



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 08:24 am GMT

PDB ID : 5LMX  
EMDB ID : EMD-4088  
Title : Monomeric RNA polymerase I at 4.9 Å resolution  
Authors : Torreira, E.; Louro, J.A.; Gil-Carton, D.; Gallego, O.; Calvo, O.; Fernandez-Tornero, C.  
Deposited on : 2016-08-02  
Resolution : 4.90 Å(reported)

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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.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) : 2.31.2

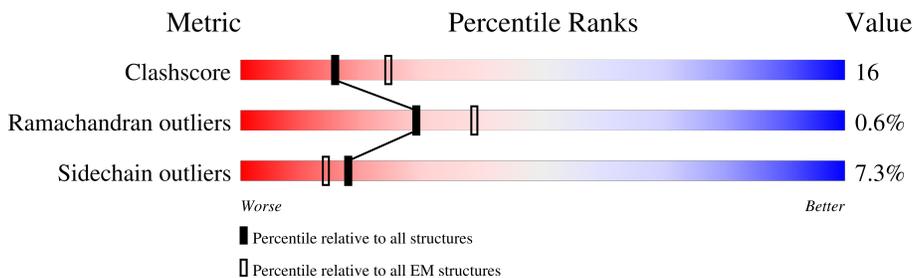
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.90 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

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	1664	
2	B	1203	
3	C	380	
4	D	137	
5	E	215	
6	F	155	
7	G	326	
8	H	146	

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Mol	Chain	Length	Quality of chain
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	ZN	L	101	-	-	X	-

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31118 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 RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1420	Total	C	N	O	S	0	0
			11207	7087	1942	2118	60		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1115	Total	C	N	O	S	0	0
			8868	5618	1546	1656	48		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	304	Total	C	N	O	S	0	0
			2418	1536	414	460	8		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	18	Total	C	N	O	0	0
			133	84	23	26		

- 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	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

- 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	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

- 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	89	706	465	113	123	5	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	134	1072	676	181	211	4	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	64	472	295	78	95	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	69	569	362	101	100	6	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	101	792	496	130	161	5	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	359	221	71	63	4	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	105	831	528	137	166	0	0

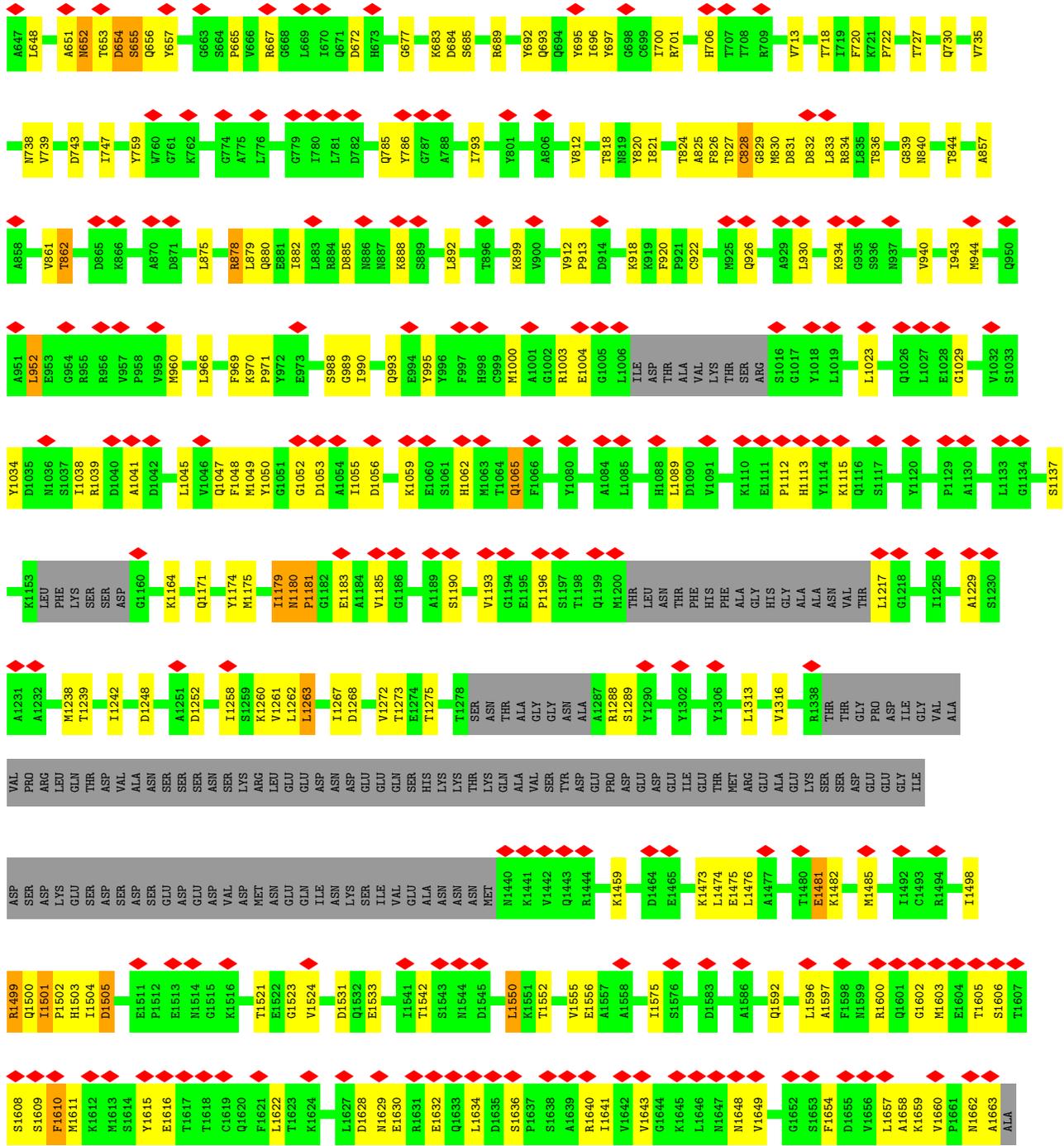
- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	139	1103	706	179	214	4	0	0

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

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





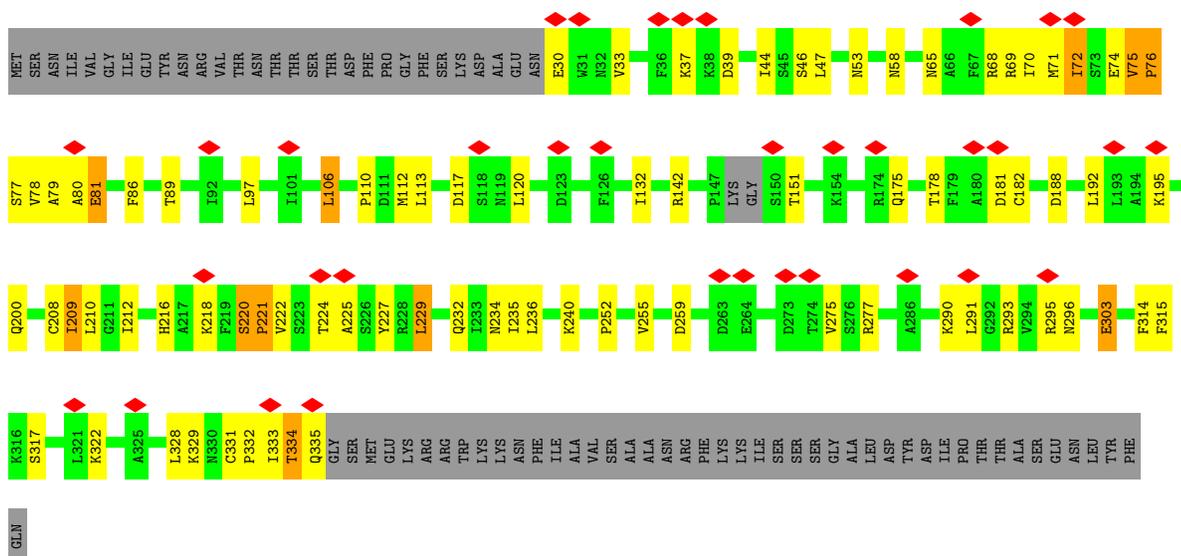
● Molecule 2: DNA-directed RNA polymerase I subunit RPA135



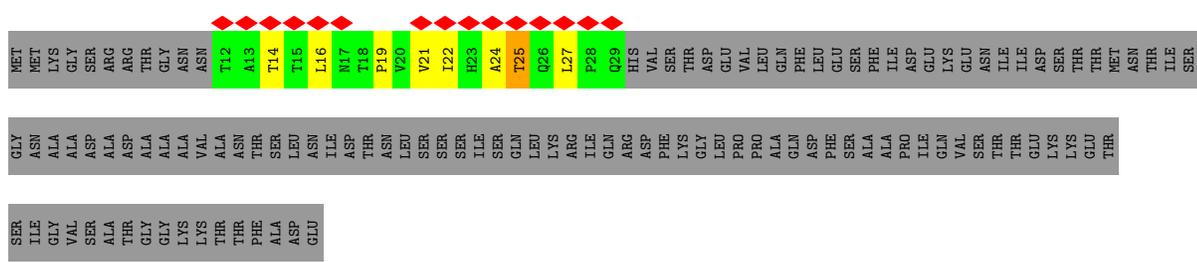




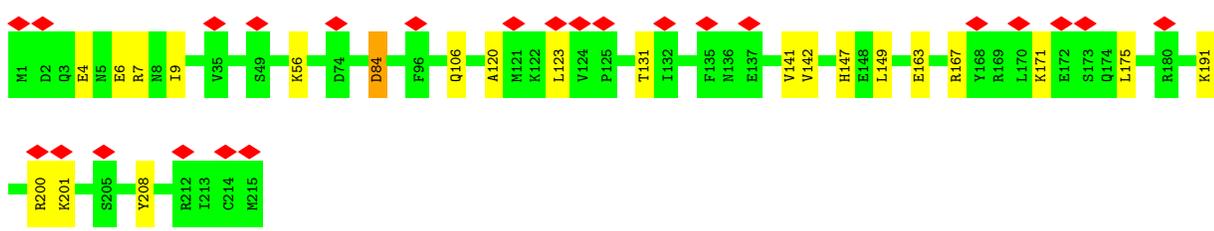
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1, DNA-directed RNA polymerases I and III subunit RPAC1



- Molecule 4: DNA-directed RNA polymerase I subunit RPA14



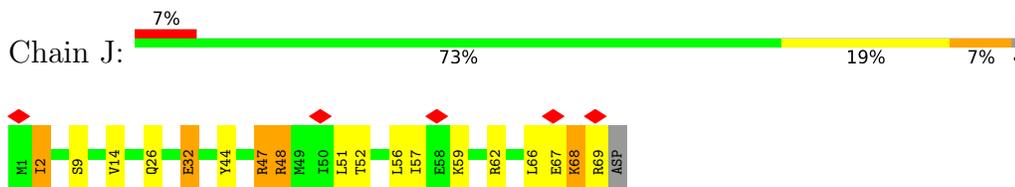
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



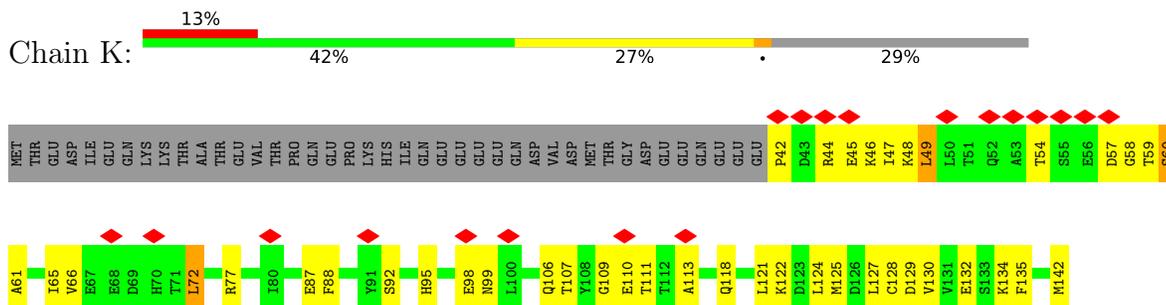
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



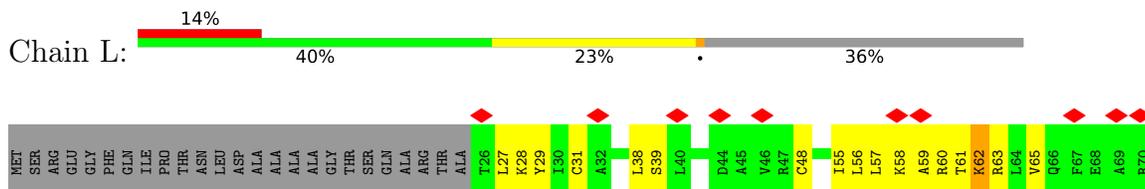
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



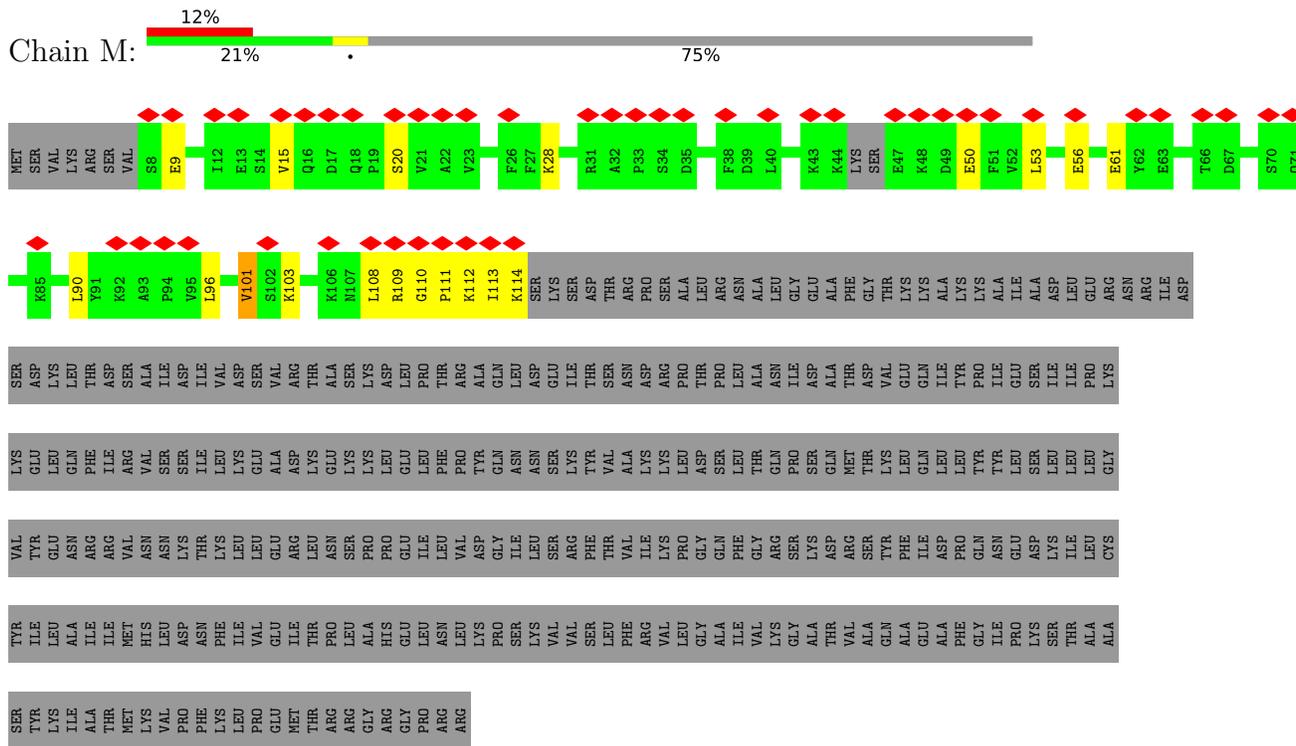
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



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



- Molecule 13: DNA-directed RNA polymerase I subunit RPA49



- Molecule 14: DNA-directed RNA polymerase I subunit RPA34



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	122348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	68.0	Depositor
Minimum defocus (nm)	1900.0	Depositor
Maximum defocus (nm)	4200.0	Depositor
Magnification	79096	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.408	Depositor
Minimum map value	-0.180	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.14	Depositor
Map size ( $\text{\AA}$ )	286.74, 286.74, 286.74	wwPDB
Map dimensions	162, 162, 162	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.77, 1.77, 1.77	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	1/11408 (0.0%)	0.57	3/15405 (0.0%)
2	B	0.39	1/9062 (0.0%)	0.59	2/12249 (0.0%)
3	C	0.42	0/2469	0.62	2/3347 (0.1%)
4	D	0.37	0/135	0.62	0/188
5	E	0.40	0/1795	0.55	0/2416
6	F	0.39	0/838	0.54	0/1129
7	G	0.40	0/725	0.60	0/990
8	H	0.39	0/1090	0.57	0/1476
9	I	0.37	0/478	0.53	0/647
10	J	0.40	0/578	0.62	0/775
11	K	0.38	0/803	0.57	0/1083
12	L	0.35	0/361	0.56	0/478
13	M	0.38	0/846	0.53	0/1136
14	N	0.44	0/1124	0.56	2/1512 (0.1%)
All	All	0.40	2/31712 (0.0%)	0.58	9/42831 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1181	PRO	N-CD	5.30	1.55	1.47
2	B	693	PRO	N-CD	5.26	1.55	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	220	SER	C-N-CD	6.06	141.13	128.40
1	A	1501	ILE	C-N-CD	6.05	141.12	128.40
3	C	75	VAL	C-N-CD	6.04	141.09	128.40
14	N	160	VAL	C-N-CD	6.04	141.07	128.40
1	A	507	TYR	C-N-CD	6.03	141.07	128.40

There are no chirality outliers.

There are no planarity outliers.

## 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	11207	0	11249	527	0
2	B	8868	0	8734	466	0
3	C	2418	0	2401	145	0
4	D	133	0	138	5	0
5	E	1759	0	1788	14	0
6	F	823	0	841	28	0
7	G	706	0	721	59	0
8	H	1072	0	1042	15	0
9	I	472	0	473	9	0
10	J	569	0	585	58	0
11	K	792	0	790	93	0
12	L	359	0	384	17	0
13	M	831	0	820	19	0
14	N	1103	0	1106	27	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	2	0
All	All	31118	0	31072	1011	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 16.

The worst 5 of 1011 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:697:LEU:HD11	2:B:984:TRP:CH2	1.23	1.65
2:B:697:LEU:HD11	2:B:984:TRP:CZ3	1.31	1.59
1:A:5:LYS:CB	2:B:1100:GLN:NE2	1.67	1.57
1:A:1660:VAL:CG2	7:G:105:ILE:HG23	1.10	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:LYS:HG3	11:K:134:LYS:CE	1.33	1.55

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	1394/1664 (84%)	1309 (94%)	76 (6%)	9 (1%)	25	65
2	B	1099/1203 (91%)	1020 (93%)	73 (7%)	6 (0%)	29	68
3	C	300/380 (79%)	273 (91%)	24 (8%)	3 (1%)	15	54
4	D	16/137 (12%)	14 (88%)	2 (12%)	0	100	100
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
6	F	98/155 (63%)	96 (98%)	2 (2%)	0	100	100
7	G	85/326 (26%)	80 (94%)	5 (6%)	0	100	100
8	H	130/146 (89%)	119 (92%)	10 (8%)	1 (1%)	19	60
9	I	62/125 (50%)	53 (86%)	8 (13%)	1 (2%)	9	44
10	J	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
11	K	99/142 (70%)	91 (92%)	6 (6%)	2 (2%)	7	39
12	L	43/70 (61%)	38 (88%)	5 (12%)	0	100	100
13	M	101/415 (24%)	93 (92%)	8 (8%)	0	100	100
14	N	131/233 (56%)	114 (87%)	15 (12%)	2 (2%)	10	46
All	All	3838/5281 (73%)	3564 (93%)	250 (6%)	24 (1%)	29	65

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	652	ASN

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Mol	Chain	Res	Type
1	A	655	SER
1	A	505	LEU
1	A	654	ASP
1	A	1499	ARG

### 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	1250/1465 (85%)	1184 (95%)	66 (5%)	22	49
2	B	973/1053 (92%)	876 (90%)	97 (10%)	7	28
3	C	269/334 (80%)	243 (90%)	26 (10%)	8	29
4	D	16/116 (14%)	11 (69%)	5 (31%)	0	2
5	E	197/197 (100%)	192 (98%)	5 (2%)	47	68
6	F	90/137 (66%)	86 (96%)	4 (4%)	28	53
7	G	80/291 (28%)	75 (94%)	5 (6%)	18	44
8	H	116/128 (91%)	111 (96%)	5 (4%)	29	54
9	I	56/110 (51%)	48 (86%)	8 (14%)	3	17
10	J	64/65 (98%)	57 (89%)	7 (11%)	6	25
11	K	91/130 (70%)	83 (91%)	8 (9%)	10	33
12	L	40/57 (70%)	37 (92%)	3 (8%)	13	39
13	M	94/371 (25%)	89 (95%)	5 (5%)	22	49
14	N	128/220 (58%)	118 (92%)	10 (8%)	12	38
All	All	3464/4674 (74%)	3210 (93%)	254 (7%)	18	40

5 of 254 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	542	LEU
10	J	2	ILE
2	B	897	GLU

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Mol	Chain	Res	Type
9	I	53	ASP
12	L	27	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	646	HIS
2	B	975	HIS
11	K	95	HIS
2	B	683	ASN
2	B	724	GLN

### 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 monosaccharides 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 [i](#)

There are no chain breaks in this entry.

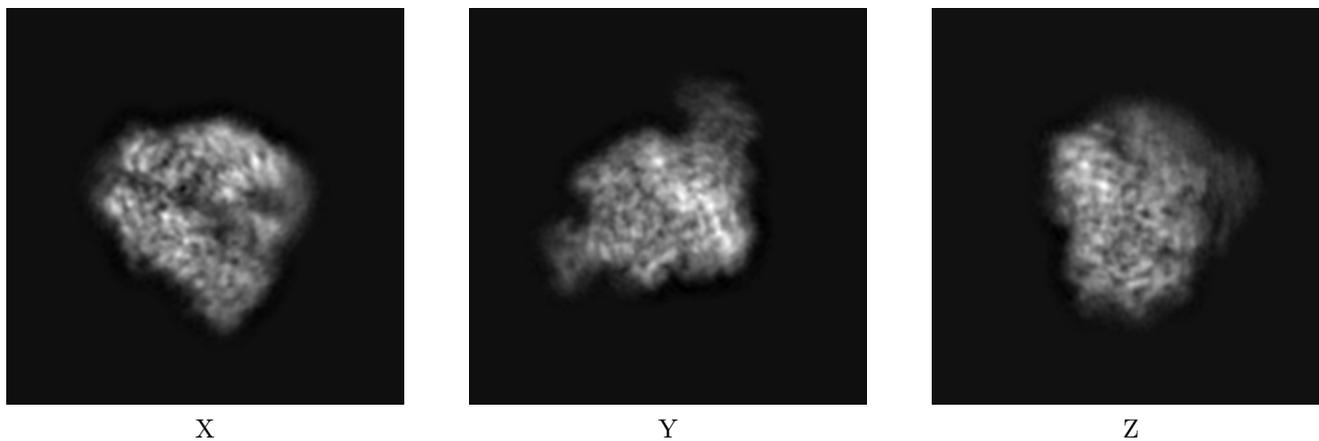
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4088. 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](#)

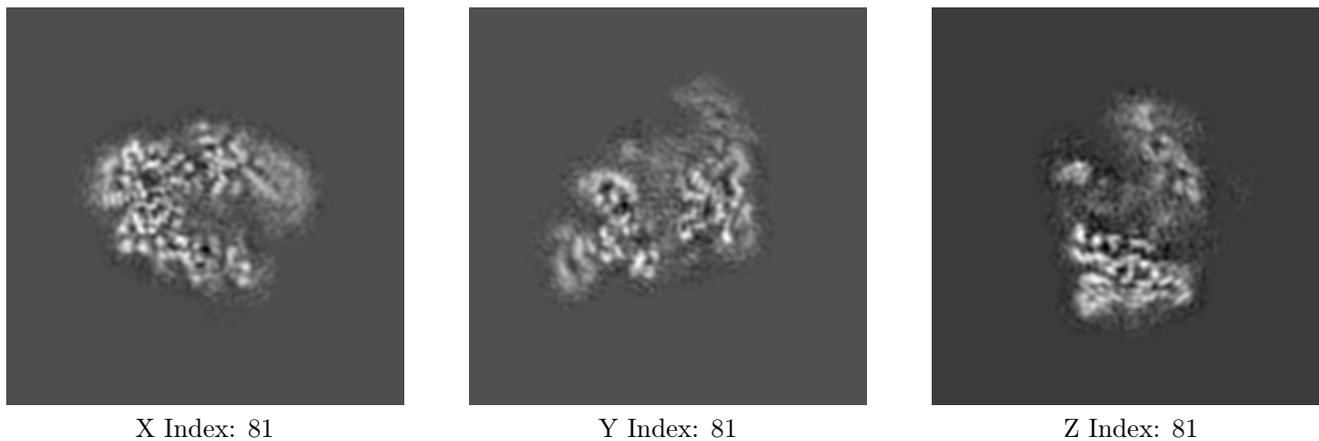
#### 6.1.1 Primary map



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

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

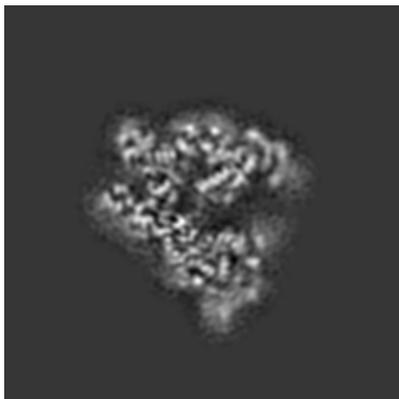
#### 6.2.1 Primary map



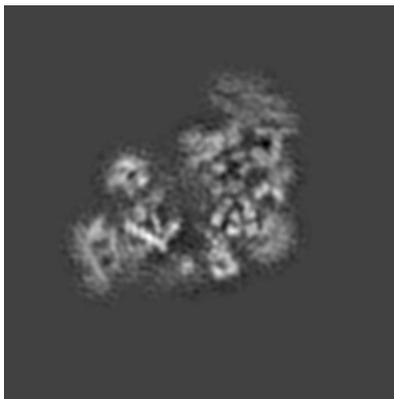
The images above show central slices of the map in three orthogonal directions.

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

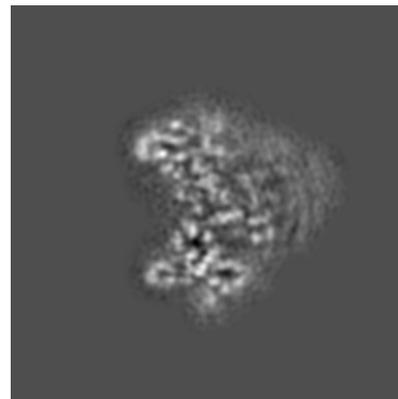
### 6.3.1 Primary map



X Index: 69



Y Index: 89

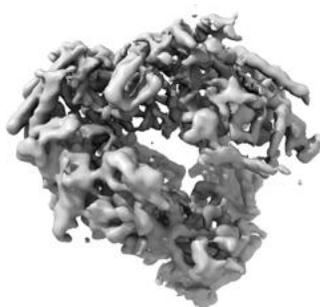


Z Index: 98

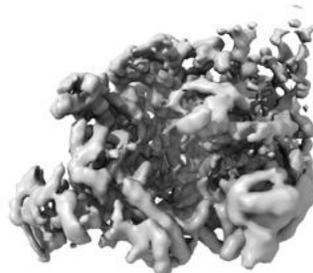
The images above show the largest variance slices of the map in three orthogonal directions.

## 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 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

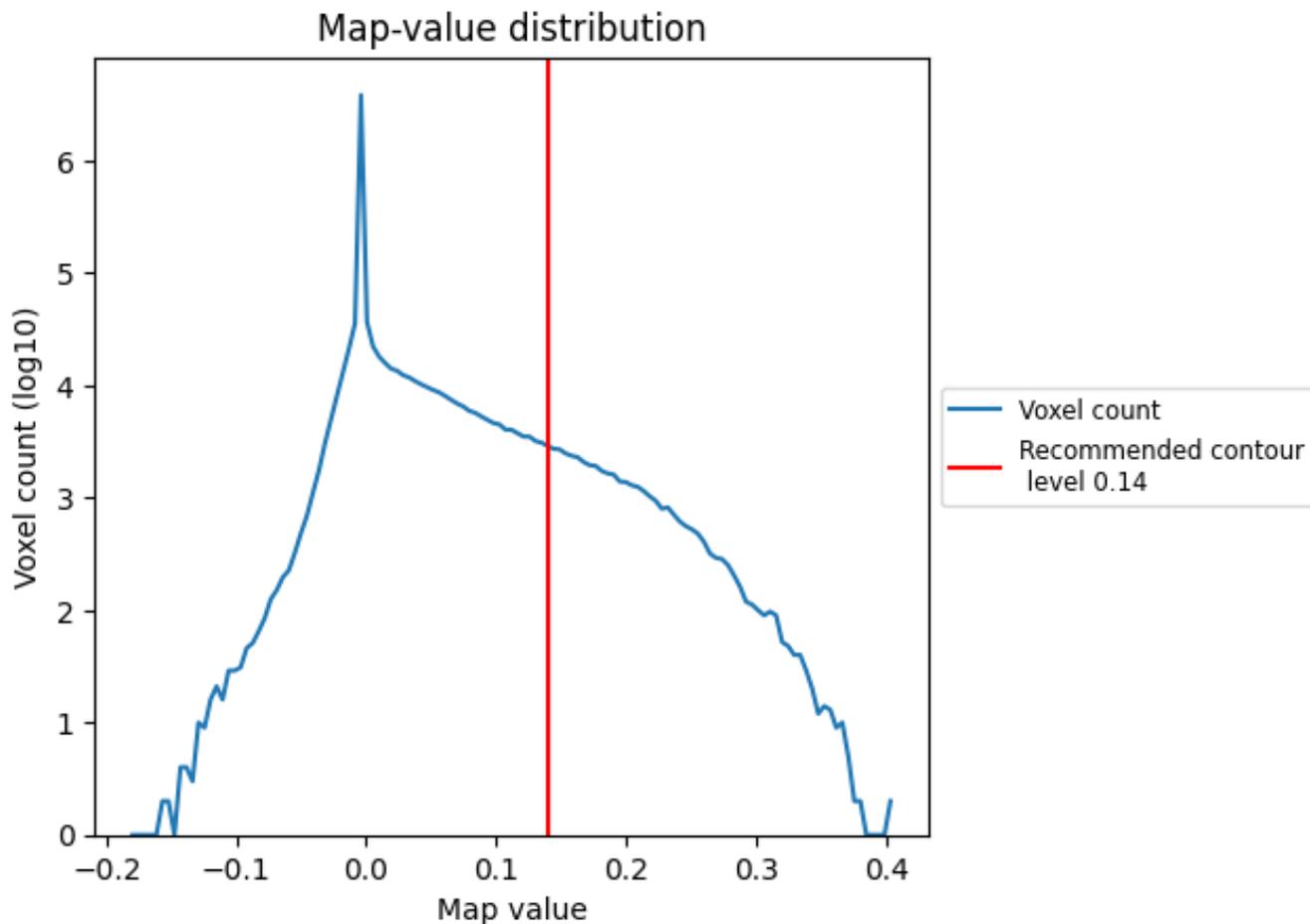
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

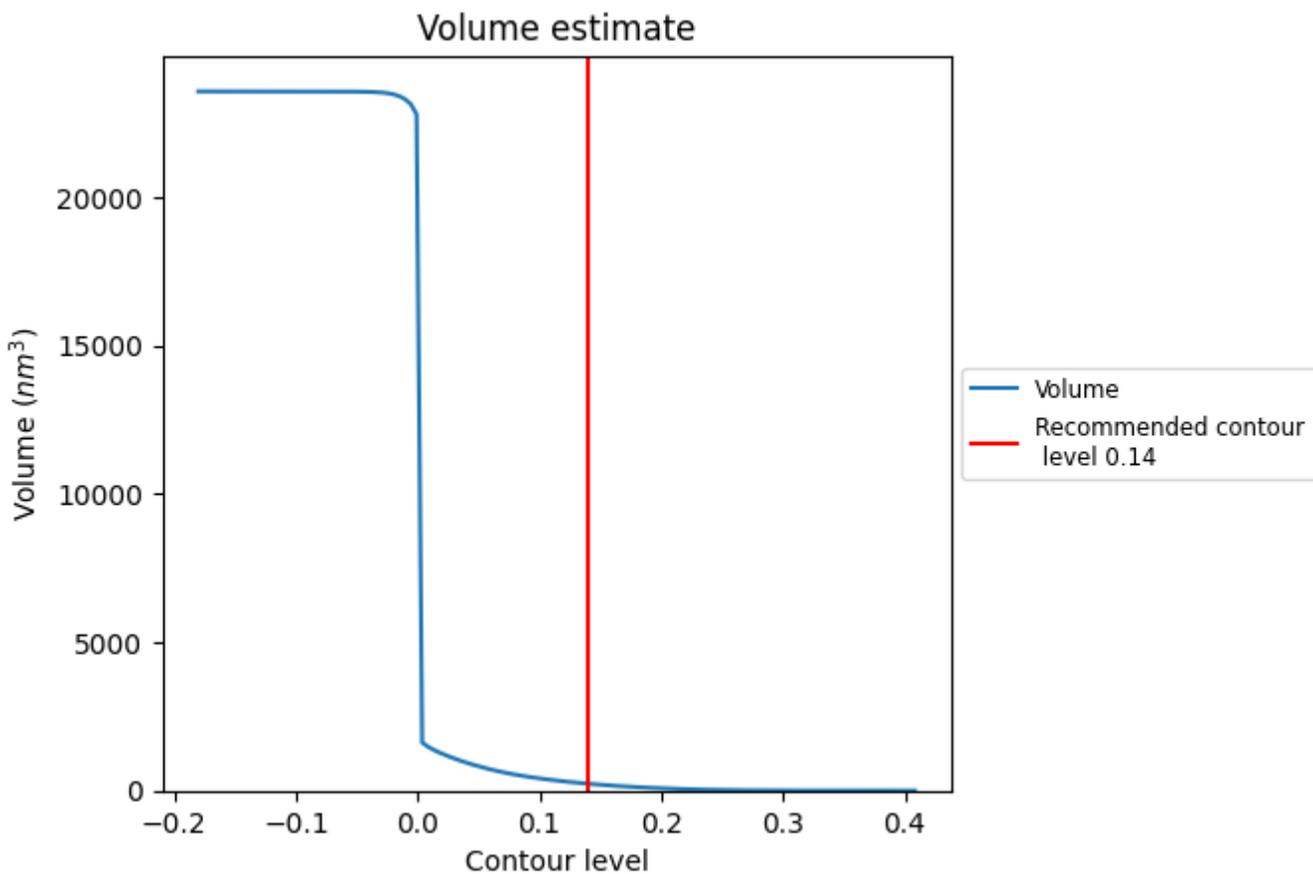
This section contains the results of statistical analysis of the map.

### 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.

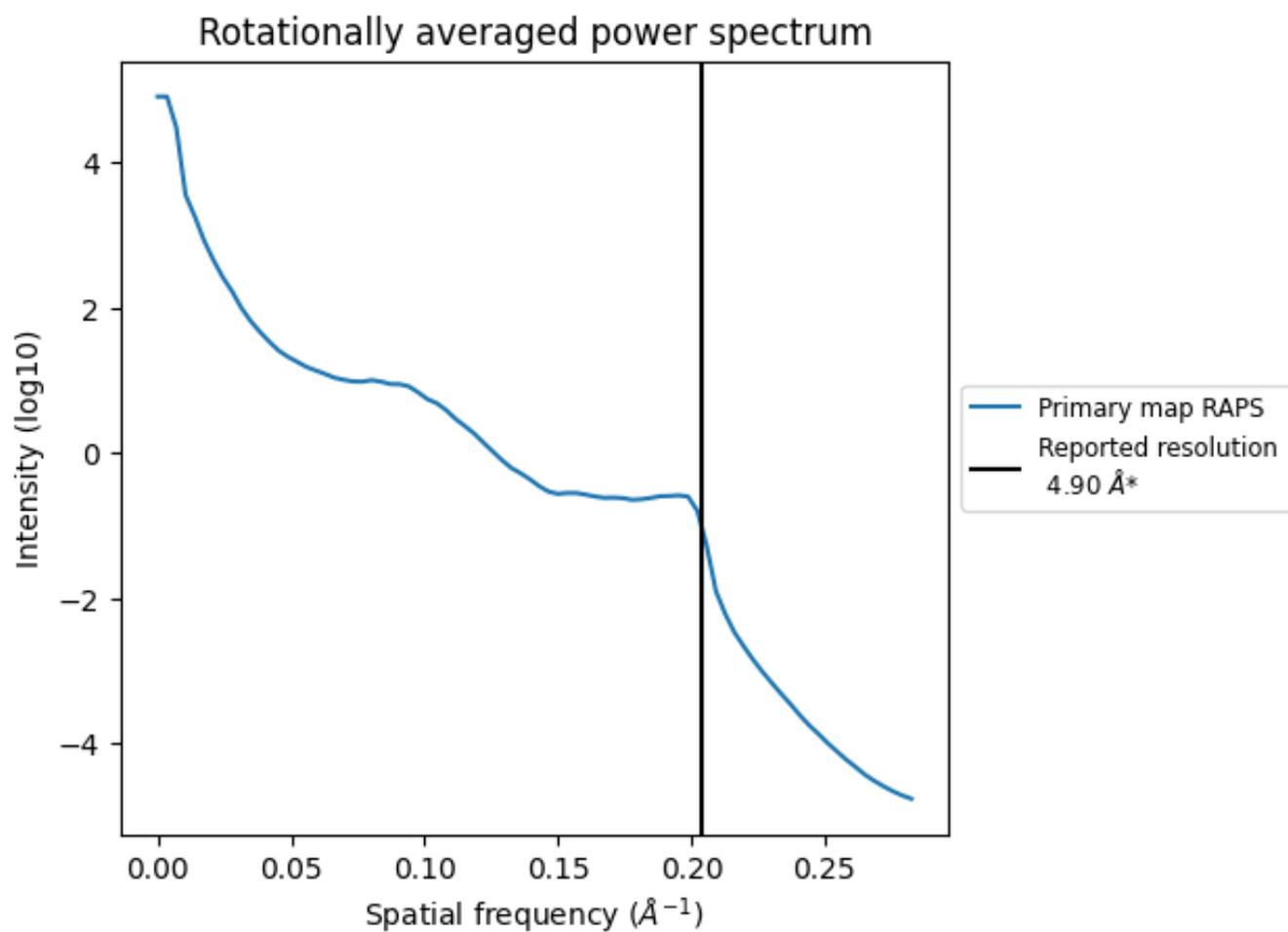
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 233 nm<sup>3</sup>; this corresponds to an approximate mass of 210 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  $0.204 \text{\AA}^{-1}$

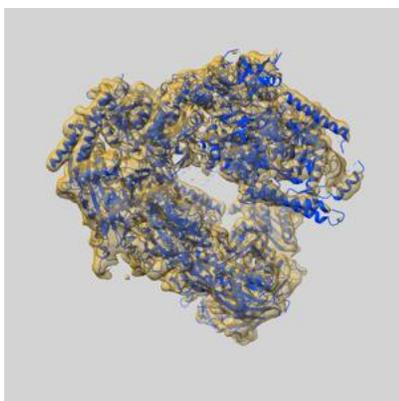
## 8 Fourier-Shell correlation

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

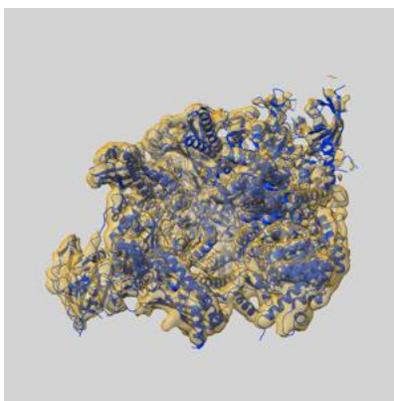
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4088 and PDB model 5LMX. Per-residue inclusion information can be found in section [3](#) on page [7](#).

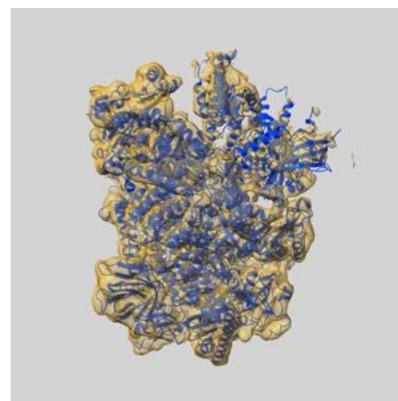
### 9.1 Map-model overlay [i](#)



X



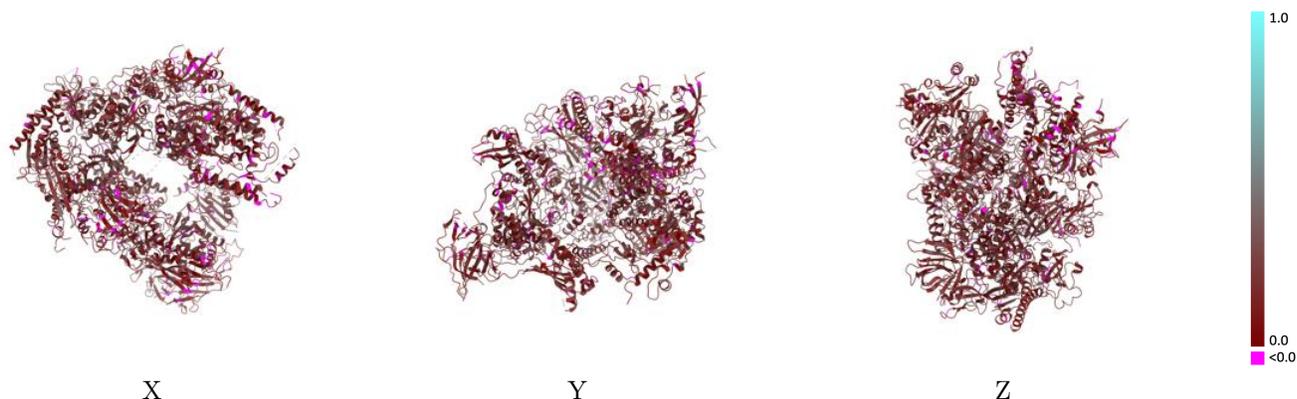
Y



Z

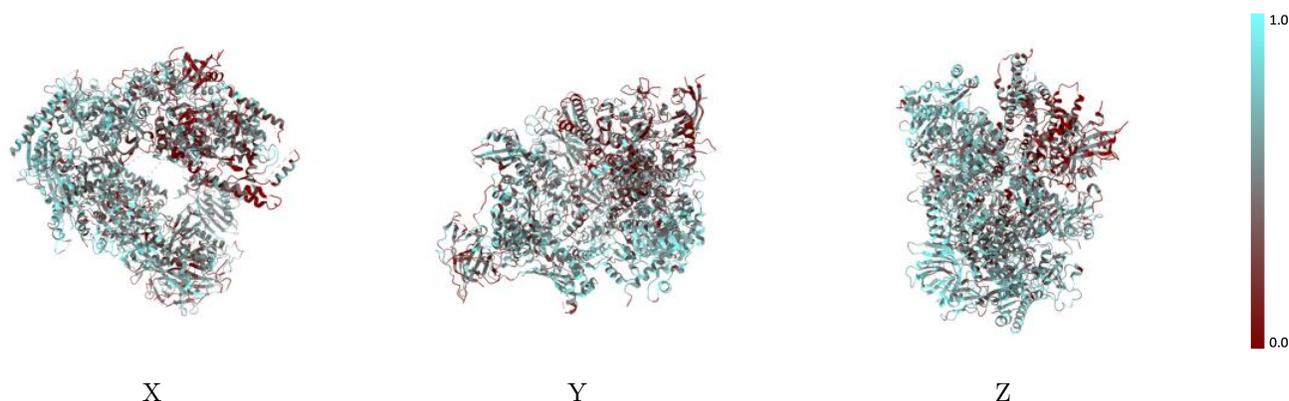
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



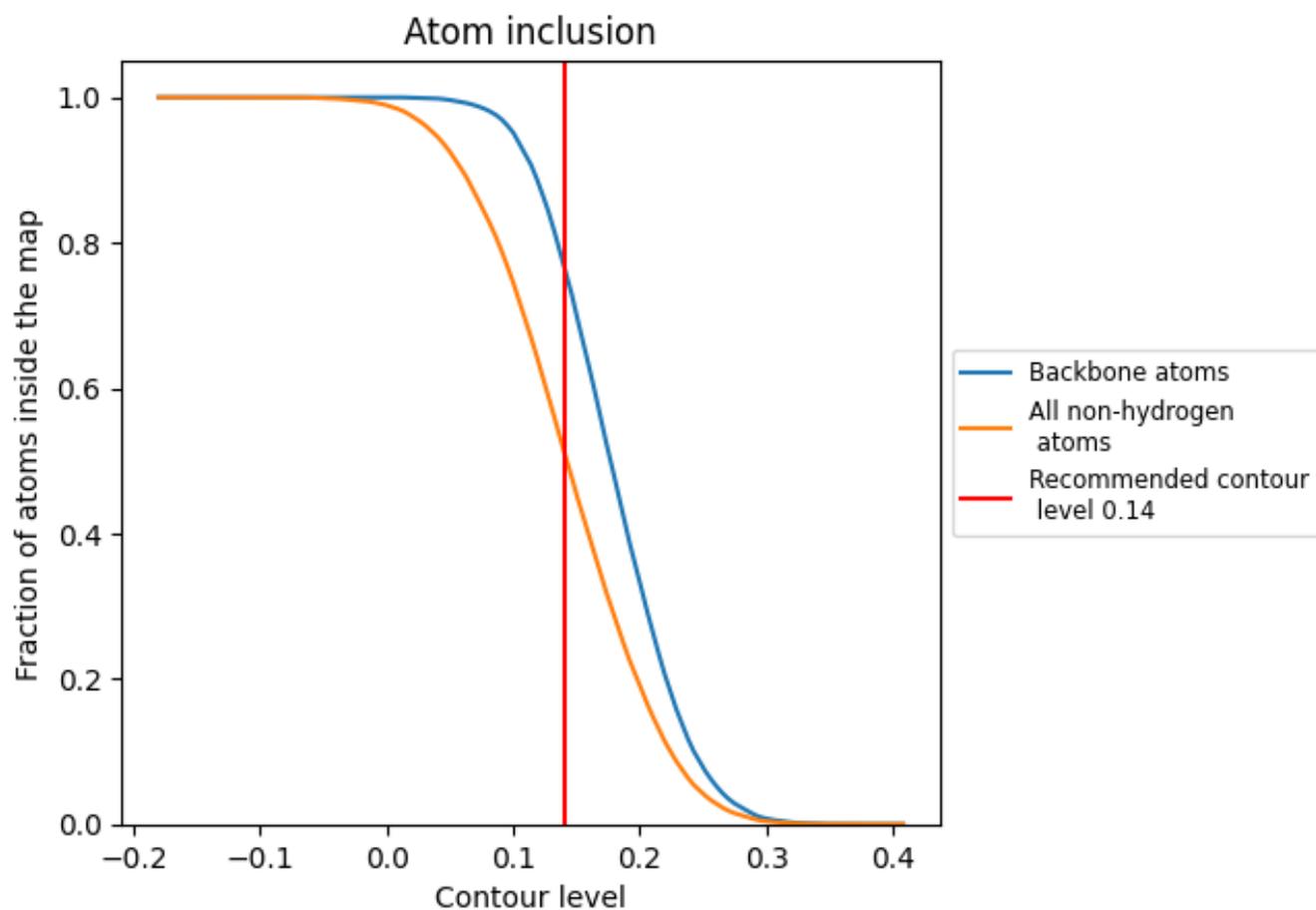
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 51% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5134	 0.1830
A	 0.4848	 0.1820
B	 0.5162	 0.1770
C	 0.6411	 0.2020
D	 0.1203	 0.2100
E	 0.6556	 0.1840
F	 0.4831	 0.1910
G	 0.2712	 0.1830
H	 0.6791	 0.2120
I	 0.4894	 0.1950
J	 0.6159	 0.1980
K	 0.5900	 0.1840
L	 0.5620	 0.1250
M	 0.4037	 0.1460
N	 0.3160	 0.1800

