wwPDB EM Validation Summary Report

Aug 23, 2026 – 10:34 pm BST

PDB ID	:	7OQ4 / pdb_00007oq4
EMDB ID	:	EMD-13026
Title	:	Cryo-EM structure of the ATV RNAP Inhibitory Protein (RIP) bound to the DNA-binding channel of the host's RNA polymerase
Authors	:	Pilotto, S.; Fouqueau, T.; Lukoyanova, N.; Sheppard, C.; Lucas-Staat, S.; Diaz-Santin, L.M.; Matelska, D.; Prangishvili, D.; Cheung, A.C.M.; Werner, F.
Deposited on	:	2021-06-02
Resolution	:	3.27 Å(reported)
Based on initial models	:	3FAJ, 7OH0

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 (i) 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 (1)) were used in the production of this report:

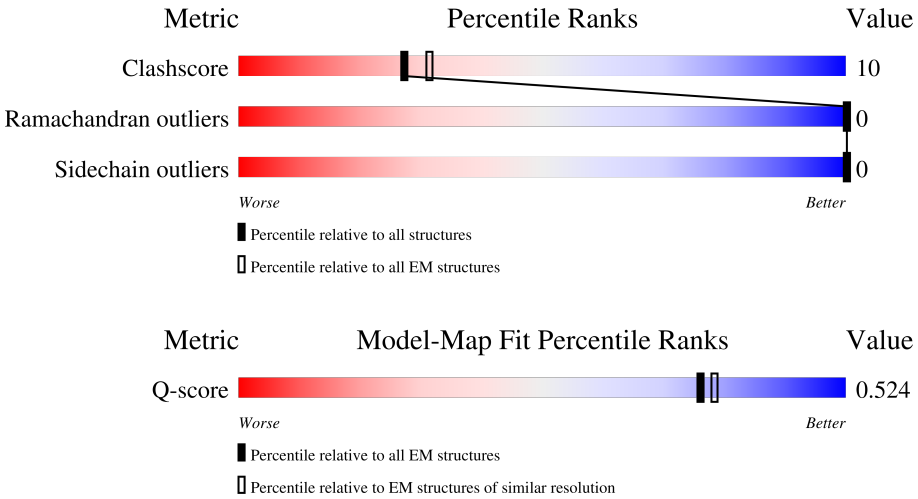
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.27 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14508 (2.77 - 3.77)

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 <=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	880	76% 24%
2	B	1126	75% 23%
3	C	393	8% 76% 24%

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Mol	Chain	Length	Quality of chain
4	D	264	75% 21%
5	E	183	7% 28% 11% 61%
6	F	114	11% 23% 76%
7	G	130	64% 29% 7%
8	H	84	73% 18% 10%
9	K	89	73% 22%
10	L	90	82% 18%
11	N	66	64% 36%
12	P	48	10% 71% 27%
13	Q	105	9% 34% 7% 59%
14	Z	149	28% 64% 15% 21%

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
17	F3S	D	301	-	-	X	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 26689 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 subunit A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	880	7006	4457	1232	1288	29	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1101	8669	5494	1518	1624	33	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ILE	VAL	variant	UNP P11513

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	393	3095	1948	535	598	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	254	2014	1290	334	379	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	72	560	363	92	104	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	27	Total	C	N	O	0	0
			186	120	30	36		

- Molecule 7 is a protein called DNA-directed RNA polymerase, subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	121	Total	C	N	O	S	0	0
			982	632	154	187	9		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	125	HIS	-	expression tag	UNP Q4JAY4
G	126	HIS	-	expression tag	UNP Q4JAY4
G	127	HIS	-	expression tag	UNP Q4JAY4
G	128	HIS	-	expression tag	UNP Q4JAY4
G	129	HIS	-	expression tag	UNP Q4JAY4
G	130	HIS	-	expression tag	UNP Q4JAY4

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	76	Total	C	N	O	0	0
			603	390	101	112		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	85	Total	C	N	O	S	0	0
			680	435	119	125	1		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	90	Total	C	N	O	S	0	0
			707	459	112	134	2		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	66	Total	C	N	O	S	0	0
			534	339	97	91	7		

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit P.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	47	Total	C	N	O	S	0	0
			376	241	67	63	5		

- Molecule 13 is a protein called Conserved protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	43	Total	C	N	O	S	0	0
			353	222	56	73	2		

- Molecule 14 is a protein called RNAP inhibitory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	118	Total	C	N	O	S	0	0
			910	587	151	170	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	146	LEU	-	expression tag	UNP Q3V4R7
Z	147	VAL	-	expression tag	UNP Q3V4R7
Z	148	PRO	-	expression tag	UNP Q3V4R7
Z	149	ARG	-	expression tag	UNP Q3V4R7

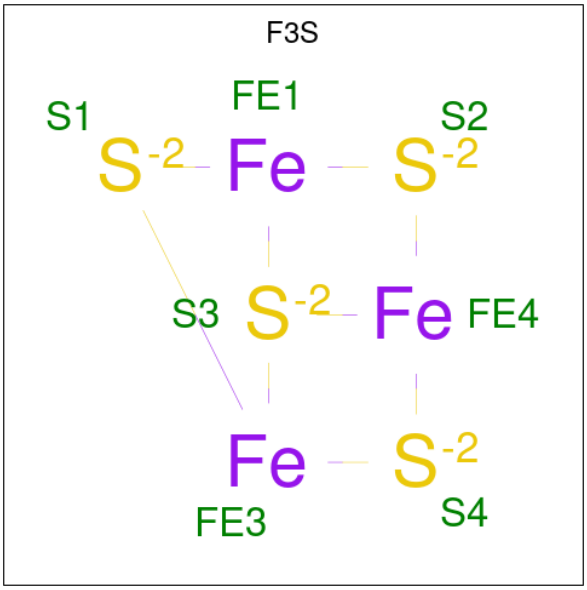
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	Mg	0
			1	1	

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	A	3	Total	Zn	0
			3	3	
16	B	1	Total	Zn	0
			1	1	
16	N	1	Total	Zn	0
			1	1	
16	P	1	Total	Zn	0
			1	1	

- Molecule 17 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).

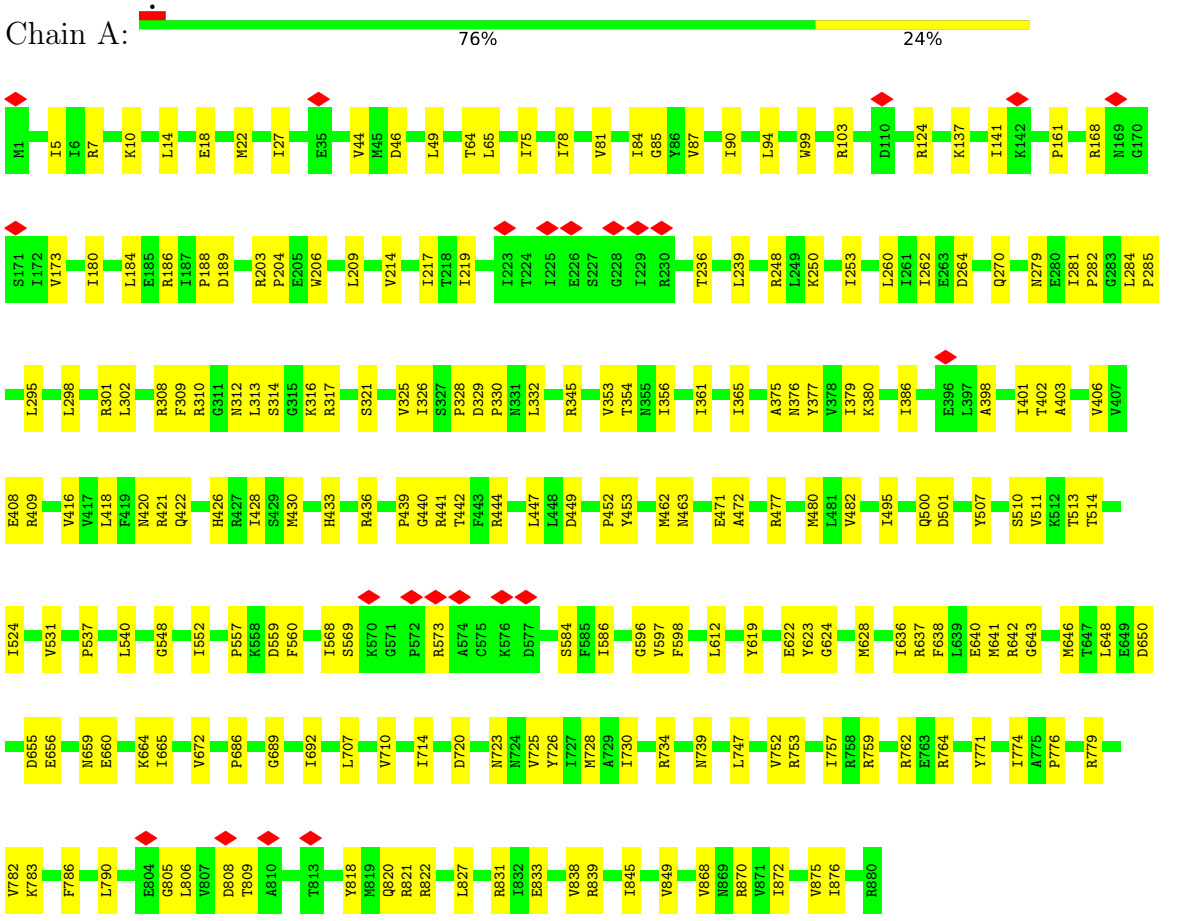


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
17	D	1	7	3	4	0

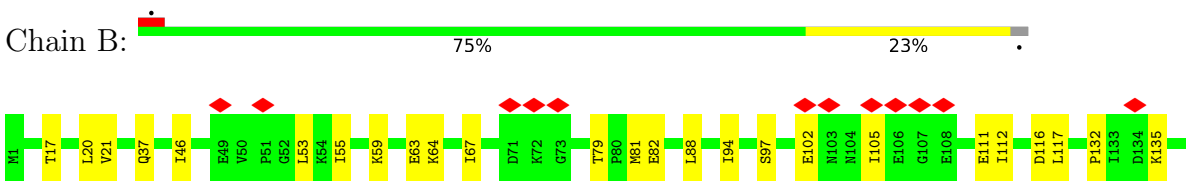
3 Residue-property plots (i)

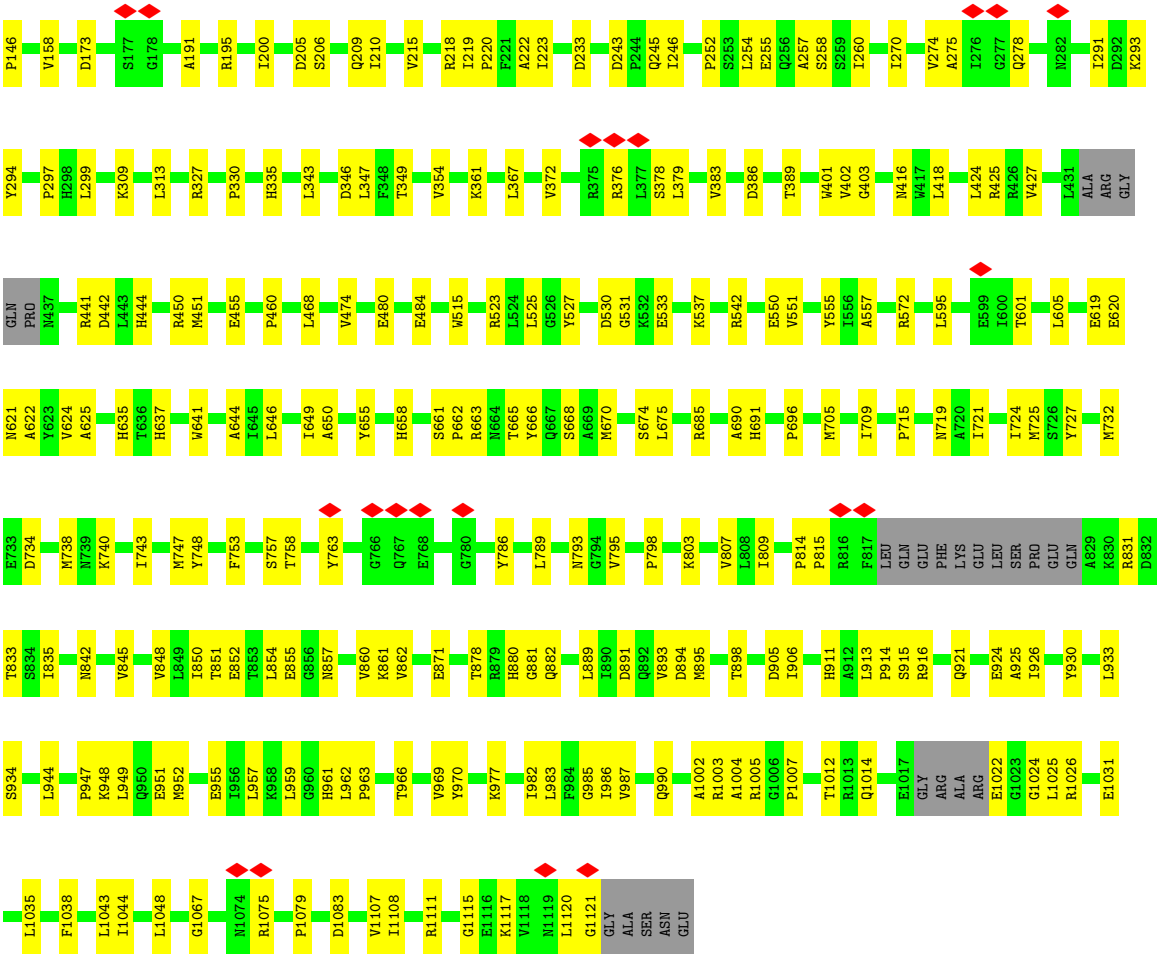
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

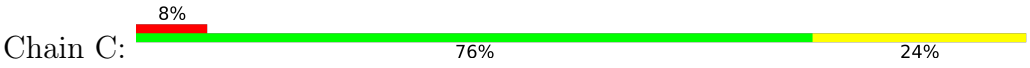


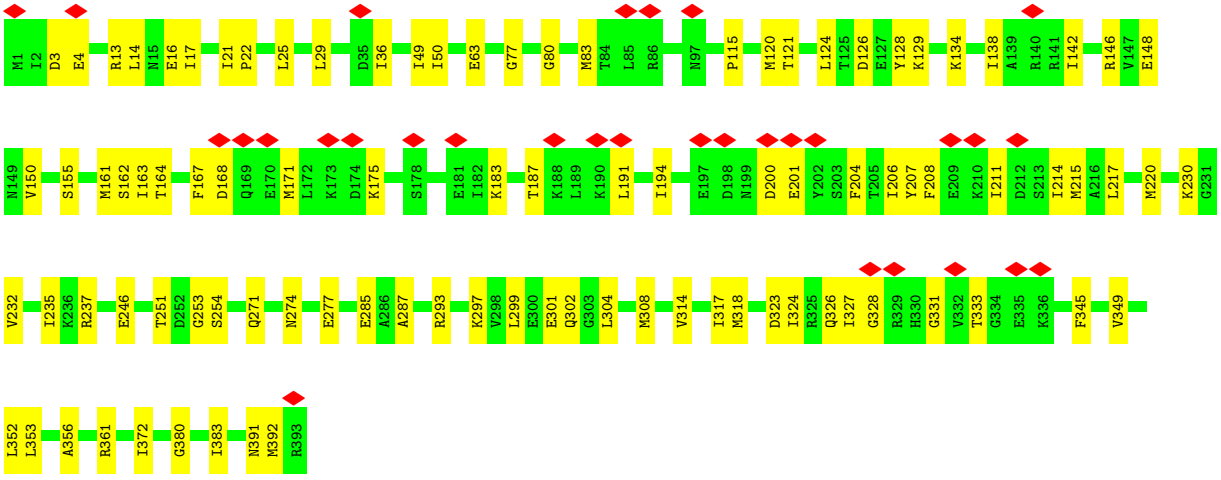
• Molecule 2: DNA-directed RNA polymerase subunit B



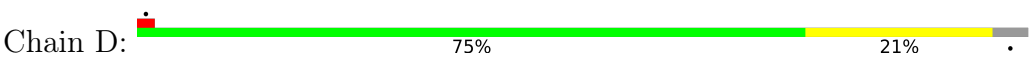


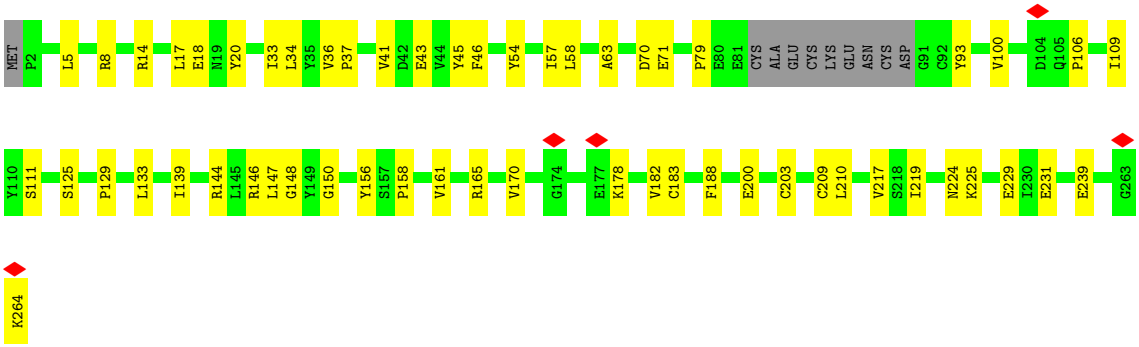
• Molecule 3: DNA-directed RNA polymerase subunit A"



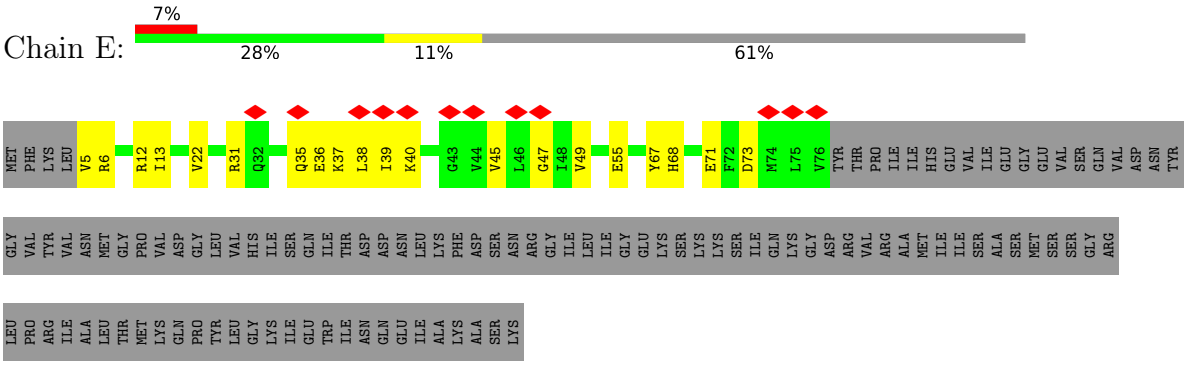


• Molecule 4: DNA-directed RNA polymerase subunit D

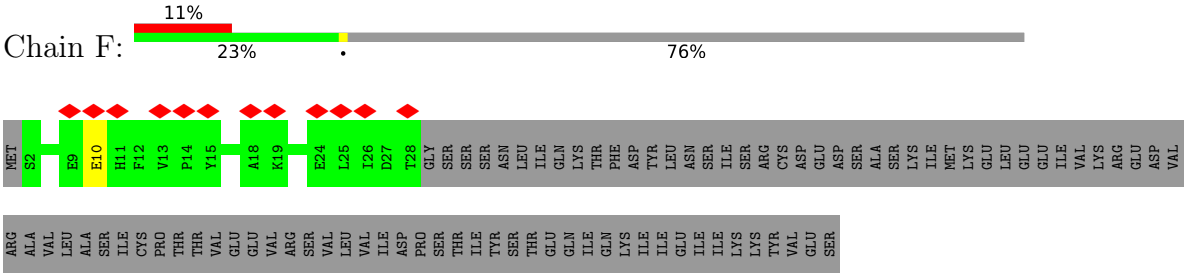




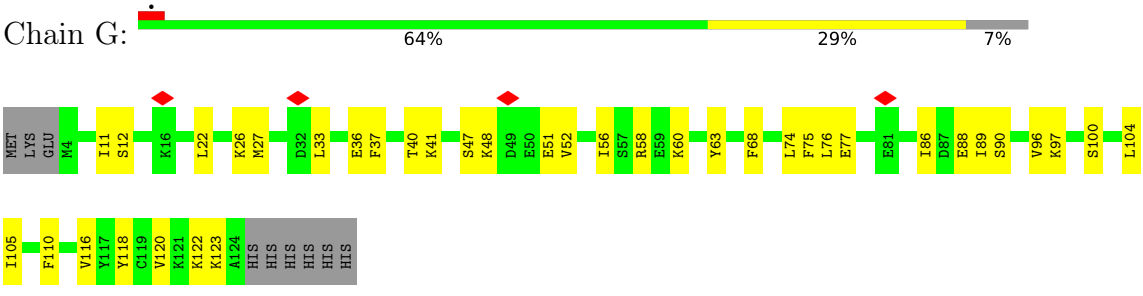
• Molecule 5: DNA-directed RNA polymerase subunit E



• Molecule 6: DNA-directed RNA polymerase, subunit F

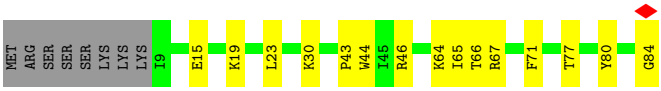


• Molecule 7: DNA-directed RNA polymerase, subunit G



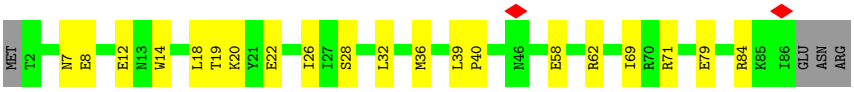
• Molecule 8: DNA-directed RNA polymerase subunit H



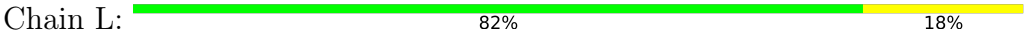


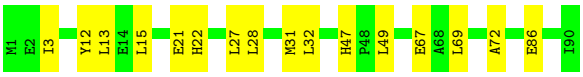
• Molecule 9: DNA-directed RNA polymerase subunit K





• Molecule 10: DNA-directed RNA polymerase subunit L





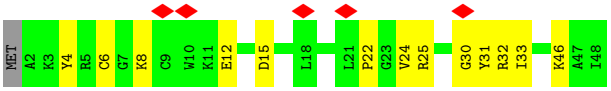
• Molecule 11: DNA-directed RNA polymerase subunit N





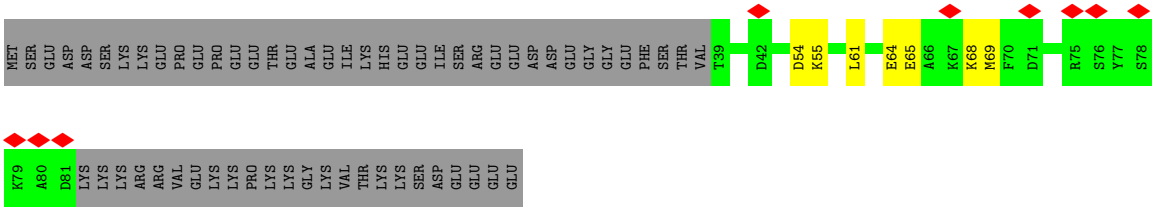
• Molecule 12: DNA-directed RNA polymerase subunit P





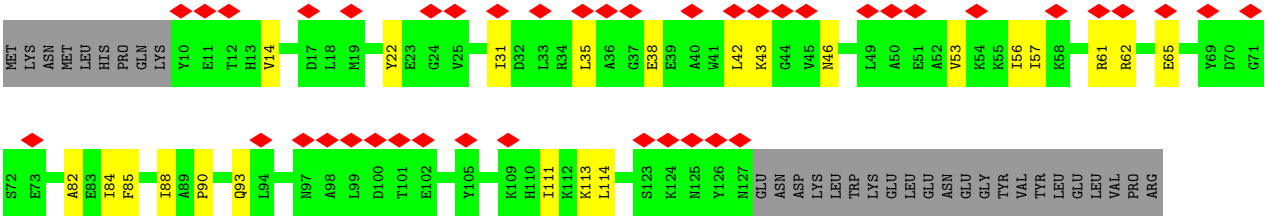
• Molecule 13: Conserved protein





• Molecule 14: RNAP inhibitory protein




MET LYS ASN MET LEU HIS PRO GLN LYS Y10 E11 T12 H13 V14 D17 L18 M19 Y22 E23 G24 V25 I31 D32 L33 R34 L35 A36 G37 E38 E39 A40 W41 L42 K43 G44 V45 N46 L49 A50 E51 A52 V53 K54 K55 I56 I57 K58 R61 R62 E65 Y69 D70 G71
S72 E73 A82 E83 I84 F85 I88 A89 P90 Q93 L94 N97 A98 L99 D100 T101 E102 Y105 K109 H110 I111 K112 K113 L114 S123 K124 N125 Y126 N127 GLU ASN ASP LYS LEU TRP LYS GLU LEU GLU ASN GLU GLY TYR VAL TYR LEU GLU LEU VAL PRO ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	151237	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 ($e^-/Å^2$)	45.5	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.195	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	314.1, 314.1, 314.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	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, MG, F3S

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	0.13	0/7156	0.30	0/9681
2	B	0.14	0/8826	0.30	0/11938
3	C	0.22	0/3124	0.36	0/4201
4	D	0.13	0/2047	0.29	0/2764
5	E	0.16	0/569	0.45	0/766
6	F	0.11	0/190	0.23	0/260
7	G	0.14	0/997	0.36	0/1330
8	H	0.12	0/616	0.36	0/833
9	K	0.12	0/687	0.29	0/925
10	L	0.14	0/716	0.33	0/964
11	N	0.14	0/545	0.32	0/735
12	P	0.12	0/382	0.32	0/510
13	Q	0.10	0/356	0.34	0/476
14	Z	0.14	0/927	0.32	0/1255
All	All	0.15	0/27138	0.32	0/36638

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

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	7006	0	7071	177	0
2	B	8669	0	8780	184	0
3	C	3095	0	3212	82	0
4	D	2014	0	2079	41	0
5	E	560	0	559	14	0
6	F	186	0	148	1	0
7	G	982	0	997	24	0
8	H	603	0	629	12	0
9	K	680	0	728	16	0
10	L	707	0	751	14	0
11	N	534	0	545	17	0
12	P	376	0	399	14	0
13	Q	353	0	353	7	0
14	Z	910	0	904	20	0
15	A	1	0	0	0	0
16	A	3	0	0	0	0
16	B	1	0	0	0	0
16	N	1	0	0	0	0
16	P	1	0	0	0	0
17	D	7	0	0	2	0
All	All	26689	0	27155	529	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 10.

The worst 5 of 529 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:A:872:ILE:HD12	3:C:36:ILE:HD11	1.25	1.11
3:C:83:MET:HG2	3:C:302:GLN:HG3	1.52	0.91
3:C:318:MET:HG2	3:C:327:ILE:HD11	1.63	0.81
3:C:161:MET:HG2	3:C:211:ILE:HG21	1.63	0.80
2:B:809:ILE:HB	2:B:835:ILE:HD13	1.66	0.77

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	878/880 (100%)	855 (97%)	23 (3%)	0	100	100
2	B	1093/1126 (97%)	1065 (97%)	28 (3%)	0	100	100
3	C	391/393 (100%)	379 (97%)	12 (3%)	0	100	100
4	D	250/264 (95%)	241 (96%)	9 (4%)	0	100	100
5	E	70/183 (38%)	64 (91%)	6 (9%)	0	100	100
6	F	25/114 (22%)	25 (100%)	0	0	100	100
7	G	119/130 (92%)	111 (93%)	8 (7%)	0	100	100
8	H	74/84 (88%)	72 (97%)	2 (3%)	0	100	100
9	K	83/89 (93%)	82 (99%)	1 (1%)	0	100	100
10	L	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
11	N	64/66 (97%)	62 (97%)	2 (3%)	0	100	100
12	P	45/48 (94%)	41 (91%)	4 (9%)	0	100	100
13	Q	41/105 (39%)	41 (100%)	0	0	100	100
14	Z	116/149 (78%)	112 (97%)	4 (3%)	0	100	100
All	All	3337/3721 (90%)	3237 (97%)	100 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	763/768 (99%)	763 (100%)	0	100	100
2	B	944/972 (97%)	944 (100%)	0	100	100
3	C	343/348 (99%)	343 (100%)	0	100	100
4	D	230/239 (96%)	230 (100%)	0	100	100
5	E	57/157 (36%)	57 (100%)	0	100	100
6	F	15/109 (14%)	15 (100%)	0	100	100
7	G	112/121 (93%)	112 (100%)	0	100	100
8	H	67/75 (89%)	67 (100%)	0	100	100
9	K	76/81 (94%)	76 (100%)	0	100	100
10	L	78/78 (100%)	78 (100%)	0	100	100
11	N	60/60 (100%)	60 (100%)	0	100	100
12	P	41/43 (95%)	41 (100%)	0	100	100
13	Q	40/98 (41%)	40 (100%)	0	100	100
14	Z	93/132 (70%)	93 (100%)	0	100	100
All	All	2919/3281 (89%)	2919 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	75	HIS
8	H	20	HIS
14	Z	117	ASN
10	L	26	ASN
1	A	798	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 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	F3S	D	301	4	0,9,9	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	F3S	D	301	4	-	-	0/3/3/3

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	301	F3S	2	0

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.

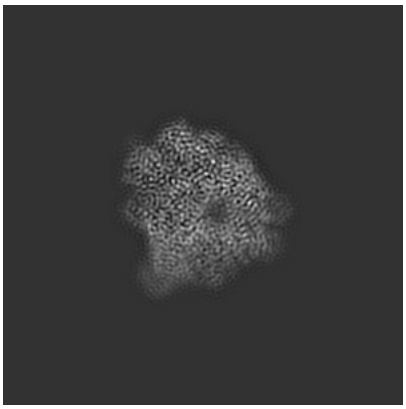
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13026. These allow visual inspection of the internal detail of the map and identification of artifacts.

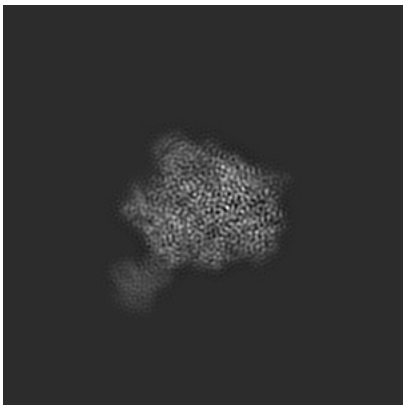
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

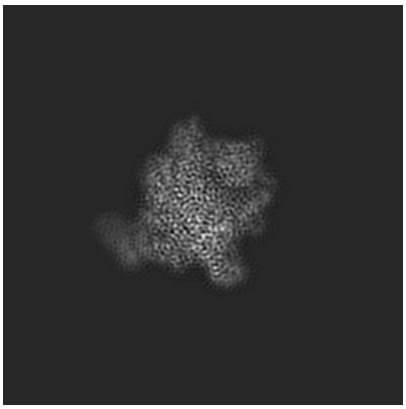
6.1.1 Primary map



X

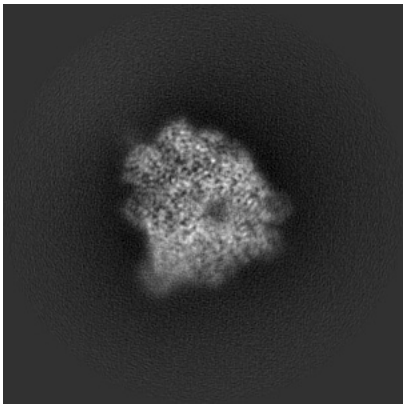


Y

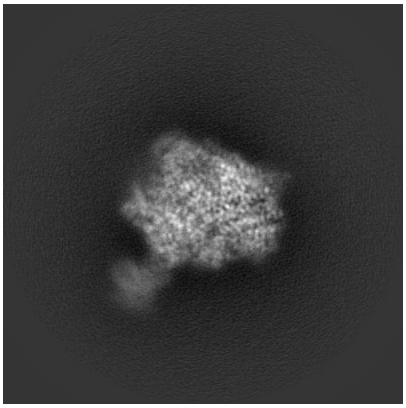


Z

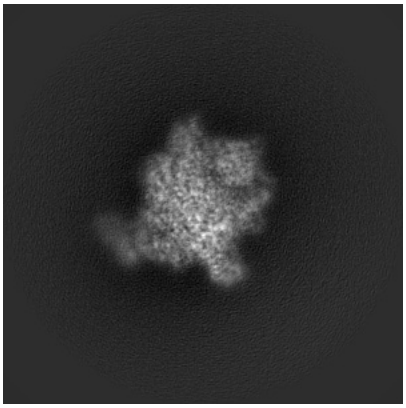
6.1.2 Raw map



X



Y

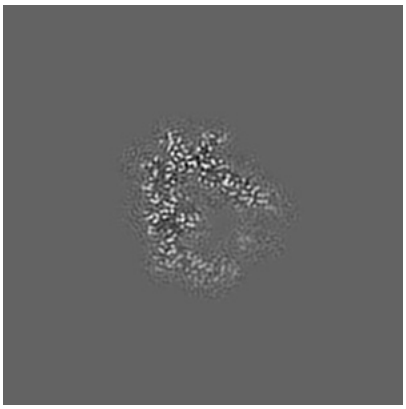


Z

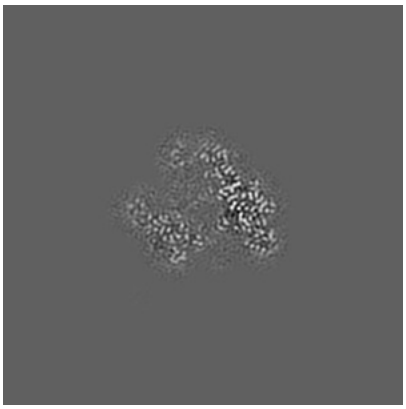
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

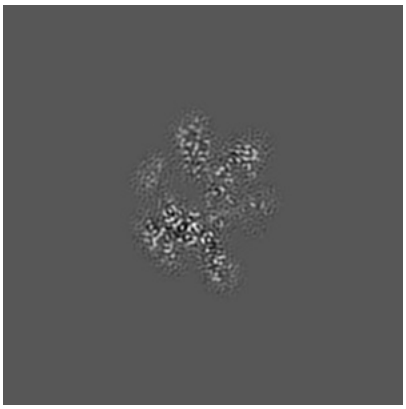
6.2.1 Primary map



X Index: 150

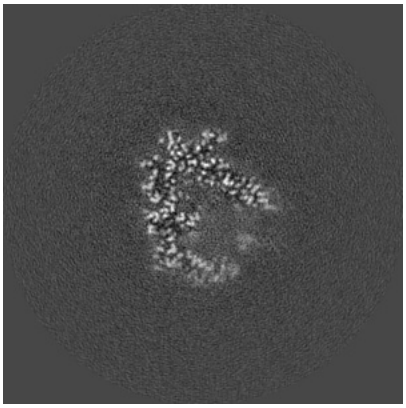


Y Index: 150

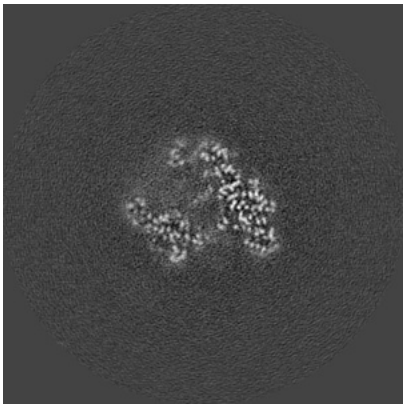


Z Index: 150

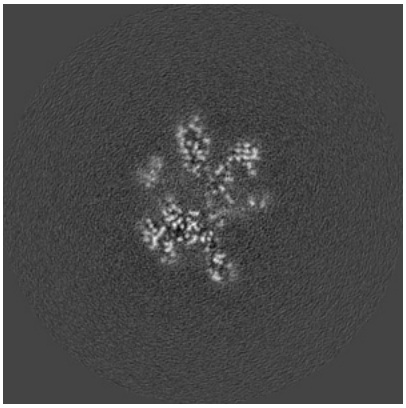
6.2.2 Raw map



X Index: 150



Y Index: 150

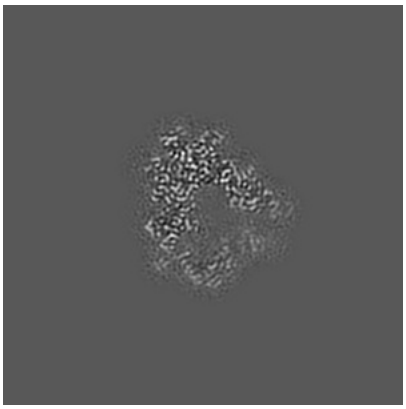


Z Index: 150

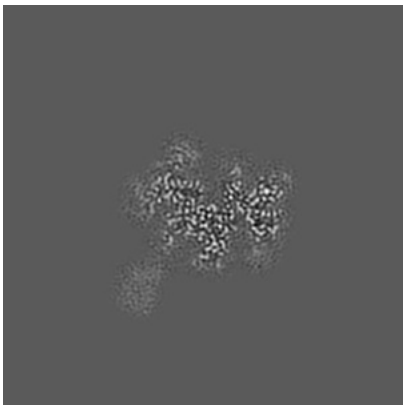
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

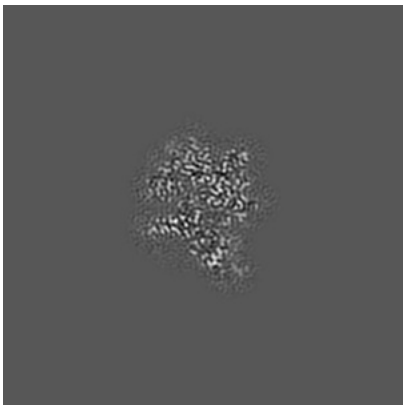
6.3.1 Primary map



X Index: 146

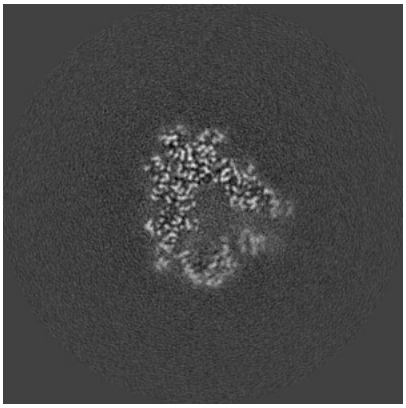


Y Index: 133

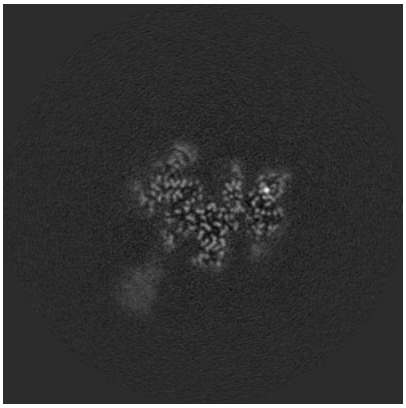


Z Index: 164

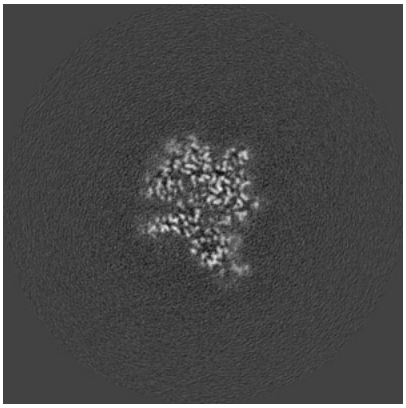
6.3.2 Raw map



X Index: 146



Y Index: 132

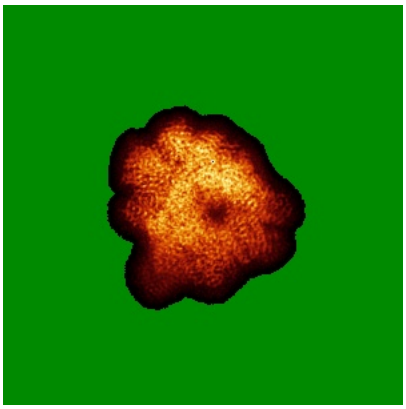


Z Index: 164

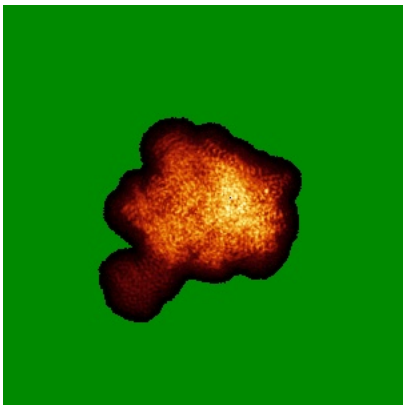
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

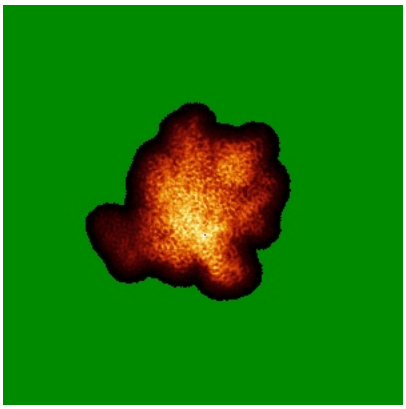
6.4.1 Primary map



X

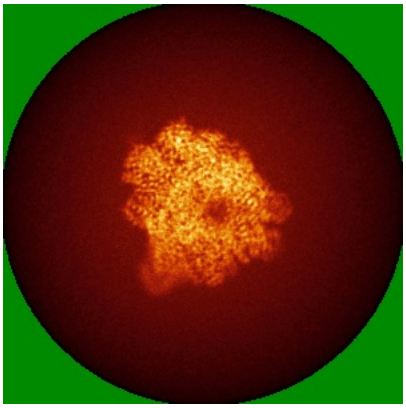


Y

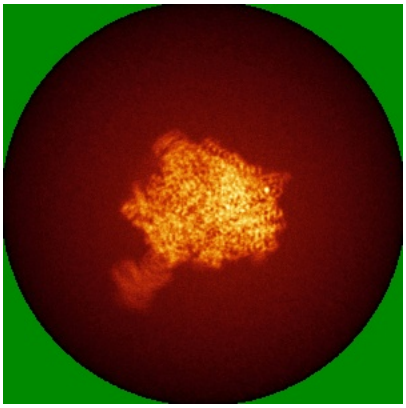


Z

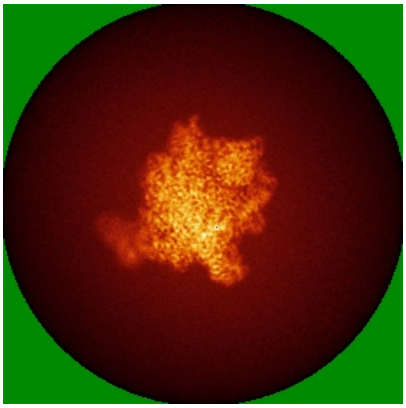
6.4.2 Raw map



X



Y

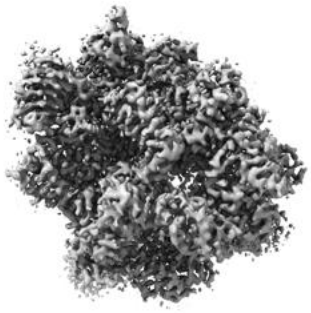


Z

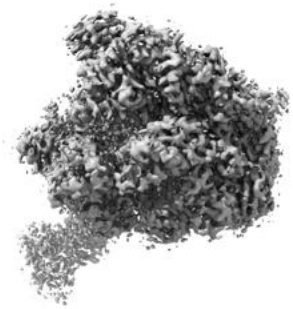
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X



Y



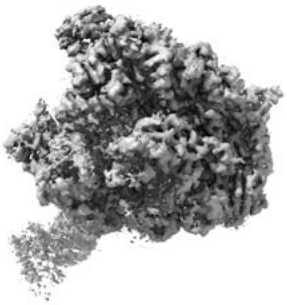
Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

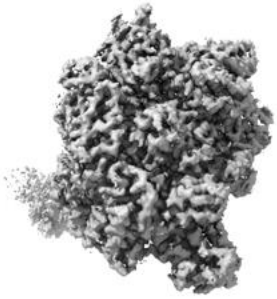
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

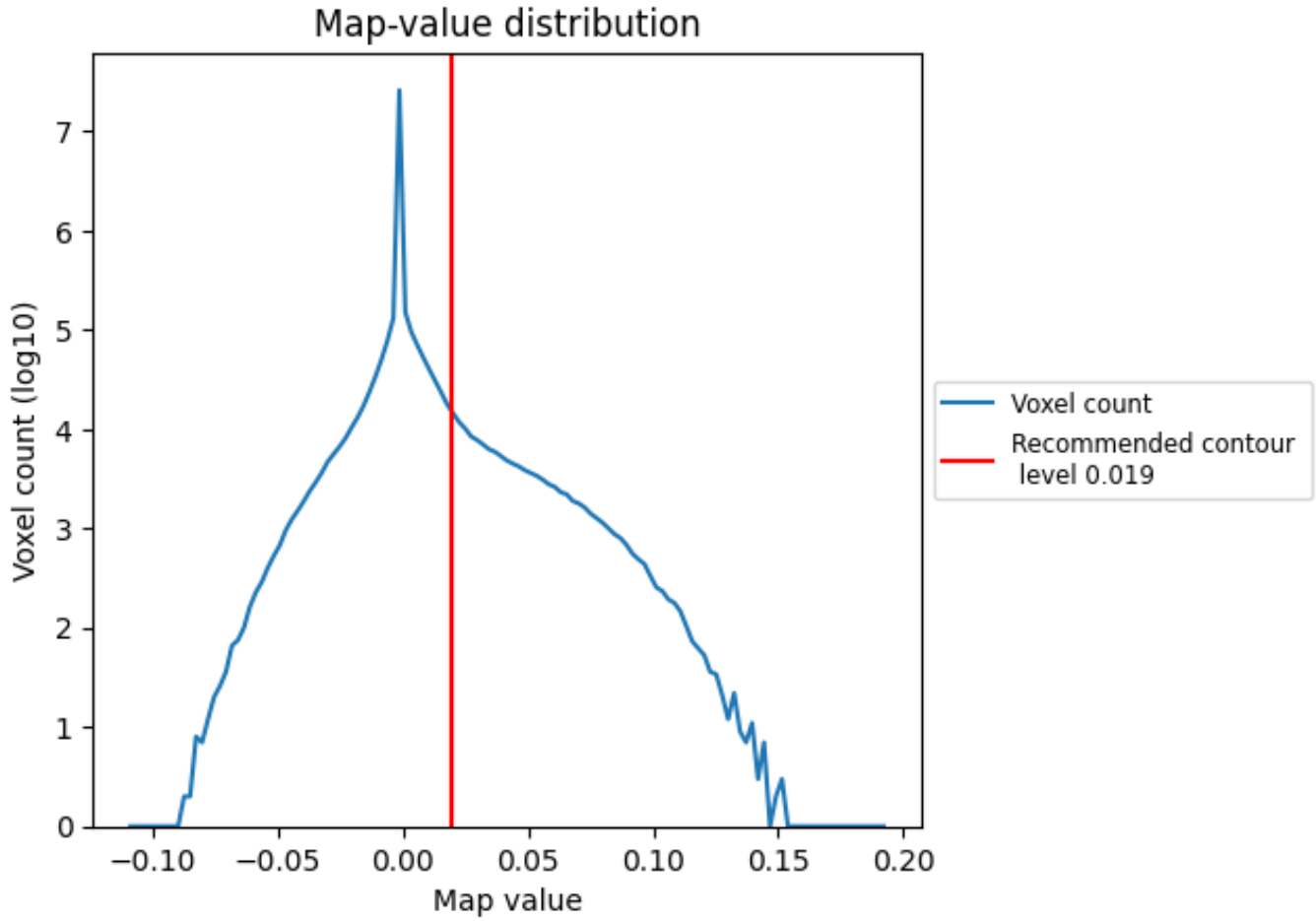
6.6 Mask visualisation (i)

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

7 Map analysis

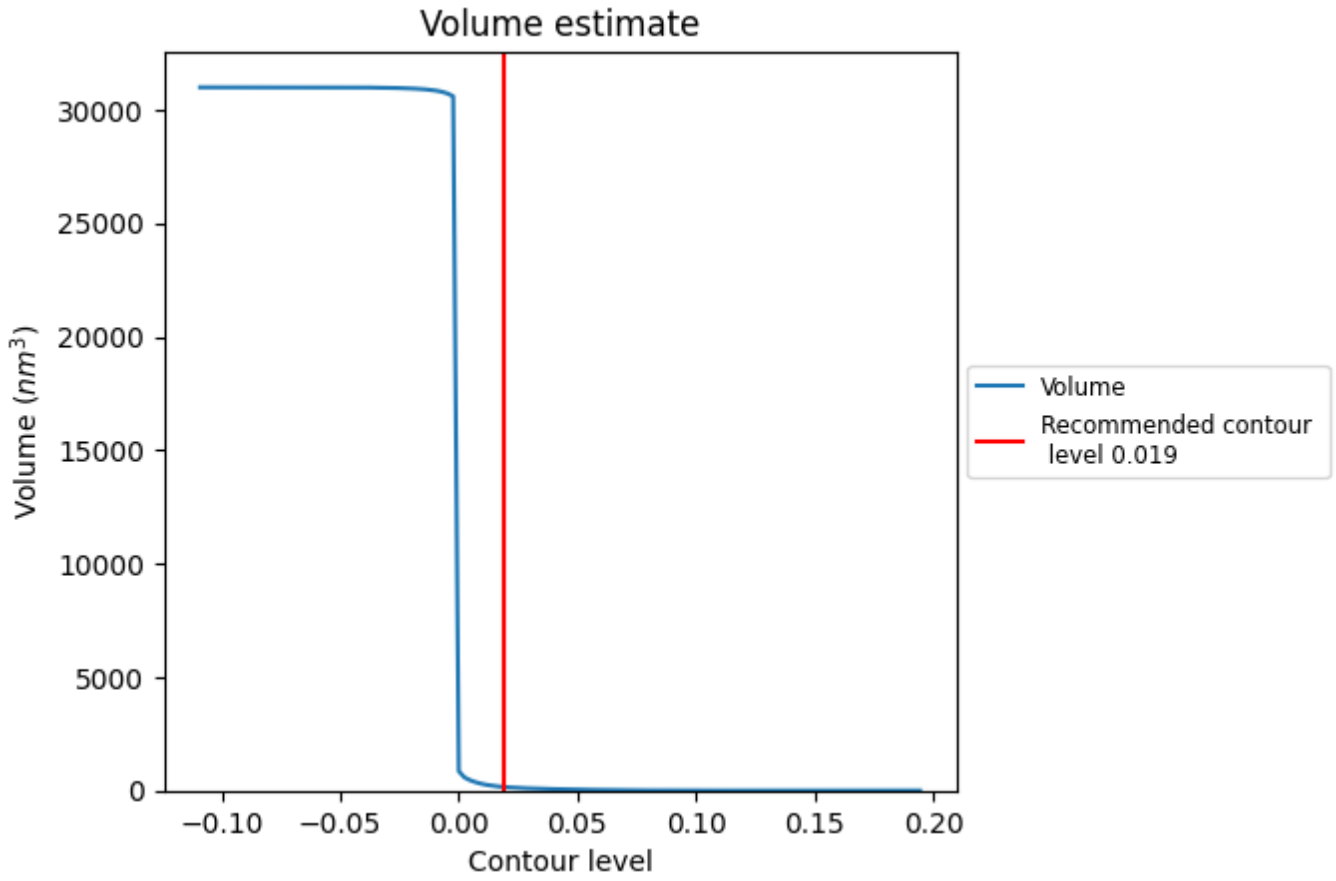
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

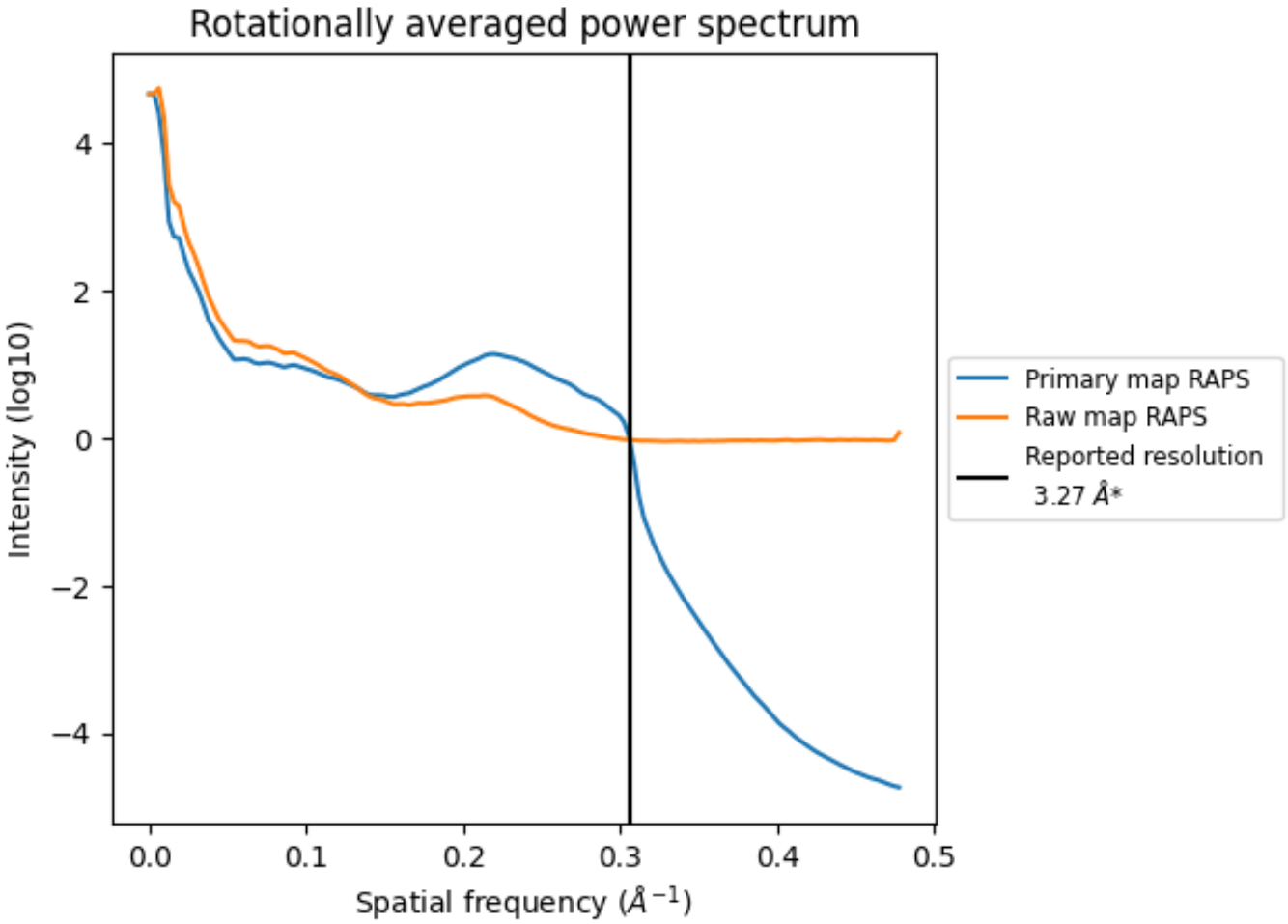
7.2 Volume estimate (i)



The volume at the recommended contour level is 158 nm^3; this corresponds to an approximate mass of 142 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)

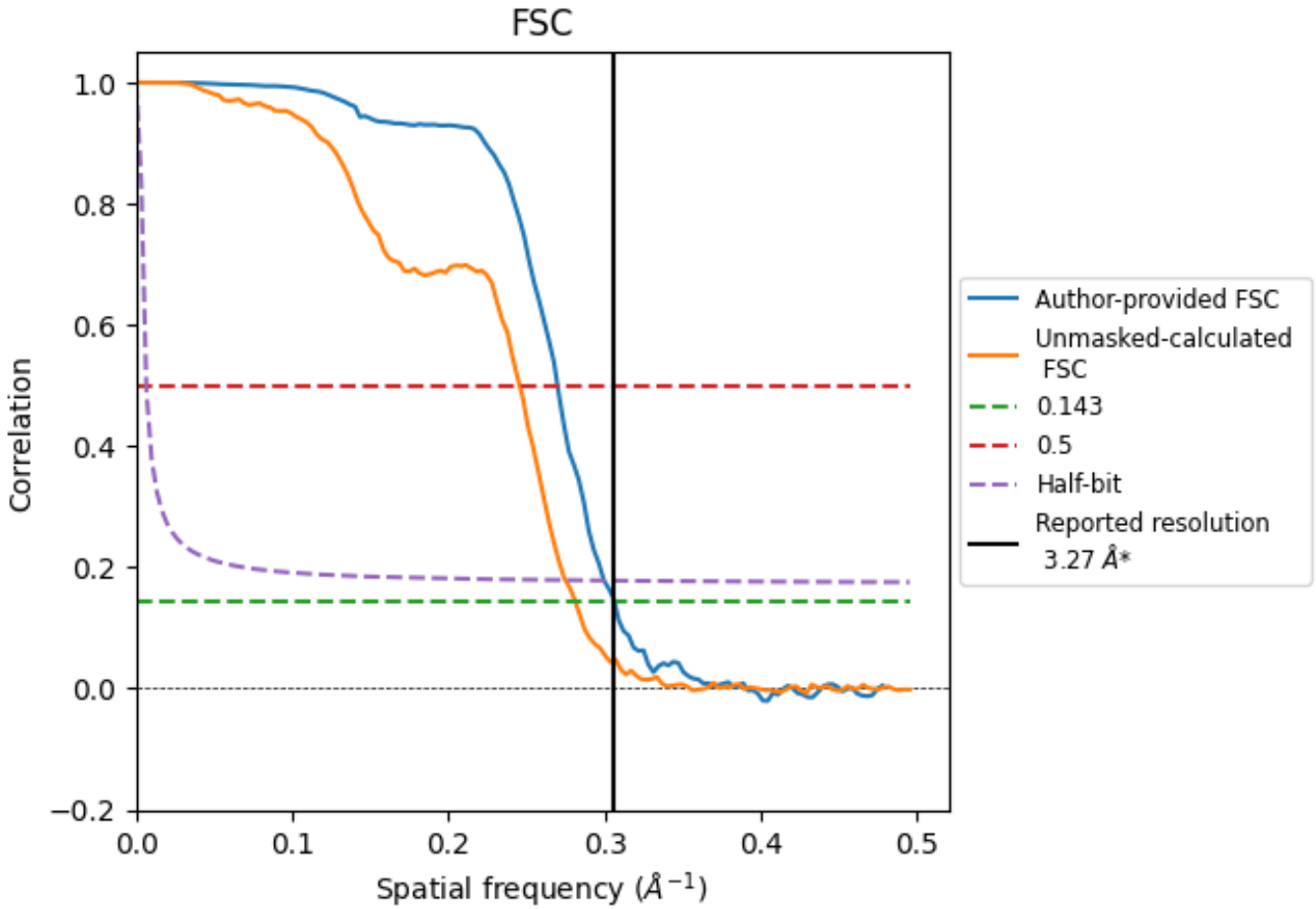


*Reported resolution corresponds to spatial frequency of 0.306 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.306 Å^{-1}

8.2 Resolution estimates (i)

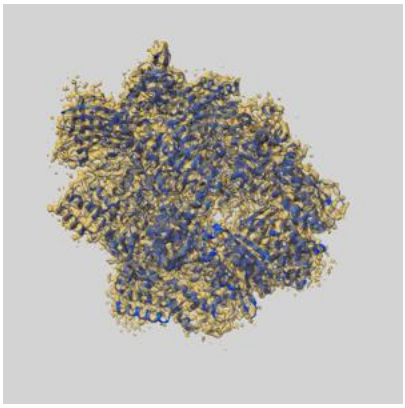
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	3.27	3.71	3.34
Unmasked-calculated*	3.56	4.07	3.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

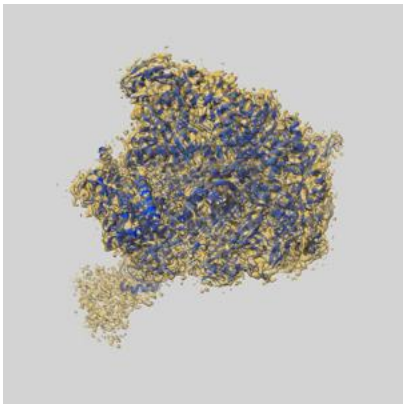
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13026 and PDB model 7OQ4. Per-residue inclusion information can be found in section 3 on page 8.

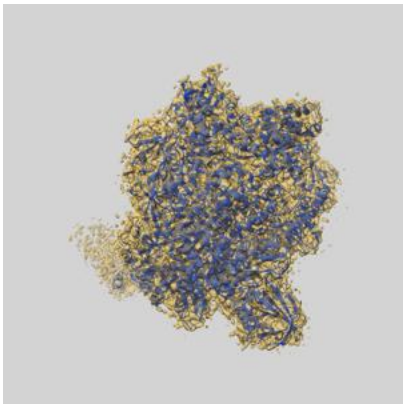
9.1 Map-model overlay



X



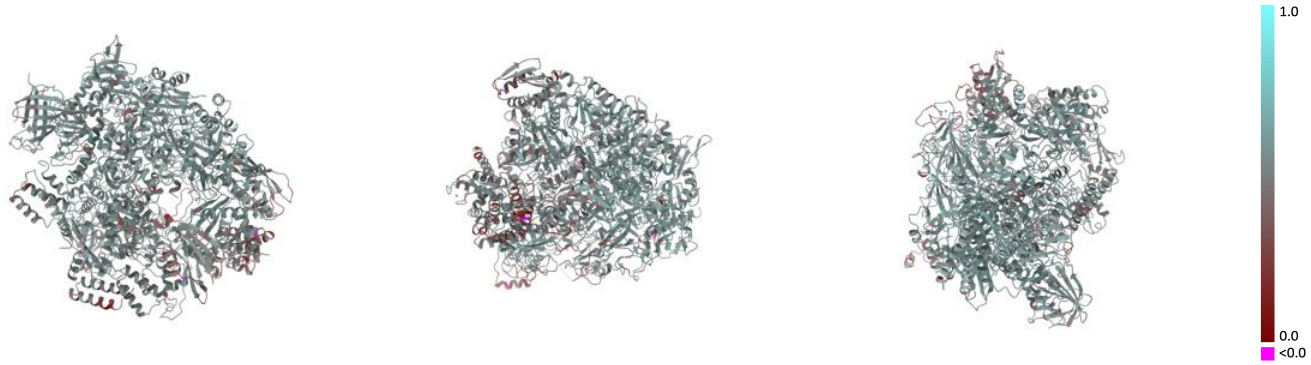
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019 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.

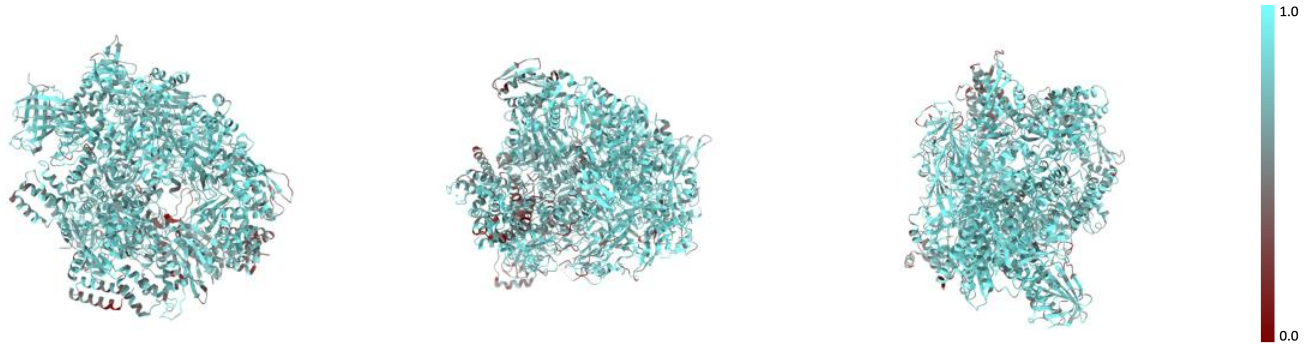
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

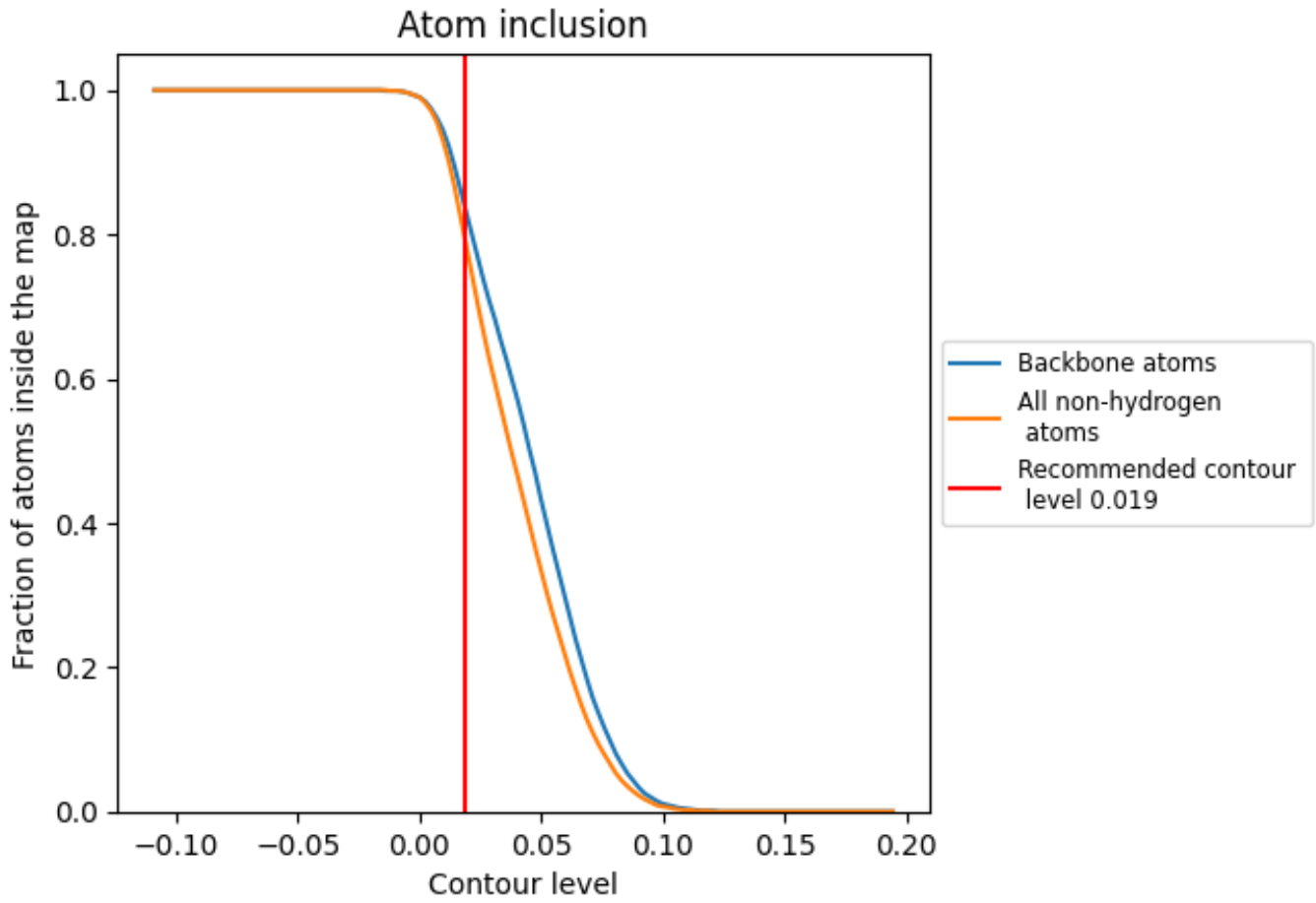
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 79% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7870	0.5240
A	0.8140	0.5370
B	0.8170	0.5370
C	0.7280	0.5010
D	0.8260	0.5480
E	0.6640	0.4640
F	0.4620	0.3070
G	0.7670	0.5280
H	0.8010	0.5410
K	0.8000	0.5330
L	0.8410	0.5440
N	0.8630	0.5660
P	0.7370	0.4890
Q	0.6080	0.4120
Z	0.5580	0.3940

