wwPDB EM Validation Summary Report

Jun 3, 2024 – 05:21 pm BST

PDB ID	:	8A40
EMDB ID	:	EMD-15129
Title	:	Structure of mammalian Pol II-TFIIS elongation complex
Authors	:	Farnung, L.; Ochmann, M.; Garg, G.; Vos, S.M.; Cramer, P.
Deposited on	:	2022-06-09
Resolution	:	3.00 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:

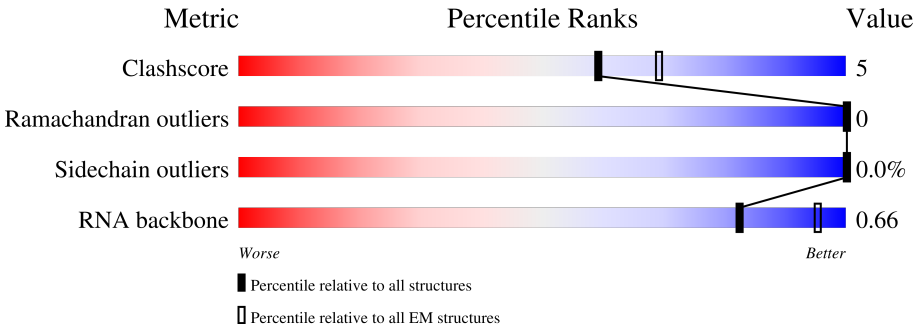
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A	1984	63% 9% 28%
2	B	1251	5% 80% 11% 9%
3	C	275	76% 17% 7%
4	D	142	90% 80% 10% 10%
5	E	210	87% 13%
6	F	127	5% 58% 6% 35%
7	G	172	77% 78% 22%

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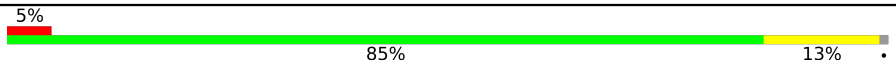
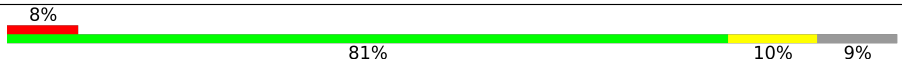
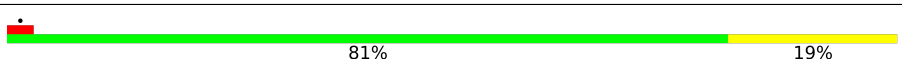
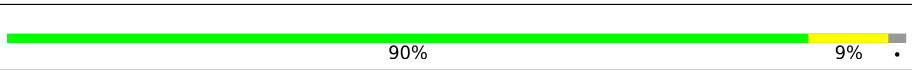
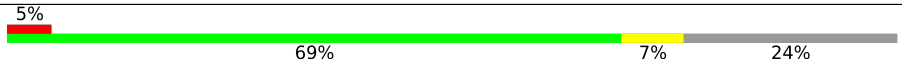
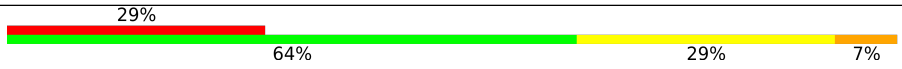
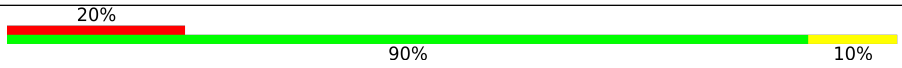
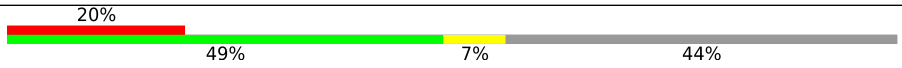
Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	48	
14	P	14	
15	T	41	
16	U	304	

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 34177 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1427	11291	7102	2021	2096	72	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1134	9062	5732	1595	1671	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	257	2059	1294	351	408	6	0	0

- Molecule 4 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	128	1005	632	172	197	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	209	1711	1084	300	319	8	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	32	GLY	GLU	conflict	UNP A0A4X1VTX4
E	46	GLY	ASP	conflict	UNP A0A4X1VTX4

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total 658	C 419	N 113	O 121	S 5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	126	THR	SER	conflict	UNP A0A4X1VEK9

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total 1334	C 867	N 216	O 243	S 8	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total 1186	C 750	N 194	O 237	S 5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total 927	C 571	N 166	O 179	S 11	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total 533	C 345	N 90	O 92	S 6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total 920	C 593	N 152	O 173	S 2	0	0

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 13 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	30	Total	C	N	O	P	0	0
			633	294	135	174	30		

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	14	Total	C	N	O	P	0	0
			302	135	59	94	14		

- Molecule 15 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	41	Total	C	N	O	P	0	0
			827	393	138	255	41		

- Molecule 16 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	170	Total	C	N	O	S	0	0
			1343	818	247	263	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	-2	SER	-	expression tag	UNP P23193
U	-1	ASN	-	expression tag	UNP P23193
U	0	ALA	-	expression tag	UNP P23193

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	A	5	Total	Zn	0
			5	5	
17	B	2	Total	Zn	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
17	I	3	Total Zn 3 3	0
17	U	1	Total Zn 1 1	0

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

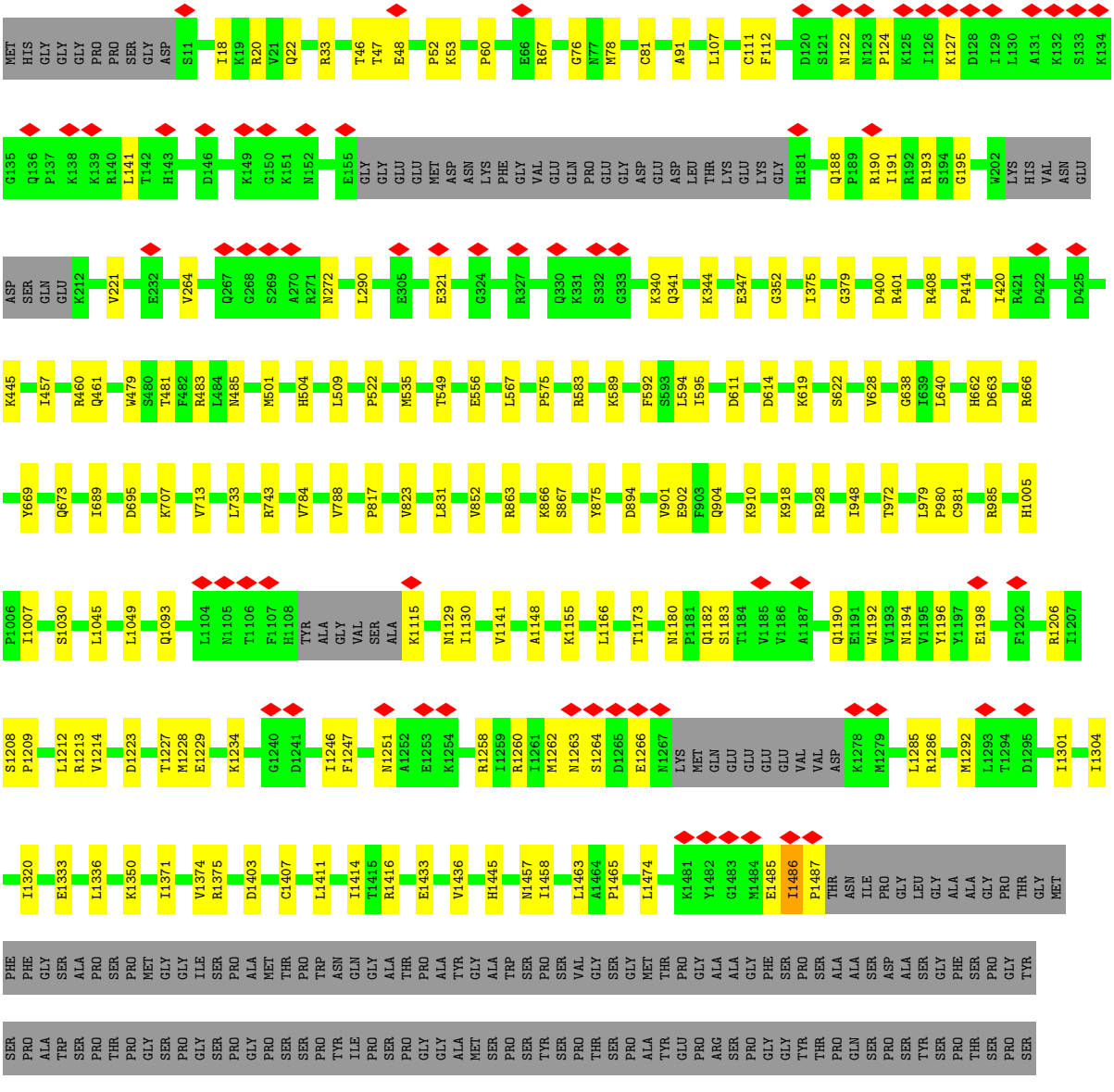
Mol	Chain	Residues	Atoms	AltConf
18	A	3	Total Mg 3 3	0

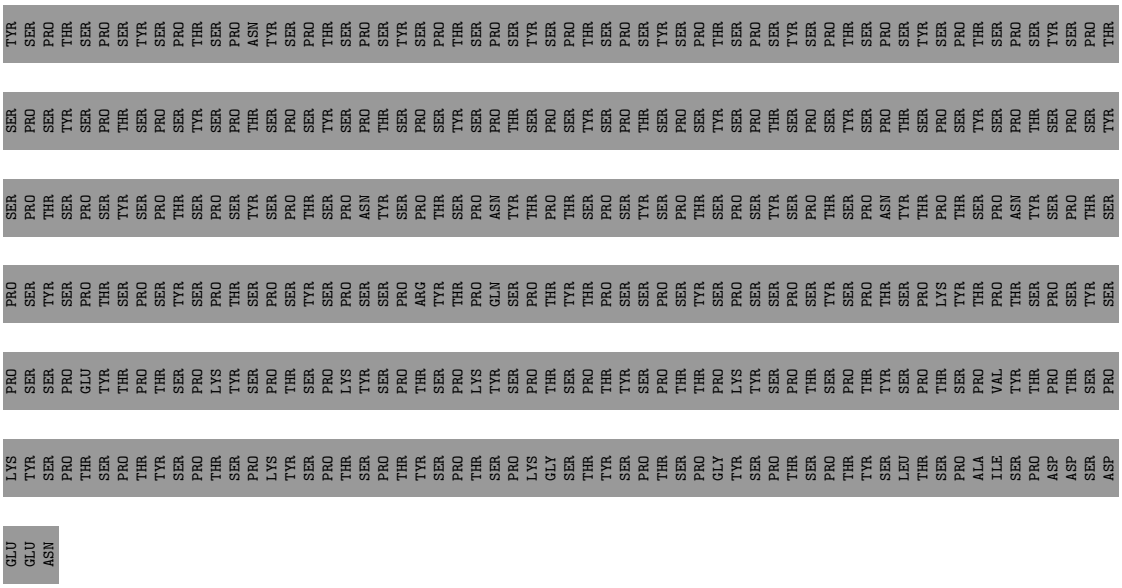
3 Residue-property plots (i)

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: DNA-directed RNA polymerase subunit

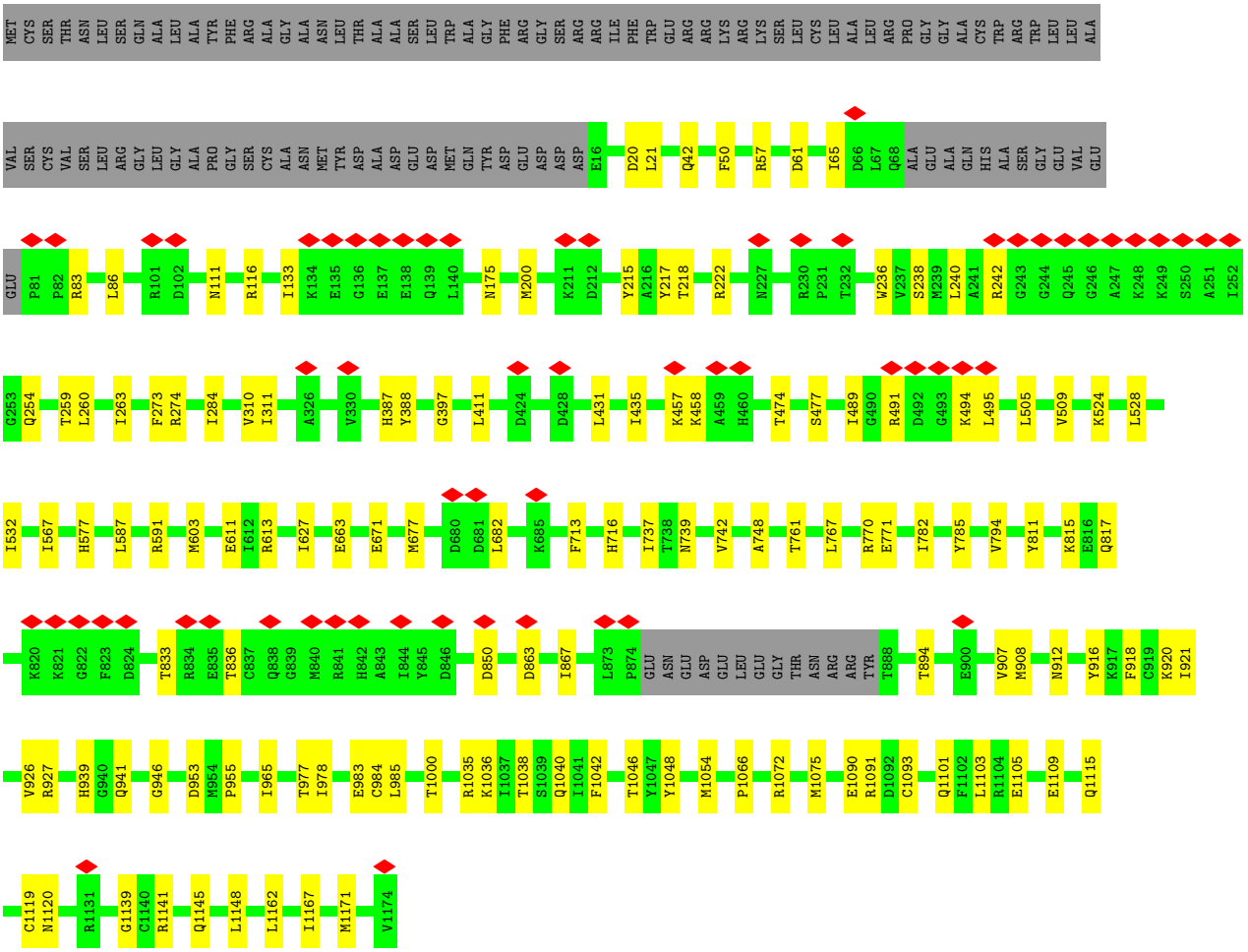
Chain A:





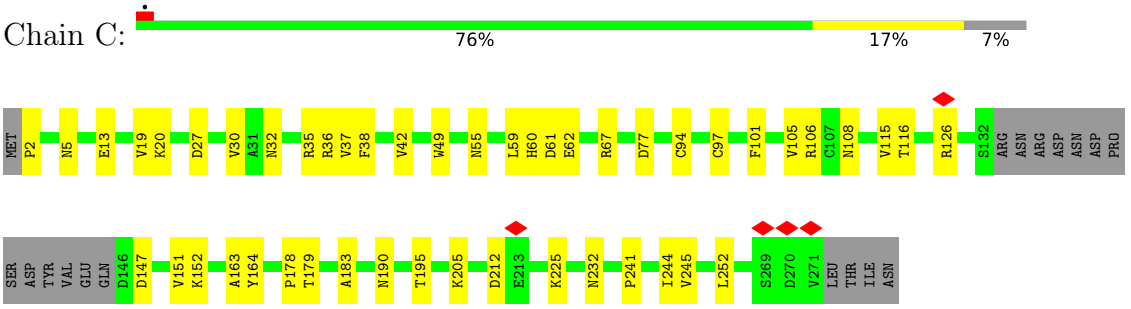
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



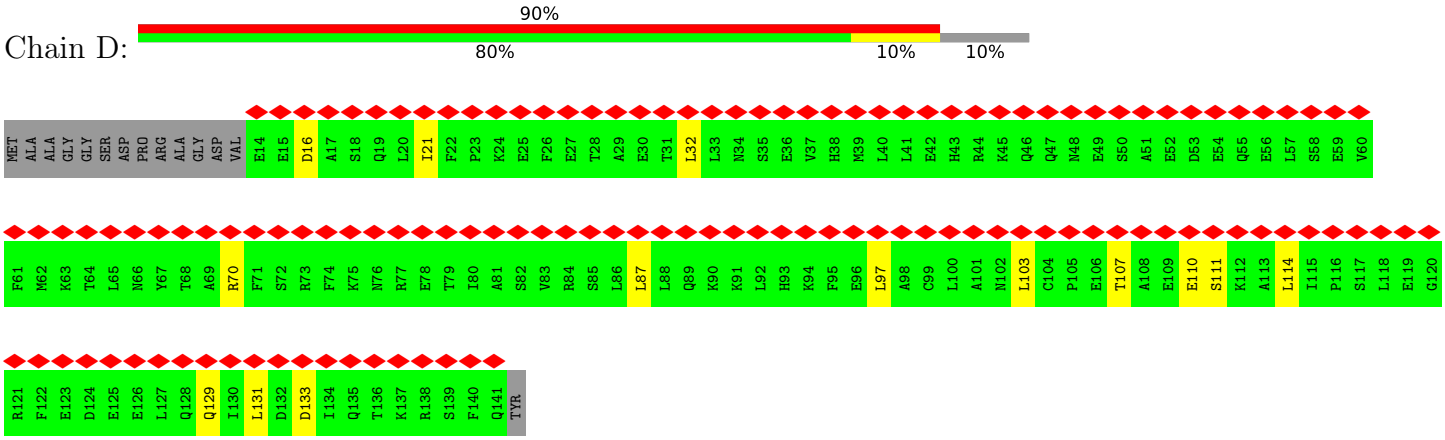
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



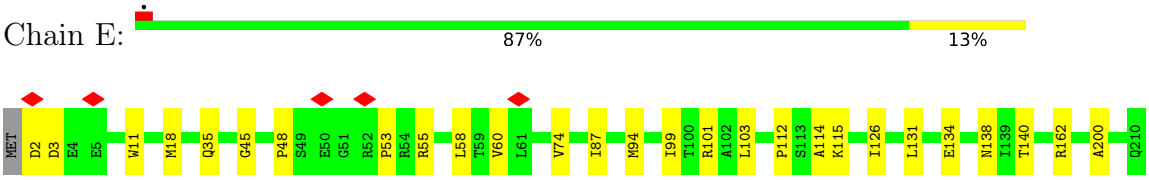
• Molecule 4: RNA polymerase II subunit D

Chain D:



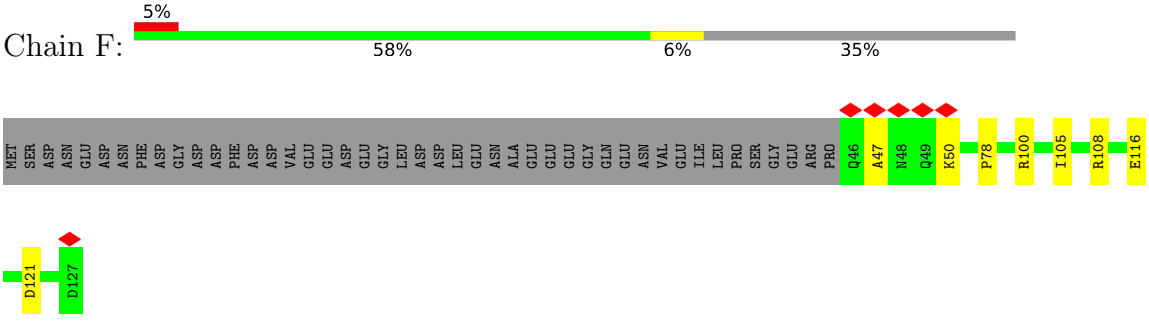
• Molecule 5: DNA-directed RNA polymerase II subunit E

Chain E:



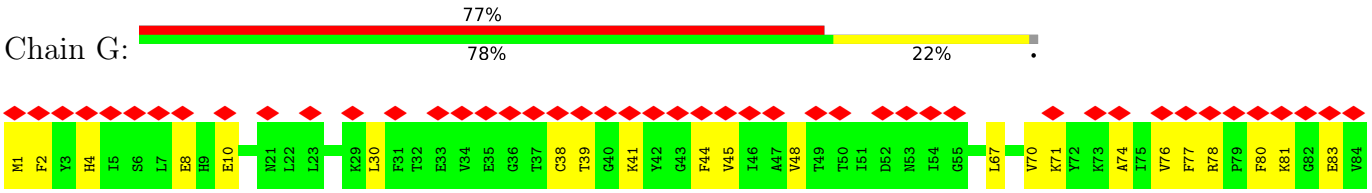
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

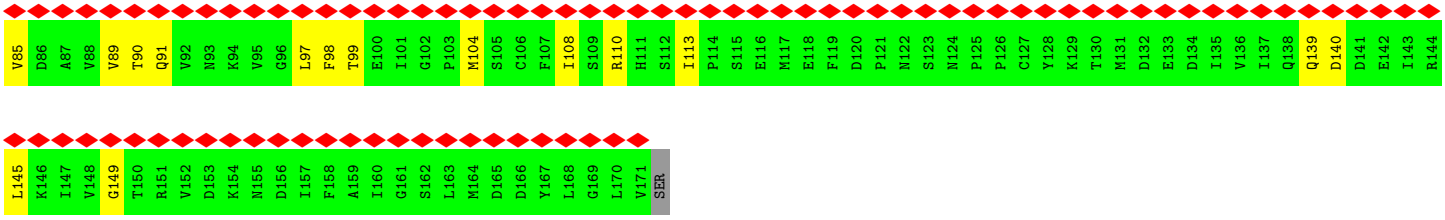
Chain F:



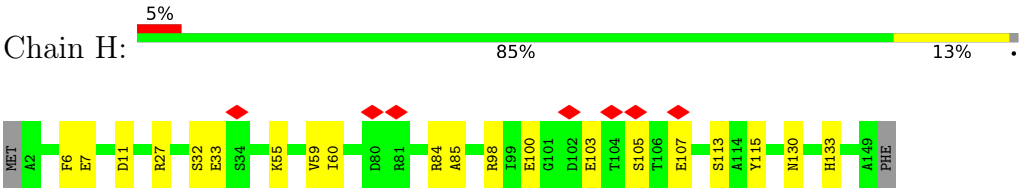
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:

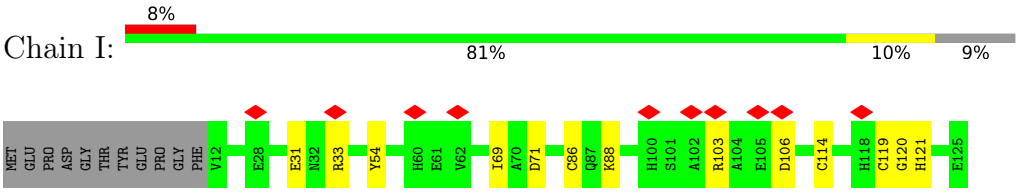




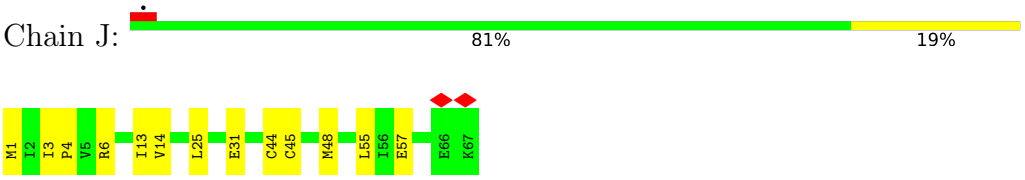
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



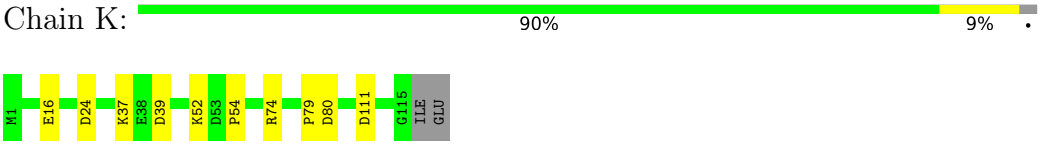
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



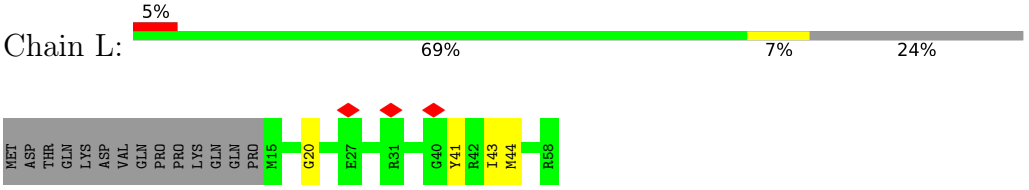
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



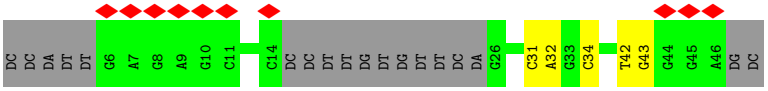
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



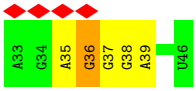
• Molecule 12: RNA polymerase II subunit K



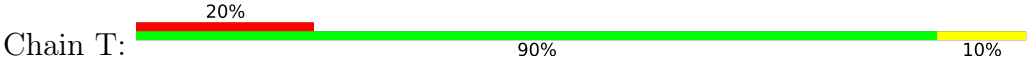
• Molecule 13: Non-template DNA

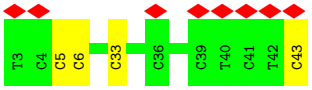


• Molecule 14: RNA

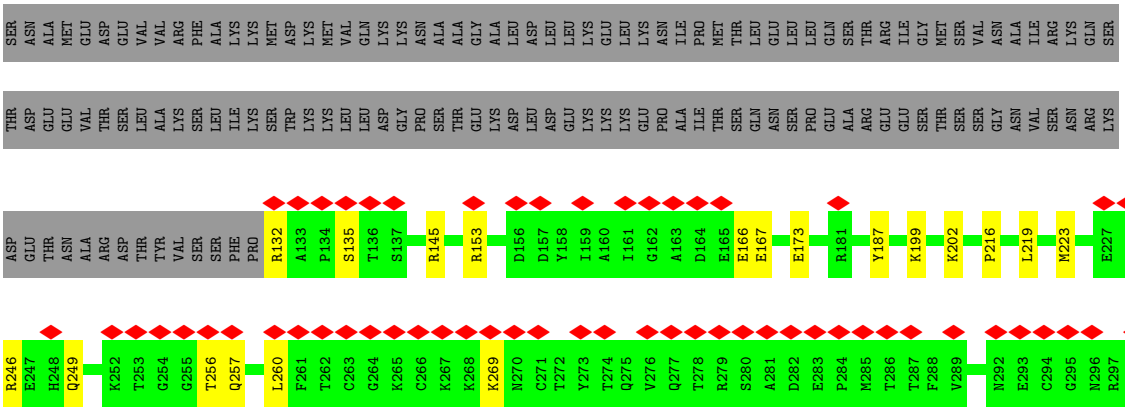


• Molecule 15: Template DNA





• Molecule 16: Transcription elongation factor A protein 1



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3000	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.021	Depositor
Minimum map value	-0.007	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	250.2, 250.2, 250.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/11495	0.55	2/15515 (0.0%)
2	B	0.29	0/9243	0.55	2/12475 (0.0%)
3	C	0.28	0/2102	0.52	0/2857
4	D	0.25	0/1019	0.49	0/1374
5	E	0.31	0/1742	0.56	0/2353
6	F	0.29	0/668	0.56	0/903
7	G	0.27	0/1365	0.53	0/1853
8	H	0.30	0/1207	0.55	0/1628
9	I	0.31	0/948	0.61	0/1284
10	J	0.30	0/542	0.51	0/730
11	K	0.30	0/939	0.59	3/1271 (0.2%)
12	L	0.33	0/377	0.74	0/500
13	N	0.46	0/714	0.75	0/1101
14	P	0.30	0/338	0.83	1/525 (0.2%)
15	T	0.54	0/921	0.94	1/1417 (0.1%)
16	U	0.27	0/1358	0.61	0/1820
All	All	0.30	0/34978	0.58	9/47606 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	863	ASP	CB-CG-OD1	7.32	124.89	118.30
11	K	80	ASP	CB-CG-OD1	6.61	124.25	118.30
14	P	36	G	P-O3'-C3'	6.40	127.38	119.70
1	A	1262	MET	CA-CB-CG	6.17	123.80	113.30
11	K	79	PRO	C-N-CA	5.52	135.51	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	910	LYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11291	0	11400	119	0
2	B	9062	0	9107	83	0
3	C	2059	0	2008	31	0
4	D	1005	0	964	10	0
5	E	1711	0	1733	15	0
6	F	658	0	686	8	0
7	G	1334	0	1333	26	0
8	H	1186	0	1147	11	0
9	I	927	0	859	9	0
10	J	533	0	557	8	0
11	K	920	0	942	5	0
12	L	372	0	378	4	0
13	N	633	0	333	3	0
14	P	302	0	153	1	0
15	T	827	0	463	2	0
16	U	1343	0	1340	18	0
17	A	5	0	0	0	0
17	B	2	0	0	0	0
17	I	3	0	0	0	0
17	U	1	0	0	0	0
18	A	3	0	0	0	0
All	All	34177	0	33403	308	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 5.

The worst 5 of 308 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)
1:A:1457:ASN:HD22	1:A:1465:PRO:HD3	1.52	0.75
1:A:479:TRP:HB2	1:A:483:ARG:HH22	1.51	0.74
1:A:1148:ALA:HB1	1:A:1333:GLU:HB3	1.74	0.68
1:A:1155:LYS:HE2	16:U:245:ILE:HD12	1.76	0.68
2:B:273:PHE:HB3	2:B:284:ILE:HD12	1.77	0.67

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1413/1984 (71%)	1357 (96%)	56 (4%)	0	100	100
2	B	1128/1251 (90%)	1086 (96%)	42 (4%)	0	100	100
3	C	253/275 (92%)	245 (97%)	8 (3%)	0	100	100
4	D	126/142 (89%)	123 (98%)	3 (2%)	0	100	100
5	E	207/210 (99%)	206 (100%)	1 (0%)	0	100	100
6	F	80/127 (63%)	78 (98%)	2 (2%)	0	100	100
7	G	169/172 (98%)	167 (99%)	2 (1%)	0	100	100
8	H	146/150 (97%)	139 (95%)	7 (5%)	0	100	100
9	I	112/125 (90%)	105 (94%)	7 (6%)	0	100	100
10	J	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	U	168/304 (55%)	158 (94%)	10 (6%)	0	100	100
All	All	4022/4982 (81%)	3878 (96%)	144 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	1252/1763 (71%)	1251 (100%)	1 (0%)	93	98
2	B	993/1084 (92%)	993 (100%)	0	100	100
3	C	234/252 (93%)	234 (100%)	0	100	100
4	D	106/126 (84%)	106 (100%)	0	100	100
5	E	189/190 (100%)	189 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	147/153 (96%)	147 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	103/112 (92%)	103 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
16	U	148/268 (55%)	148 (100%)	0	100	100
All	All	3573/4407 (81%)	3572 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1375	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1251	ASN
2	B	817	GLN
2	B	912	ASN
7	G	139	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	13/14 (92%)	3 (23%)	2 (15%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	36	G
14	P	37	G
14	P	39	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	36	G
14	P	38	G

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	831:LEU	C	832:THR	N	5.19
1	A	1195:VAL	C	1196:TYR	N	4.95

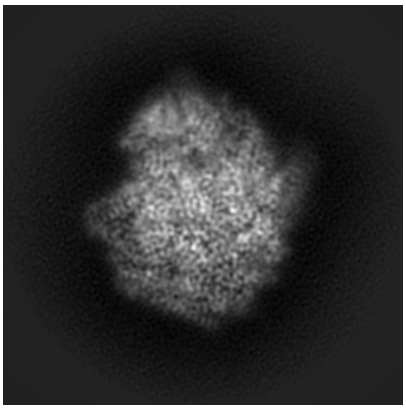
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15129. These allow visual inspection of the internal detail of the map and identification of artifacts.

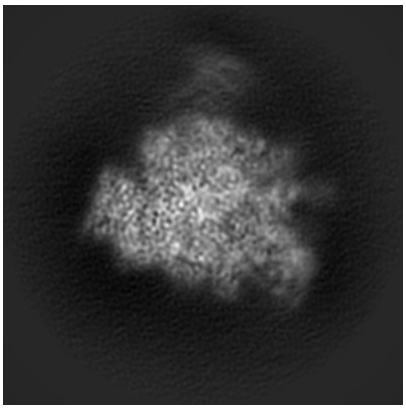
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

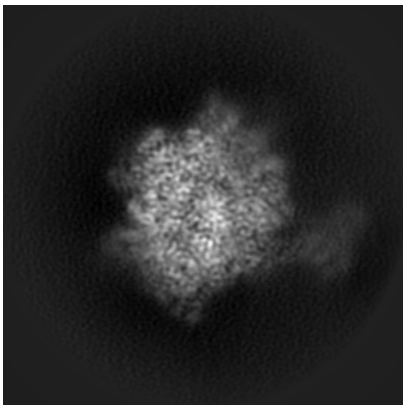
6.1.1 Primary map



X

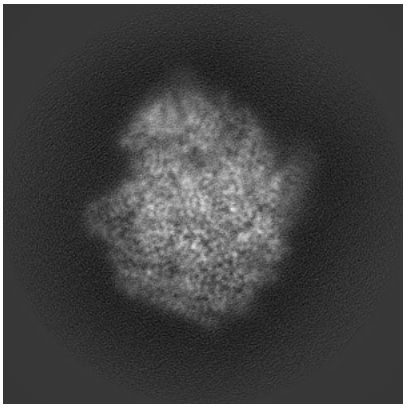


Y

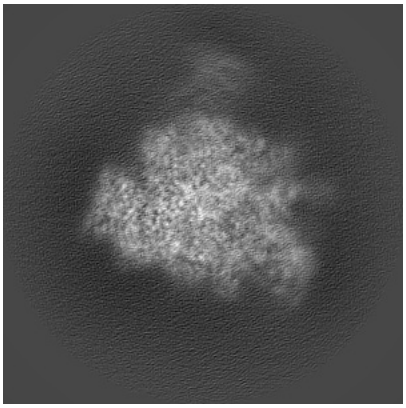


Z

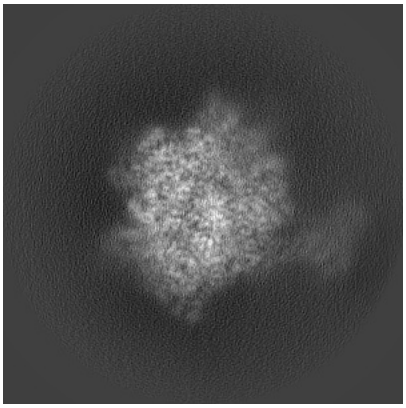
6.1.2 Raw map



X



Y

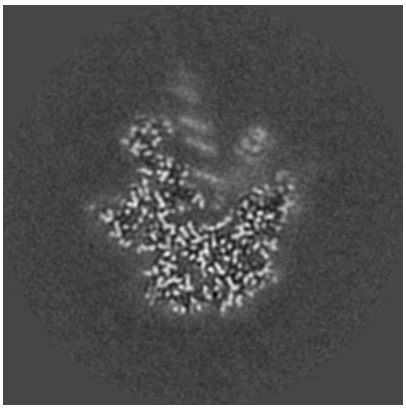


Z

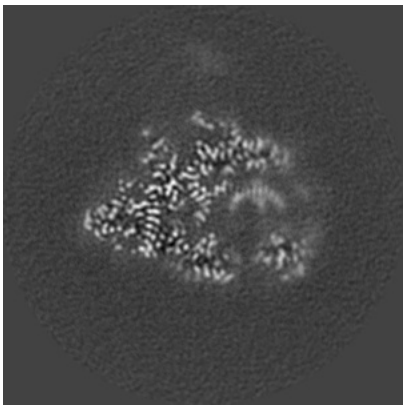
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

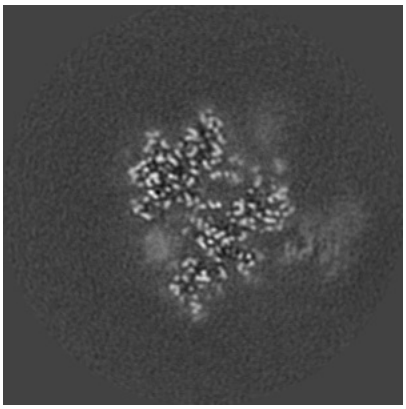
6.2.1 Primary map



X Index: 150

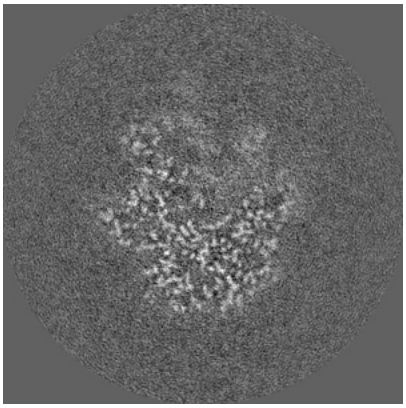


Y Index: 150

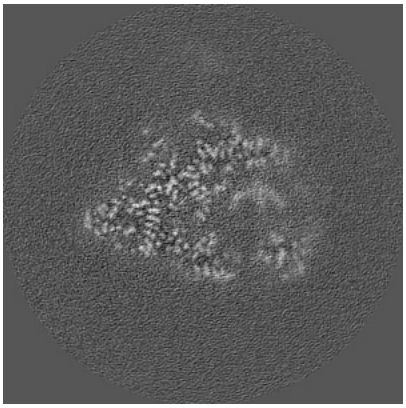


Z Index: 150

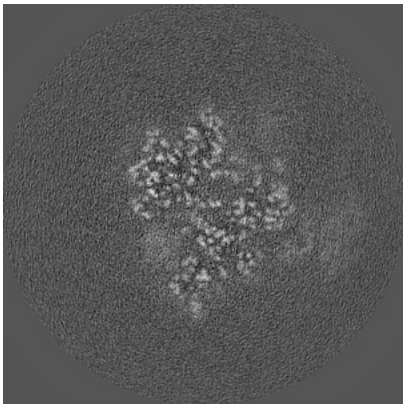
6.2.2 Raw map



X Index: 150



Y Index: 150

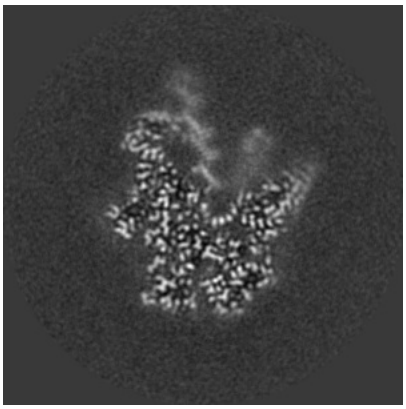


Z Index: 150

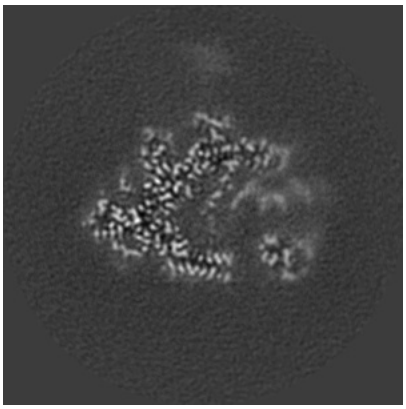
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

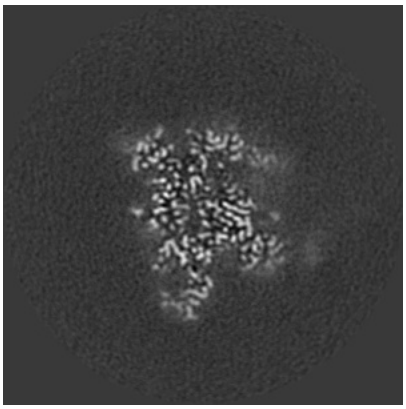
6.3.1 Primary map



X Index: 155

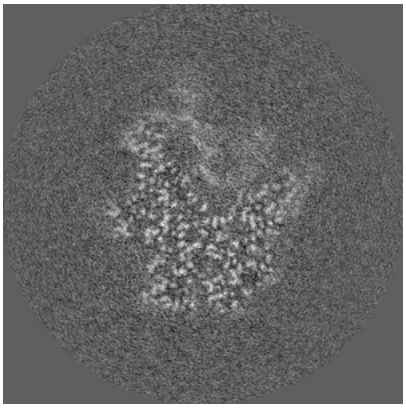


Y Index: 146

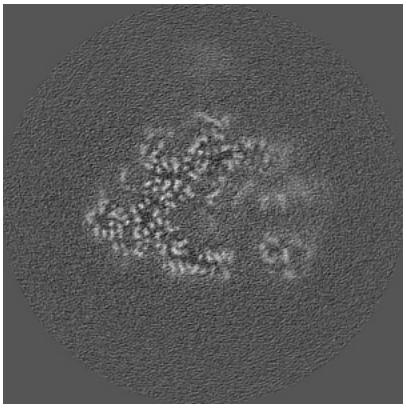


Z Index: 128

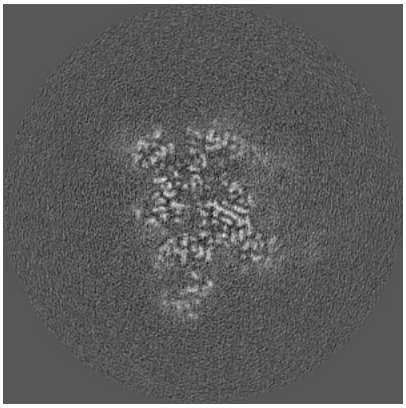
6.3.2 Raw map



X Index: 154



Y Index: 145

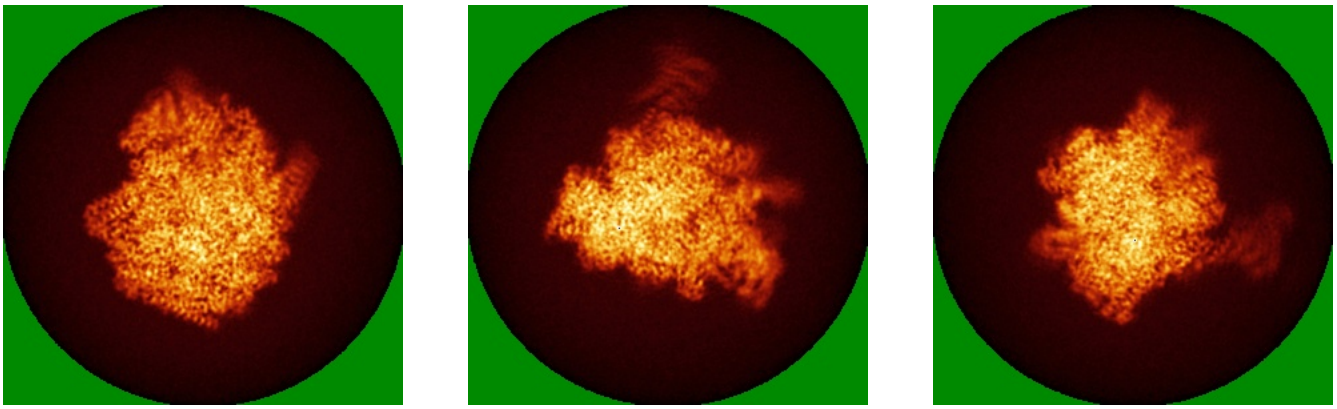


Z Index: 129

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

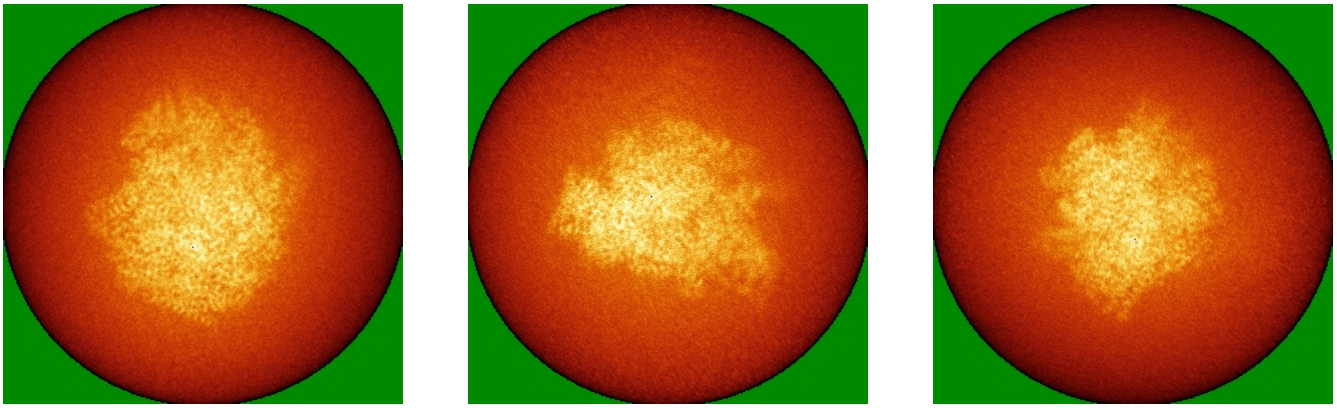
6.4 Orthogonal standard-deviation projections (False-color) (i)

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.

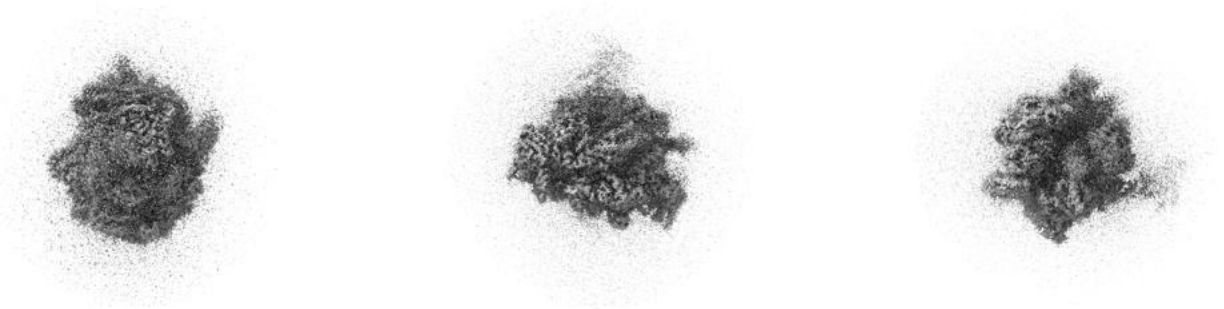
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. 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.

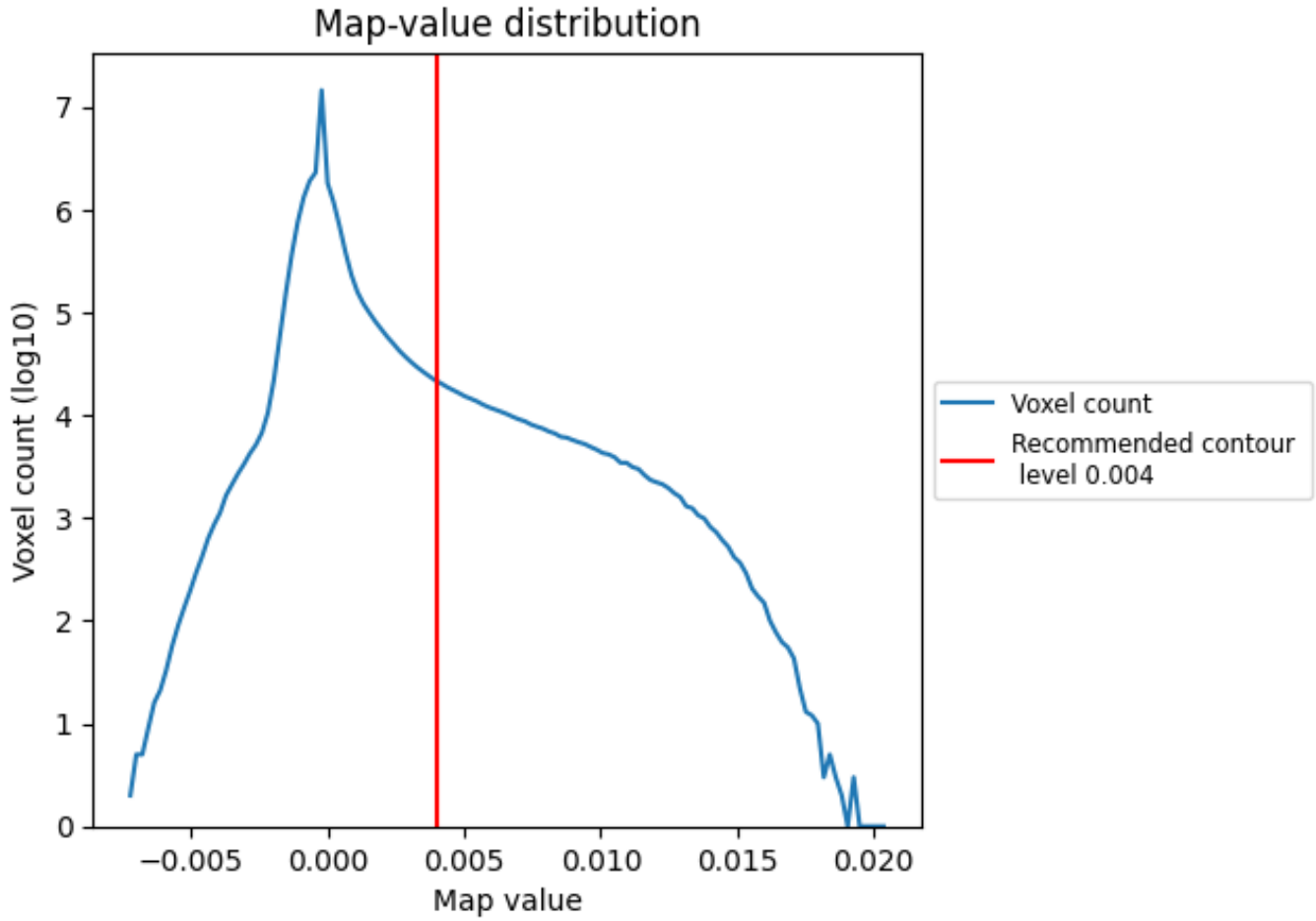
6.6 Mask visualisation (i)

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

7 Map analysis

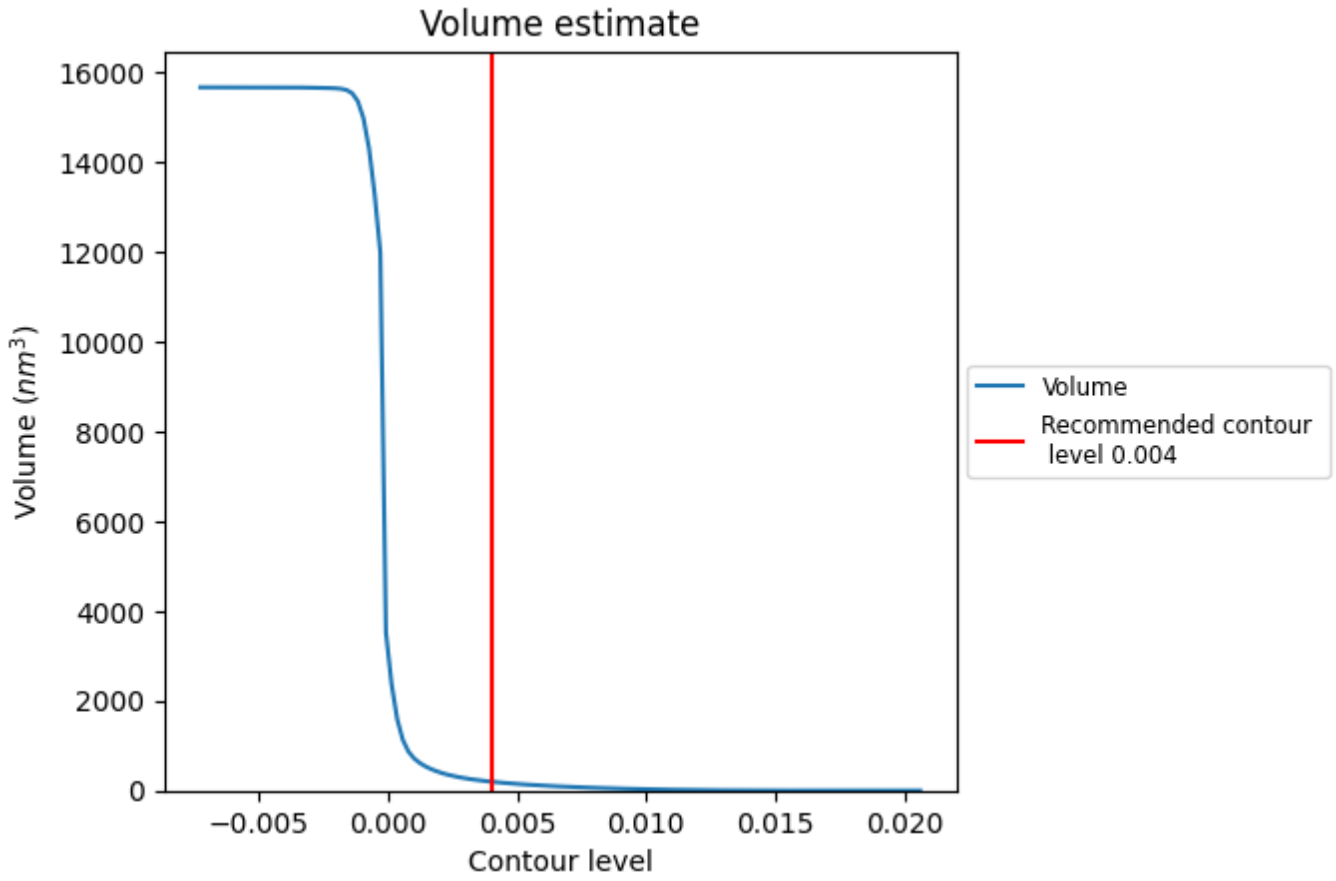
This section contains the results of statistical analysis of the map.

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.

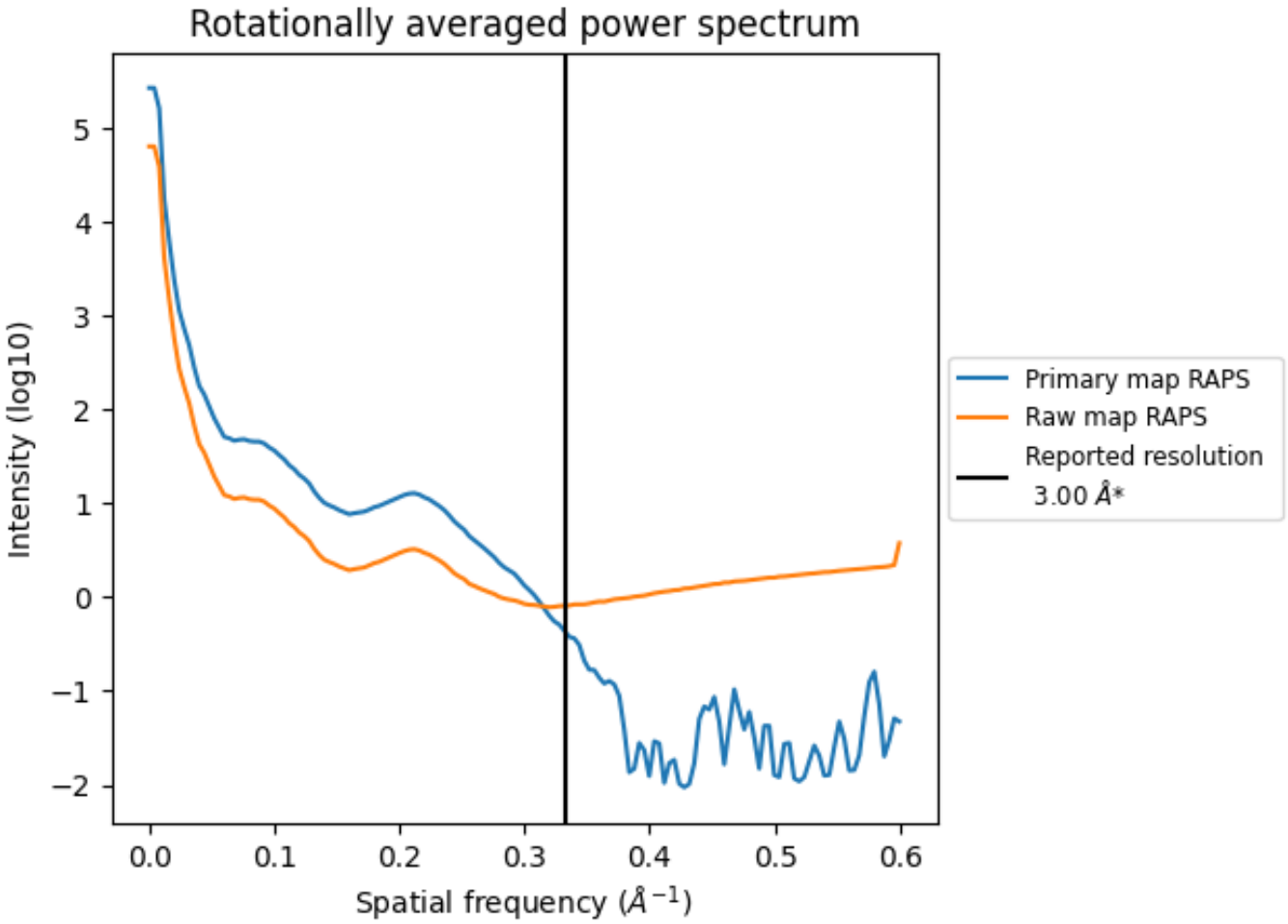
7.2 Volume estimate (i)



The volume at the recommended contour level is 198 nm^3; this corresponds to an approximate mass of 179 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)

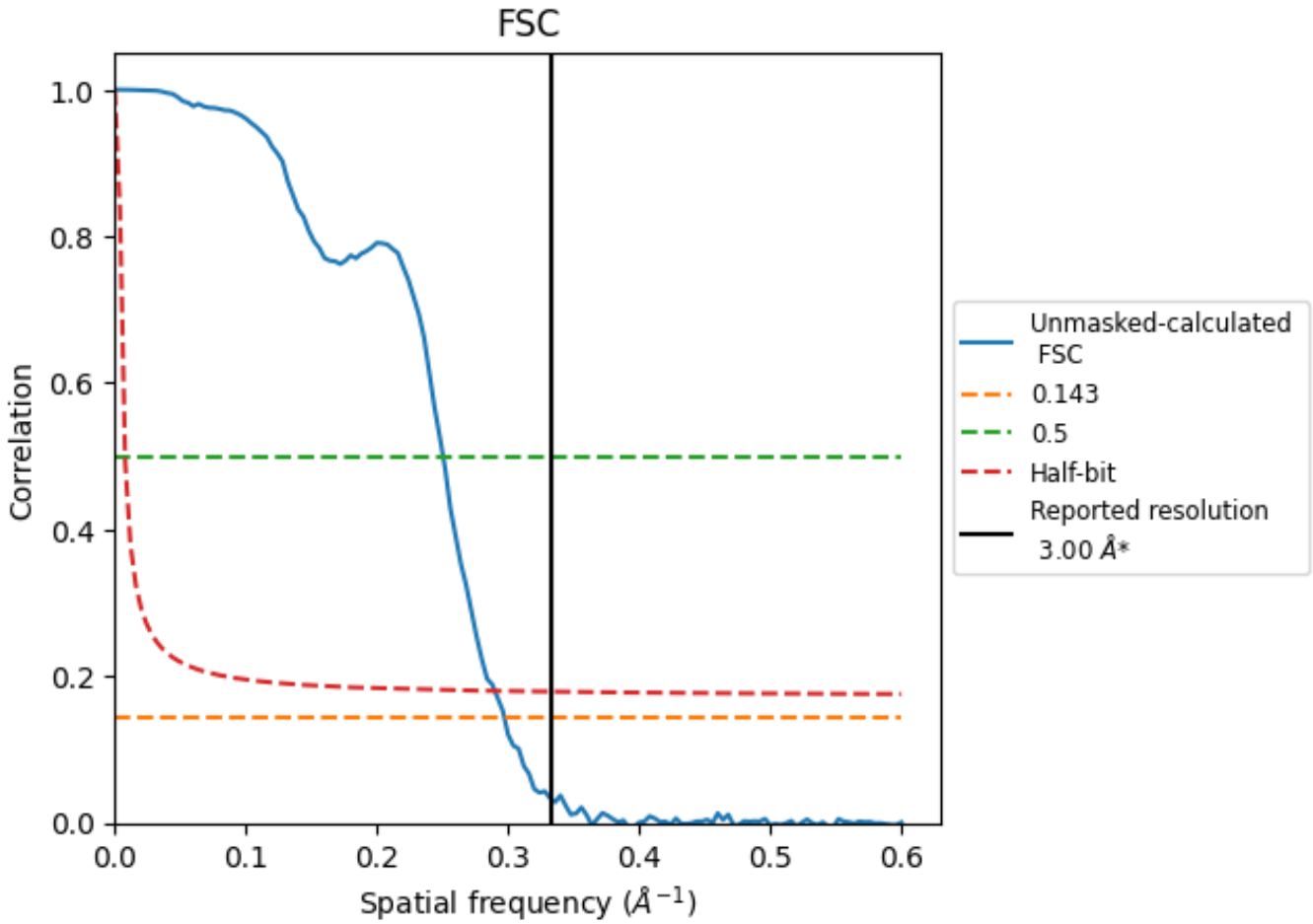


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

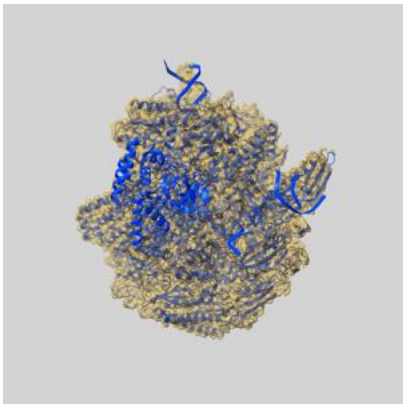
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.37	4.00	3.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.37 differs from the reported value 3.0 by more than 10 %

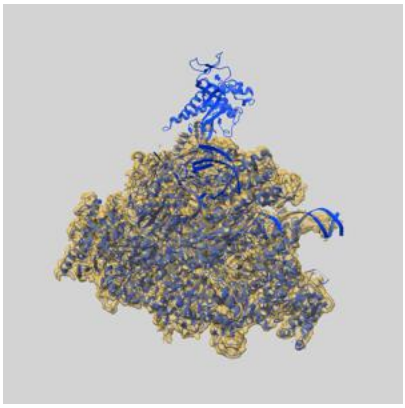
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15129 and PDB model 8A40. Per-residue inclusion information can be found in section 3 on page 8.

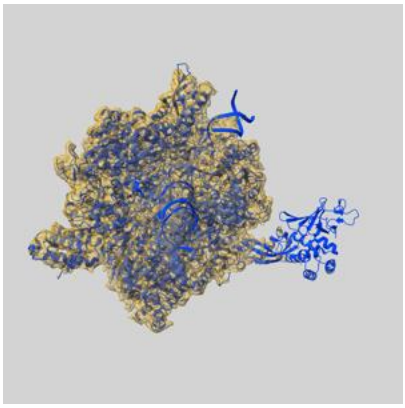
9.1 Map-model overlay



X



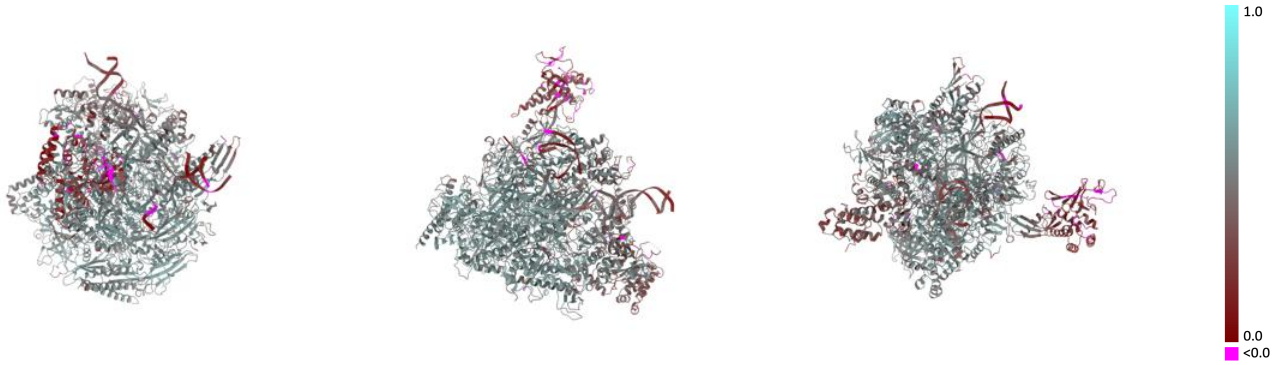
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 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.

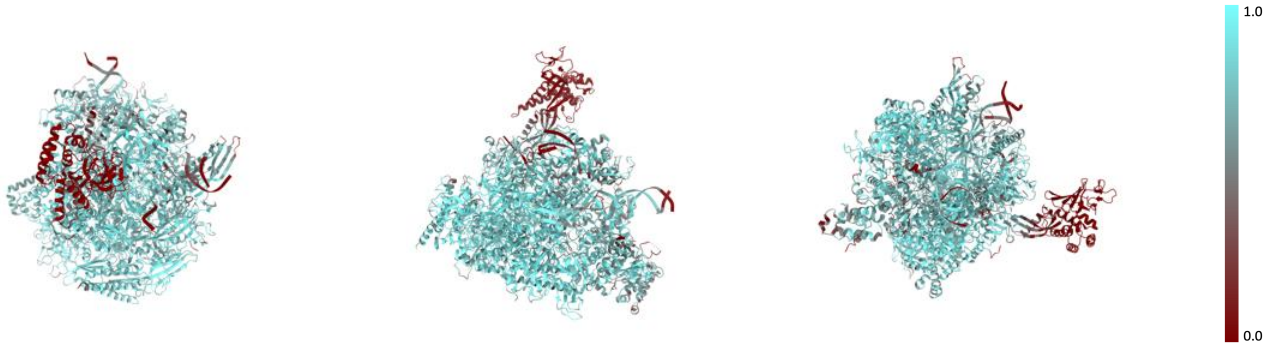
9.2 Q-score mapped to coordinate model (i)



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.

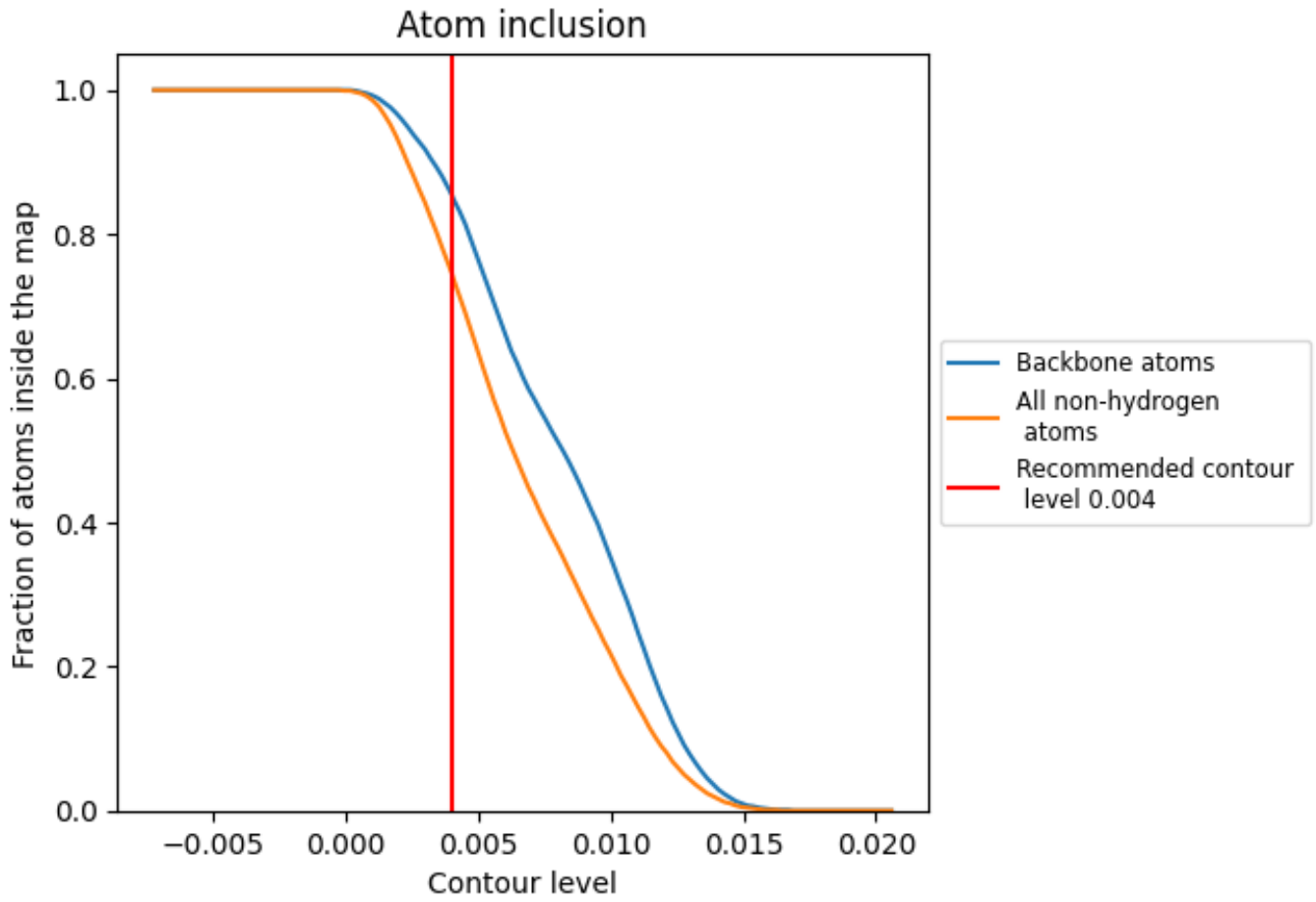
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 74% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7450	0.4860
A	0.8110	0.5190
B	0.8190	0.5300
C	0.8500	0.5460
D	0.0040	0.1800
E	0.8020	0.5020
F	0.8120	0.5270
G	0.1810	0.2750
H	0.8070	0.5190
I	0.7580	0.4900
J	0.8640	0.5630
K	0.8640	0.5520
L	0.7770	0.4930
N	0.5500	0.2920
P	0.6560	0.3980
T	0.6880	0.3940
U	0.4860	0.2760