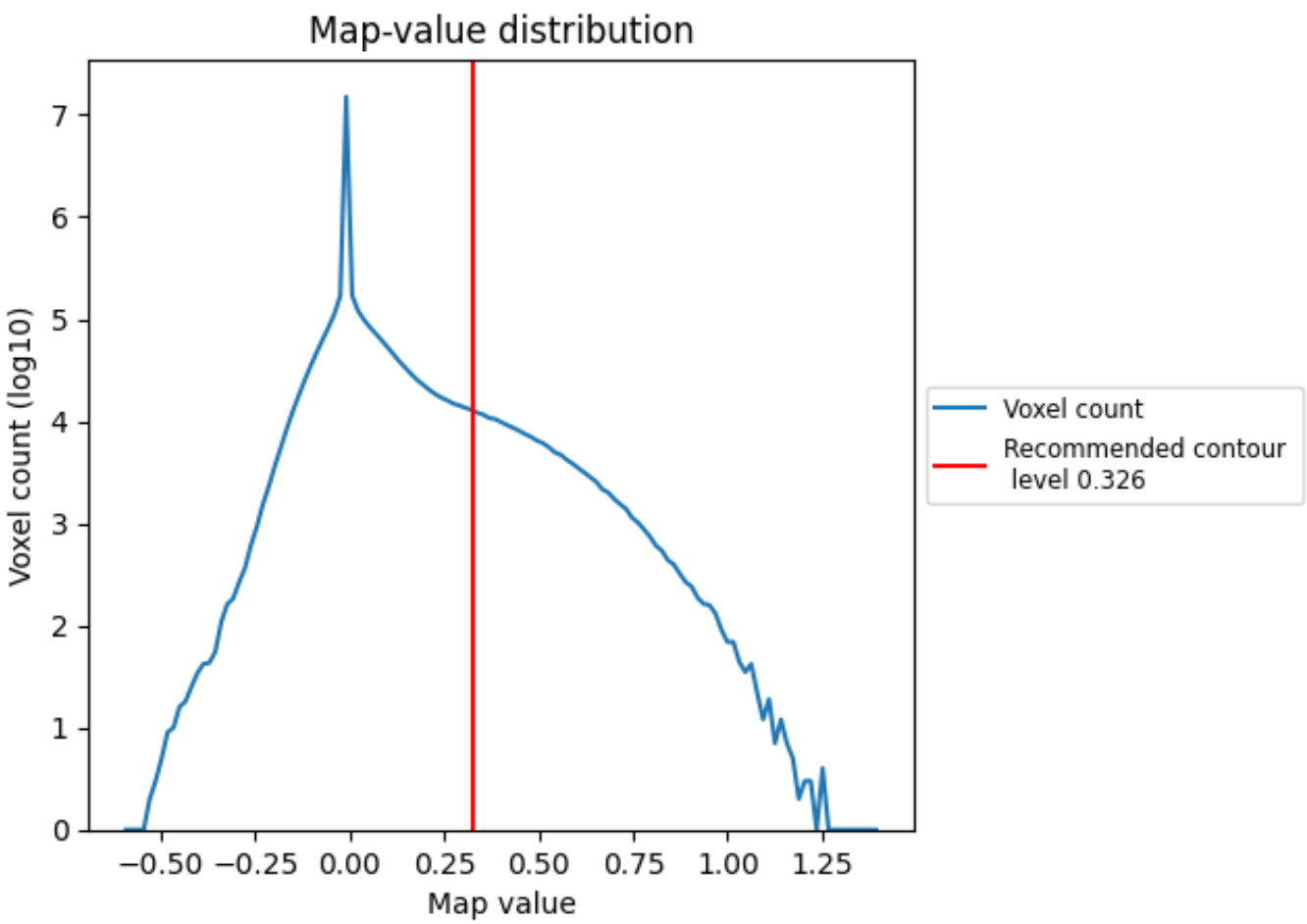
6.6 Mask visualisation (i)

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

7 Map analysis (i)

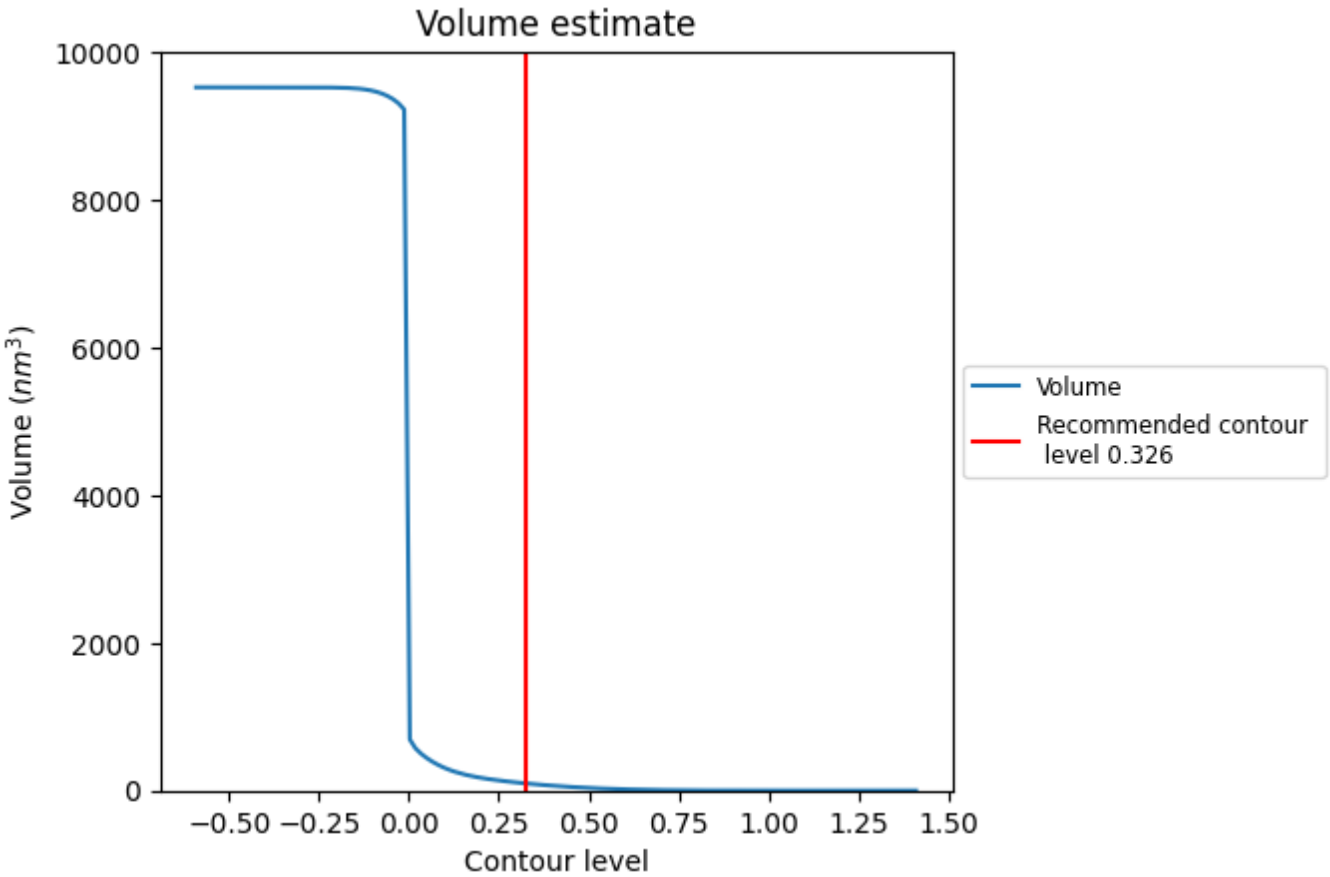
This section contains the results of statistical analysis of the map.

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.

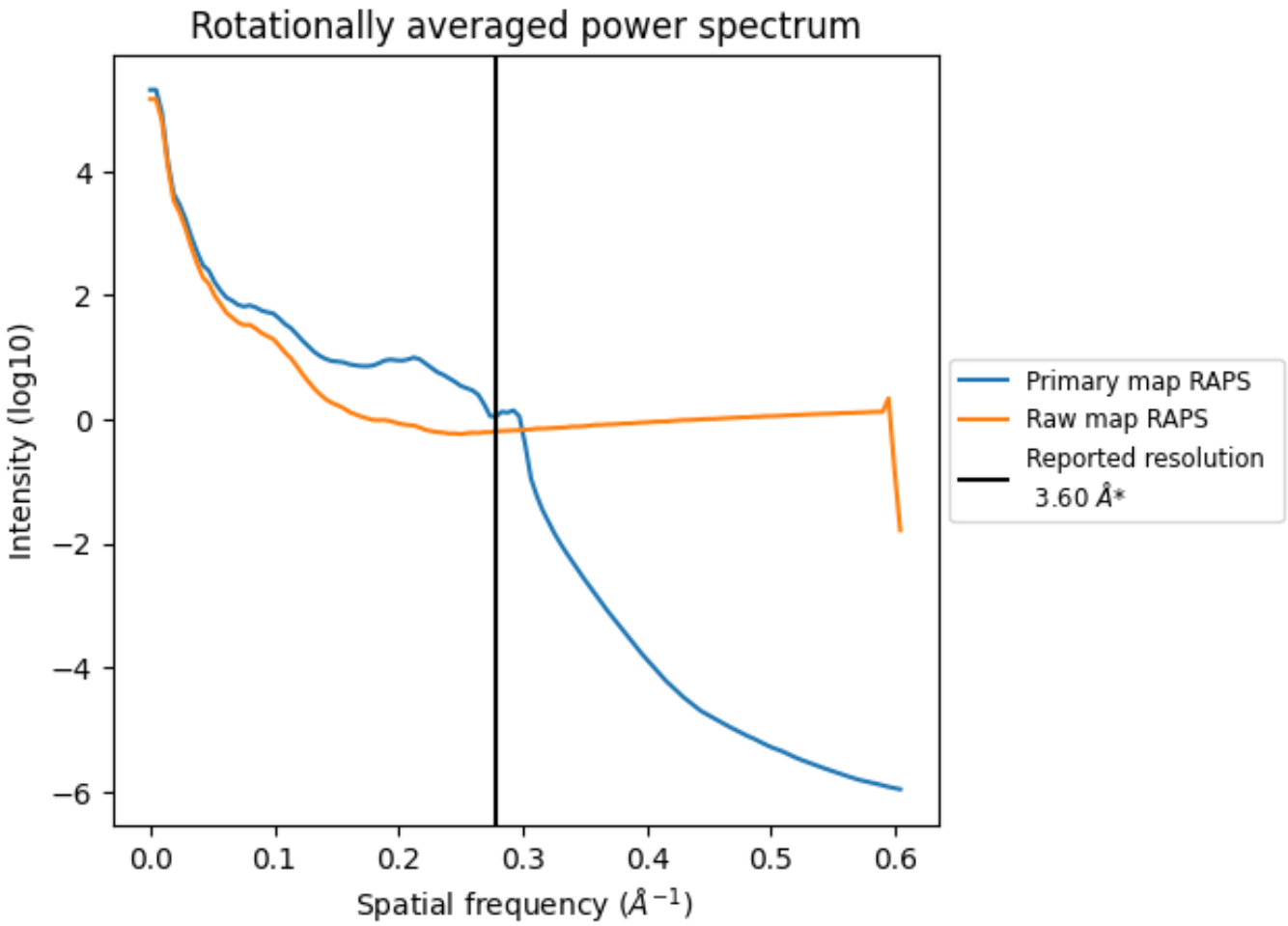
7.2 Volume estimate (i)



The volume at the recommended contour level is 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)

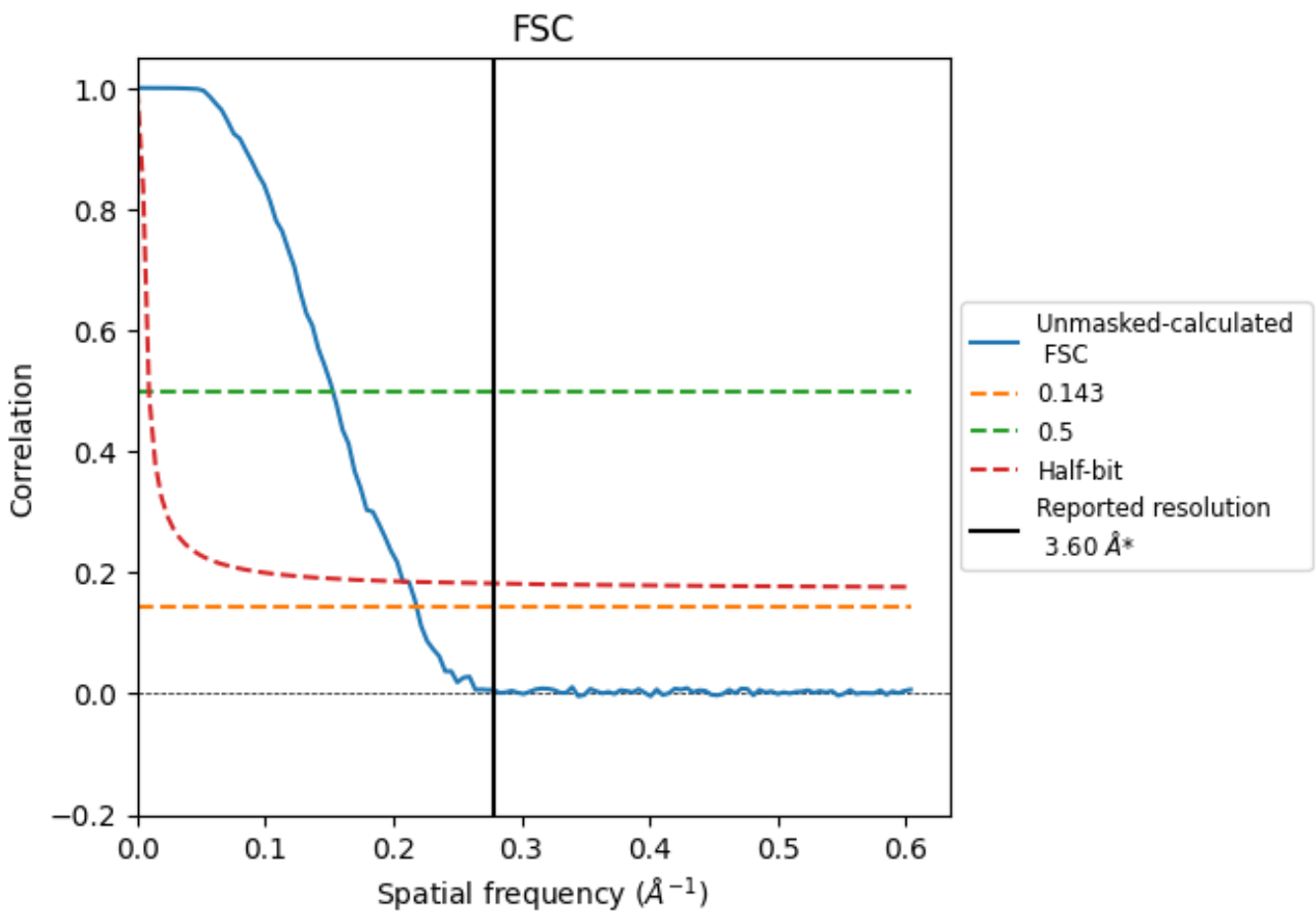


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation (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 0.278 Å^{-1}

8.2 Resolution estimates (i)

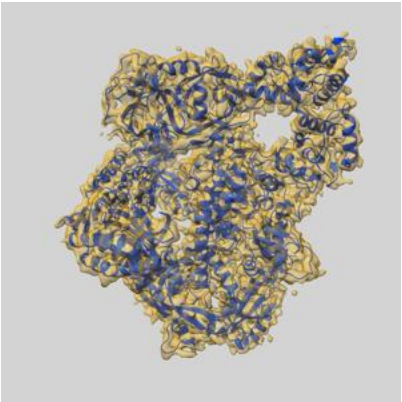
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.58	6.55	4.82

*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 %

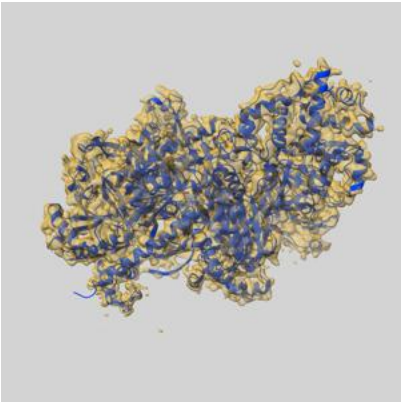
9 Map-model fit (i)

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.

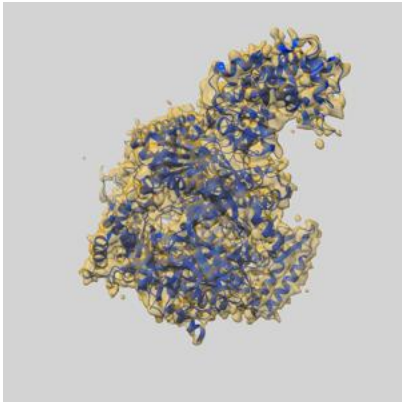
9.1 Map-model overlay (i)



X



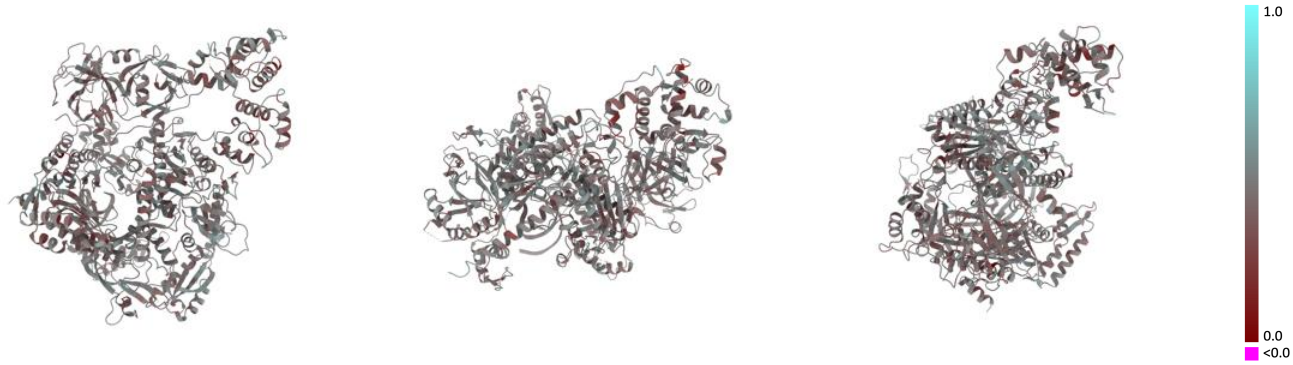
Y



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.

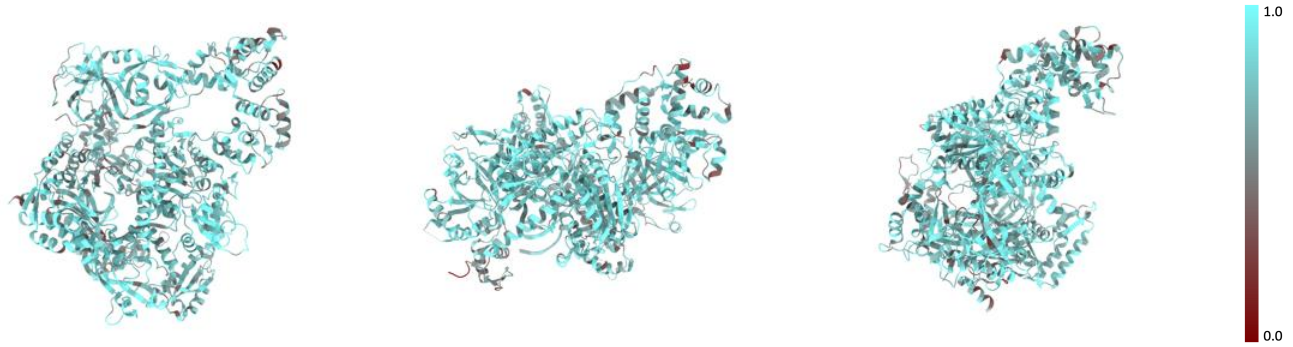
9.2 Q-score mapped to coordinate model (i)



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.

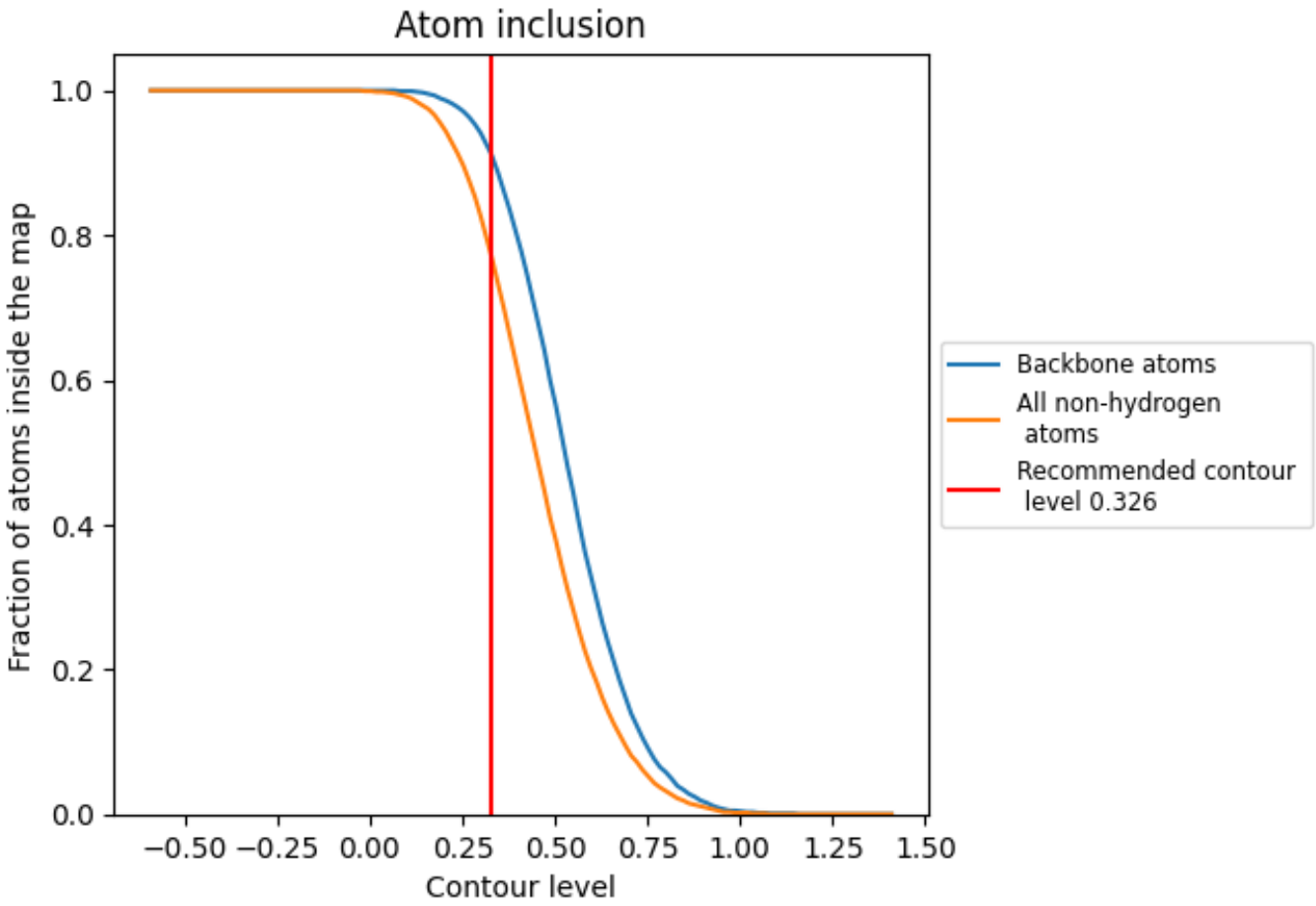
9.3 Atom inclusion mapped to coordinate model (i)



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 (i)

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