



## wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 10:09 am BST

PDB ID : 7AOC  
EMDB ID : EMD-11840  
Title : Schizosaccharomyces pombe RNA polymerase I (monomer)  
Authors : Heiss, F.; Daiss, J.; Becker, P.; Engel, C.  
Deposited on : 2020-10-14  
Resolution : 3.84 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

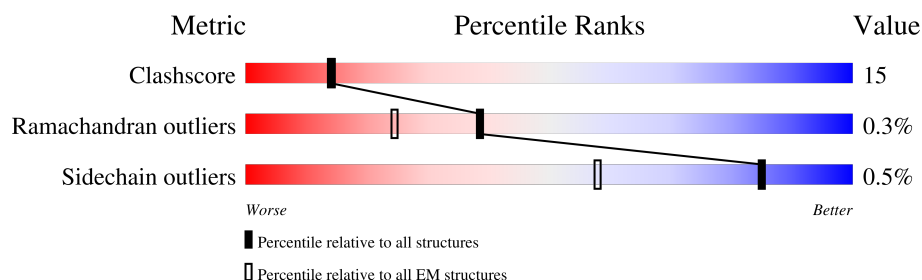
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.84 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>46%</div> <div>55%</div> <div>27%</div> <div>17%</div> </div>
2	B	1174	<div> <div>37%</div> <div>65%</div> <div>33%</div> <div>.</div> </div>
3	C	348	<div> <div>39%</div> <div>65%</div> <div>26%</div> <div>.</div> <div>9%</div> </div>
4	D	147	<div> <div>27%</div> <div>16%</div> <div>10%</div> <div>73%</div> </div>
5	E	210	<div> <div>77%</div> <div>65%</div> <div>30%</div> <div>..</div> </div>
6	F	142	<div> <div>25%</div> <div>45%</div> <div>12%</div> <div>.</div> <div>42%</div> </div>
7	G	173	<div> <div>88%</div> <div>56%</div> <div>36%</div> <div>8%</div> </div>
8	H	125	<div> <div>43%</div> <div>54%</div> <div>43%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	119	<div><div><div></div><div></div><div></div></div><div>47%34%13%52%</div></div>
10	J	71	<div><div><div></div><div></div><div></div></div><div>21%44%51%. .</div></div>
11	K	125	<div><div><div></div><div></div><div></div></div><div>24%56%20%24%</div></div>
12	L	63	<div><div><div></div><div></div><div></div></div><div>33%48%24%29%</div></div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 29724 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
1	A	1394	Total	C	N	O	S	0	0
			11051	7009	1907	2076	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1159	Total	C	N	O	S	0	0
			9148	5803	1595	1691	59		

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

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

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

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

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

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

- 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	C	N	O	S	0	0
			650	413	111	123	3		

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	A	2	Total	Zn	0
			2	2	
13	B	1	Total	Zn	0
			1	1	

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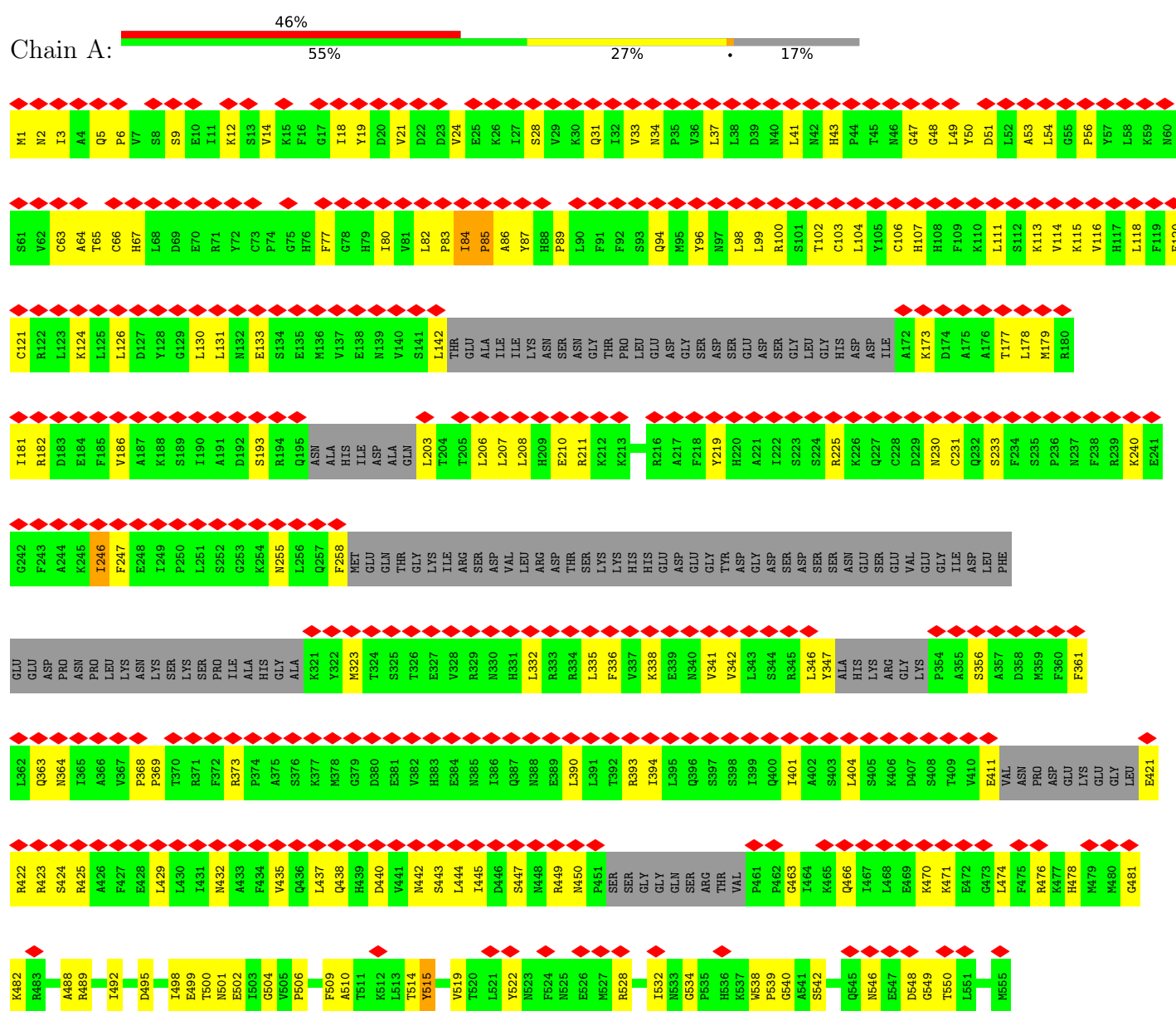
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Mol	Chain	Residues	Atoms		AltConf
13	I	1	Total 1	Zn 1	0
13	J	1	Total 1	Zn 1	0
13	L	1	Total 1	Zn 1	0

### 3 Residue-property plots

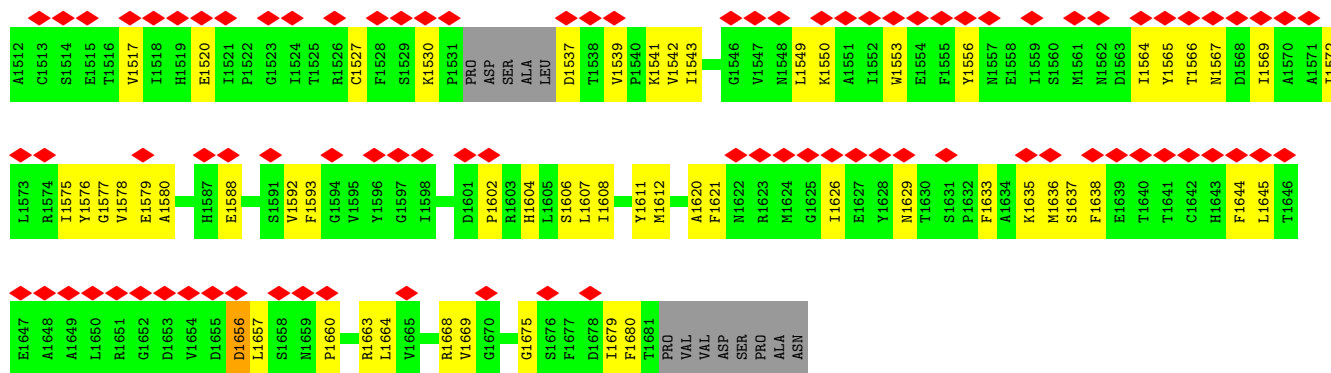
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 I subunit rpa1

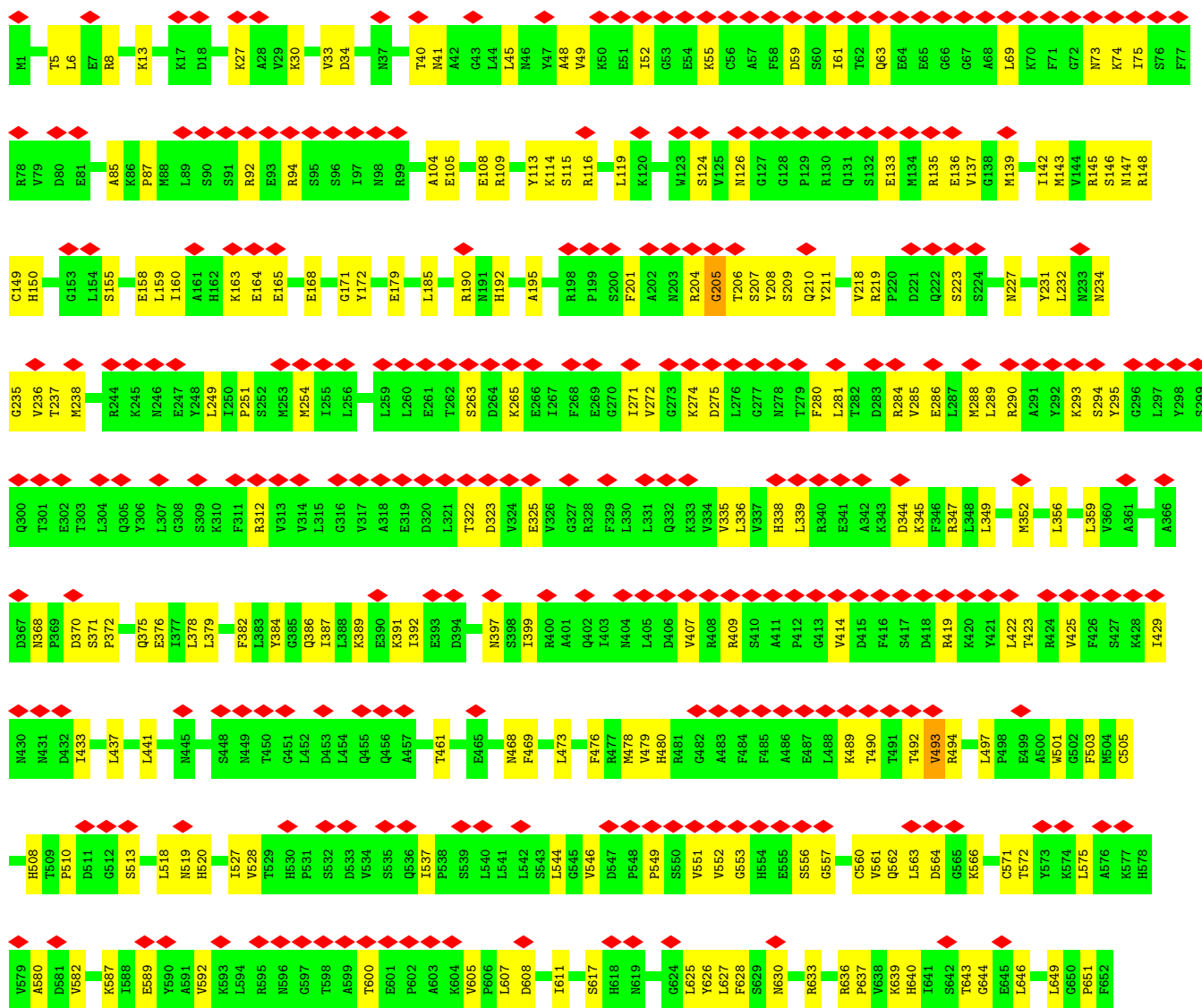


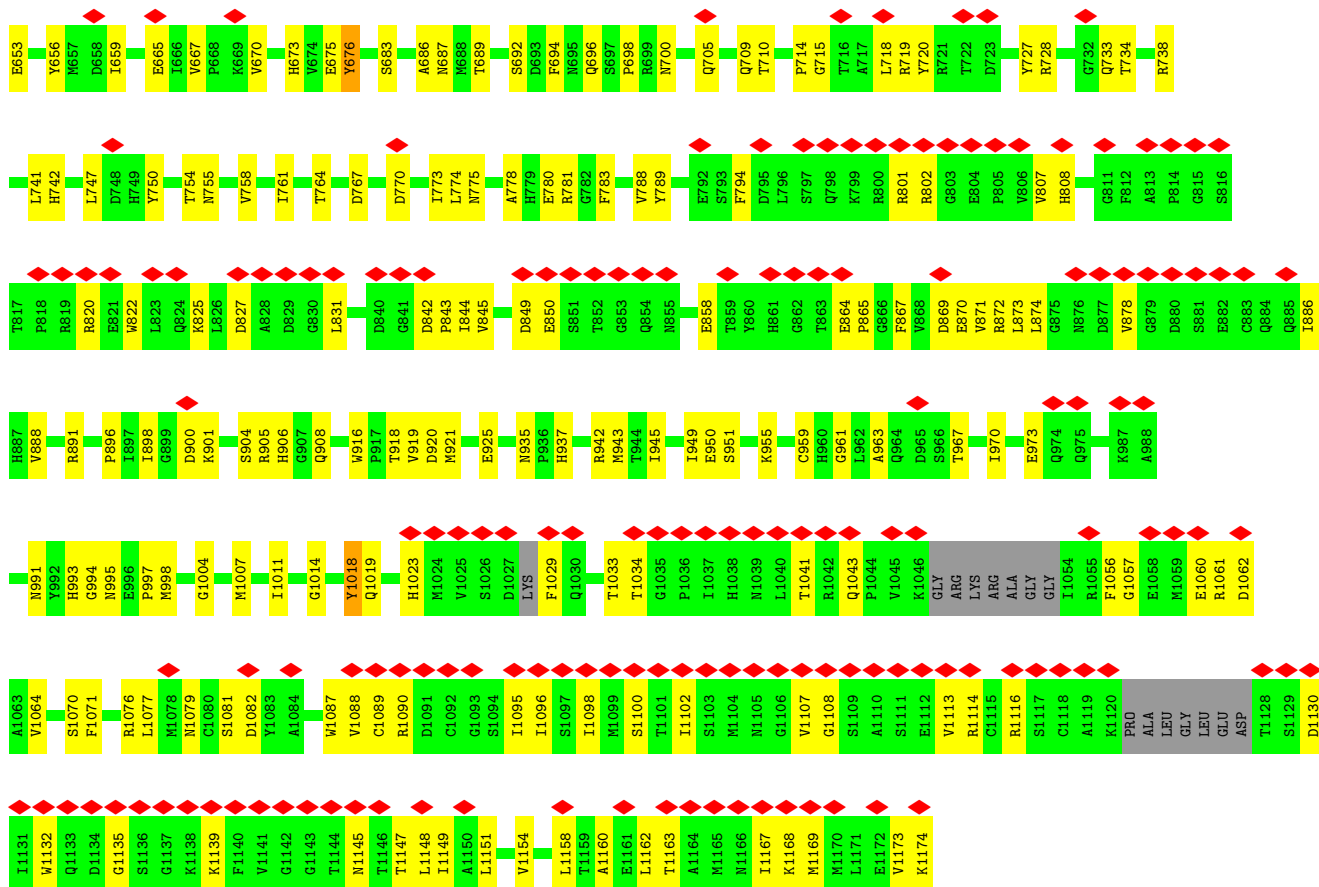




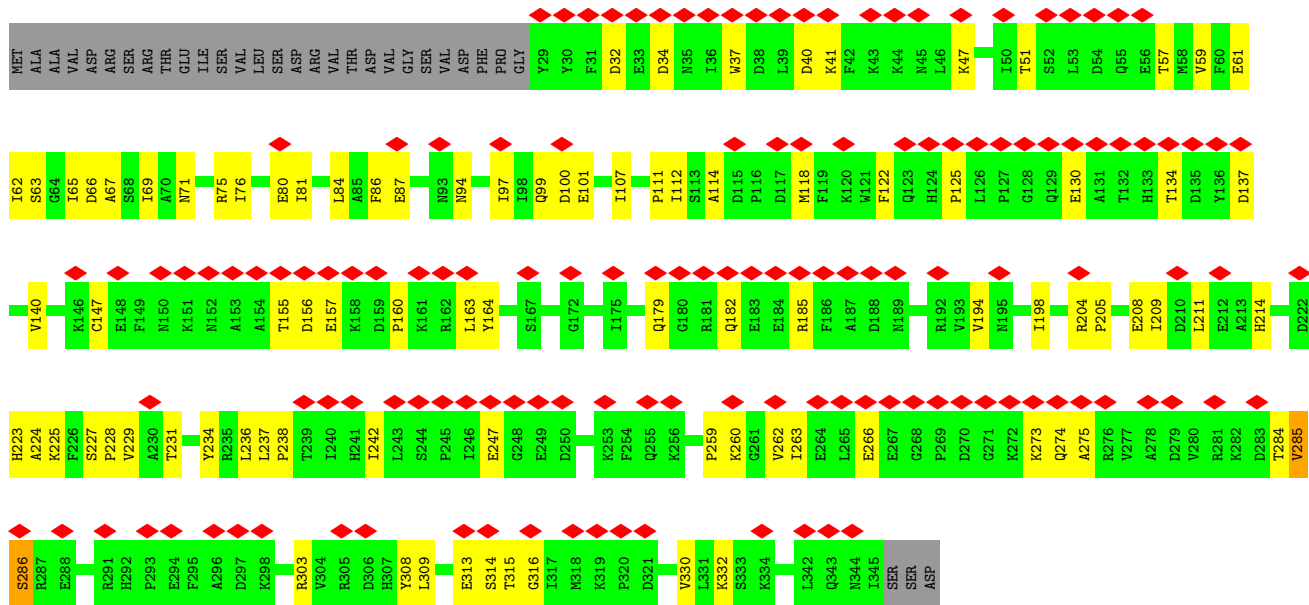
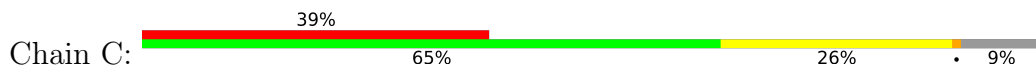


• Molecule 2: Probable DNA-directed RNA polymerase I subunit RPA2

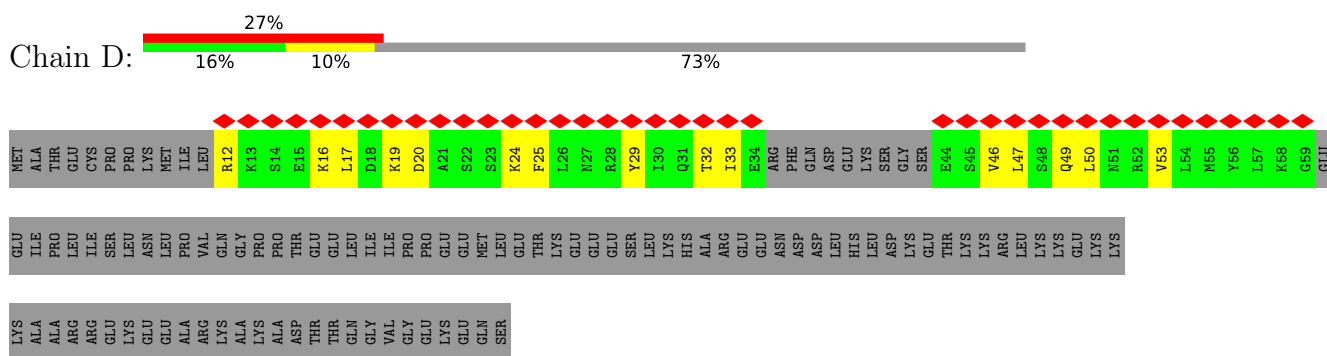




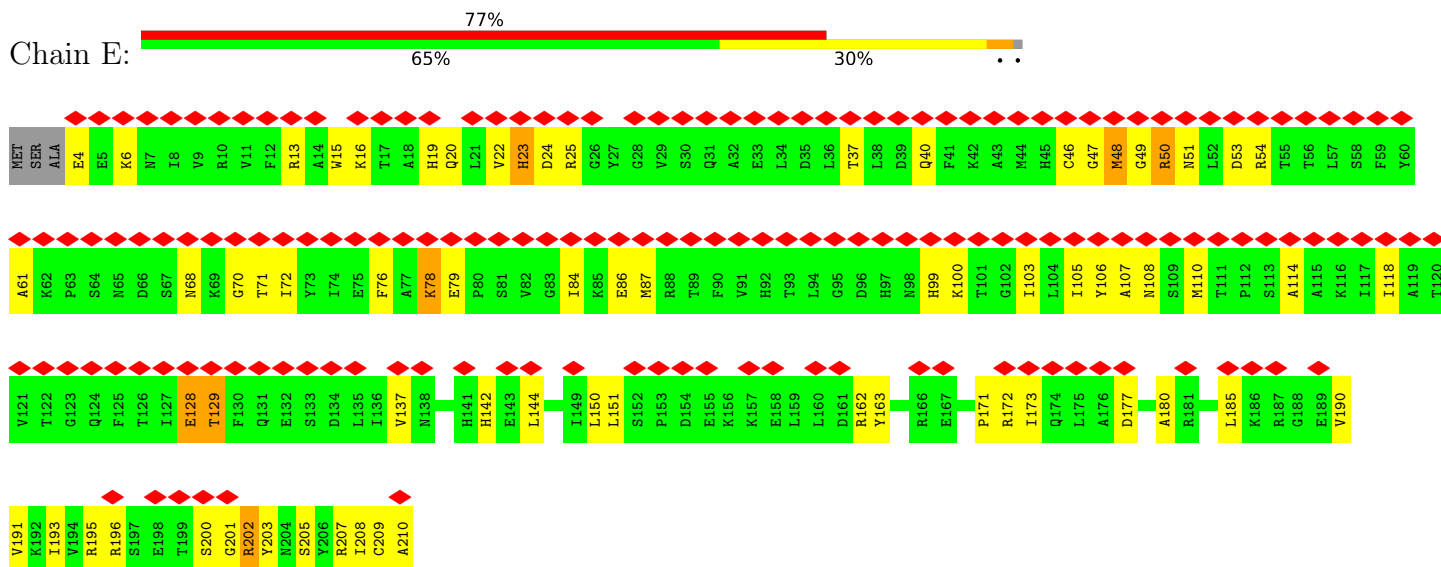
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



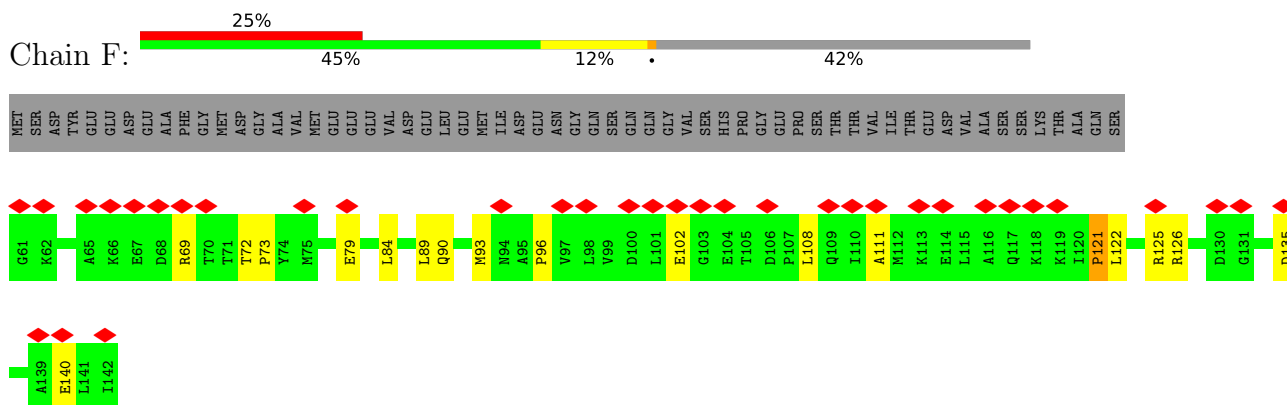
• Molecule 4: DNA-directed RNA polymerase I subunit rpa14



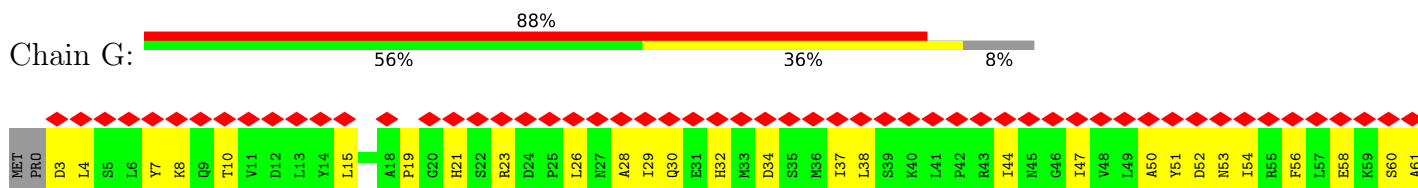
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

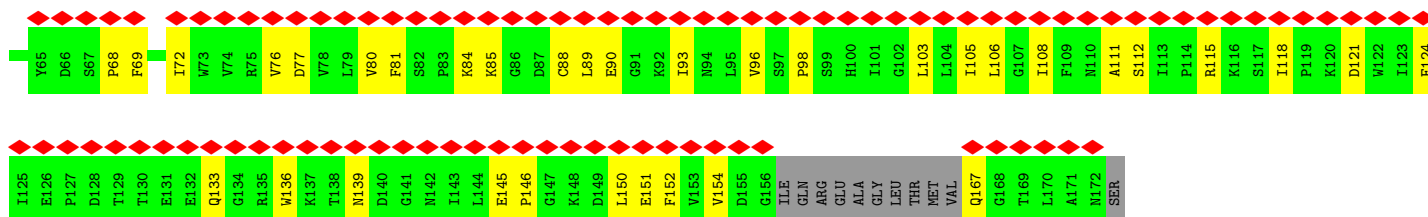


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

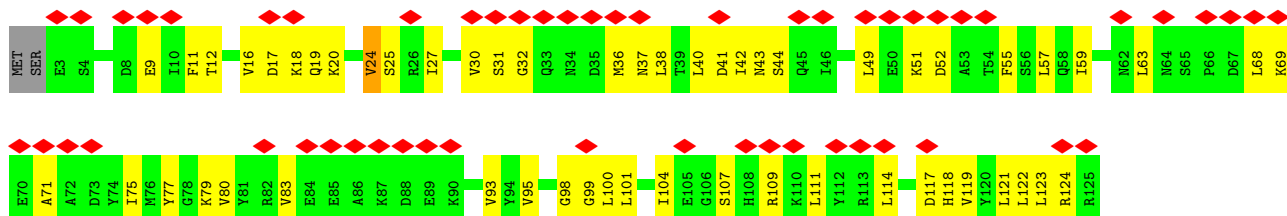
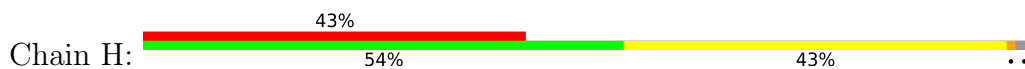


- Molecule 7: DNA-directed RNA polymerase I subunit rpa43

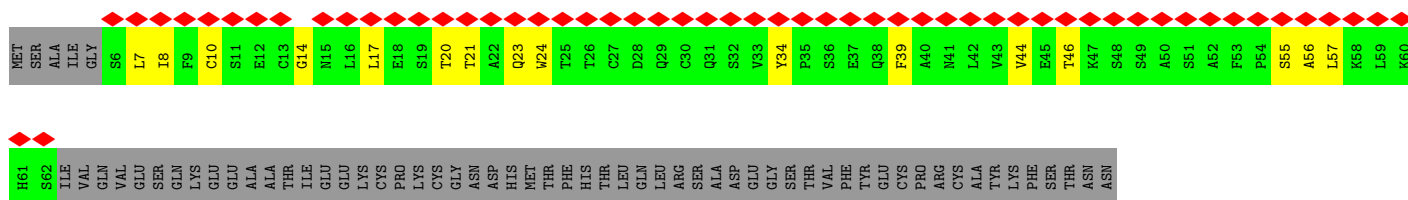
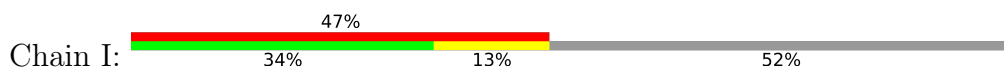




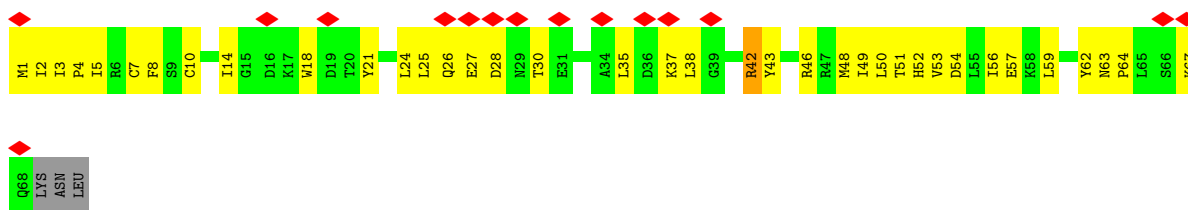
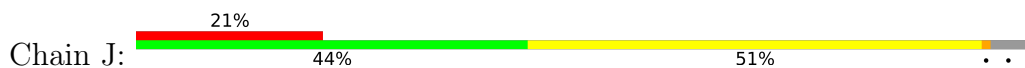
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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

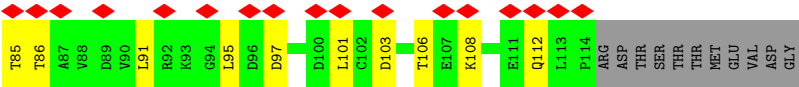


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

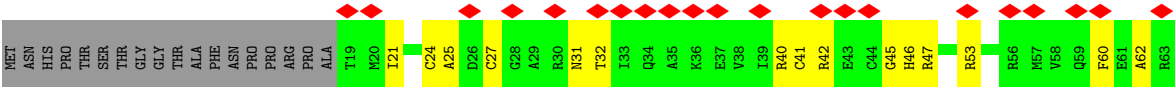


• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2





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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79313	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 ( $e^-/\text{\AA}^2$ )	86.5	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	0.501	Depositor
Minimum map value	-0.291	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.11	Depositor
Map size ( $\text{\AA}$ )	233.97002, 233.97002, 233.97002	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0635, 1.0635, 1.0635	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

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	0.39	0/11271	0.52	0/15226
2	B	0.43	0/9353	0.52	0/12644
3	C	0.40	0/2588	0.48	0/3505
4	D	0.28	0/323	0.43	0/427
5	E	0.33	0/1695	0.58	1/2287 (0.0%)
6	F	0.40	0/660	0.50	0/893
7	G	0.29	0/1295	0.48	0/1755
8	H	0.39	0/1004	0.58	0/1355
9	I	0.28	0/439	0.48	0/596
10	J	0.44	0/558	0.53	0/751
11	K	0.42	0/759	0.48	0/1030
12	L	0.39	0/371	0.49	0/491
All	All	0.40	0/30316	0.52	1/40960 (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	2
5	E	0	5
All	All	0	14

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	24	ASP	N-CA-C	5.61	126.15	111.00

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1065	GLU	Peptide
1	A	1066	ASP	Peptide
1	A	246	ILE	Peptide
1	A	84	ILE	Peptide
1	A	896	TYR	Peptide

## 5.2 Too-close contacts

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	11051	0	11047	374	0
2	B	9148	0	9109	316	0
3	C	2533	0	2540	73	0
4	D	322	0	338	19	0
5	E	1663	0	1684	58	0
6	F	650	0	674	19	0
7	G	1267	0	1278	54	0
8	H	990	0	1001	42	0
9	I	431	0	410	15	0
10	J	550	0	566	38	0
11	K	745	0	745	22	0
12	L	368	0	377	15	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	I	1	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
All	All	29724	0	29769	915	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 15.

The worst 5 of 915 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)
5:E:23:HIS:HA	5:E:25:ARG:H	1.27	0.97
1:A:1324:PHE:O	1:A:1328:PHE:HB3	1.72	0.90
1:A:103:CYS:SG	1:A:106:CYS:HB3	1.86	0.90
8:H:17:ASP:HA	8:H:18:LYS:HB2	1.58	0.84
1:A:56:PRO:HG3	1:A:63:CYS:HB2	1.58	0.84

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	1368/1689 (81%)	1235 (90%)	130 (10%)	3 (0%)	44	75
2	B	1151/1174 (98%)	993 (86%)	155 (14%)	3 (0%)	37	70
3	C	315/348 (90%)	290 (92%)	23 (7%)	2 (1%)	22	57
4	D	35/147 (24%)	35 (100%)	0	0	100	100
5	E	205/210 (98%)	176 (86%)	29 (14%)	0	100	100
6	F	80/142 (56%)	74 (92%)	5 (6%)	1 (1%)	10	41
7	G	156/173 (90%)	141 (90%)	15 (10%)	0	100	100
8	H	121/125 (97%)	94 (78%)	26 (22%)	1 (1%)	16	51
9	I	55/119 (46%)	51 (93%)	4 (7%)	0	100	100
10	J	66/71 (93%)	50 (76%)	16 (24%)	0	100	100
11	K	93/125 (74%)	84 (90%)	9 (10%)	0	100	100
12	L	43/63 (68%)	42 (98%)	1 (2%)	0	100	100
All	All	3688/4386 (84%)	3265 (88%)	413 (11%)	10 (0%)	38	70

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	206	THR

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Mol	Chain	Res	Type
2	B	493	VAL
1	A	782	GLY
3	C	286	SER
1	A	968	ARG

### 5.3.2 Protein sidechains ⓘ

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	1233/1484 (83%)	1225 (99%)	8 (1%)	84	88
2	B	1004/1013 (99%)	999 (100%)	5 (0%)	86	90
3	C	281/308 (91%)	281 (100%)	0	100	100
4	D	37/134 (28%)	37 (100%)	0	100	100
5	E	182/184 (99%)	179 (98%)	3 (2%)	58	73
6	F	70/121 (58%)	70 (100%)	0	100	100
7	G	143/154 (93%)	142 (99%)	1 (1%)	81	86
8	H	112/114 (98%)	112 (100%)	0	100	100
9	I	51/105 (49%)	51 (100%)	0	100	100
10	J	63/66 (96%)	62 (98%)	1 (2%)	58	73
11	K	86/111 (78%)	86 (100%)	0	100	100
12	L	39/53 (74%)	39 (100%)	0	100	100
All	All	3301/3847 (86%)	3283 (100%)	18 (0%)	85	90

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	78	LYS
10	J	42	ARG
7	G	56	PHE
2	B	676	TYR
5	E	48	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	99	HIS
7	G	30	GLN
10	J	63	ASN
1	A	1317	GLN
1	A	1075	HIS

### 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](#)

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

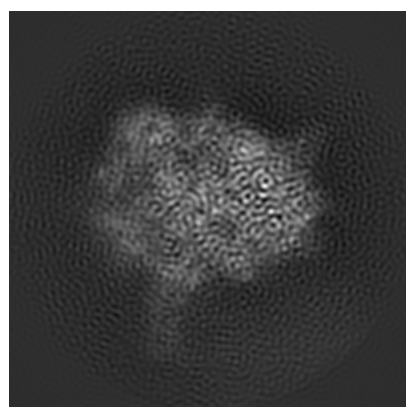
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11840. These allow visual inspection of the internal detail of the map and identification of artifacts.

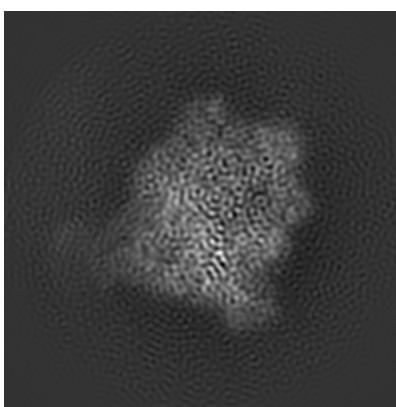
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

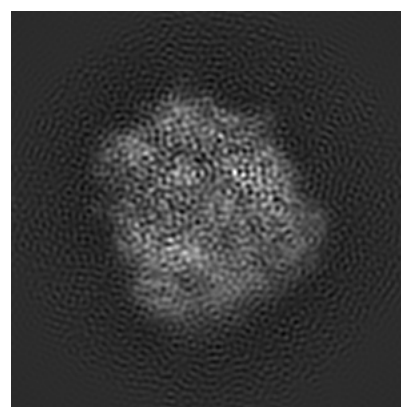
#### 6.1.1 Primary map



X



Y

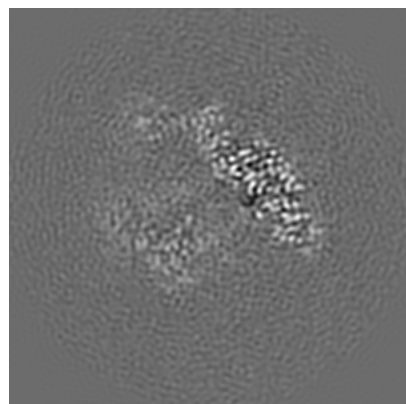


Z

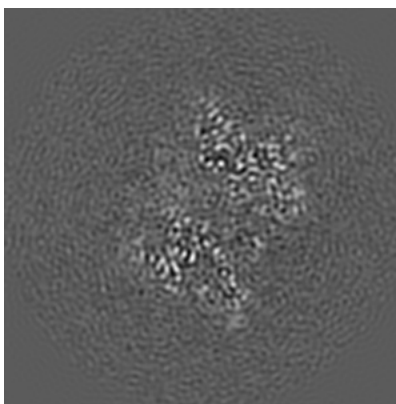
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

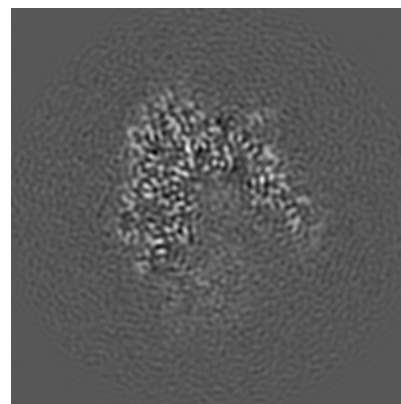
#### 6.2.1 Primary map



X Index: 110



Y Index: 110

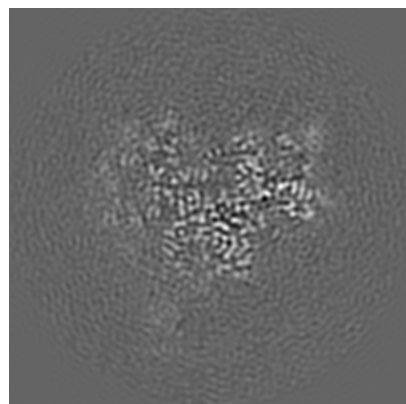


Z Index: 110

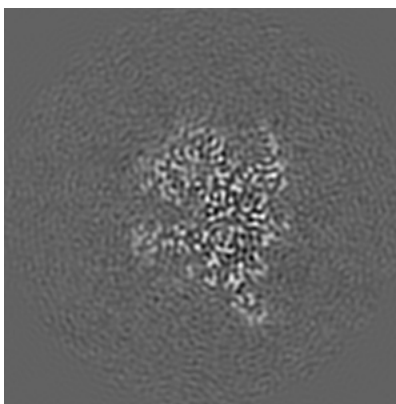
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

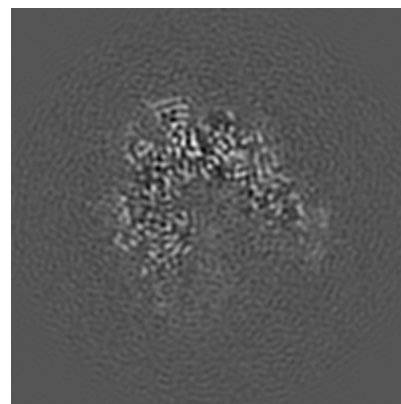
### 6.3.1 Primary map



X Index: 91



Y Index: 129

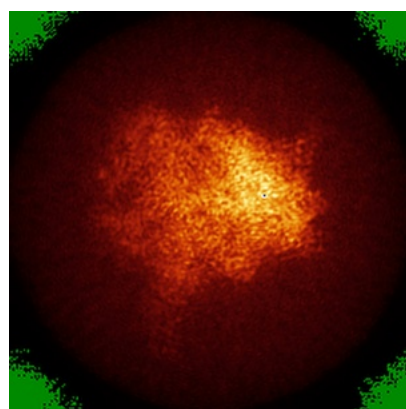


Z Index: 118

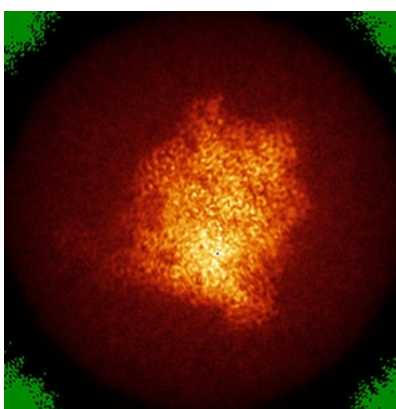
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

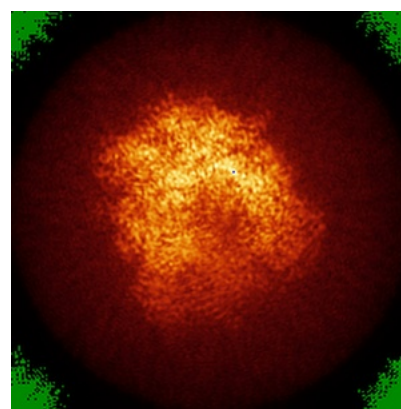
### 6.4.1 Primary map



X



Y

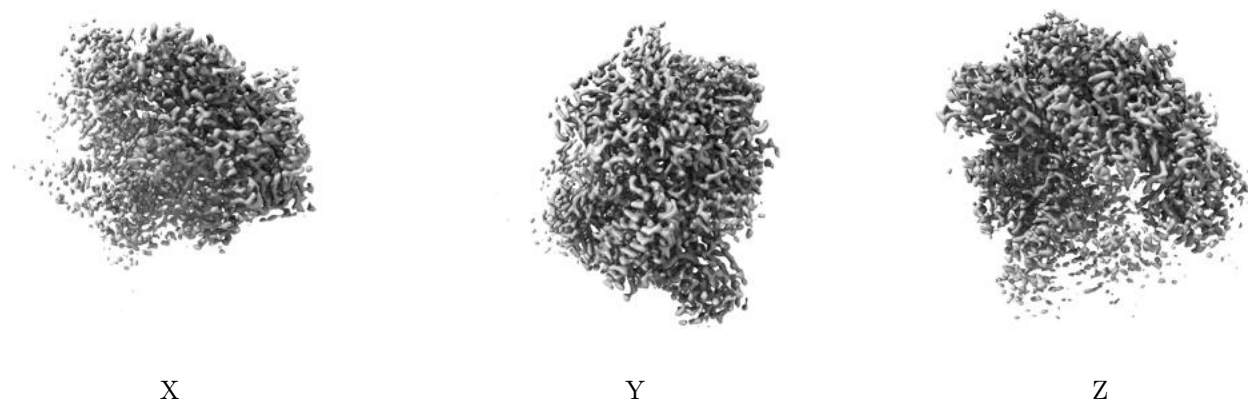


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

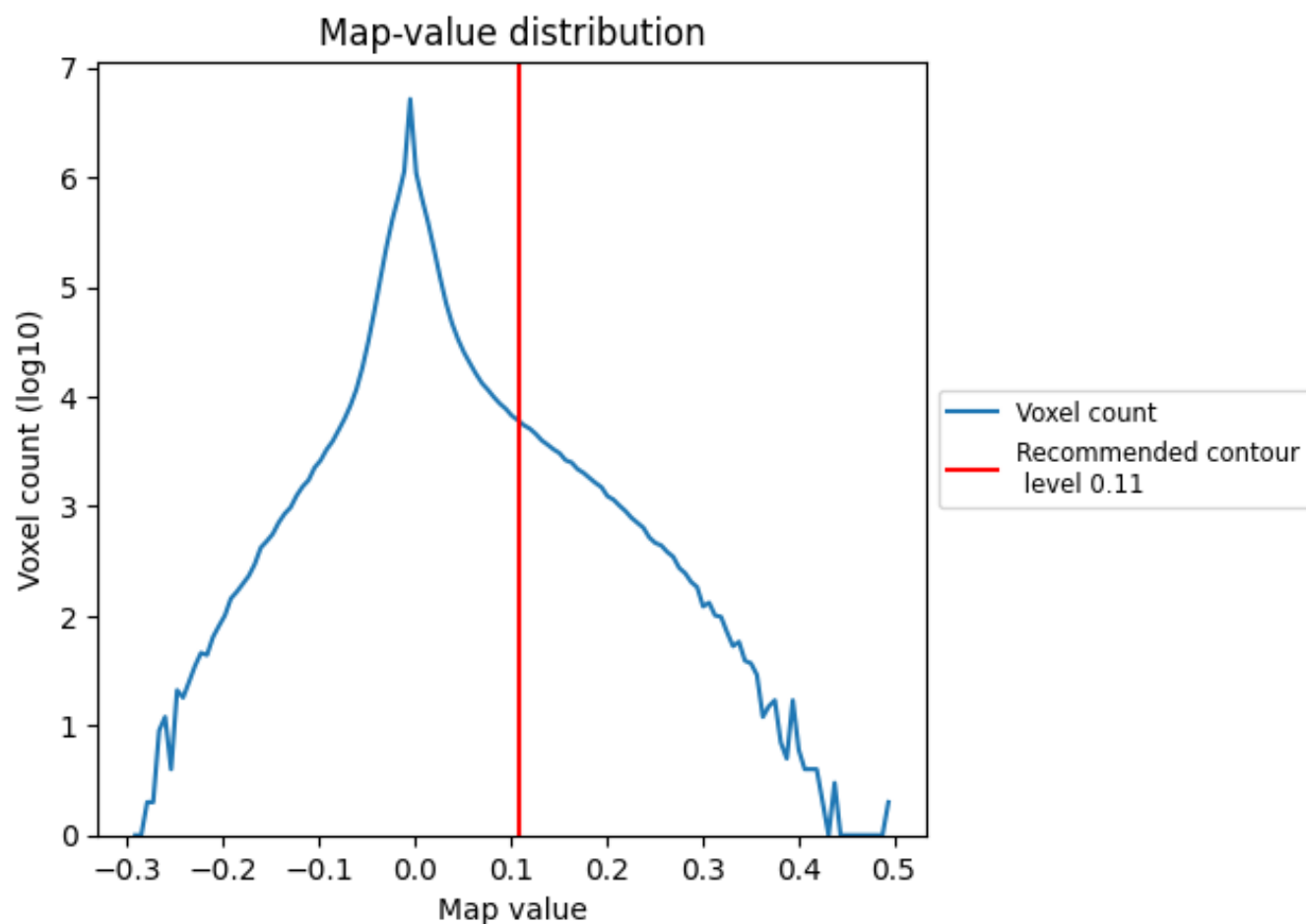
## 6.6 Mask visualisation [i](#)

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.

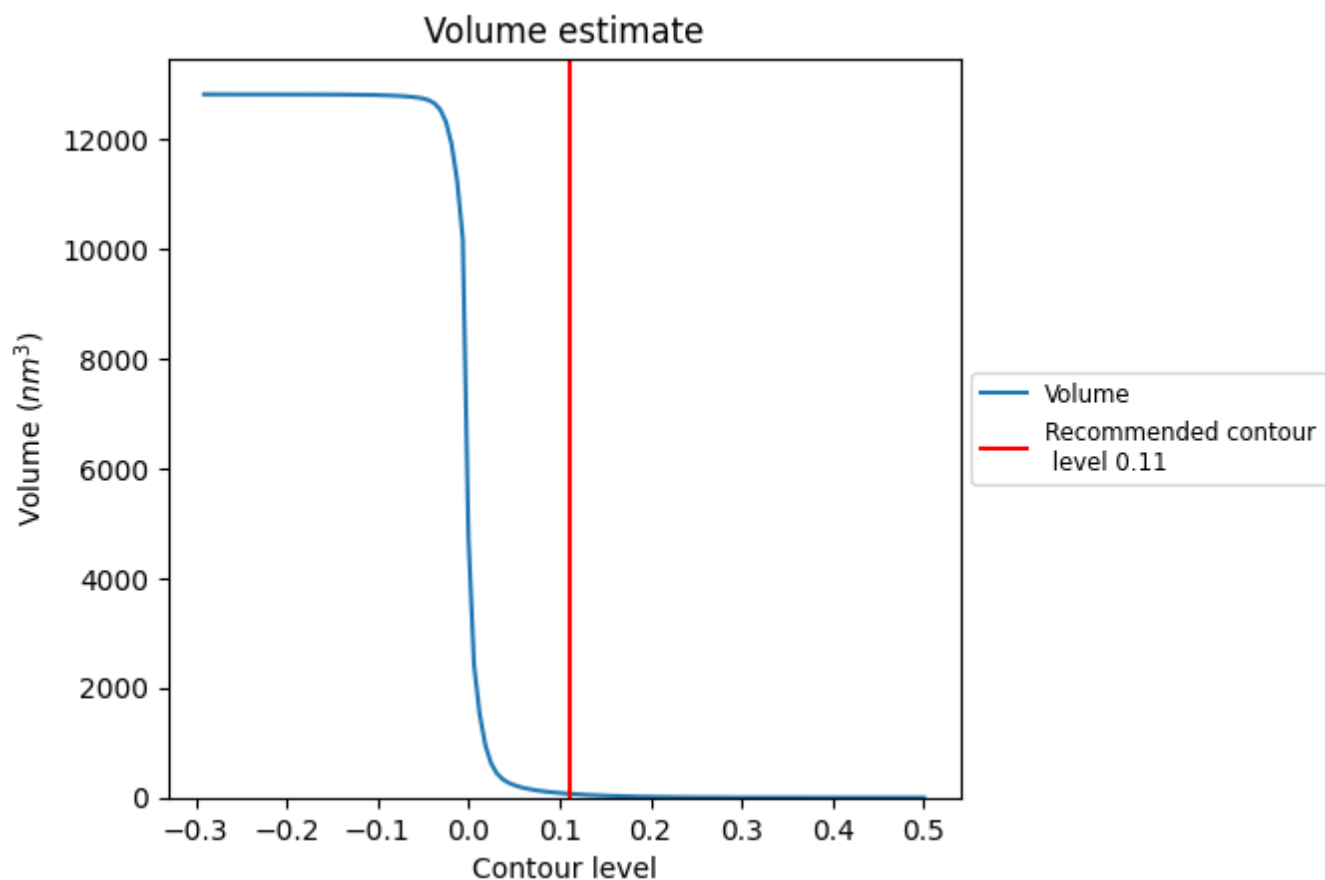
### 7.1 Map-value distribution [i](#)



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.



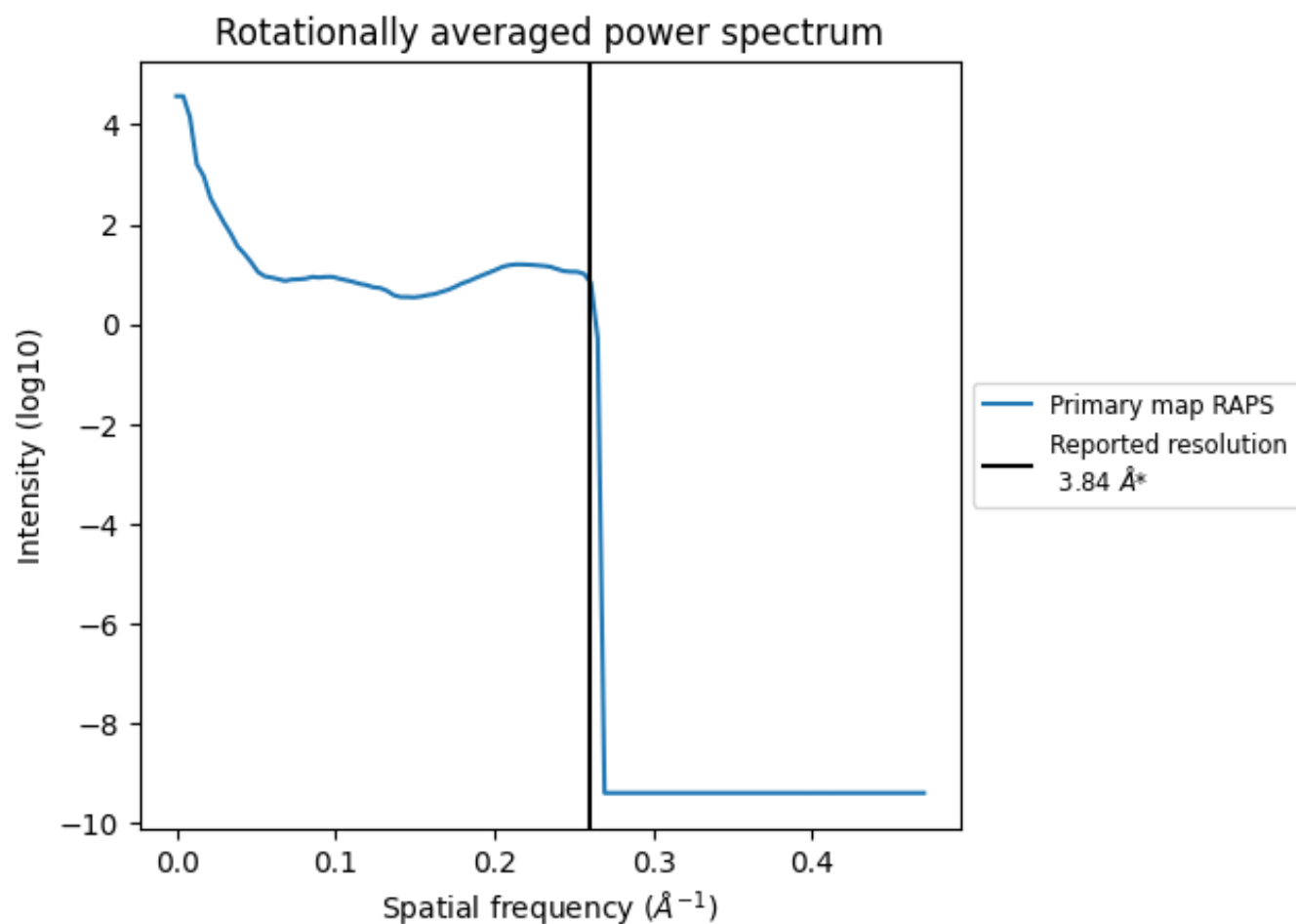
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69 nm<sup>3</sup>; this corresponds to an approximate mass of 63 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.260 Å<sup>-1</sup>

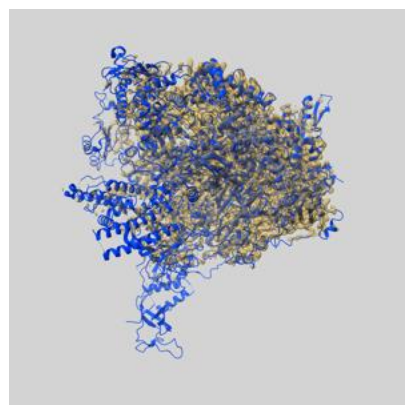
## 8 Fourier-Shell correlation

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

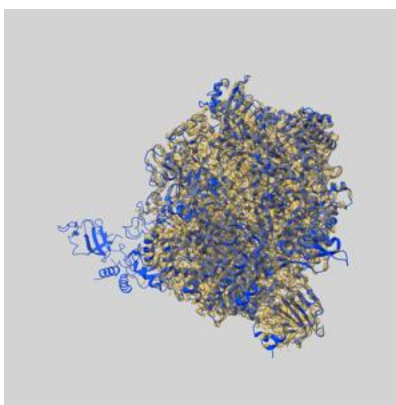
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11840 and PDB model 7AOC. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

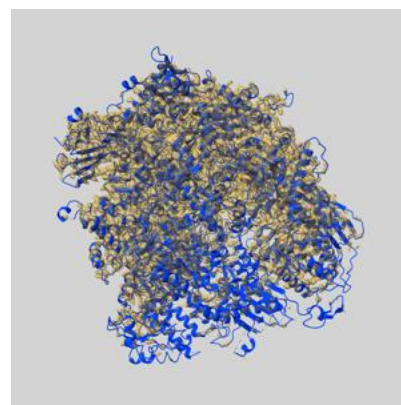
### 9.1 Map-model overlay [i](#)



X



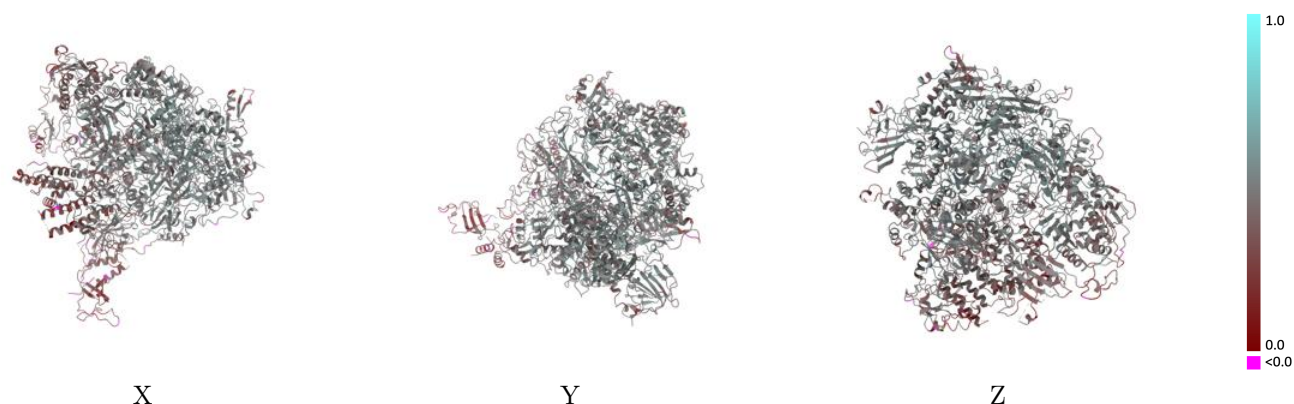
Y



Z

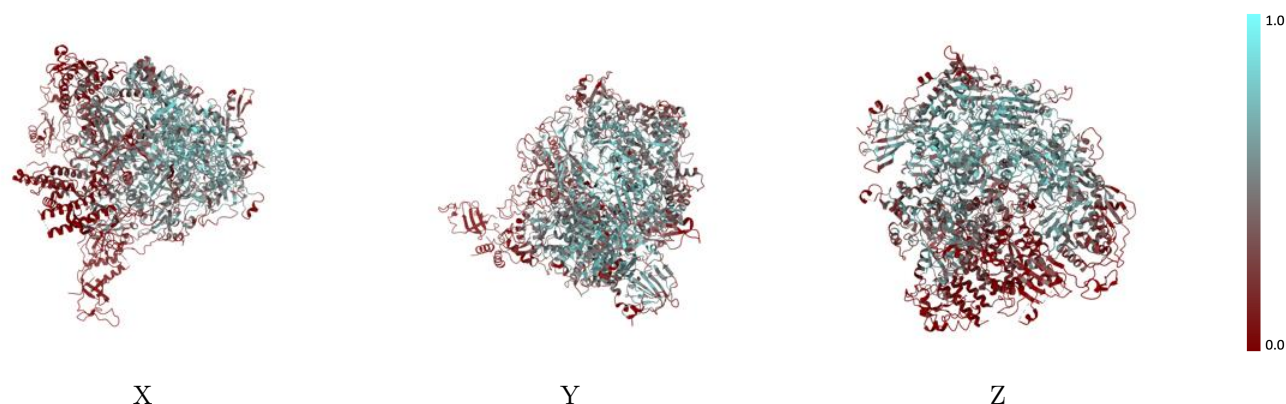
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



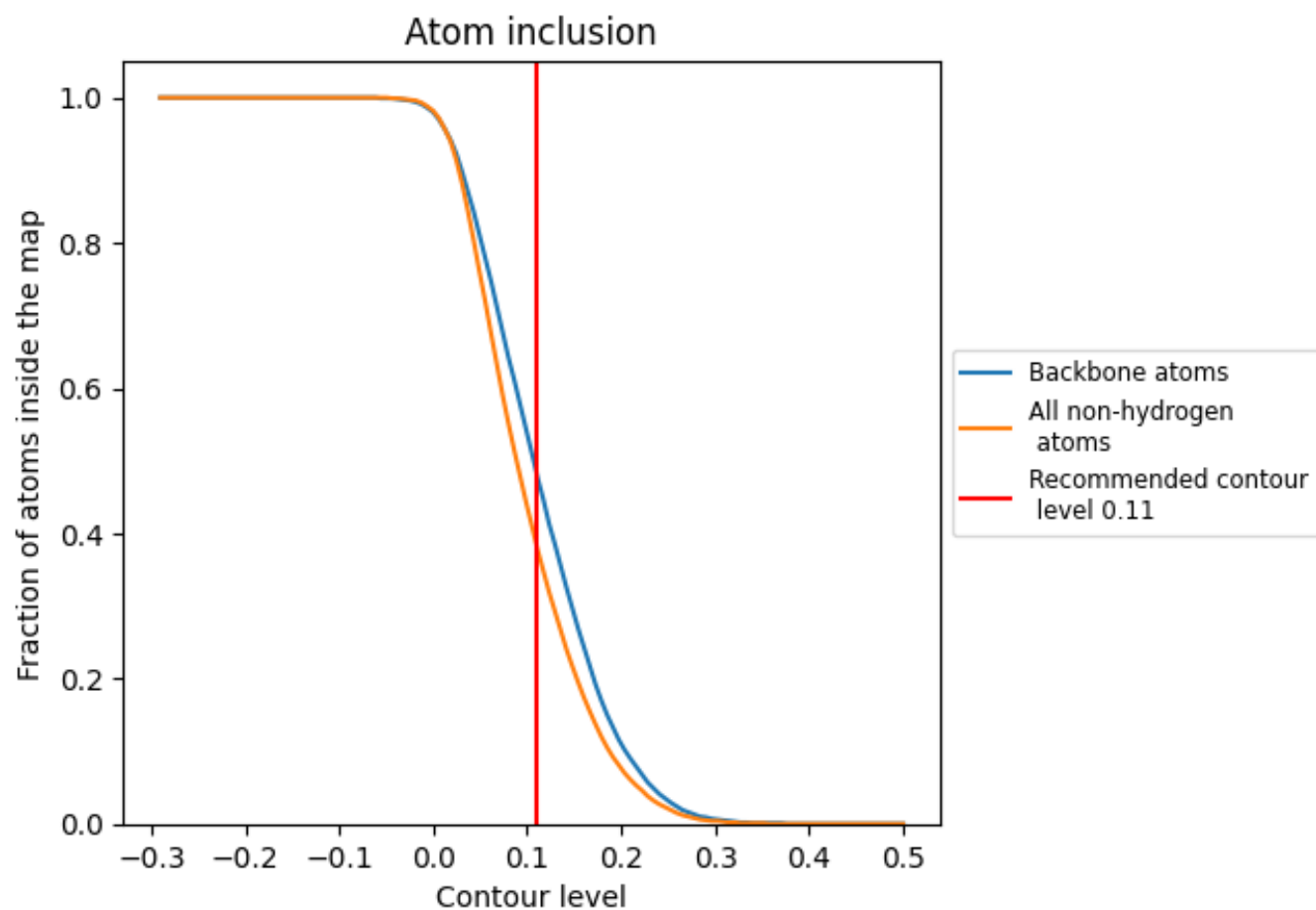
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 38% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3830	<div></div> 0.4490
A	<div></div> 0.3510	<div></div> 0.4410
B	<div></div> 0.4770	<div></div> 0.4760
C	<div></div> 0.4280	<div></div> 0.4710
D	<div></div> 0.0000	<div></div> 0.2440
E	<div></div> 0.2120	<div></div> 0.4140
F	<div></div> 0.4690	<div></div> 0.4850
G	<div></div> 0.0660	<div></div> 0.3150
H	<div></div> 0.4210	<div></div> 0.4760
I	<div></div> 0.0280	<div></div> 0.3530
J	<div></div> 0.5830	<div></div> 0.5020
K	<div></div> 0.5320	<div></div> 0.4940
L	<div></div> 0.4420	<div></div> 0.4940

