



wwPDB EM Validation Summary Report ⓘ

Mar 11, 2024 – 06:32 AM EDT

PDB ID : 6PMI
EMDB ID : EMD-20394
Title : Sigm28-transcription initiation complex with specific promoter at the state 1
Authors : Liu, B.; Shi, W.
Deposited on : 2019-07-02
Resolution : 3.86 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.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

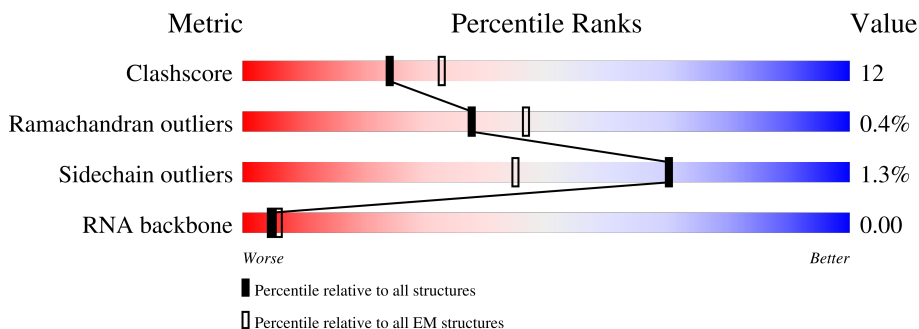
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.86 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	329	53% (green), 17% (yellow), 30% (grey)
1	B	329	51% (green), 17% (yellow), 31% (grey), 5% (red)
2	C	1342	69% (green), 30% (yellow), 1% (red)
3	D	1407	68% (green), 27% (yellow), 5% (grey), 5% (red)
4	E	91	63% (green), 21% (yellow), 13% (grey), 6% (red)
5	F	247	69% (green), 25% (yellow), 6% (red)
6	1	54	61% (green), 35% (yellow), 4% (red)

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	2	54	 63% 35%
8	3	3	 33% 67%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 57996 atoms, of which 28621 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	230	Total	C	H	N	O	S	0	0
			3599	1112	1813	317	351	6		
1	B	228	Total	C	H	N	O	S	0	0
			3556	1100	1789	312	349	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	C	1340	Total	C	H	N	O	S	0	0
			21152	6631	10582	1841	2055	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	D	1337	Total	C	H	N	O	S	0	0
			21011	6531	10615	1853	1962	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	E	79	Total	C	H	N	O	S	0	0
			1261	382	634	118	126	1		

- Molecule 5 is a protein called RNA polymerase sigma factor FliA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	F	239	Total	C	H	N	O	S	0	0
			3871	1201	1936	356	374	4		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	240	LEU	-	expression tag	UNP P0AEM6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	241	GLU	-	expression tag	UNP P0AEM6
F	242	HIS	-	expression tag	UNP P0AEM6
F	243	HIS	-	expression tag	UNP P0AEM6
F	244	HIS	-	expression tag	UNP P0AEM6
F	245	HIS	-	expression tag	UNP P0AEM6
F	246	HIS	-	expression tag	UNP P0AEM6
F	247	HIS	-	expression tag	UNP P0AEM6

- Molecule 6 is a DNA chain called SYNTHETIC NONTEMPLATE STRAND DNA (54-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	1	54	1712	526	611	194	327	54	0	0

- Molecule 7 is a DNA chain called SYNTHETIC TEMPLATE STRAND DNA (54-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
7	2	54	1724	530	607	214	319	54	0	0

- Molecule 8 is a RNA chain called Nascent RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
8	3	3	107	29	34	13	26	5	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

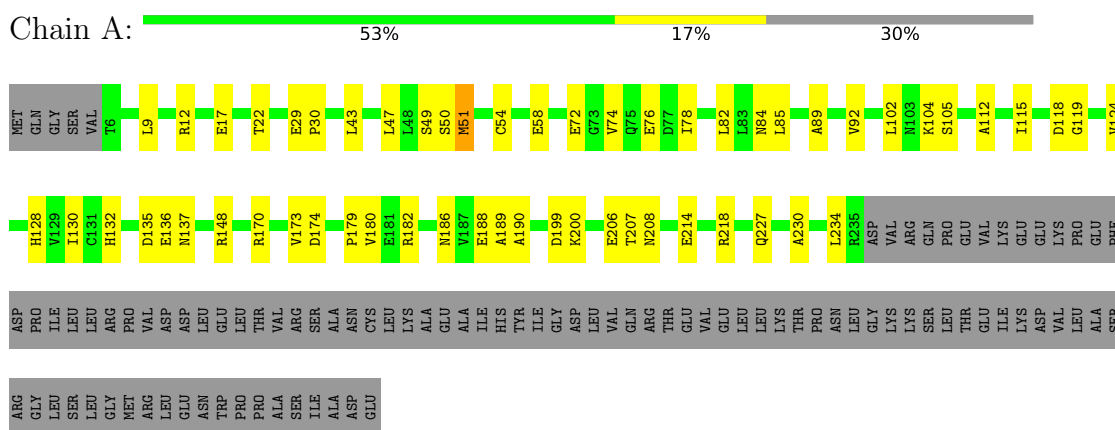
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

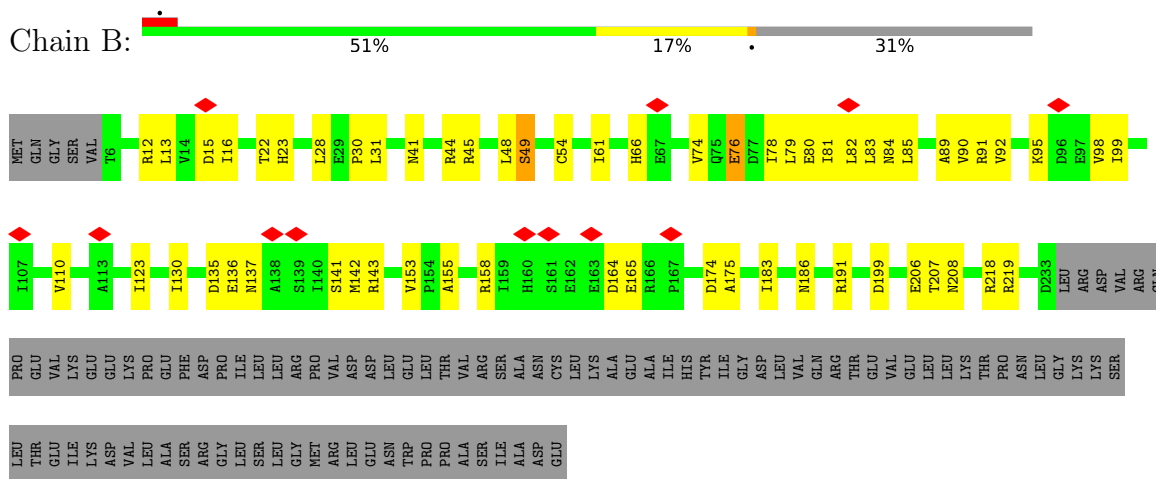
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

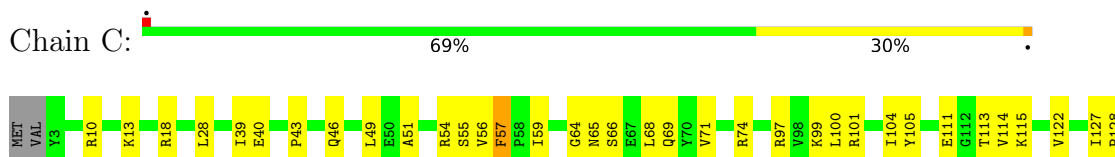
- Molecule 1: DNA-directed RNA polymerase subunit alpha

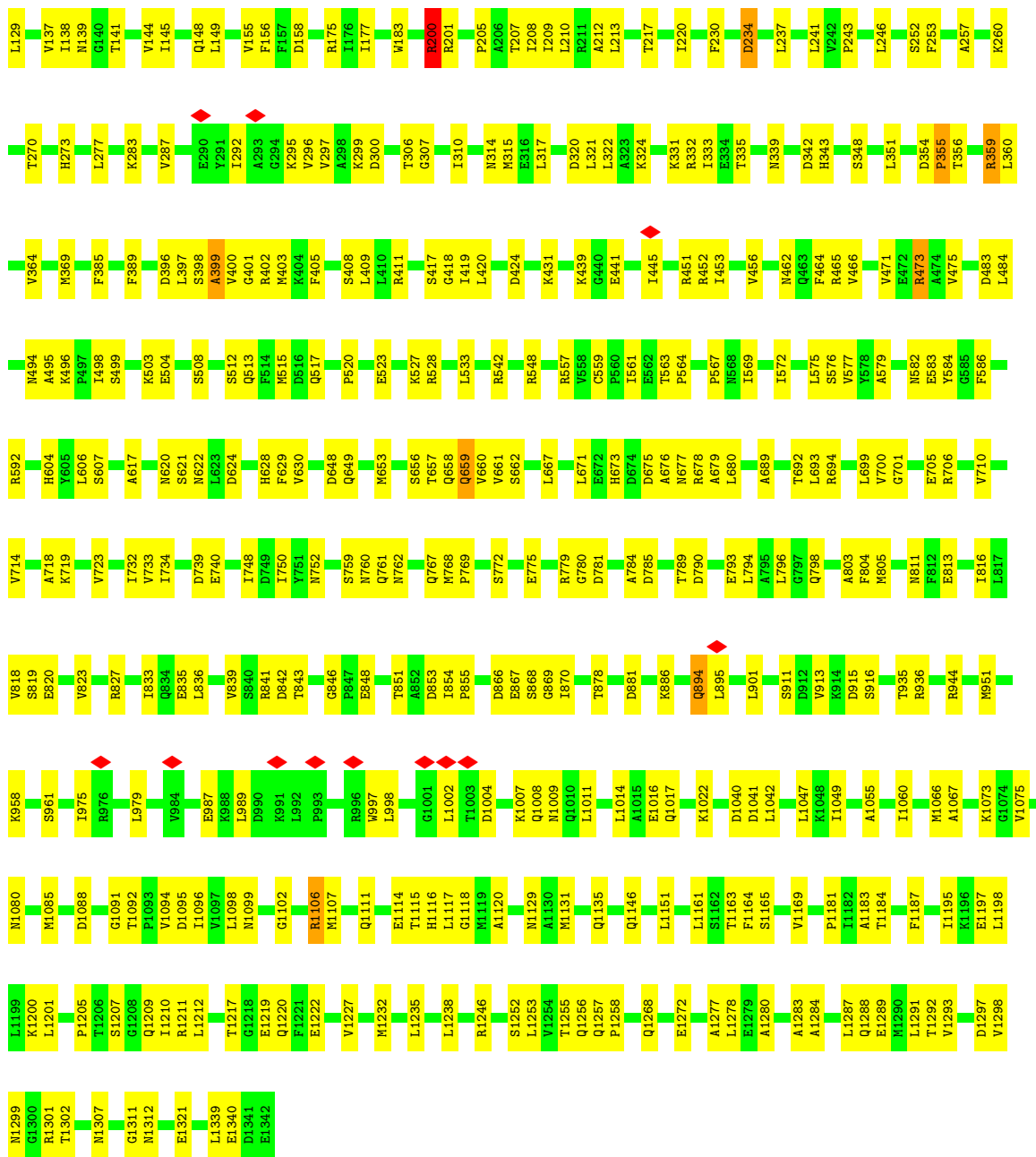


- Molecule 1: DNA-directed RNA polymerase subunit alpha

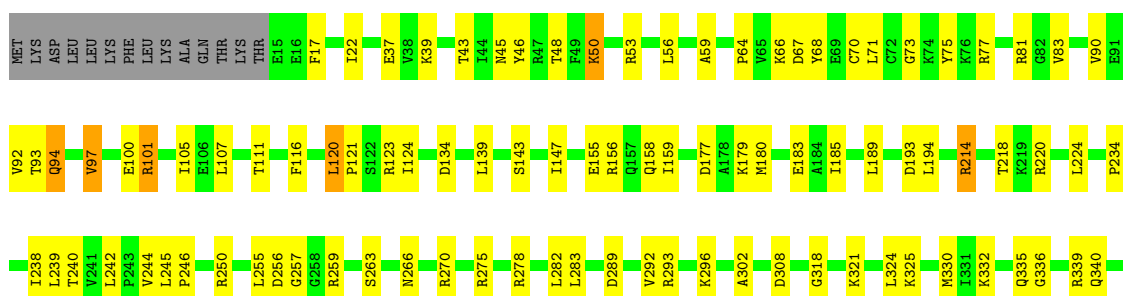


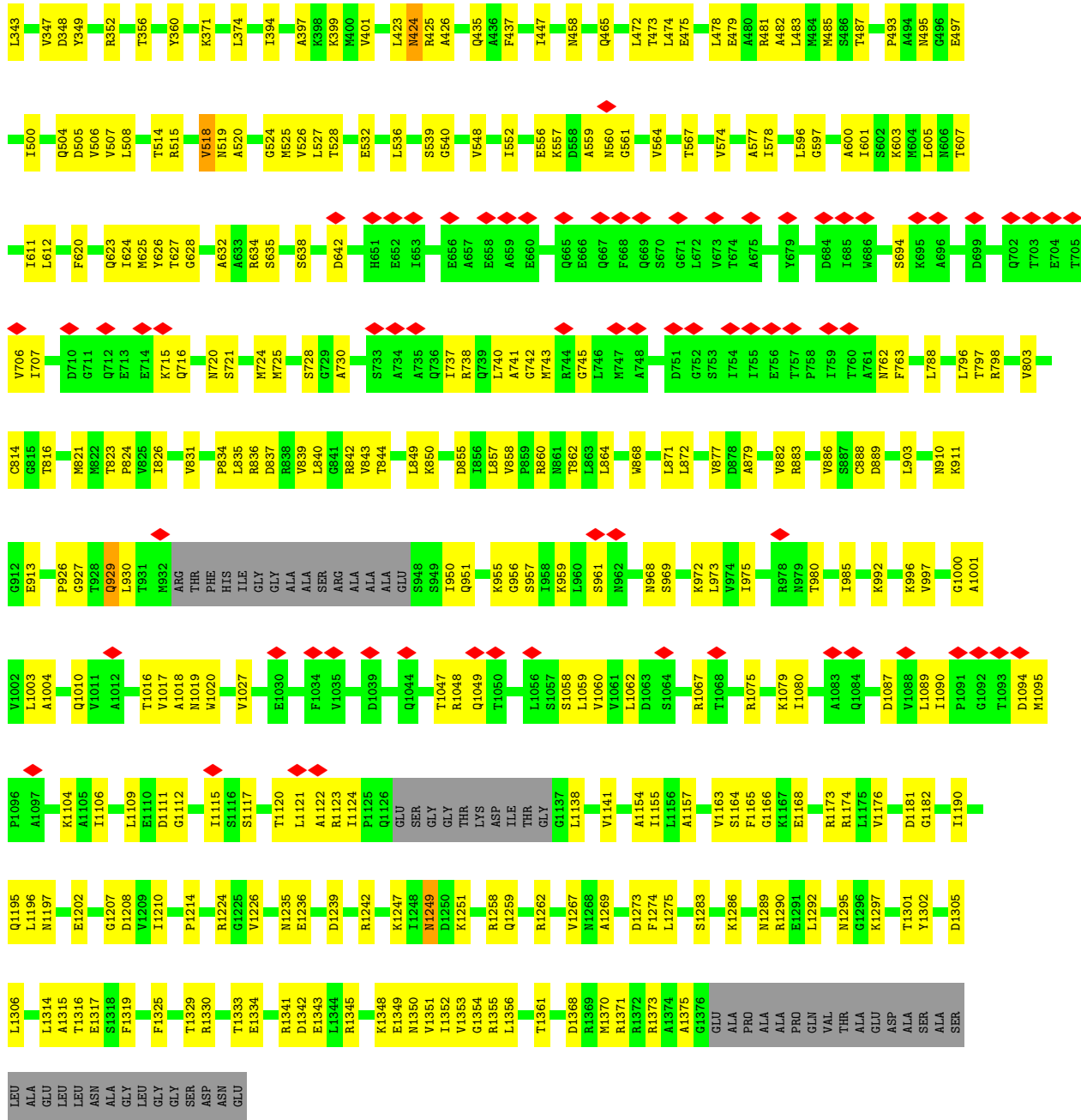
- Molecule 2: DNA-directed RNA polymerase subunit beta



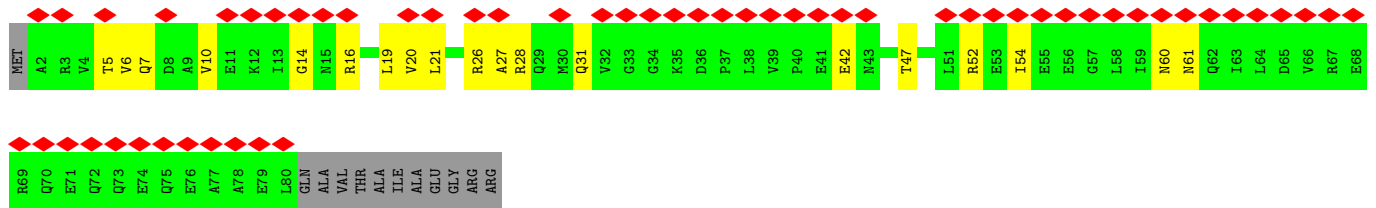


● Molecule 3: DNA-directed RNA polymerase subunit beta'

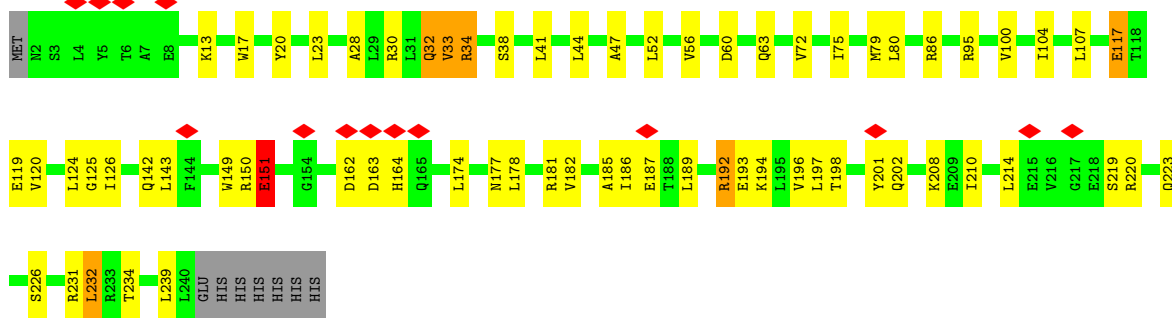




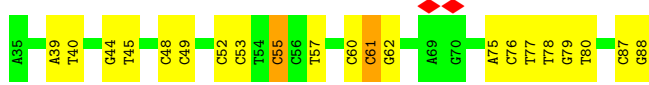
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor FliA



● Molecule 6: SYNTHETIC NONTEMPLATE STRAND DNA (54-MER)



● Molecule 7: SYNTHETIC TEMPLATE STRAND DNA (54-MER)



● Molecule 8: Nascent RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	43838	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	6.363	Depositor
Minimum map value	-2.941	Depositor
Average map value	-0.018	Depositor
Map value standard deviation	0.345	Depositor
Recommended contour level	0.8	Depositor
Map size (\AA)	291.6, 291.6, 291.6	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.90000004, 0.90000004, 0.90000004	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: ATP, MG, 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	0.52	0/1808	0.70	0/2450
1	B	0.47	0/1789	0.74	1/2425 (0.0%)
2	C	0.59	1/10739 (0.0%)	0.74	2/14489 (0.0%)
3	D	0.55	0/10553	0.75	2/14248 (0.0%)
4	E	0.32	0/629	0.62	0/847
5	F	0.57	0/1960	0.82	1/2649 (0.0%)
6	1	1.09	0/1232	1.18	7/1898 (0.4%)
7	2	1.20	0/1256	1.12	5/1938 (0.3%)
8	3	0.52	0/46	0.95	0/69
All	All	0.63	1/30012 (0.0%)	0.79	18/41013 (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	B	0	3
2	C	0	6
3	D	0	6
5	F	0	4
All	All	0	19

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	813	GLU	CA-CB	-5.17	1.42	1.53

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	2	45	DC	O4'-C1'-N1	6.99	112.89	108.00
6	1	62	DG	O5'-P-OP1	-6.87	99.52	105.70
7	2	45	DC	O4'-C4'-C3'	-6.34	101.96	104.50
6	1	45	DT	O4'-C4'-C3'	-6.28	101.99	104.50
3	D	270	ARG	NE-CZ-NH1	6.22	123.41	120.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	191	ARG	Peptide
1	B	49	SER	Peptide
1	B	76	GLU	Peptide
2	C	234	ASP	Peptide
2	C	57	PHE	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	1786	1813	1813	35	0
1	B	1767	1789	1789	40	0
2	C	10570	10582	10582	289	0
3	D	10396	10615	10614	266	0
4	E	627	634	634	25	0
5	F	1935	1936	1936	50	0
6	1	1101	611	611	16	0
7	2	1117	607	607	20	0
8	3	73	34	34	0	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	29375	28621	28620	685	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 12.

The worst 5 of 685 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)
3:D:425:ARG:NH1	3:D:426:ALA:O	2.05	0.90
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.45	0.90
5:F:189:LEU:O	5:F:194:LYS:NZ	2.08	0.87
3:D:886:VAL:O	3:D:1258:ARG:NH1	2.08	0.86
5:F:231:ARG:O	5:F:234:THR:OG1	1.95	0.85

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	228/329 (69%)	209 (92%)	19 (8%)	0	100	100
1	B	226/329 (69%)	211 (93%)	15 (7%)	0	100	100
2	C	1338/1342 (100%)	1197 (90%)	137 (10%)	4 (0%)	41	74
3	D	1331/1407 (95%)	1167 (88%)	161 (12%)	3 (0%)	47	78
4	E	77/91 (85%)	72 (94%)	5 (6%)	0	100	100
5	F	237/247 (96%)	199 (84%)	32 (14%)	6 (2%)	5	35
All	All	3437/3745 (92%)	3055 (89%)	369 (11%)	13 (0%)	38	70

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	659	GLN
5	F	33	VAL
2	C	399	ALA
5	F	117	GLU
5	F	125	GLY

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	198/286 (69%)	196 (99%)	2 (1%)	76	85
1	B	196/286 (68%)	192 (98%)	4 (2%)	55	74
2	C	1155/1157 (100%)	1142 (99%)	13 (1%)	73	84
3	D	1120/1168 (96%)	1106 (99%)	14 (1%)	69	81
4	E	67/75 (89%)	66 (98%)	1 (2%)	65	80
5	F	208/216 (96%)	205 (99%)	3 (1%)	67	81
All	All	2944/3188 (92%)	2907 (99%)	37 (1%)	70	81

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	834	PRO
5	F	151	GLU
3	D	836	ARG
3	D	1289	ASN
2	C	894	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	424	ASN
3	D	560	ASN
5	F	139	ASN
3	D	458	ASN
3	D	623	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	3	2/3 (66%)	1 (50%)	1 (50%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	3	3	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	3	1	ATP

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.

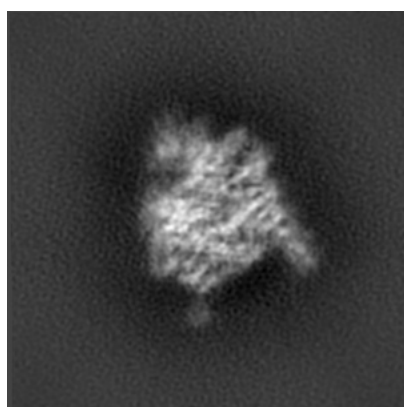
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20394. These allow visual inspection of the internal detail of the map and identification of artifacts.

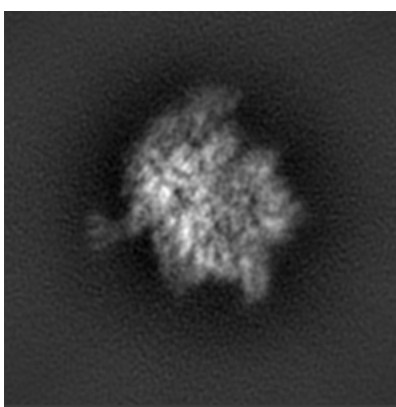
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

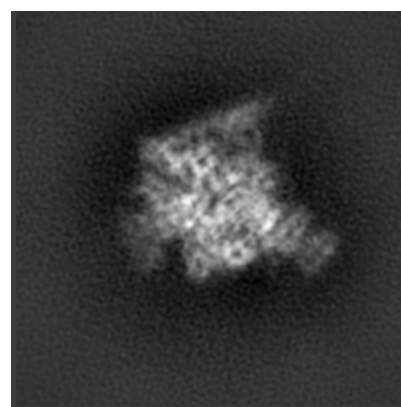
6.1.1 Primary map



X



Y

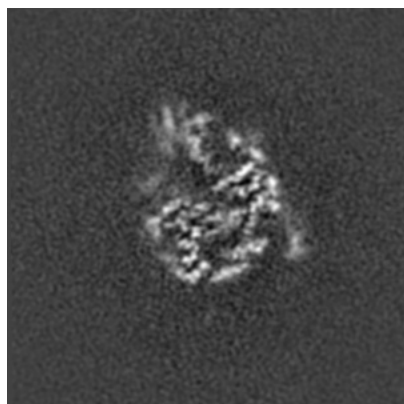


Z

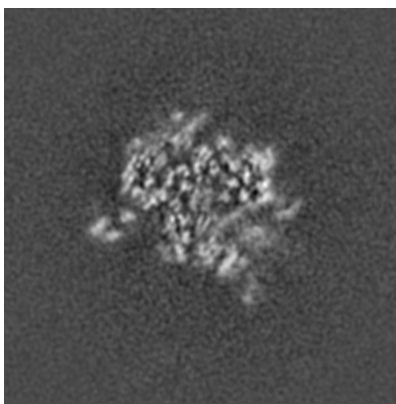
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

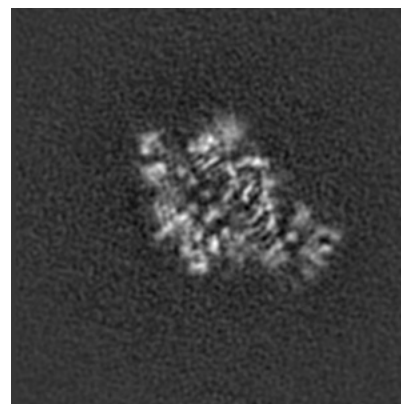
6.2.1 Primary map



X Index: 162



Y Index: 162

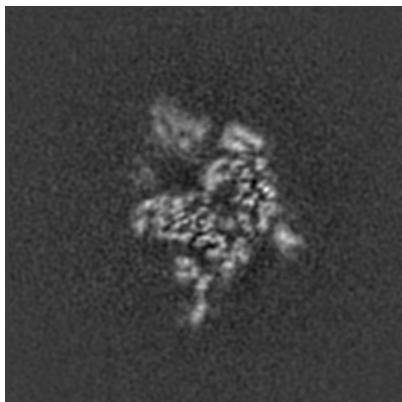


Z Index: 162

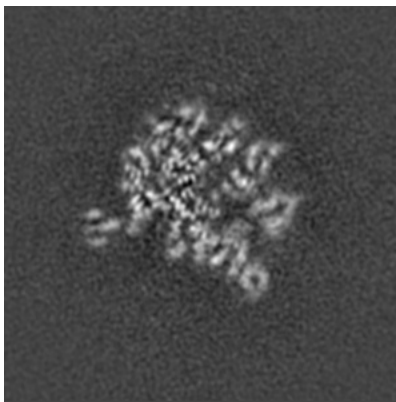
The images above show central slices of the map in three orthogonal directions.

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

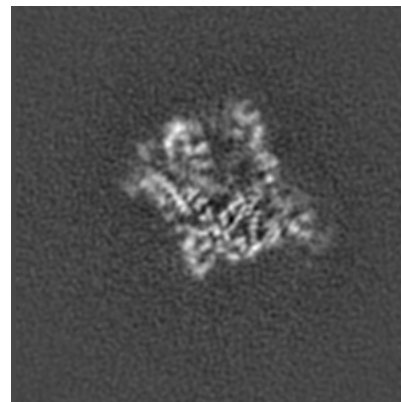
6.3.1 Primary map



X Index: 153



Y Index: 152

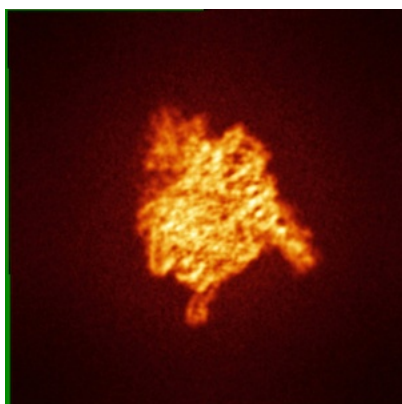


Z Index: 146

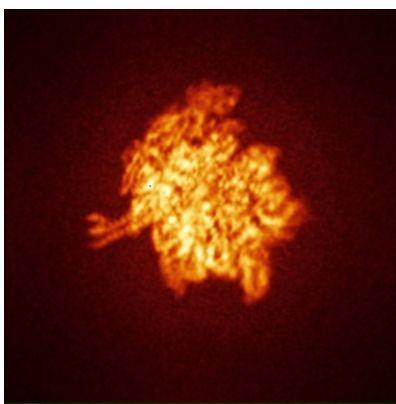
The images above show the largest variance slices of the map in three orthogonal directions.

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

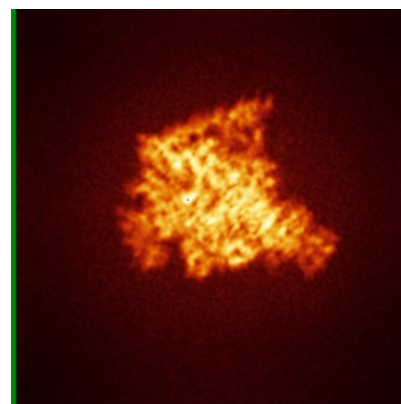
6.4.1 Primary map



X



Y

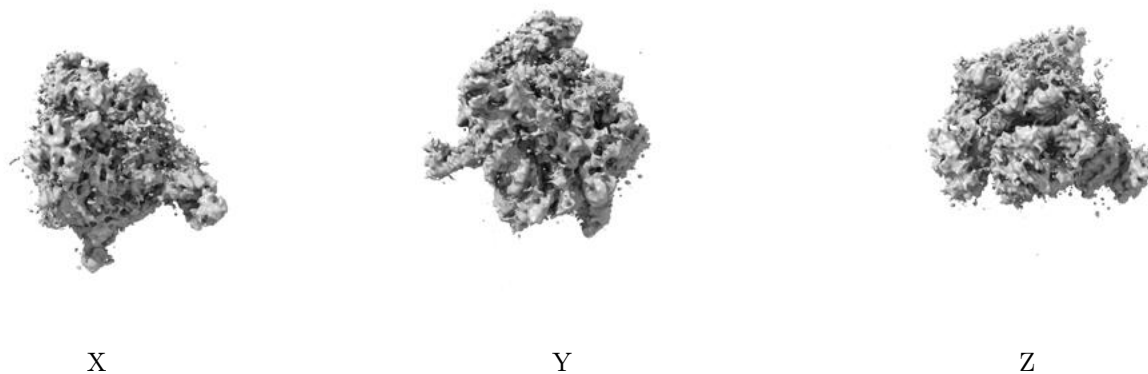


Z

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

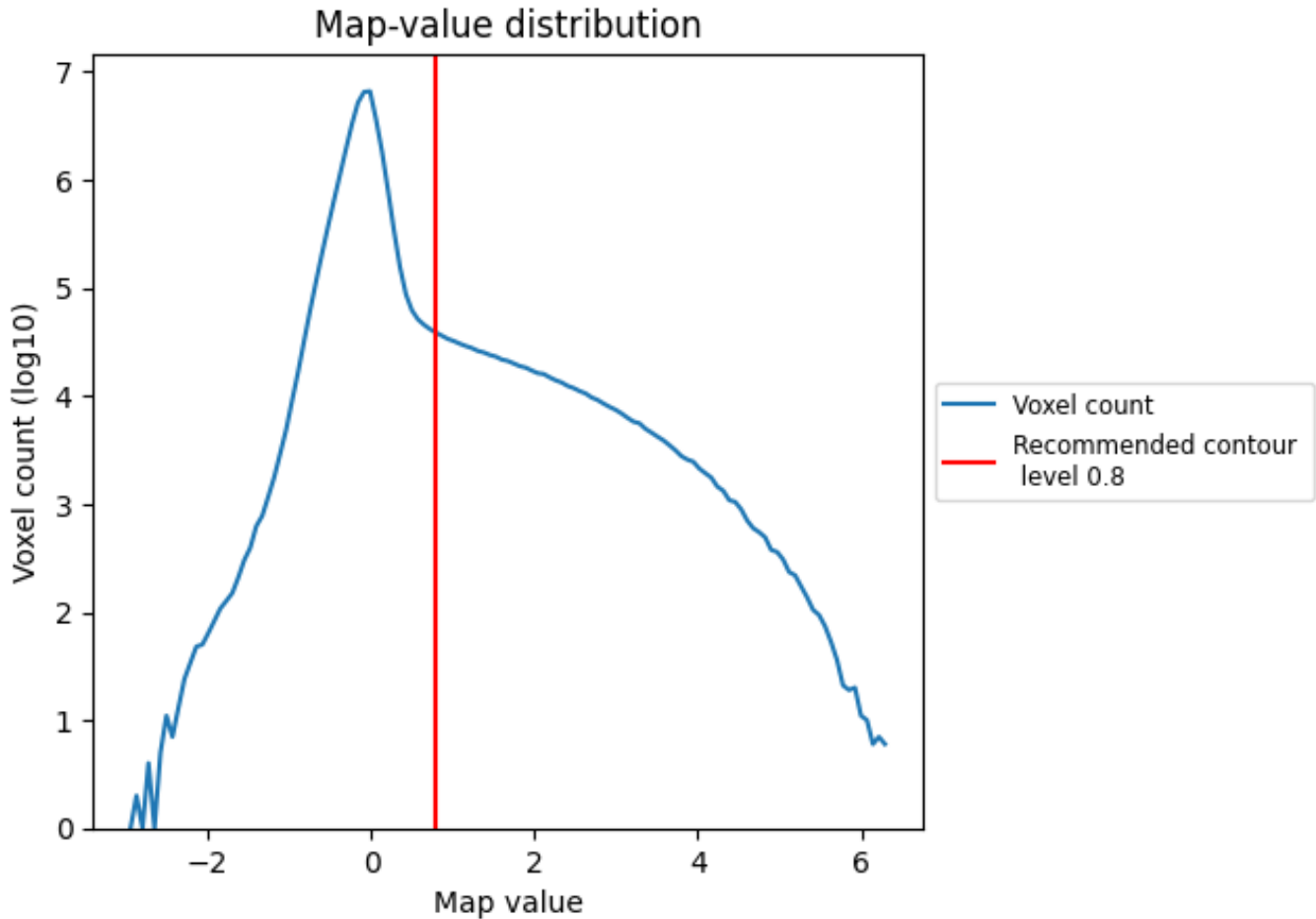
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

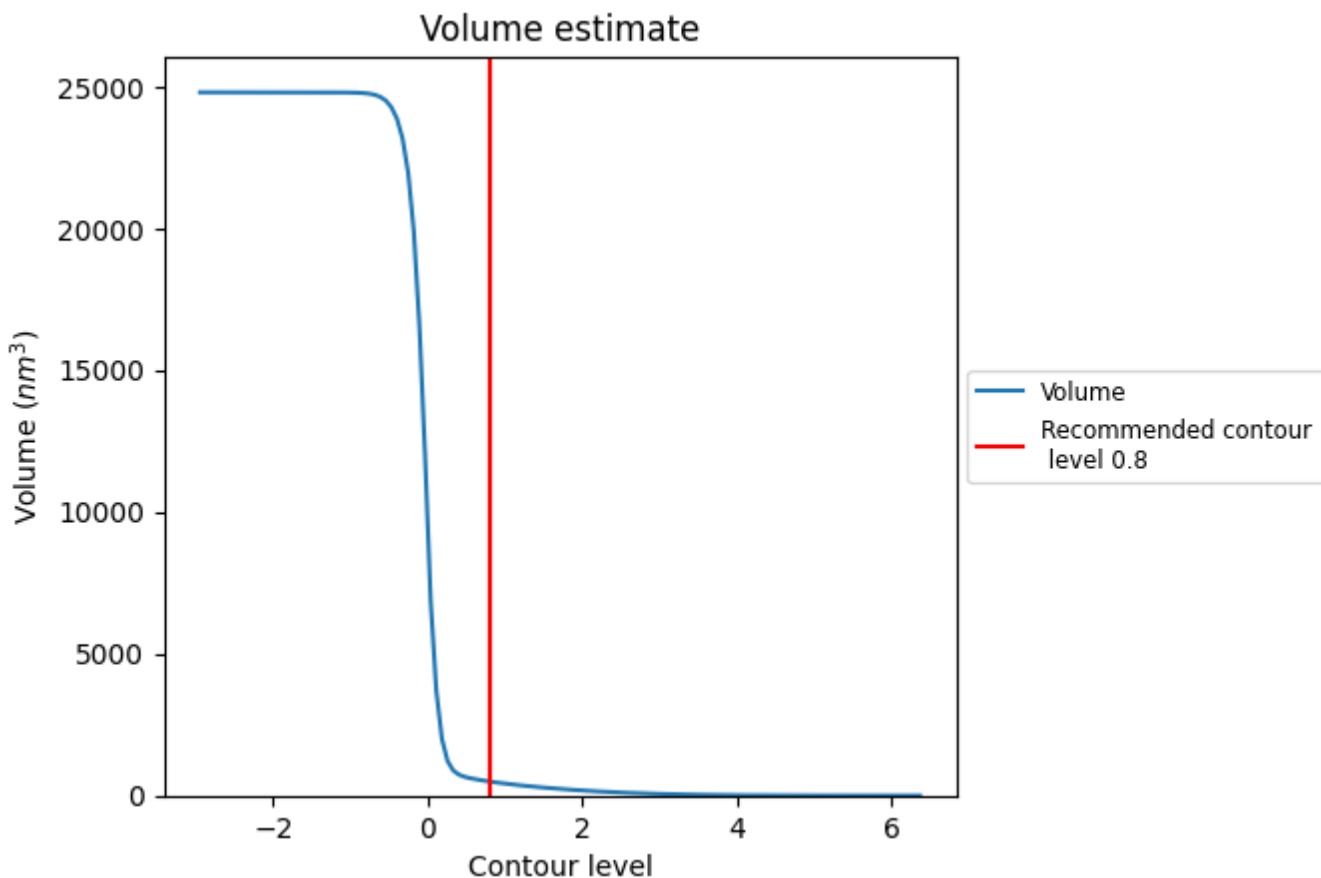
This section contains the results of statistical analysis of the map.

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.

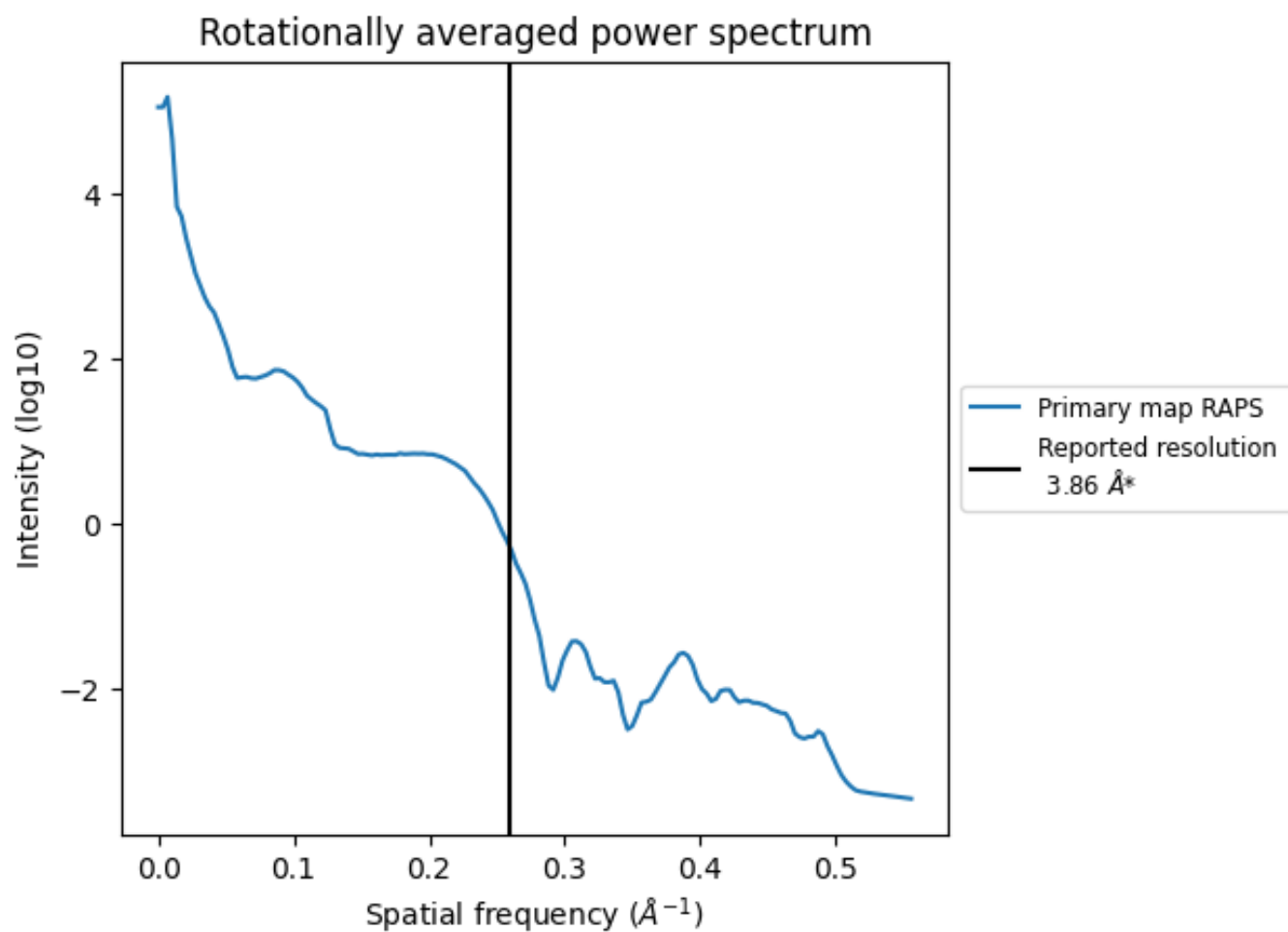
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 494 nm^3 ; this corresponds to an approximate mass of 447 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 0.259\AA^{-1}

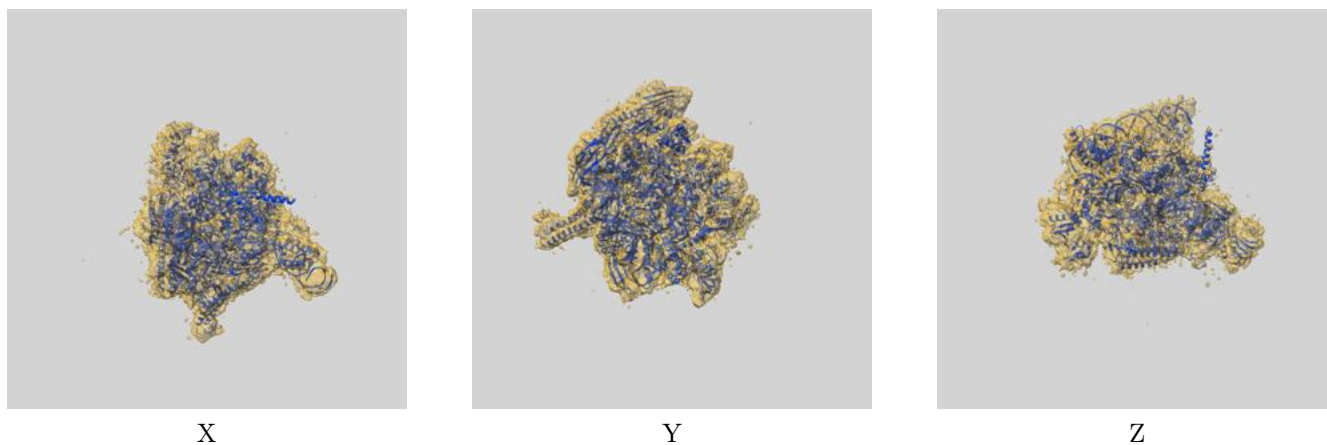
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

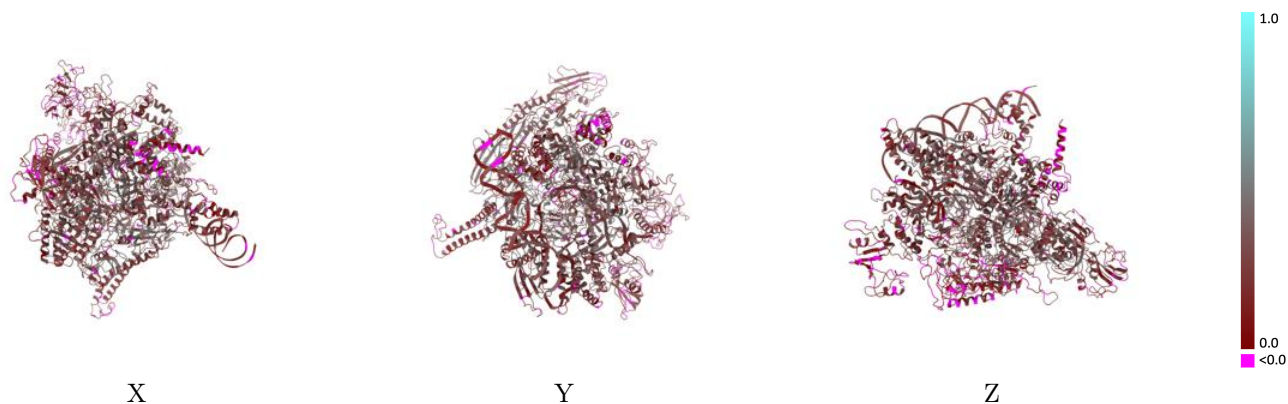
This section contains information regarding the fit between EMDB map EMD-20394 and PDB model 6PMI. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



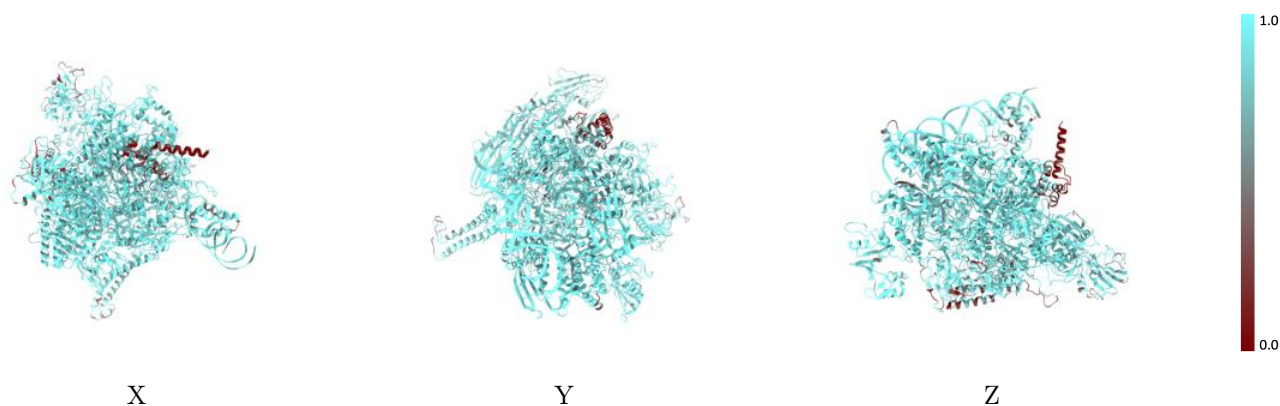
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



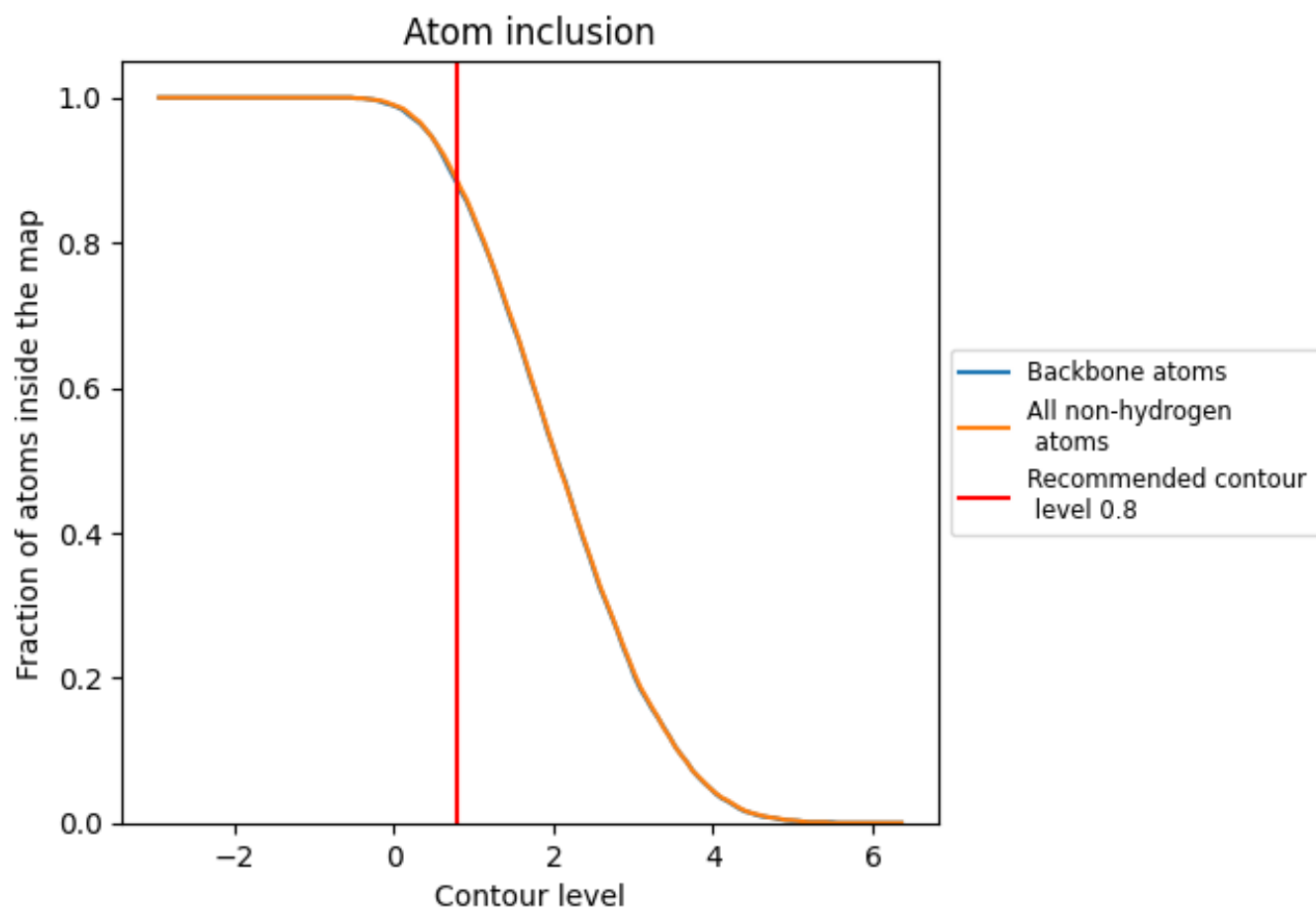
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8840	 0.2480
1	 0.8950	 0.1980
2	 0.9250	 0.2190
3	 0.8630	 0.3080
A	 0.9260	 0.2950
B	 0.8510	 0.2010
C	 0.9340	 0.2820
D	 0.8790	 0.2420
E	 0.2830	 0.0400
F	 0.8590	 0.1970

