



wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 01:52 pm GMT

PDB ID : 7AOE
EMDB ID : EMD-11842
Title : Schizosaccharomyces pombe RNA polymerase I (elongation complex)
Authors : Heiss, F.; Daiss, J.; Becker, P.; Engel, C.
Deposited on : 2020-10-14
Resolution : 3.90 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

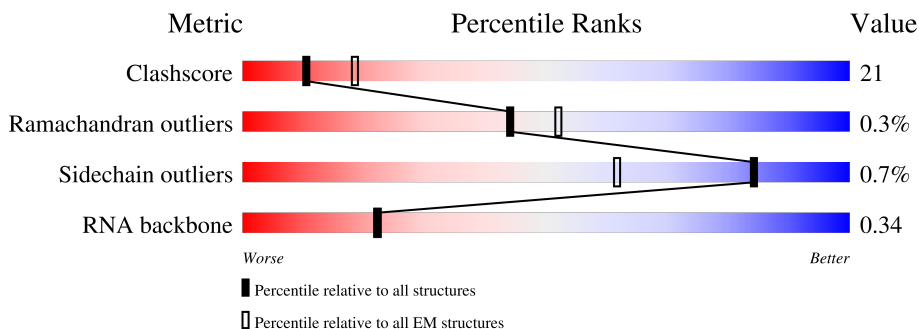
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.90 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1689	
2	B	1174	
3	C	348	
4	D	147	
5	E	210	
6	F	142	
7	G	173	

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Mol	Chain	Length	Quality of chain
8	H	125	<p>6% 47% 50%</p>
9	I	119	<p>36% 33% 15% 52%</p>
10	J	71	<p>6% 54% 41%</p>
11	K	125	<p>6% 54% 22% 24%</p>
12	L	63	<p>6% 44% 27% 29%</p>
13	U	39	<p>36% 13% 23% 64%</p>
14	T	39	<p>33% 15% 49% 36%</p>
15	R	20	<p>15% 15% 5% 65%</p>

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 30828 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 I subunit rpa1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1401	11102	7039	1918	2086	59	0	0

- Molecule 2 is a protein called Probable DNA-directed RNA polymerase I subunit RPA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1174	9254	5867	1618	1710	59	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	317	2533	1621	430	475	7	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit rpa14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	39	322	203	57	61	1	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	207	1663	1050	301	306	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	82	650	413	111	123	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit rpa43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	160	1267	817	210	236	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	123	990	628	166	193	3	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	57	431	269	69	89	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	68	550	350	93	100	7	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	95	745	472	123	146	4	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	45	368	225	74	61	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	U	14	285	138	51	83	13	0	0

- Molecule 14 is a DNA chain called template DNA.

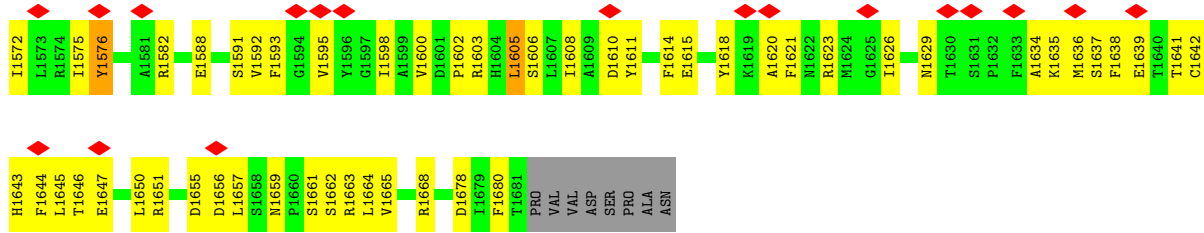
Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	25	Total	C	N	O	P	0	0
			509	244	95	146	24		

- Molecule 15 is a RNA chain called RNA.

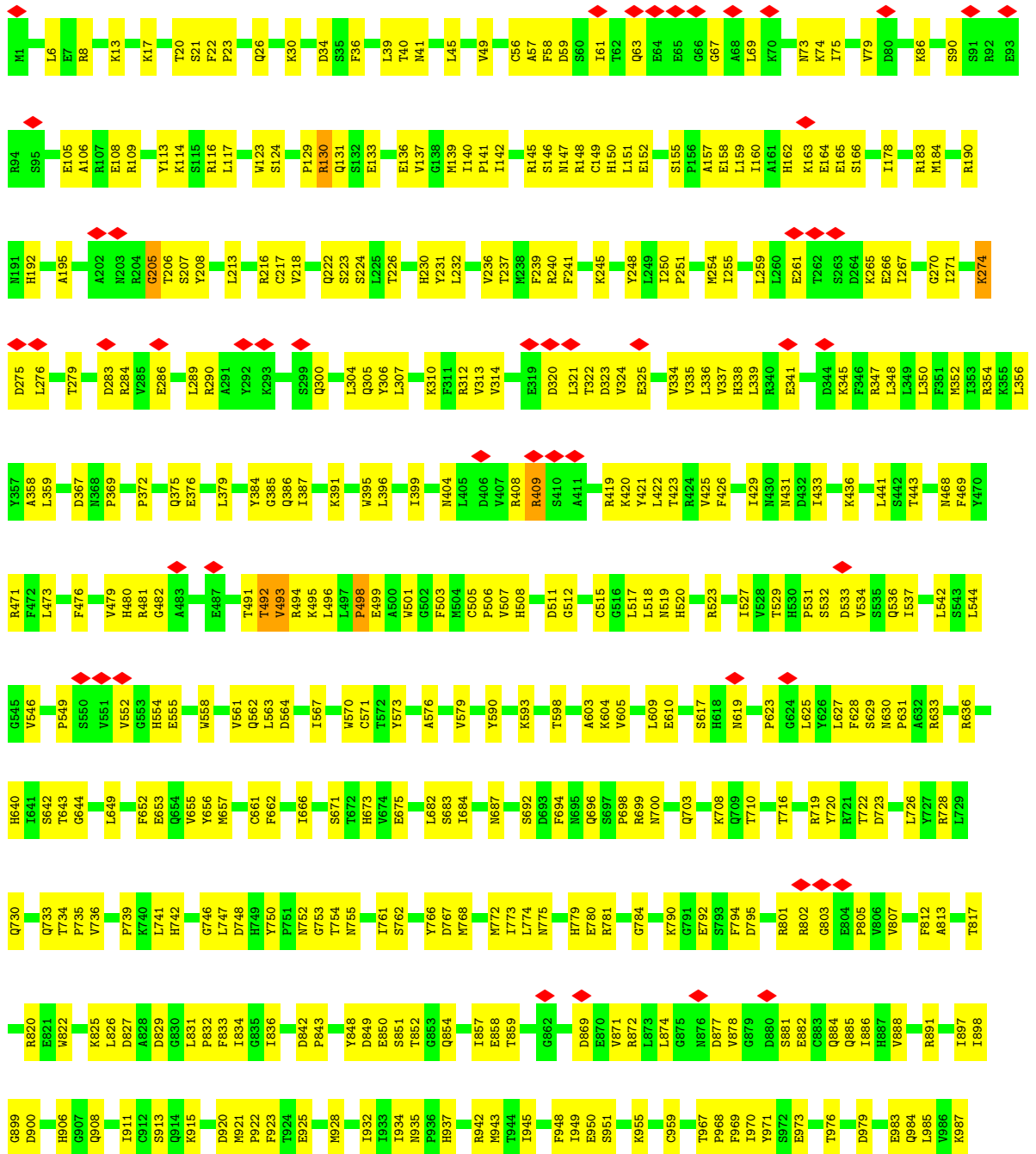
Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	7	Total	C	N	O	P	0	0
			153	68	31	47	7		

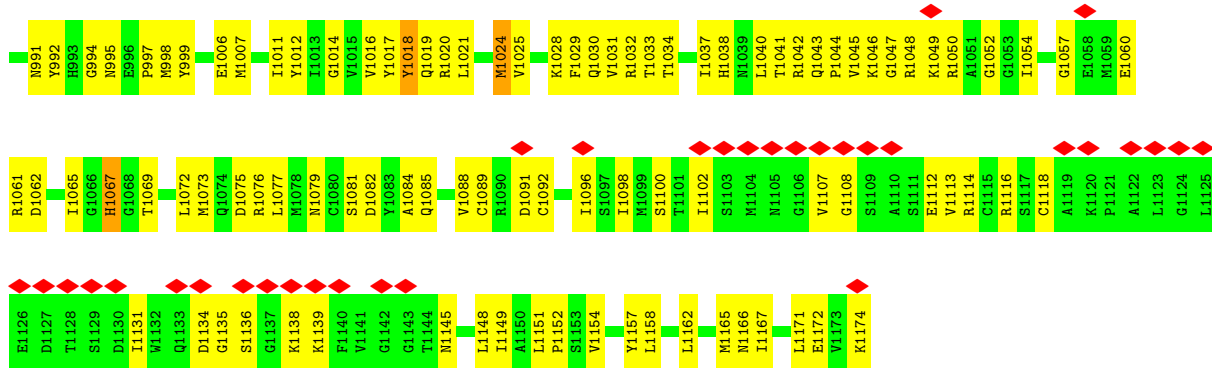
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	A	2	Total	Zn	0
			2	2	
16	B	1	Total	Zn	0
			1	1	
16	I	1	Total	Zn	0
			1	1	
16	J	1	Total	Zn	0
			1	1	
16	L	1	Total	Zn	0
			1	1	

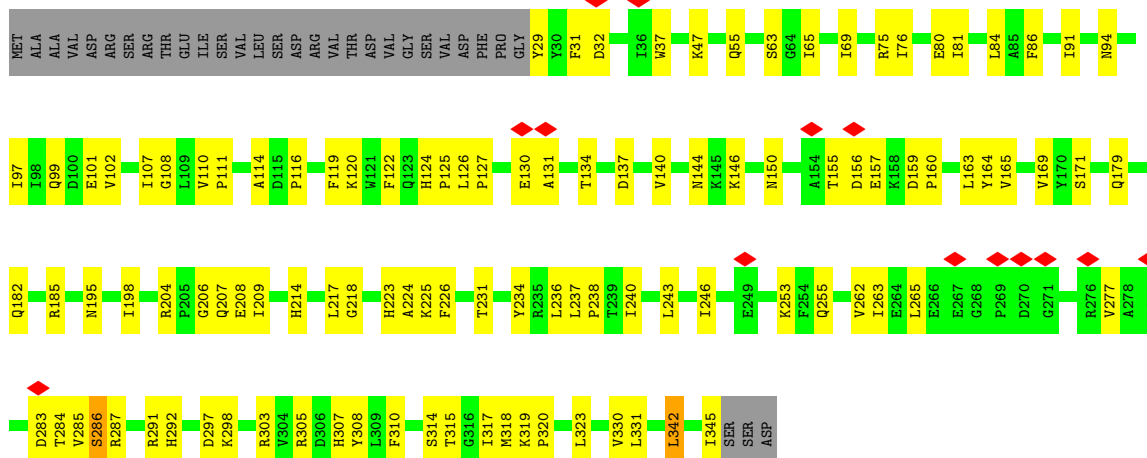


• Molecule 2: Probable DNA-directed RNA polymerase I subunit RPA2

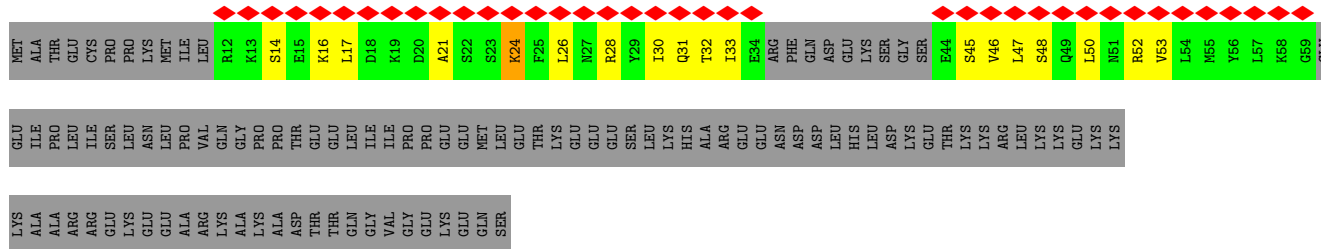




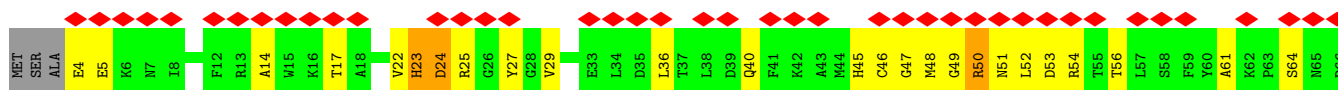
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPA C1

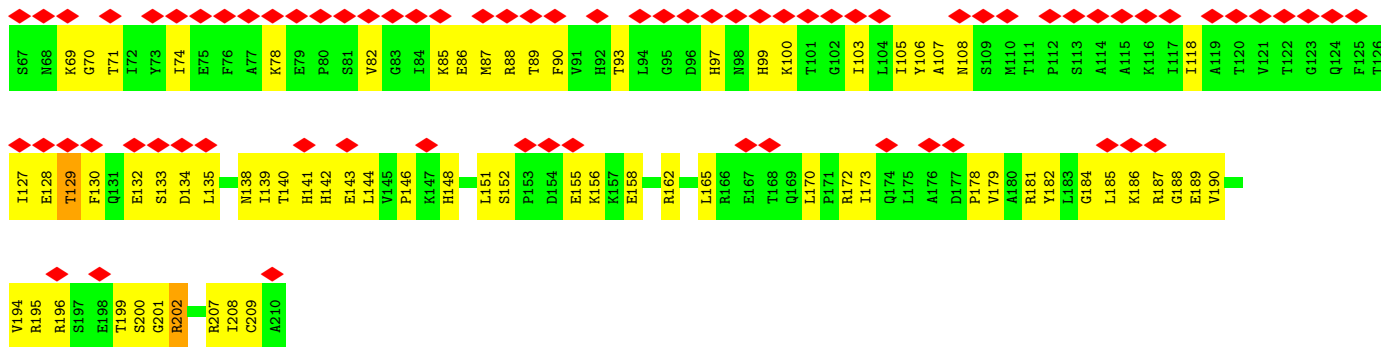


• Molecule 4: DNA-directed RNA polymerase I subunit rpa14

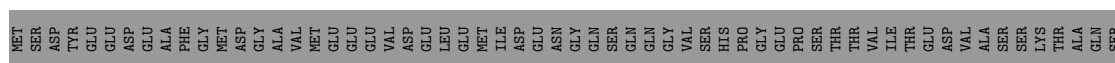


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPA BC1

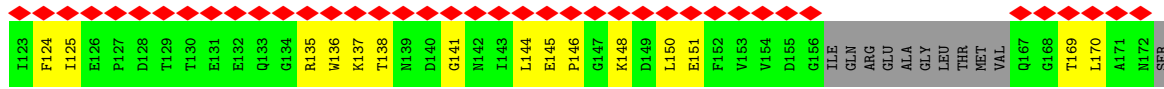
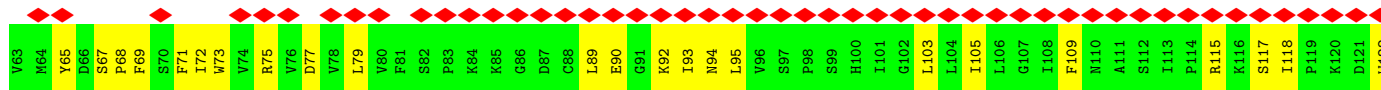
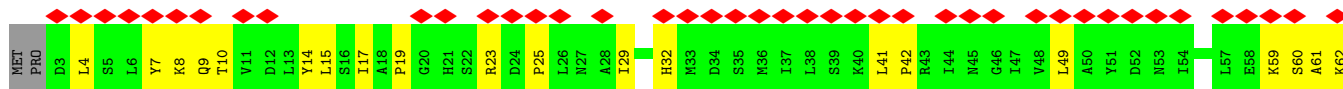
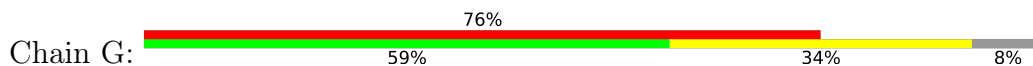




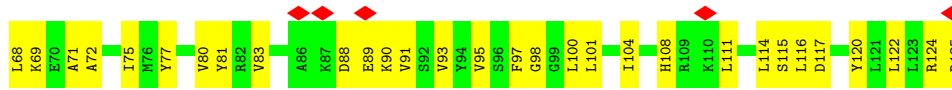
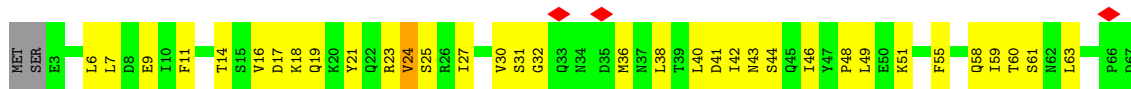
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



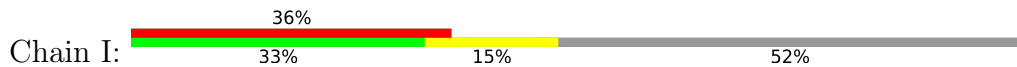
• Molecule 7: DNA-directed RNA polymerase I subunit rpa43

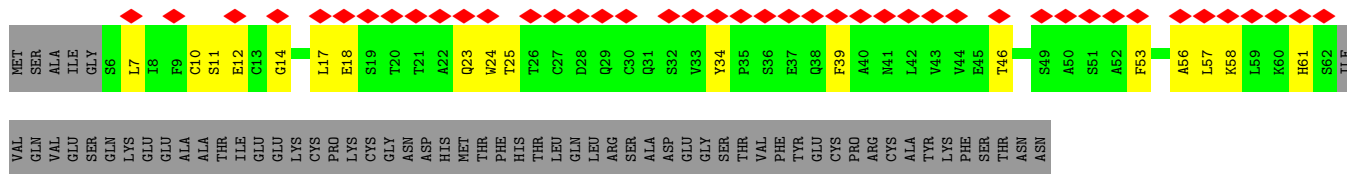


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 9: DNA-directed RNA polymerase I subunit RPA12

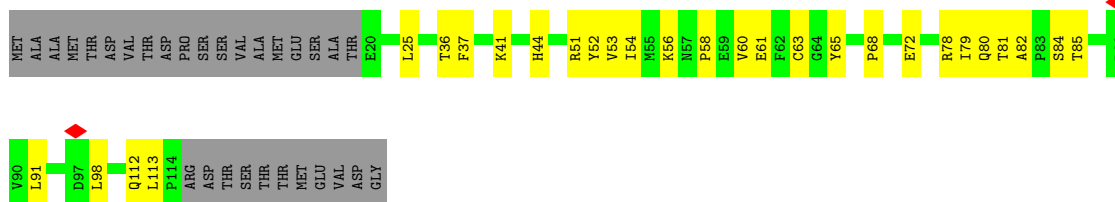




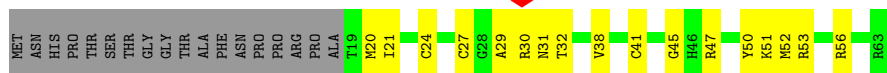
● Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



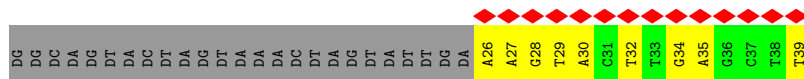
● Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



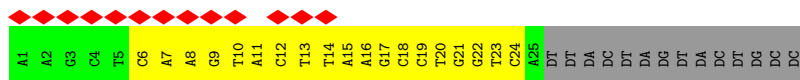
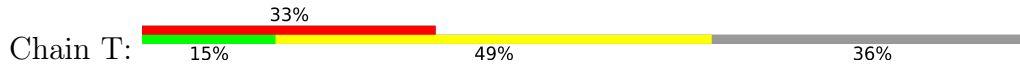
● Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



● Molecule 13: non-template DNA



● Molecule 14: template DNA



● Molecule 15: RNA



U	A	U	C	U	G	C	A	U	G	U	A	G13	A14	C15	A17	G18	G19	C
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	88.28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.371	Depositor
Minimum map value	-0.231	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	272.256, 272.256, 272.256	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0635, 1.0635, 1.0635	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:
ZN

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	0.40	0/11323	0.53	1/15297 (0.0%)
2	B	0.44	0/9463	0.53	0/12794
3	C	0.41	0/2588	0.51	0/3505
4	D	0.26	0/323	0.40	0/427
5	E	0.31	0/1695	0.54	1/2287 (0.0%)
6	F	0.38	0/660	0.48	0/893
7	G	0.31	0/1295	0.50	0/1755
8	H	0.39	0/1004	0.59	0/1355
9	I	0.28	0/439	0.48	0/596
10	J	0.48	0/558	0.55	0/751
11	K	0.43	0/759	0.51	1/1030 (0.1%)
12	L	0.42	0/371	0.50	0/491
13	U	0.59	0/319	0.97	0/491
14	T	0.74	0/571	0.93	0/879
15	R	0.64	0/171	1.11	0/265
All	All	0.42	0/31539	0.55	3/42816 (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	7
2	B	0	5
5	E	0	3
All	All	0	15

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	735	GLN	C-N-CA	-5.15	108.84	121.70
11	K	112	GLN	C-N-CA	-5.13	108.87	121.70
5	E	24	ASP	N-CA-C	5.10	124.78	111.00

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1068	LEU	Peptide
1	A	246	ILE	Peptide
1	A	6	PRO	Peptide
1	A	686	ILE	Peptide
1	A	84	ILE	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	11102	0	11105	570	0
2	B	9254	0	9225	447	0
3	C	2533	0	2540	97	0
4	D	322	0	338	20	0
5	E	1663	0	1684	80	0
6	F	650	0	674	29	0
7	G	1267	0	1278	53	0
8	H	990	0	1001	54	0
9	I	431	0	410	16	0
10	J	550	0	566	35	0
11	K	745	0	745	27	0
12	L	368	0	377	20	0
13	U	285	0	161	8	0
14	T	509	0	283	20	0
15	R	153	0	78	3	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	1	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30828	0	30465	1295	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 21.

The worst 5 of 1295 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)
2:B:1092:CYS:HB3	2:B:1118:CYS:SG	1.94	1.08
1:A:1297:TYR:HB3	1:A:1494:LEU:O	1.61	1.00
1:A:466:GLN:O	1:A:470:LYS:HB2	1.63	0.96
1:A:1297:TYR:OH	1:A:1505:MET:SD	2.24	0.94
5:E:23:HIS:HA	5:E:25:ARG:H	1.34	0.93

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	1377/1689 (82%)	1229 (89%)	143 (10%)	5 (0%)	34 71
2	B	1172/1174 (100%)	1022 (87%)	145 (12%)	5 (0%)	34 71
3	C	315/348 (90%)	290 (92%)	24 (8%)	1 (0%)	41 75
4	D	35/147 (24%)	33 (94%)	2 (6%)	0	100 100
5	E	205/210 (98%)	178 (87%)	27 (13%)	0	100 100
6	F	80/142 (56%)	71 (89%)	9 (11%)	0	100 100
7	G	156/173 (90%)	143 (92%)	13 (8%)	0	100 100
8	H	121/125 (97%)	92 (76%)	28 (23%)	1 (1%)	19 57
9	I	55/119 (46%)	50 (91%)	5 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	66/71 (93%)	46 (70%)	20 (30%)	0	100	100
11	K	93/125 (74%)	88 (95%)	5 (5%)	0	100	100
12	L	43/63 (68%)	41 (95%)	2 (5%)	0	100	100
All	All	3718/4386 (85%)	3283 (88%)	423 (11%)	12 (0%)	44	75

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1067	SER
2	B	493	VAL
2	B	206	THR
1	A	782	GLY
3	C	286	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	A	1239/1484 (84%)	1230 (99%)	9 (1%)	84	90
2	B	1013/1013 (100%)	1003 (99%)	10 (1%)	76	86
3	C	281/308 (91%)	280 (100%)	1 (0%)	91	94
4	D	37/134 (28%)	36 (97%)	1 (3%)	44	67
5	E	182/184 (99%)	181 (100%)	1 (0%)	88	93
6	F	70/121 (58%)	70 (100%)	0	100	100
7	G	143/154 (93%)	143 (100%)	0	100	100
8	H	112/114 (98%)	111 (99%)	1 (1%)	78	87
9	I	51/105 (49%)	51 (100%)	0	100	100
10	J	63/66 (96%)	62 (98%)	1 (2%)	62	79
11	K	86/111 (78%)	86 (100%)	0	100	100
12	L	39/53 (74%)	39 (100%)	0	100	100
All	All	3316/3847 (86%)	3292 (99%)	24 (1%)	84	90

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	820	ARG
2	B	1024	MET
2	B	1018	TYR
2	B	1067	HIS
1	A	1025	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	908	GLN
5	E	138	ASN
2	B	1019	GLN
3	C	182	GLN
7	G	167	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	6/20 (30%)	2 (33%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	15	C
15	R	17	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

There are no chain breaks in this entry.

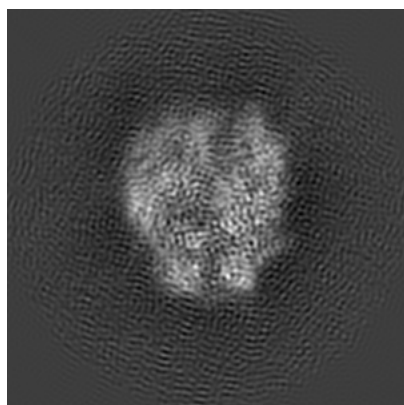
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11842. These allow visual inspection of the internal detail of the map and identification of artifacts.

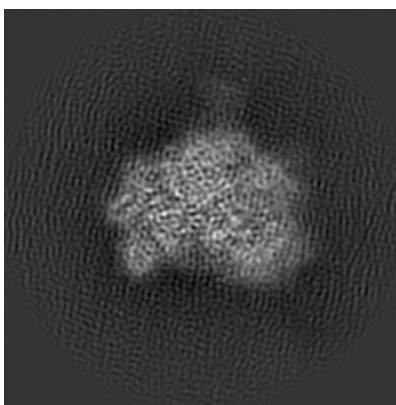
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

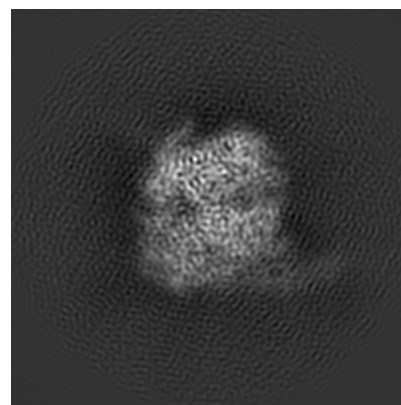
6.1.1 Primary map



X



Y

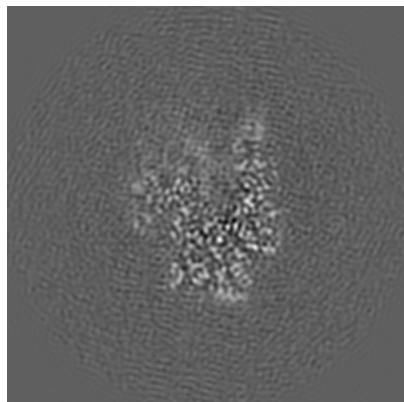


Z

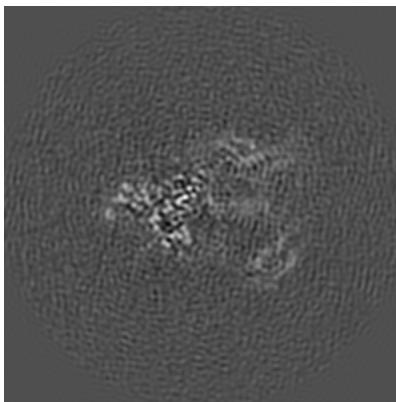
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

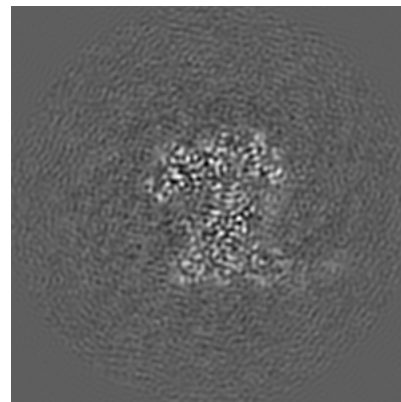
6.2.1 Primary map



X Index: 128



Y Index: 128

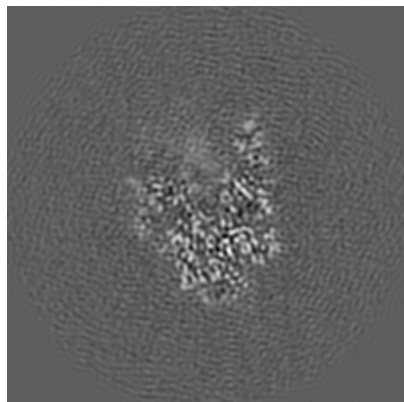


Z Index: 128

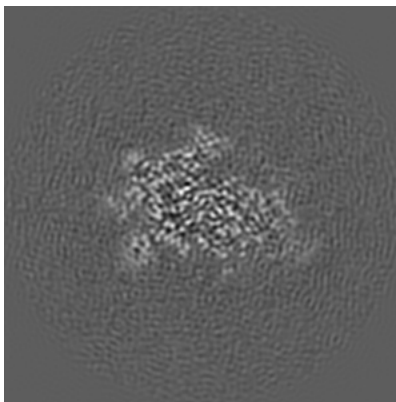
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

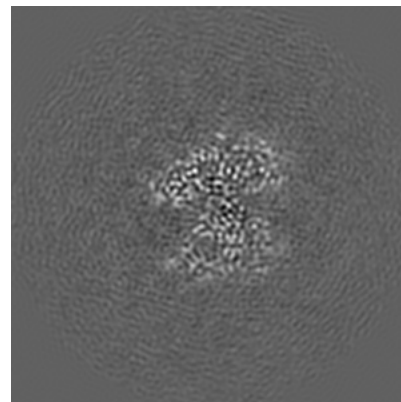
6.3.1 Primary map



X Index: 125



Y Index: 151



Z Index: 118

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

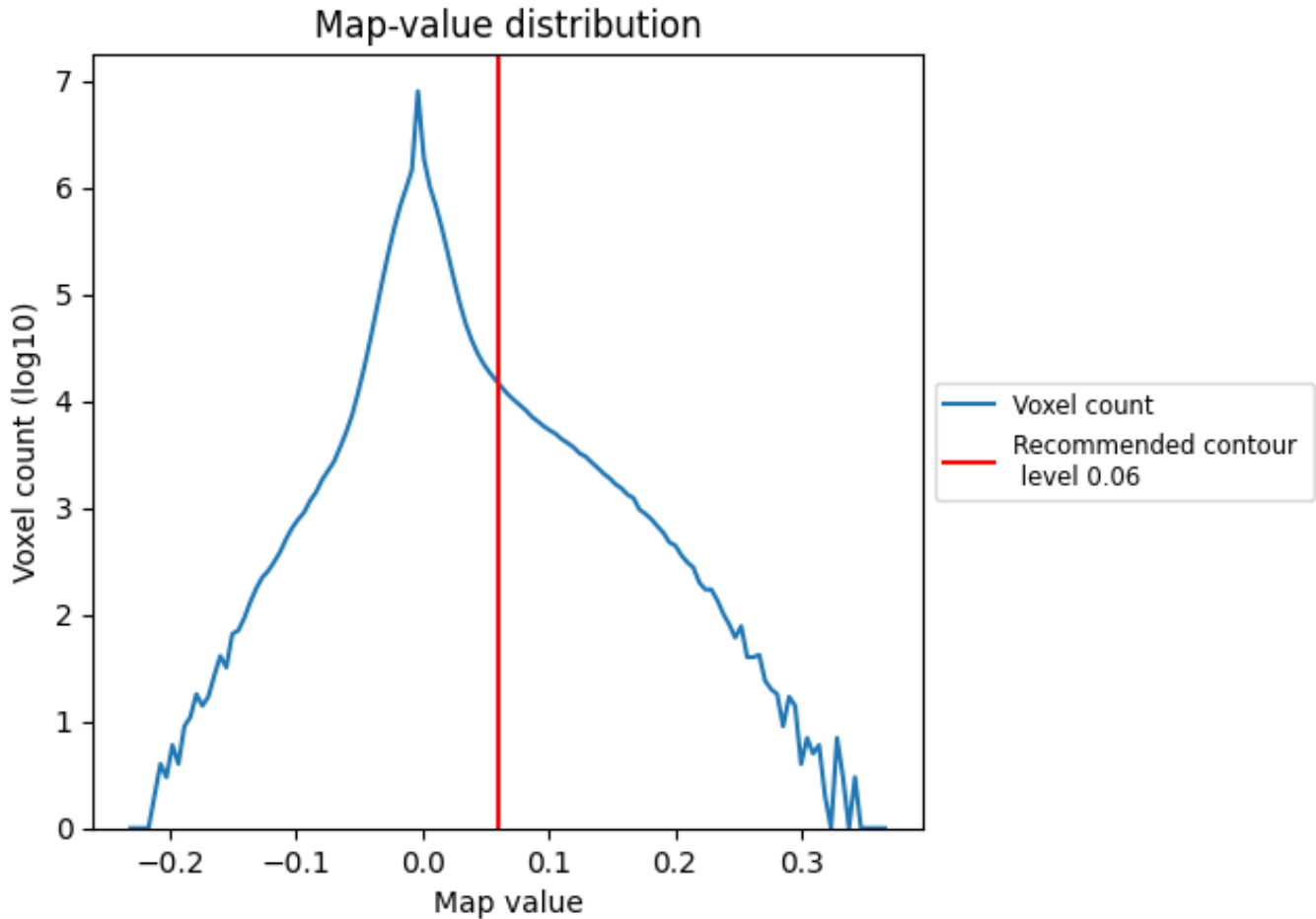
6.5 Mask visualisation

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

7 Map analysis [i](#)

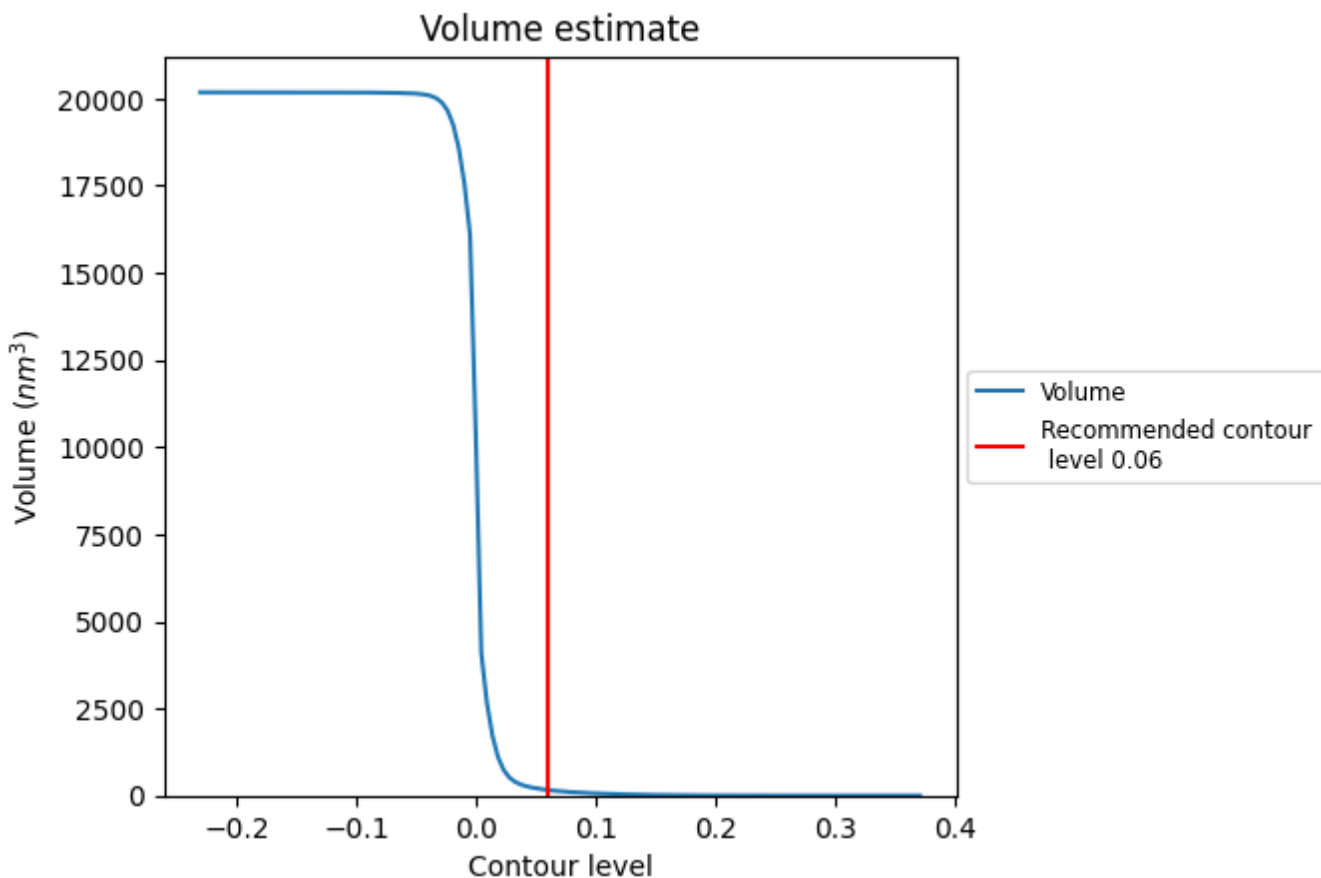
This section contains the results of statistical analysis of the map.

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.

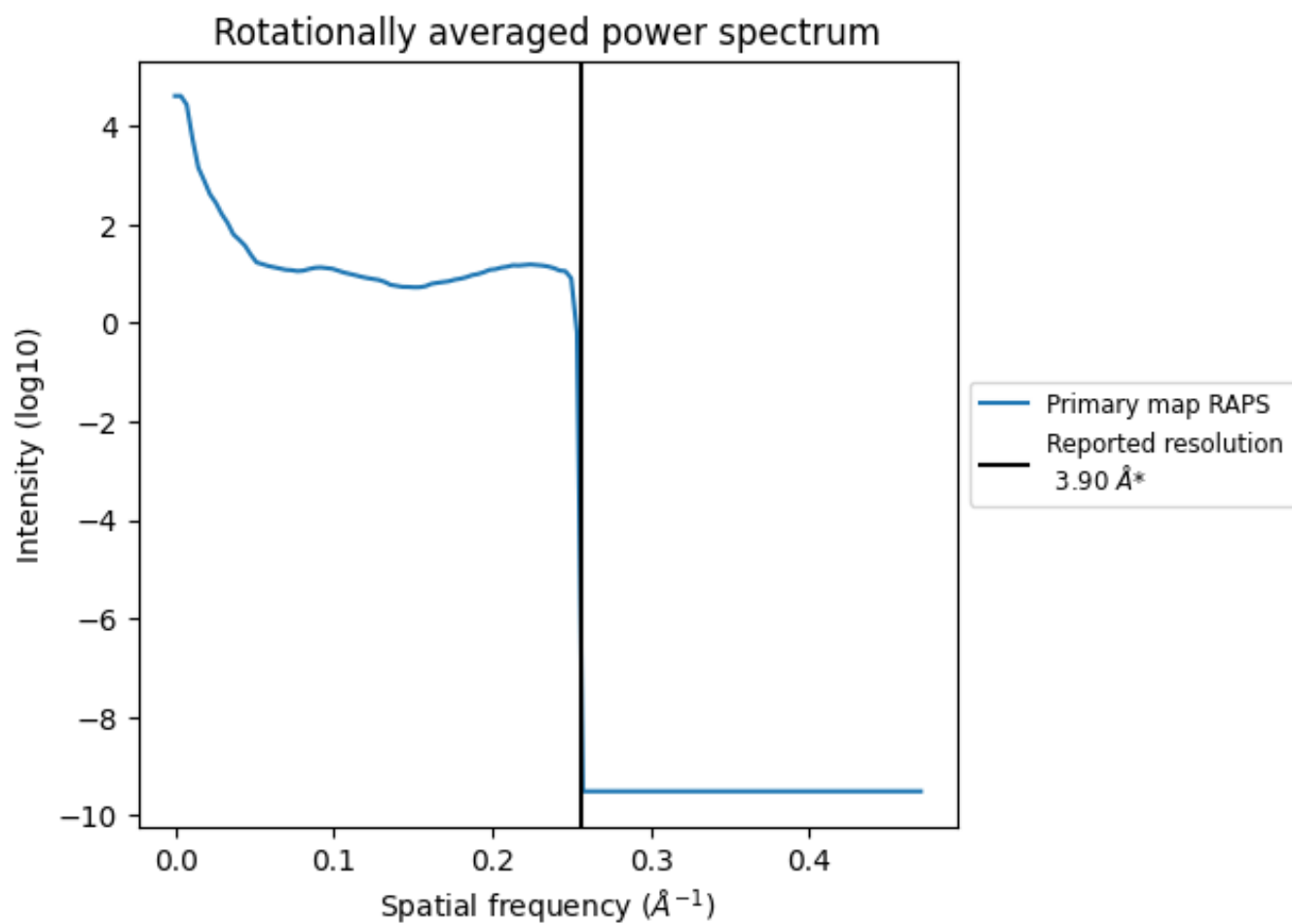
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm³; this corresponds to an approximate mass of 144 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 0.256 Å⁻¹

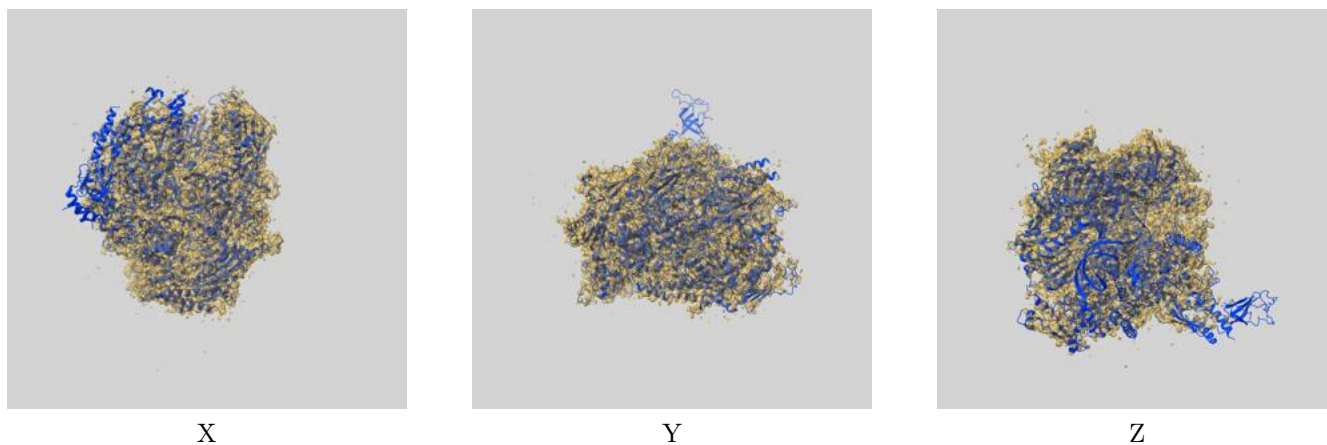
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

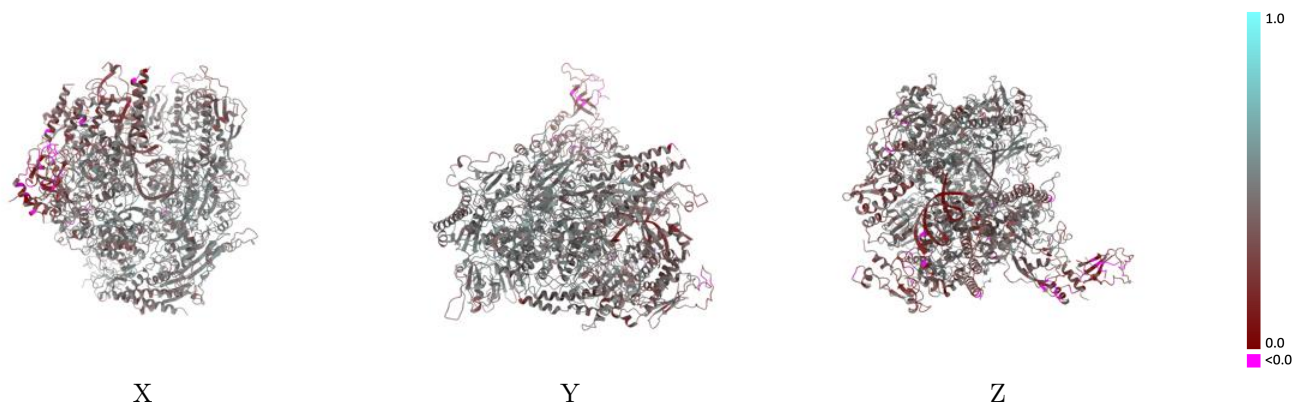
This section contains information regarding the fit between EMDB map EMD-11842 and PDB model 7AOE. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



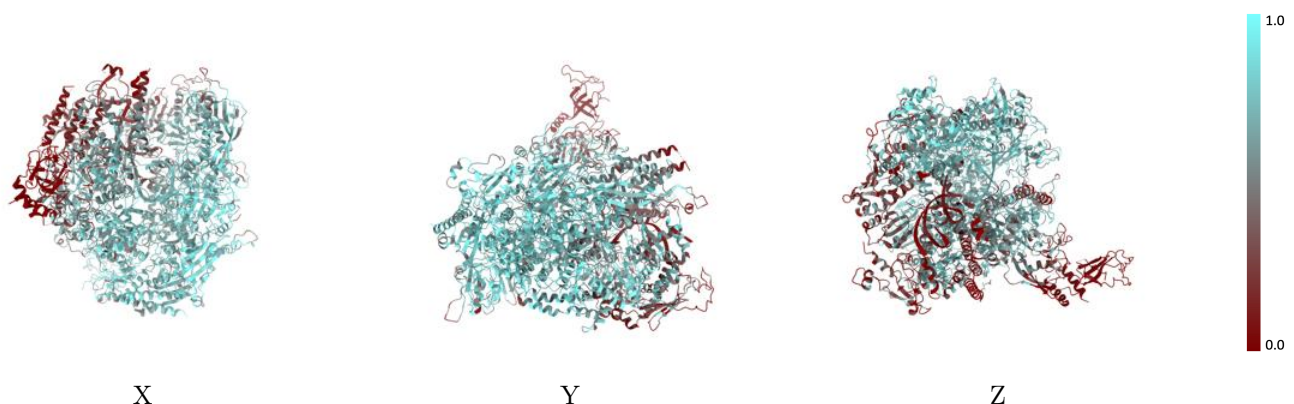
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



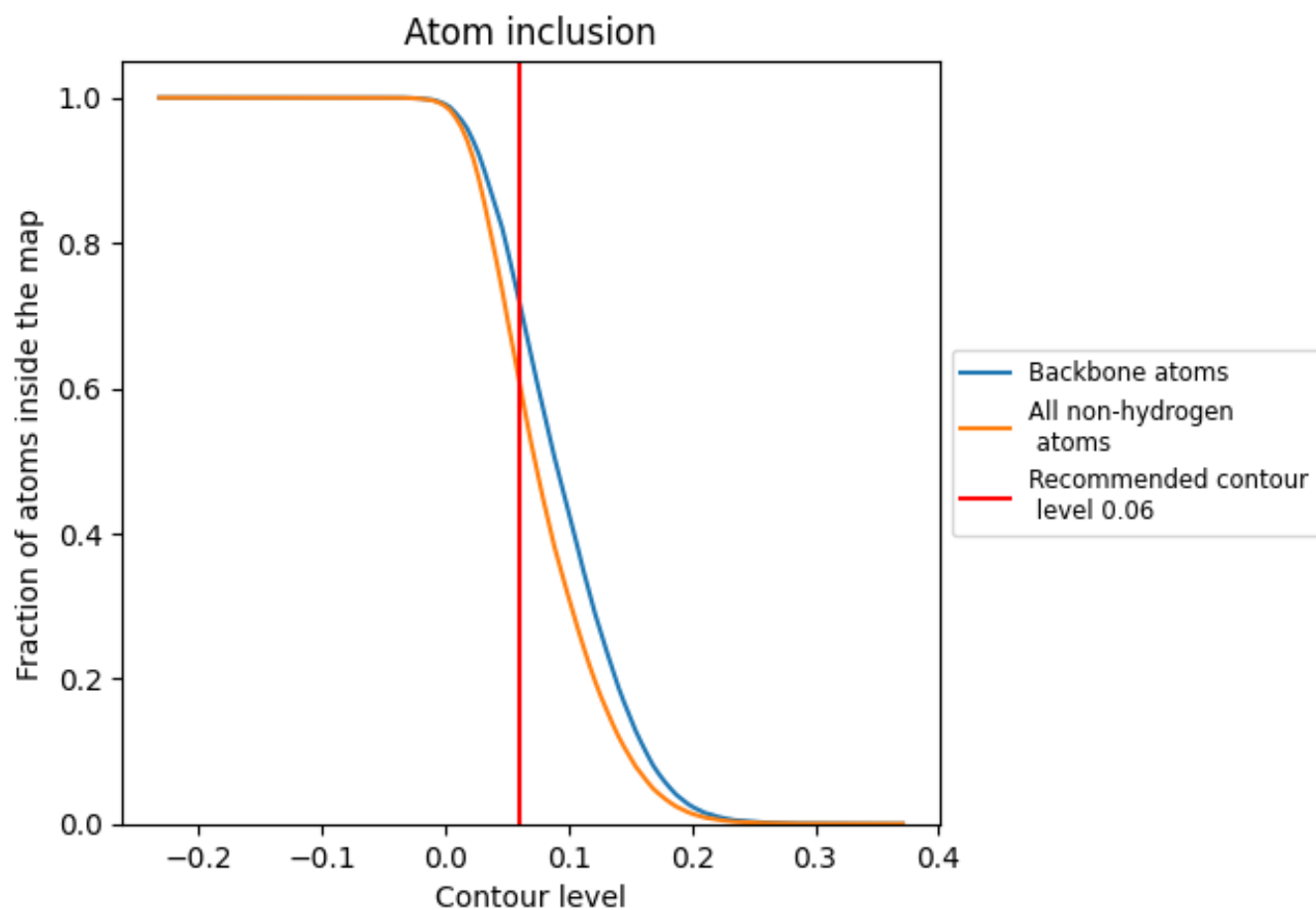
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 61% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6117	 0.4220
A	 0.5746	 0.4190
B	 0.7329	 0.4630
C	 0.7476	 0.4580
D	 0.0032	 0.2100
E	 0.3787	 0.3490
F	 0.6746	 0.4550
G	 0.1763	 0.2540
H	 0.7397	 0.4640
I	 0.2163	 0.3490
J	 0.8219	 0.4870
K	 0.7924	 0.4730
L	 0.7847	 0.4680
R	 0.8105	 0.4310
T	 0.4067	 0.2750
U	 0.0912	 0.1450

