



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 04:28 PM JST

PDB ID : 7C97  
EMDB ID : EMD-30307  
Title : Cryo-EM structure of an Escherichia coli RNAP-promoter open complex (RPo) with SspA  
Authors : Lin, W.; Feng, Y.  
Deposited on : 2020-06-05  
Resolution : 3.68 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>.

---

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

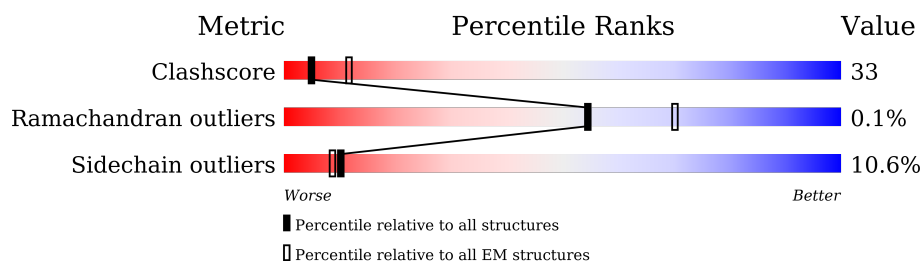
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.68 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	H	63	<div> <div>37%</div> <div>35%</div> <div>65%</div> </div>
2	I	212	<div> <div>34%</div> <div>39%</div> <div>53%</div> <div>5%</div> </div>
2	J	212	<div> <div>29%</div> <div>35%</div> <div>55%</div> <div>5%</div> <div>5%</div> </div>
3	A	329	<div> <div>5%</div> <div>35%</div> <div>31%</div> <div>30%</div> </div>
3	B	329	<div> <div>8%</div> <div>34%</div> <div>30%</div> <div>5%</div> <div>31%</div> </div>
3	K	329	<div> <div>20%</div> <div>13%</div> <div>6%</div> <div>80%</div> </div>
4	C	1342	<div> <div>9%</div> <div>49%</div> <div>45%</div> <div>6%</div> </div>
5	D	1407	<div> <div>16%</div> <div>47%</div> <div>43%</div> <div>6%</div> <div>5%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	E	91	<div><div><div></div><div></div><div></div><div></div></div><div>9%43%41%•13%</div></div>
7	F	613	<div><div><div></div><div></div><div></div><div></div></div><div>27%28%42%7%23%</div></div>
8	G	63	<div><div><div></div><div></div><div></div><div></div></div><div>24%14%62%24%</div></div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 35581 atoms, of which 532 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 DNA chain called DNA (63-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	63	Total	C	N	O	P	0	0
			1312	623	256	370	63		

- Molecule 2 is a protein called Stringent starvation protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	206	Total	C	N	O	S	0	0
			1663	1066	279	310	8		
2	J	201	Total	C	N	O	S	0	0
			1629	1046	272	303	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	K	67	Total	C	H	N	O	S	0	0
			1050	328	532	88	100	2		
3	A	230	Total	C	N	O	S		0	0
			1787	1112	317	352	6			
3	B	226	Total	C	N	O	S		0	0
			1755	1094	310	345	6			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1340	Total	C	N	O	S	0	0
			10569	6632	1841	2053	43		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	engineered mutation	UNP P0A8V2

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	1343	Total	C	N	O	S	0	0
			10368	6512	1846	1960	50		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 7 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	472	Total	C	N	O	S	0	0
			3845	2408	685	729	23		

- Molecule 8 is a DNA chain called DNA (63-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	48	Total	C	N	O	P	0	0
			973	469	161	295	48		

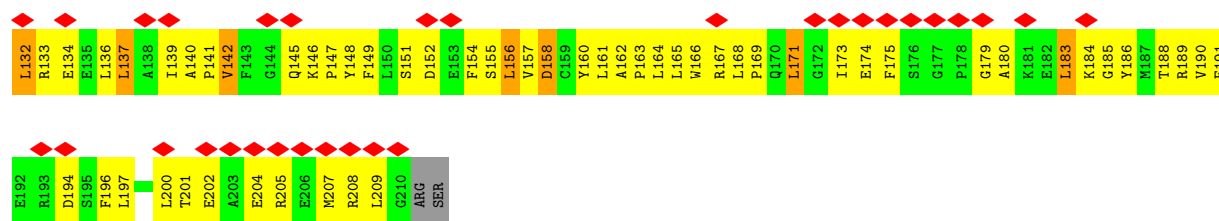
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total	Mg	0
			1	1	

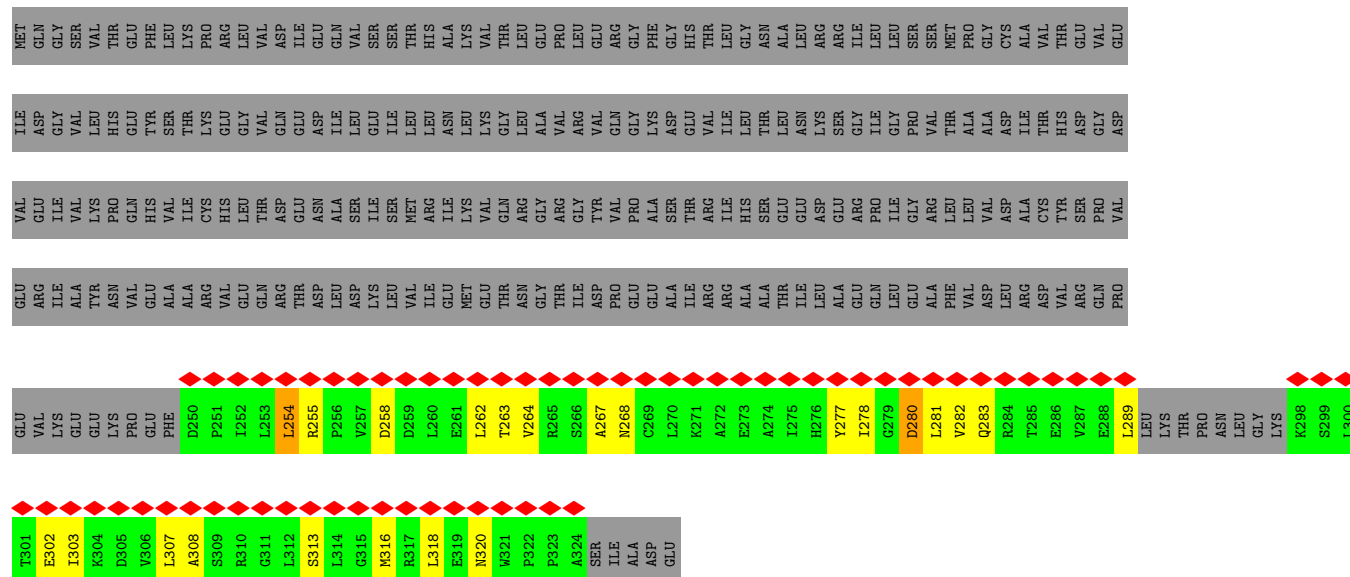
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	

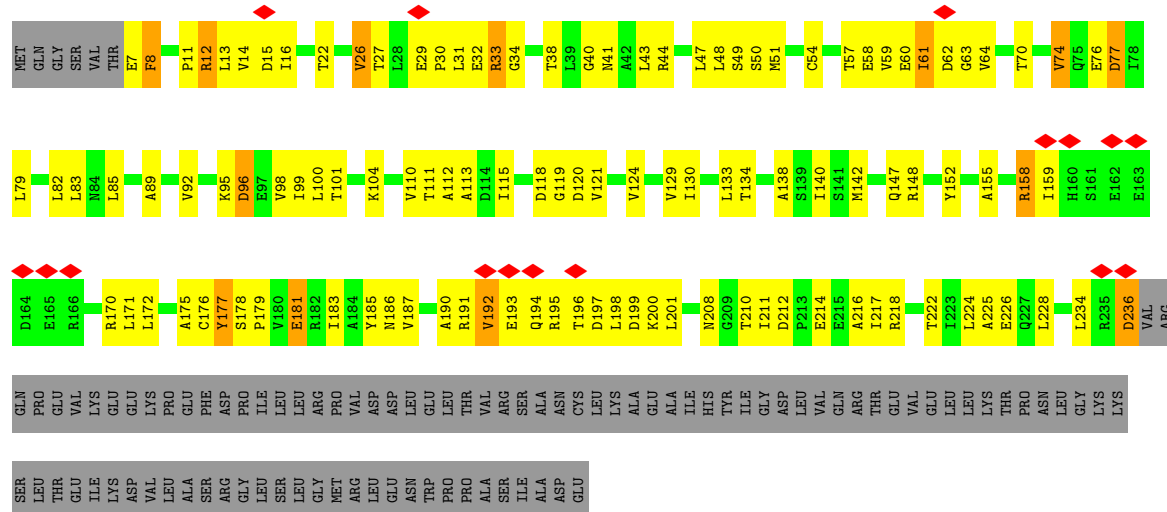




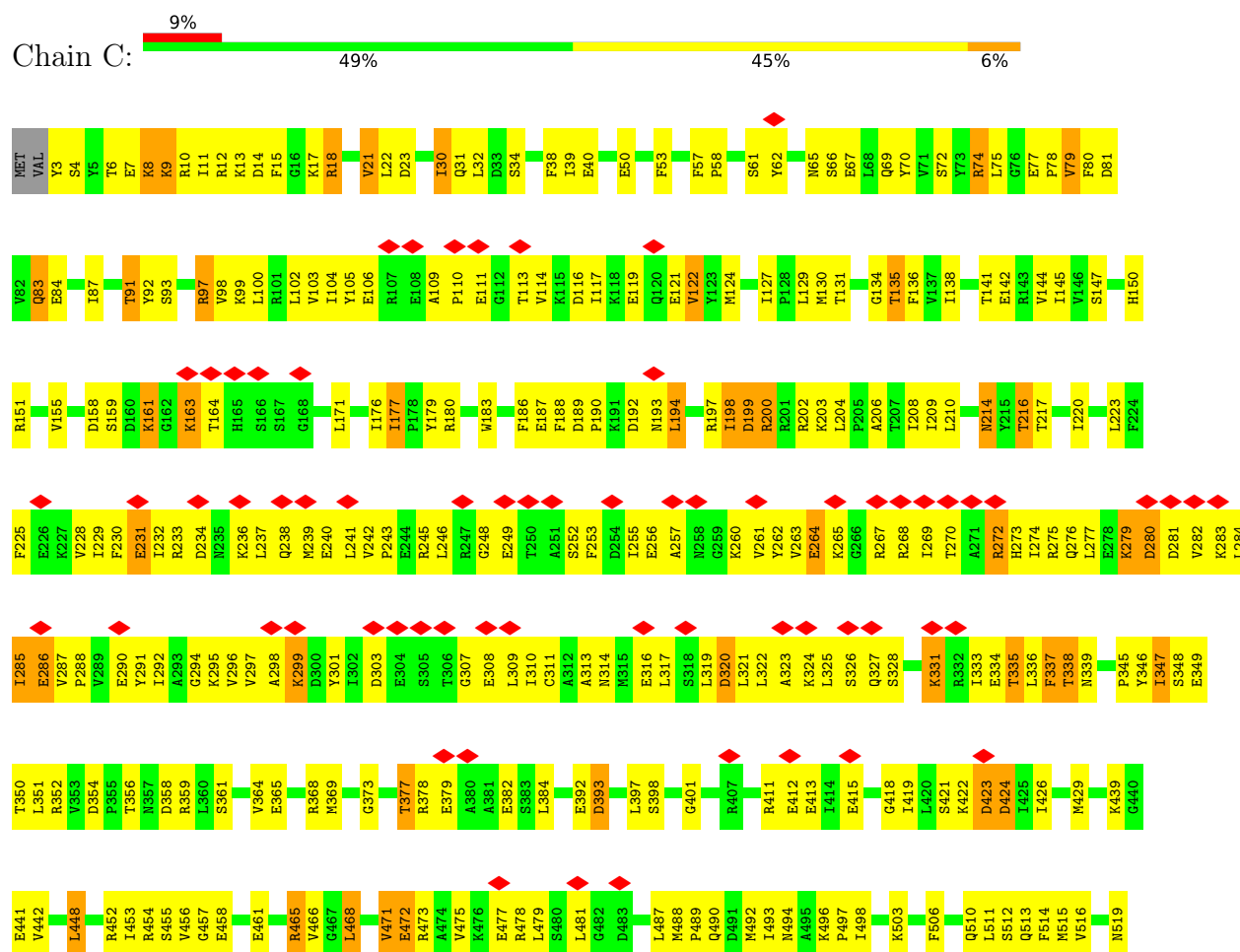
• Molecule 3: DNA-directed RNA polymerase subunit alpha



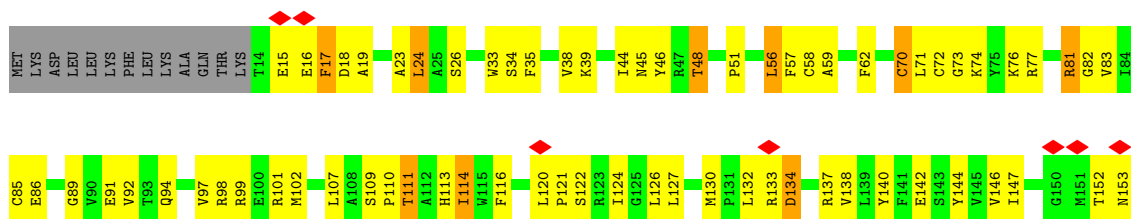
• Molecule 3: DNA-directed RNA polymerase subunit alpha

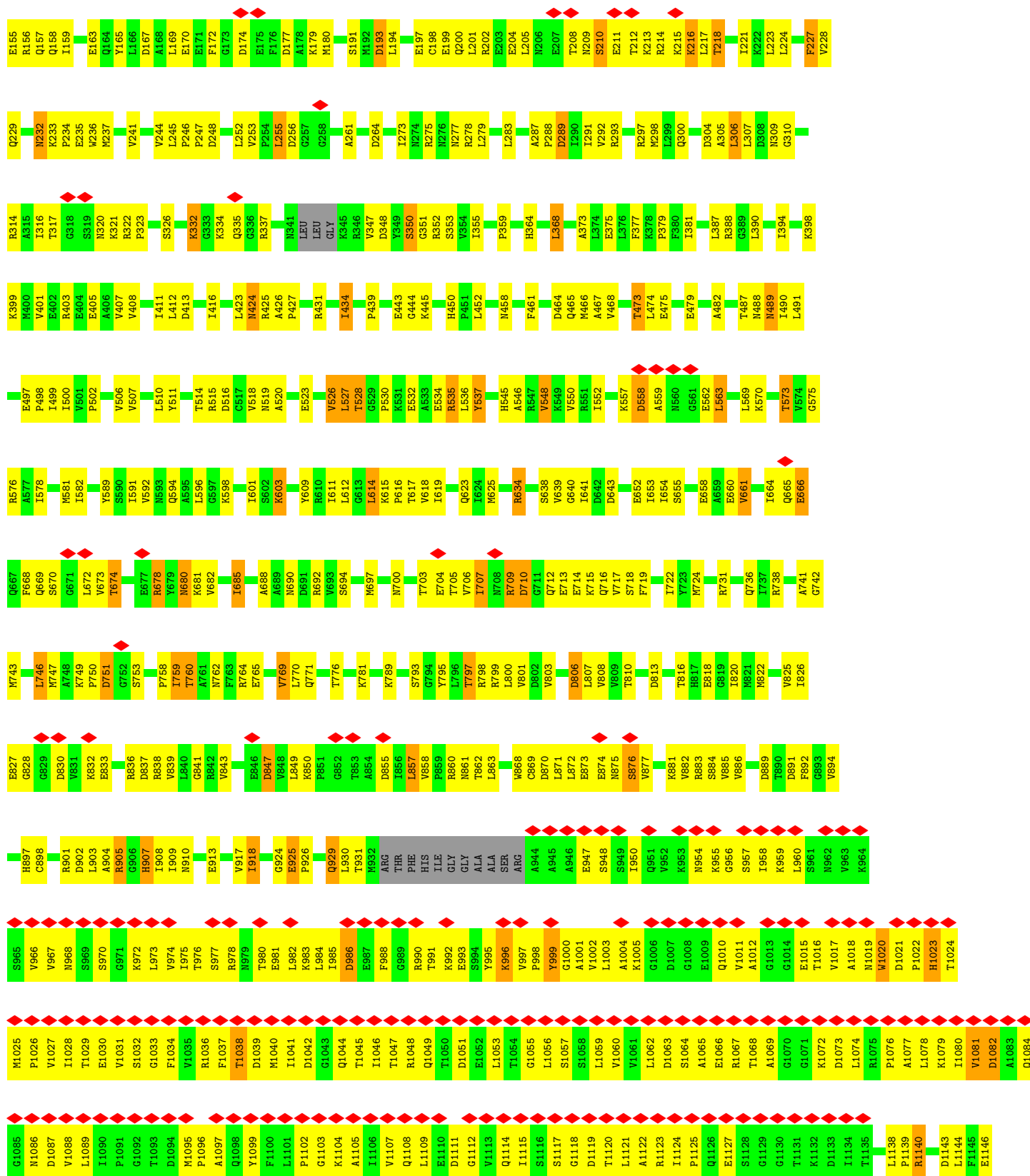


• Molecule 3: DNA-directed RNA polymerase subunit alpha

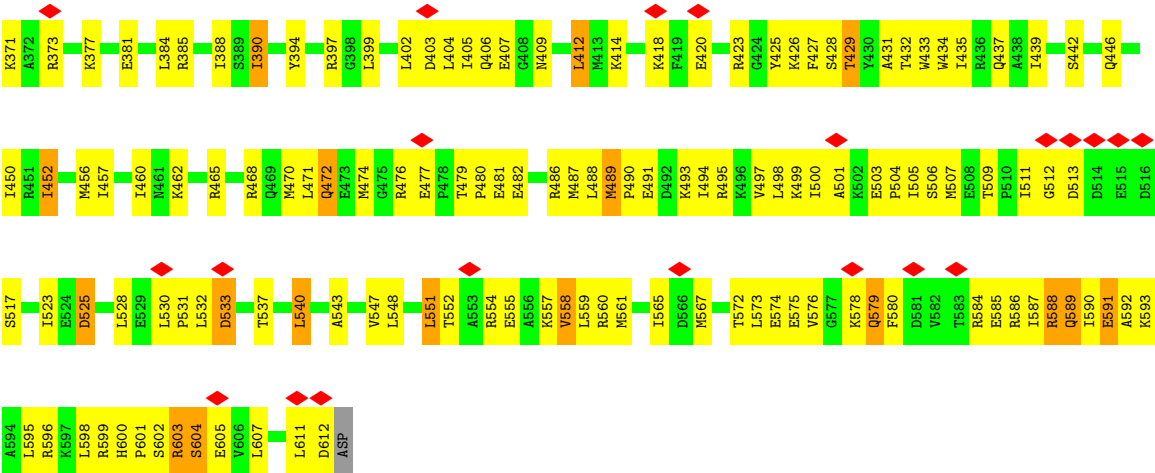




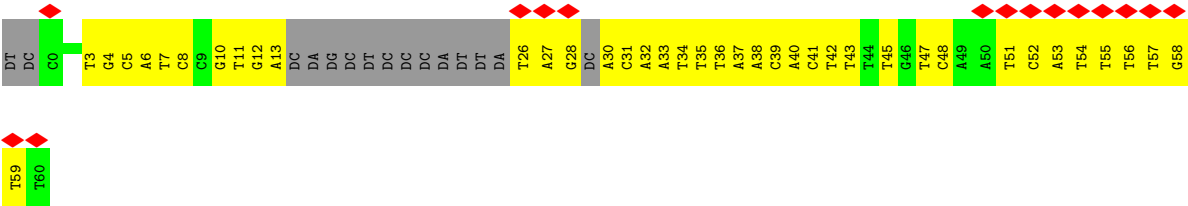
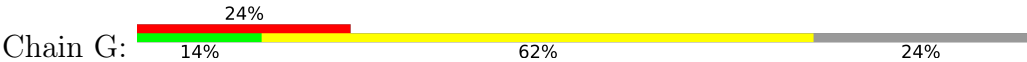








● Molecule 8: DNA (63-mer)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60145	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 ( $e^-/\text{\AA}^2$ )	59	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.170	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	261.4, 261.4, 261.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3069999, 1.3069999, 1.3069999	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, 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	H	0.62	0/1478	0.92	0/2283
2	I	0.30	0/1704	0.45	0/2313
2	J	0.30	0/1670	0.44	0/2267
3	A	0.39	0/1809	0.49	0/2451
3	B	0.34	0/1776	0.51	0/2406
3	K	0.31	0/524	0.68	0/711
4	C	0.41	0/10738	0.49	0/14488
5	D	0.40	0/10521	0.49	0/14208
6	E	0.37	0/629	0.47	0/847
7	F	0.30	0/3896	0.44	0/5236
8	G	0.60	0/1084	0.99	0/1664
All	All	0.40	0/35829	0.54	0/48874

There are no bond length outliers.

There are no bond angle outliers.

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	H	1312	0	709	81	0
2	I	1663	0	1646	144	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1629	0	1613	150	0
3	A	1787	0	1810	105	0
3	B	1755	0	1778	115	0
3	K	518	532	531	13	0
4	C	10569	0	10587	647	0
5	D	10368	0	10517	700	0
6	E	627	0	634	34	0
7	F	3845	0	3913	400	0
8	G	973	0	550	47	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	35049	532	34288	2276	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 33.

The worst 5 of 2276 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:H:42:DG:O6	7:F:106:GLY:HA3	1.36	1.21
5:D:1089:LEU:HA	5:D:1096:PRO:HA	1.30	1.11
7:F:476:ARG:HG2	7:F:477:GLU:HG2	1.37	1.06
4:C:993:PRO:HG2	4:C:996:ARG:HB3	1.41	1.03
2:I:12:THR:HB	2:I:63:VAL:HB	1.44	1.00

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
2	I	204/212 (96%)	184 (90%)	19 (9%)	1 (0%)	29 66

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	199/212 (94%)	179 (90%)	19 (10%)	1 (0%)	29	66
3	A	228/329 (69%)	202 (89%)	26 (11%)	0	100	100
3	B	222/329 (68%)	191 (86%)	31 (14%)	0	100	100
3	K	63/329 (19%)	58 (92%)	5 (8%)	0	100	100
4	C	1338/1342 (100%)	1152 (86%)	183 (14%)	3 (0%)	47	78
5	D	1333/1407 (95%)	1159 (87%)	174 (13%)	0	100	100
6	E	77/91 (85%)	70 (91%)	6 (8%)	1 (1%)	12	47
7	F	466/613 (76%)	422 (91%)	44 (9%)	0	100	100
All	All	4130/4864 (85%)	3617 (88%)	507 (12%)	6 (0%)	54	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	200	ARG
2	J	72	SER
4	C	198	ILE
4	C	1164	PHE
2	I	72	SER

### 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	
2	I	182/187 (97%)	166 (91%)	16 (9%)	10	38
2	J	179/187 (96%)	166 (93%)	13 (7%)	14	44
3	A	198/286 (69%)	177 (89%)	21 (11%)	6	30
3	B	194/286 (68%)	172 (89%)	22 (11%)	6	28
3	K	58/286 (20%)	51 (88%)	7 (12%)	5	24
4	C	1155/1157 (100%)	1030 (89%)	125 (11%)	6	29
5	D	1104/1168 (94%)	987 (89%)	117 (11%)	6	30
6	E	67/75 (89%)	61 (91%)	6 (9%)	9	37

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	F	420/540 (78%)	369 (88%)	51 (12%)	5	24
All	All	3557/4172 (85%)	3179 (89%)	378 (11%)	10	30

5 of 378 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	300	GLN
5	D	876	SER
5	D	387	LEU
5	D	617	THR
5	D	1045	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
4	C	1268	GLN
5	D	477	GLN
7	F	455	HIS
4	C	1336	ASN
5	D	229	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 3 ligands modelled in this entry, 3 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.

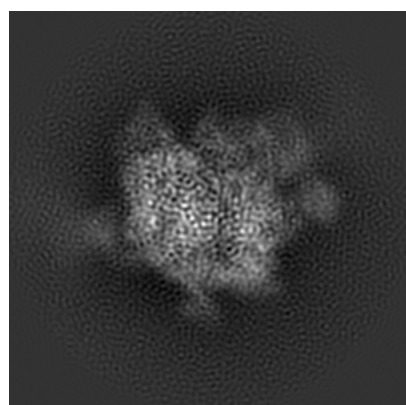
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30307. These allow visual inspection of the internal detail of the map and identification of artifacts.

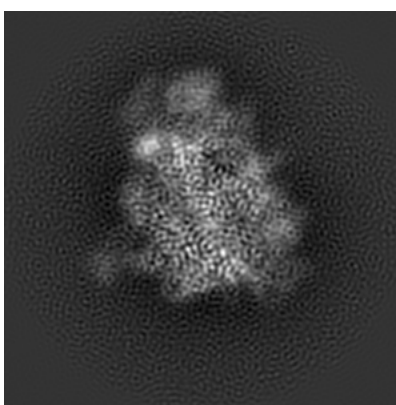
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

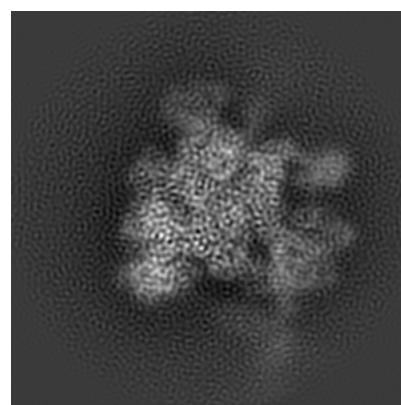
#### 6.1.1 Primary map



X



Y

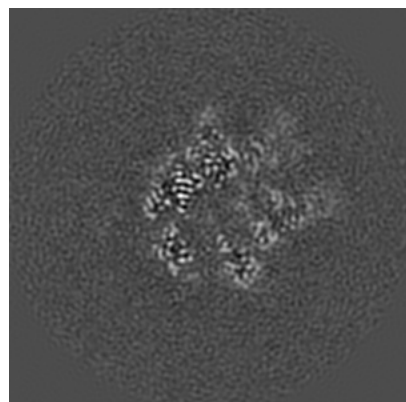


Z

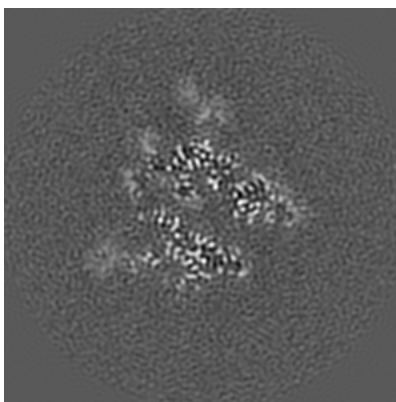
The images above show the map projected in three orthogonal directions.

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

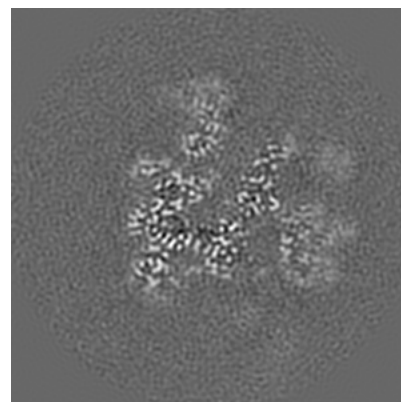
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

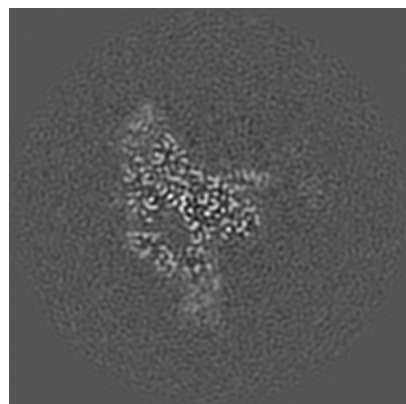


Z Index: 100

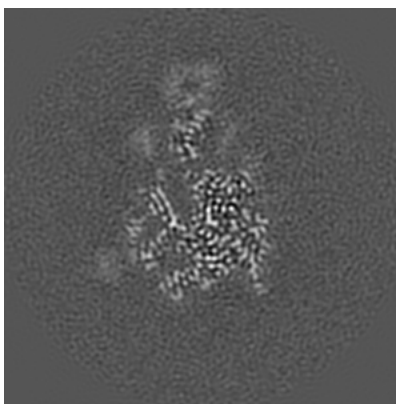
The images above show central slices of the map in three orthogonal directions.

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

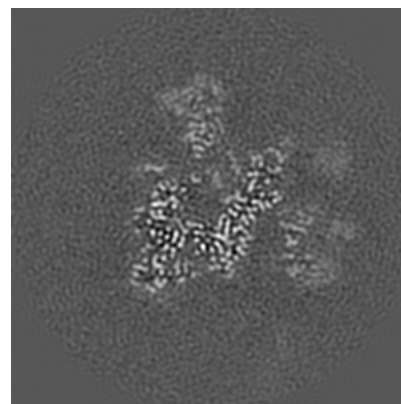
### 6.3.1 Primary map



X Index: 74



Y Index: 87



Z Index: 103

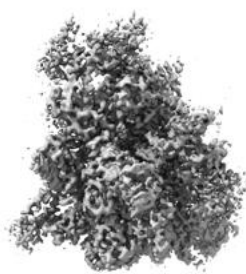
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

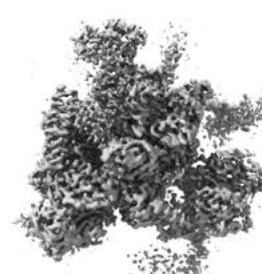
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

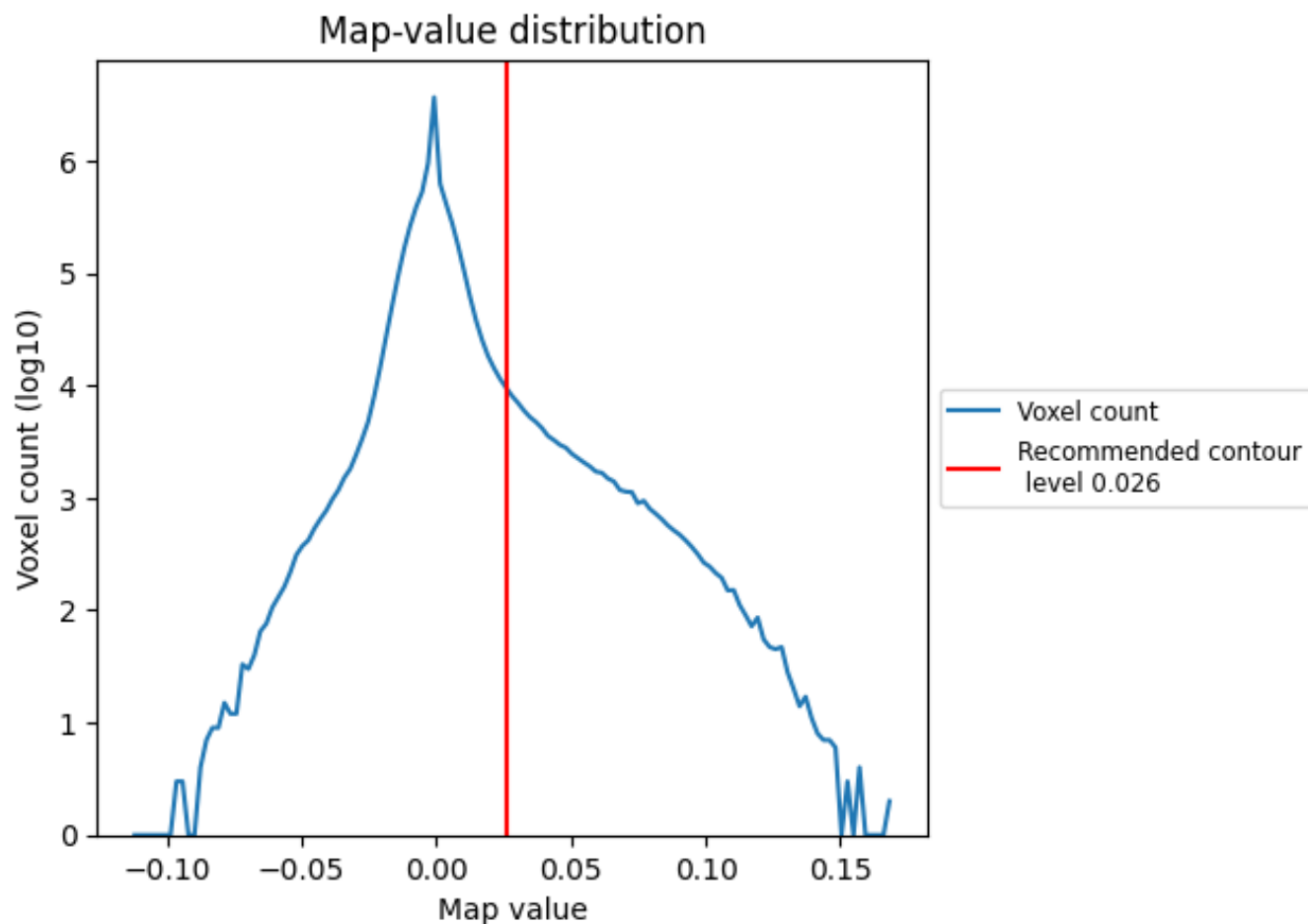
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

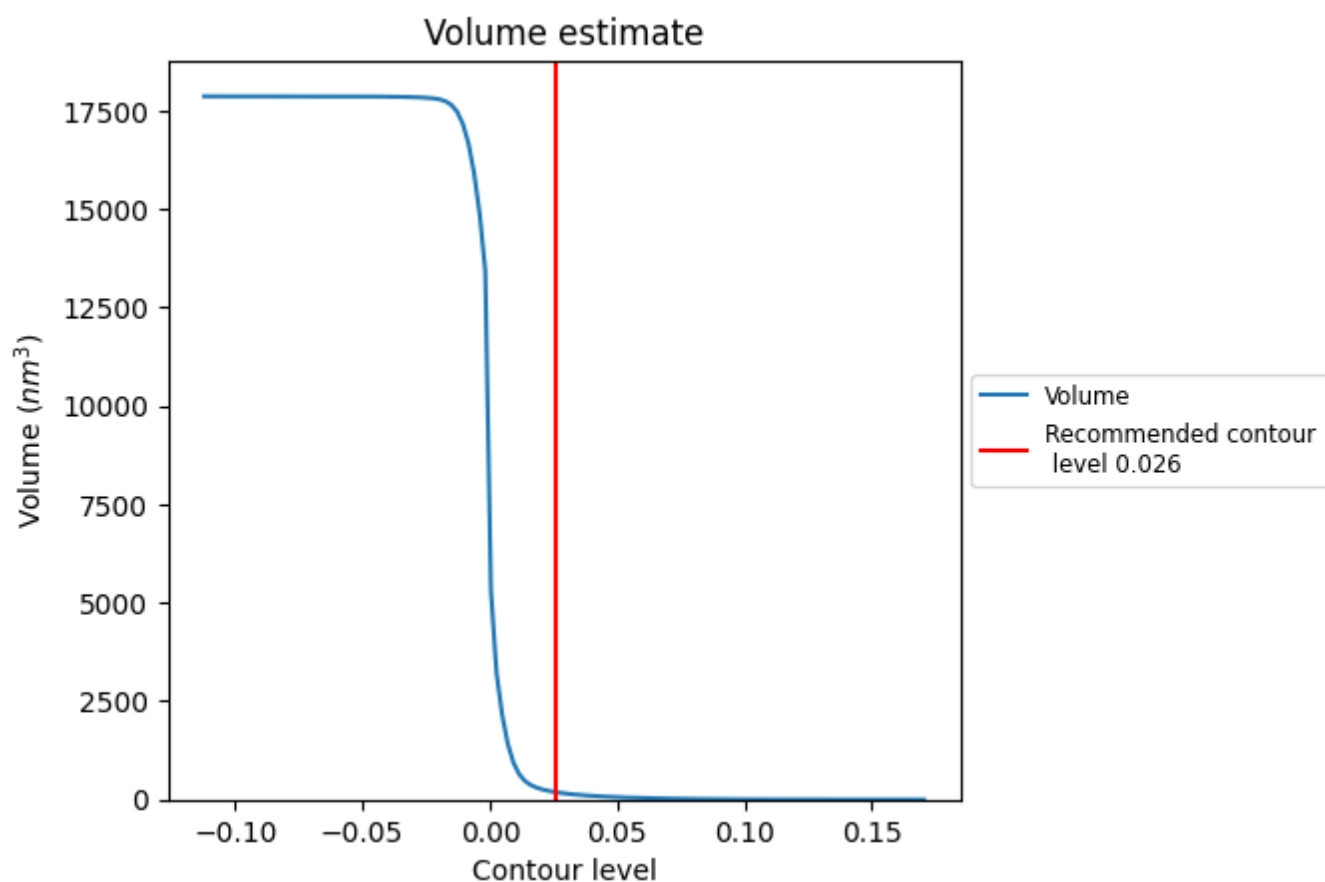
This section contains the results of statistical analysis of the map.

### 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.

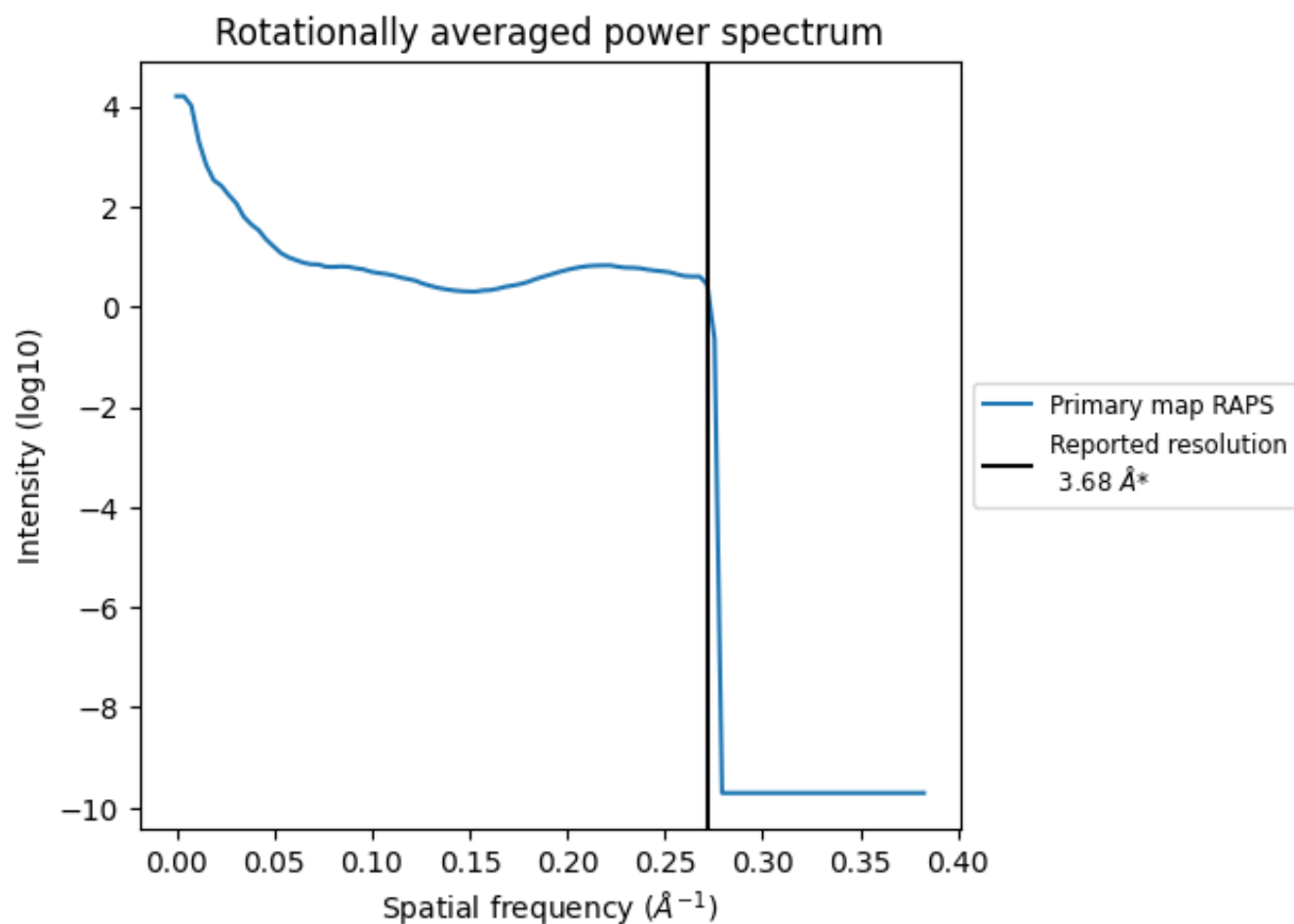
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 186 nm<sup>3</sup>; this corresponds to an approximate mass of 168 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 0.272  $\text{\AA}^{-1}$



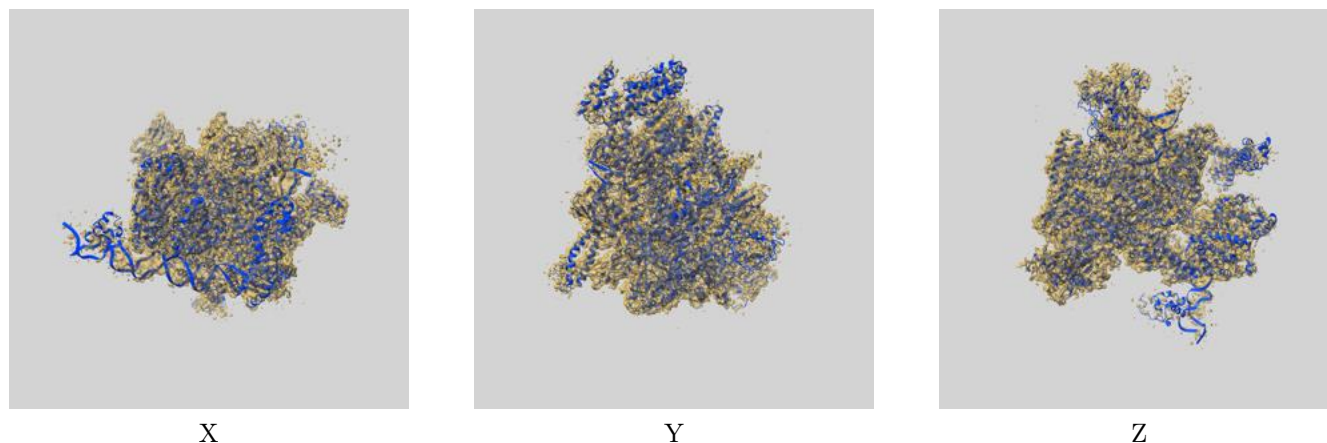
## 8 Fourier-Shell correlation

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

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

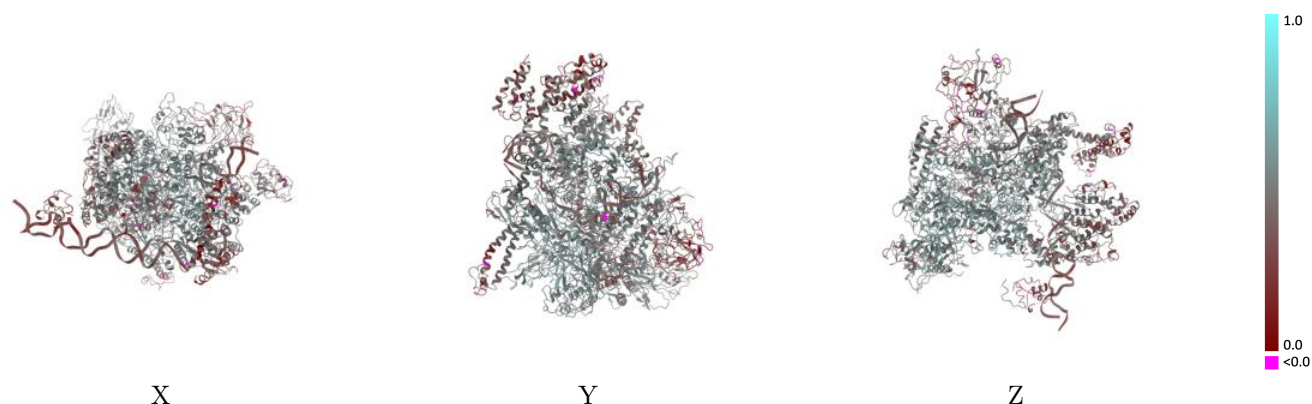
This section contains information regarding the fit between EMDB map EMD-30307 and PDB model 7C97. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



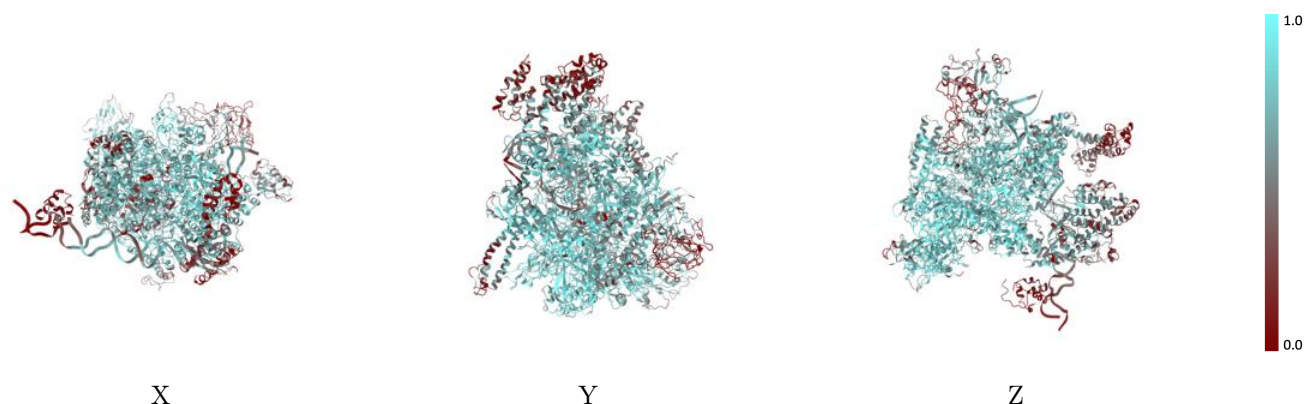
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



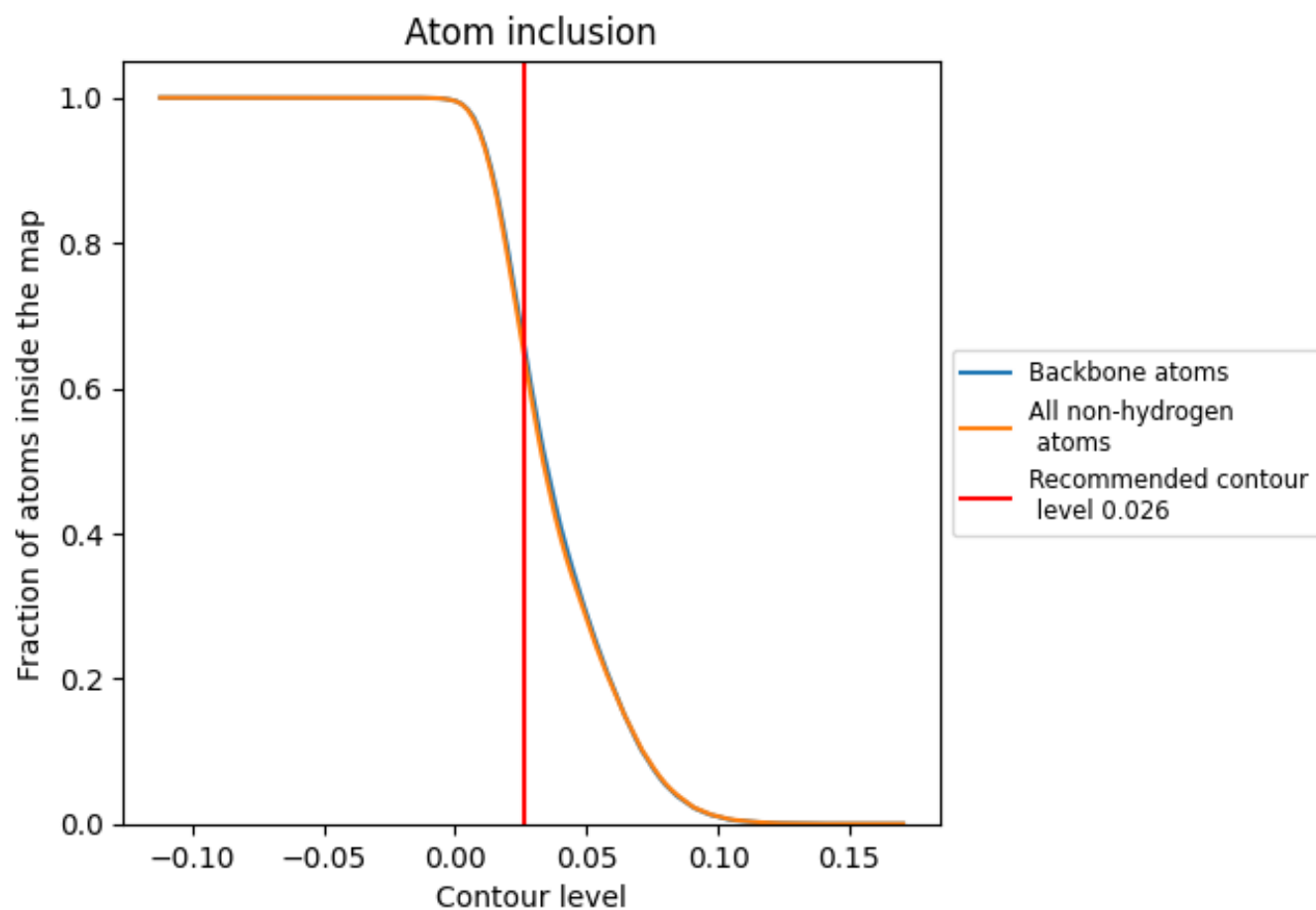
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.026).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 65% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6510	<div></div> 0.4610
A	<div></div> 0.7696	<div></div> 0.5210
B	<div></div> 0.6853	<div></div> 0.4780
C	<div></div> 0.7425	<div></div> 0.4990
D	<div></div> 0.6899	<div></div> 0.4800
E	<div></div> 0.7332	<div></div> 0.5020
F	<div></div> 0.5091	<div></div> 0.4020
G	<div></div> 0.5283	<div></div> 0.3400
H	<div></div> 0.4939	<div></div> 0.3570
I	<div></div> 0.5166	<div></div> 0.4190
J	<div></div> 0.5270	<div></div> 0.4150
K	<div></div> 0.0630	<div></div> 0.2430

1.0

0.0

<0.0