



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 04:07 PM UTC

PDB ID : 8P4F / pdb_00008p4f
EMDB ID : EMD-17408
Title : Structural insights into human co-transcriptional capping - structure 6
Authors : Garg, G.; Dienemann, C.; Farnung, L.; Schwarz, J.; Linden, A.; Urlaub, H.; Cramer, P.
Deposited on : 2023-05-20
Resolution : 4.00 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:

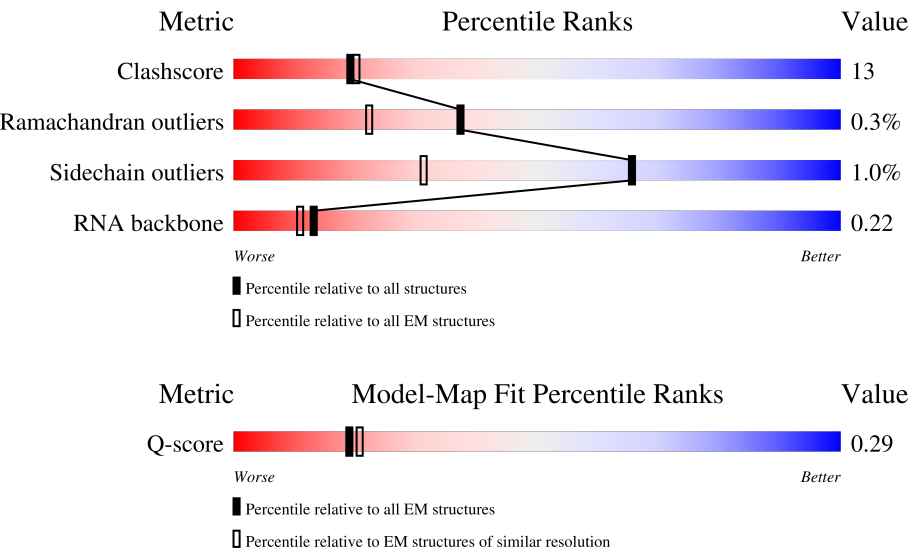
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 4.00 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.



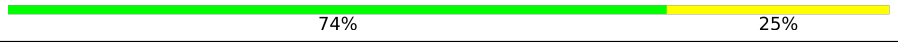
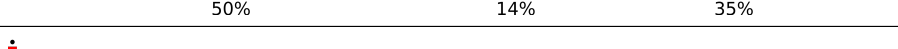
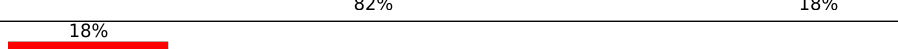
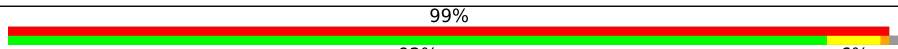
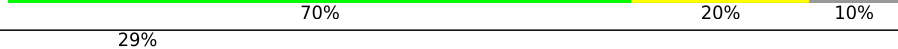
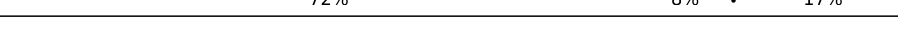
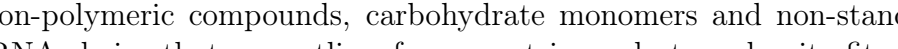
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	P	29	
2	A	1970	
3	B	1174	

Continued on next page...

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Mol	Chain	Length	Quality of chain
4	C	275	
5	E	210	
6	F	127	
7	H	150	
8	I	125	
9	J	67	
10	K	117	
11	L	58	
12	N	38	
13	T	38	
14	Y	117	
15	Z	1087	
16	G	172	
17	D	142	
18	O	835	

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
22	SAM	O	901	-	-	X	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 43686 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 RNA chain called RNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	29	Total	C	N	O	P	0	0
			622	281	124	189	28		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1421	Total	C	N	O	S	0	0
			11261	7084	2015	2090	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	1147	Total	C	N	O	S	0	0
			9142	5780	1612	1686	64		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	259	Total	C	N	O	S	0	0
			2079	1305	357	411	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1711	1084	300	319	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			658	419	113	121	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	126	THR	SER	conflict	UNP F1SKN8

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	117	Total	C	N	O	S	0	0
			946	584	169	182	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	11	ILE	PHE	conflict	UNP P60899

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 11 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	45	Total	C	N	O	S	0	0
			379	236	73	64	6		

- Molecule 12 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	38	Total	C	N	O	P	0	9
			610	287	112	173	38		

- Molecule 13 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	38	Total	C	N	O	P	0	0
			774	371	136	229	38		

- Molecule 14 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

- Molecule 15 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	488	Total	C	N	O	S	0	0
			3894	2475	686	716	17		

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	171	Total	C	N	O	S	0	0
			1341	871	218	244	8		

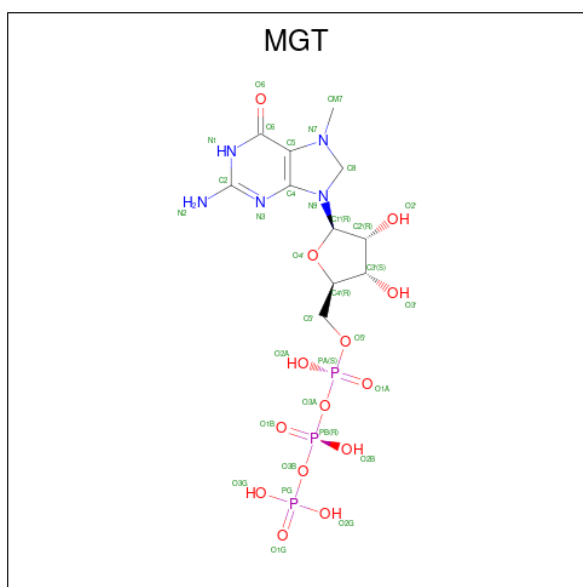
- Molecule 17 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	128	Total	C	N	O	S	0	0
			1008	635	170	199	4		

- Molecule 18 is a protein called Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	695	Total	C	N	O	S	0	0
			5643	3606	962	1040	35		

- Molecule 19 is 7N-METHYL-8-HYDROGUANOSINE-5'-TRIPHOSPHATE (CCD ID: MGT) (formula: C₁₁H₂₀N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
19	P	1	Total	C	N	O	P	0
			32	11	5	13	3	

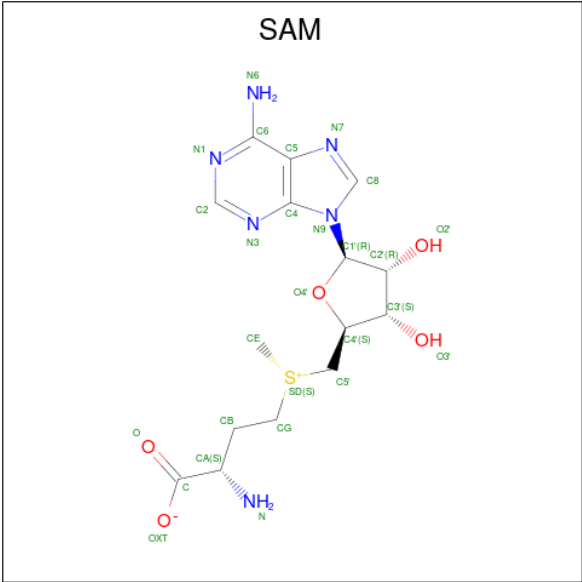
- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 22 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).



Mol	Chain	Residues	Atoms					AltConf
22	O	1	Total	C	N	O	S	0
			27	15	6	5	1	

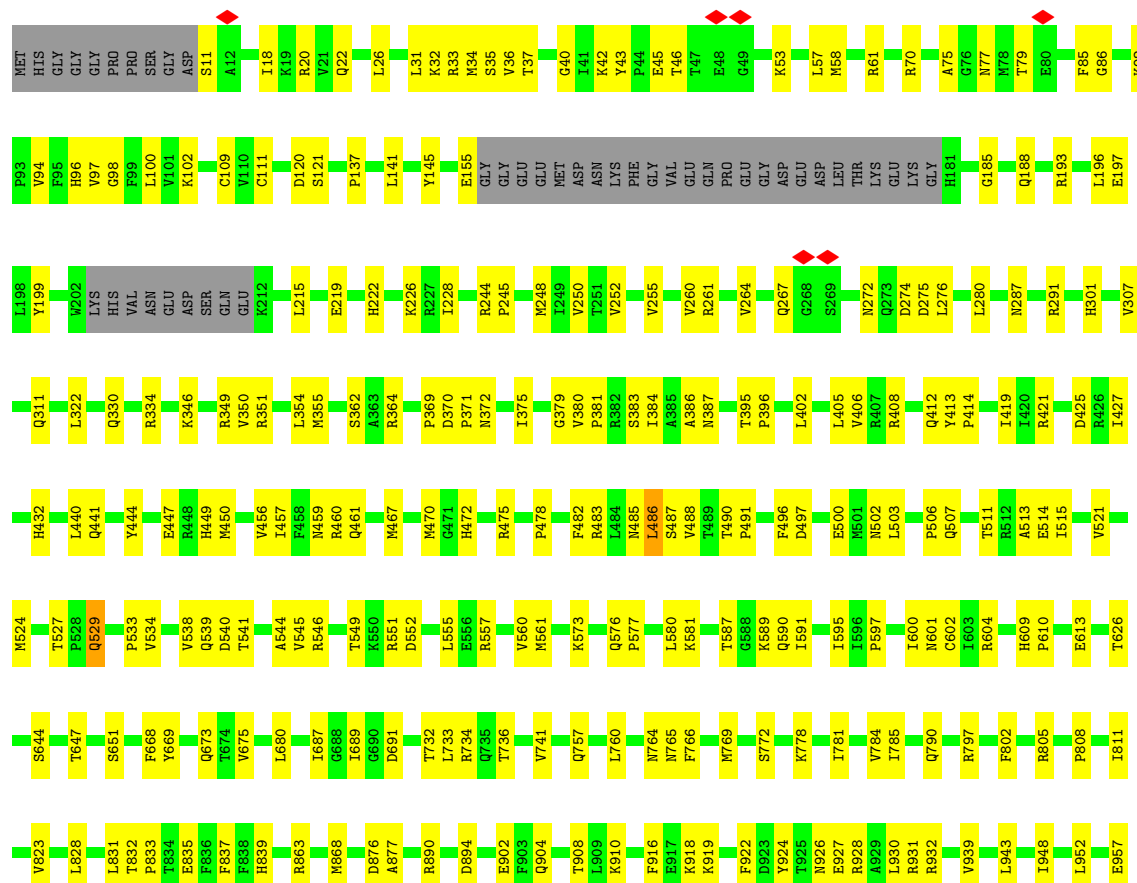
3 Residue-property plots

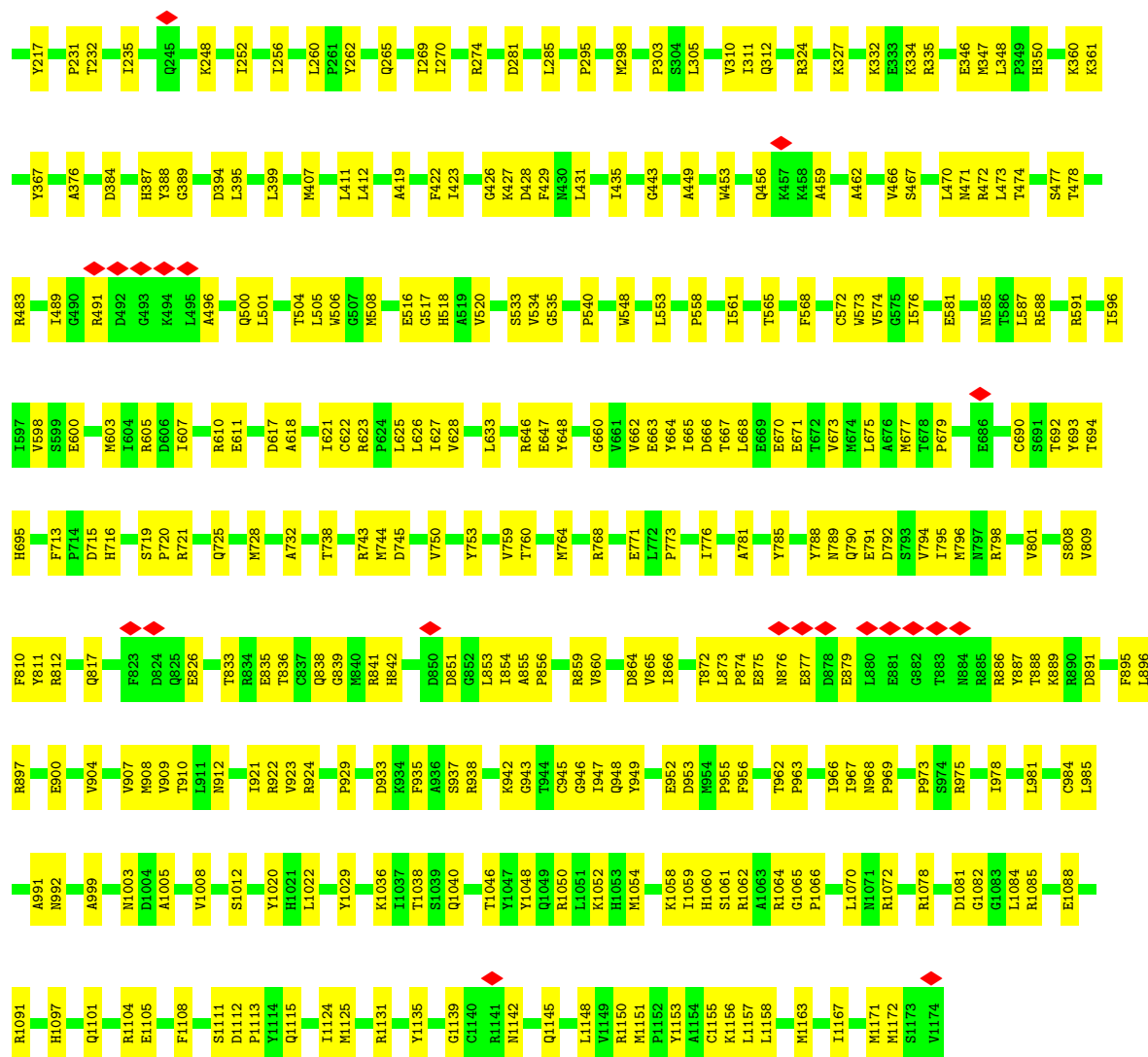
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: RNA (29-MER)



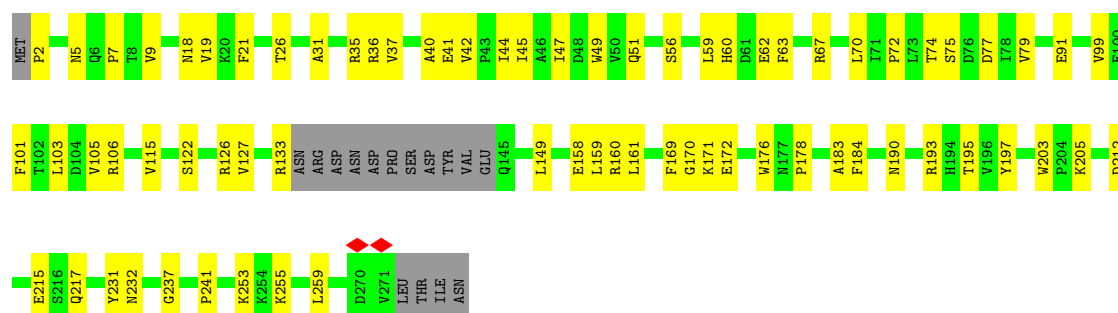
• Molecule 2: DNA-directed RNA polymerase II subunit RPB1





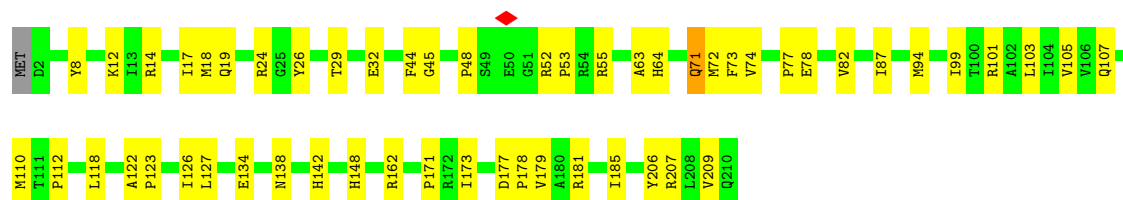
• Molecule 4: DNA-directed RNA polymerase II subunit RPB3

Chain C: 68% 26% 6%

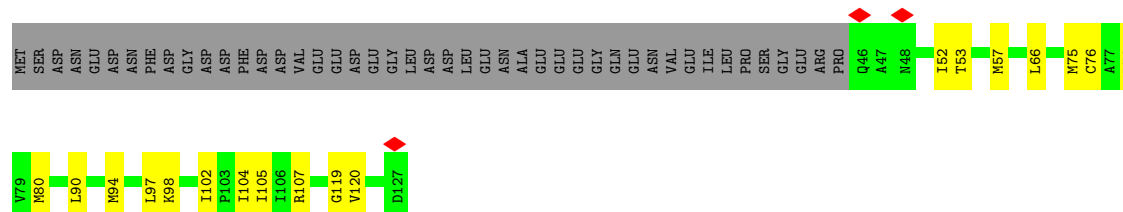


• Molecule 5: DNA-directed RNA polymerase II subunit E

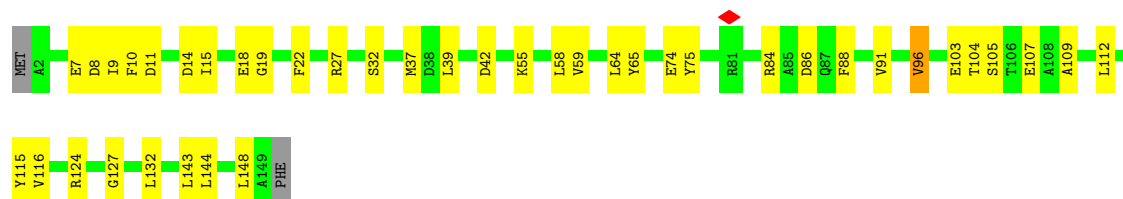
Chain E: 74% 25%



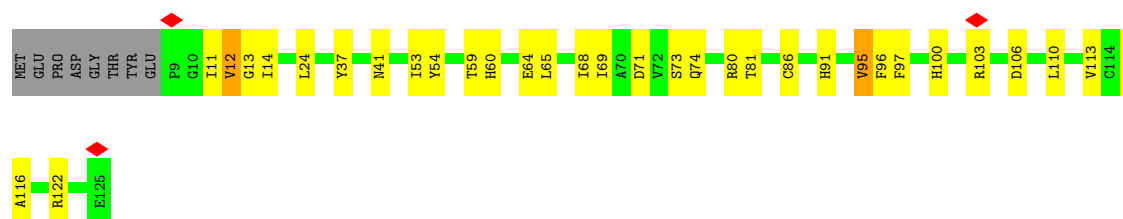
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 8: DNA-directed RNA polymerase II subunit RPB9



- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC5

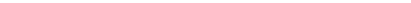


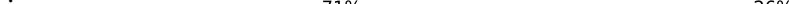
- Molecule 10: DNA-directed RNA polymerase II subunit RPB11-a

M1	N2	F10	I19	T20	I21	C31	T41	L42	I45	P54	P64	H65	P66	L67	E68	I72	F87	I91	I95	R104	F105	I109	E114	G115	I1E	GLU
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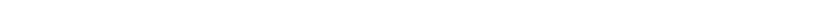
- Chain L:

MET	ASP	THR	GLN	LYS	ASP	VAL	GLN	PRO	PRO	LYS	GLN	GLN	P14	M15	I16	Y17		H23		E27	I28	K29		I34	R35	C36	R37	E38	C39	G40	Y41	R42	I43	M44	Y45	K46	K47	R48		V54		R58
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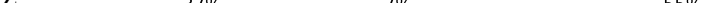
- Chain N:  29% 82% 18%

- Chain T:  18% 71% 26%

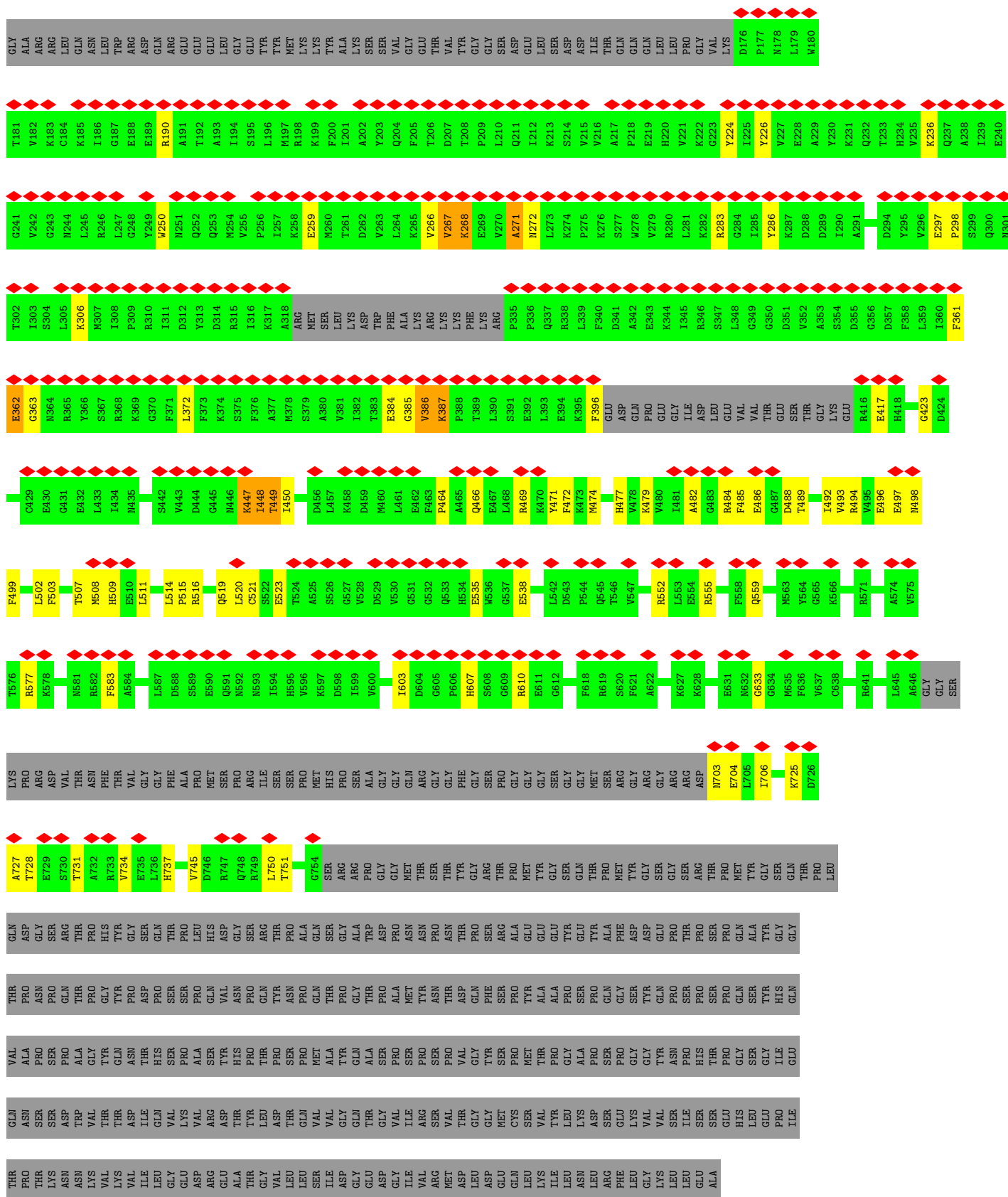
T3 T9 G21 C22 C23 T24 T29 A30 T31 A32 C33 T34 A35 A38 C39 T40

- Chain Y:  99% 92% 6%

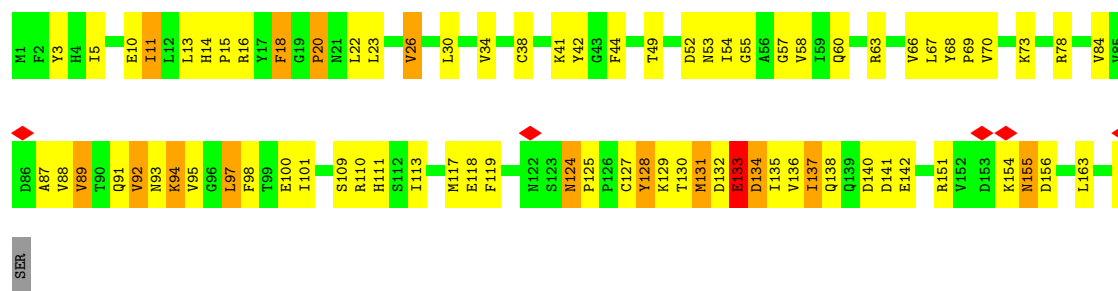
A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	A13	A14	A15	A16	A17	A18	A19	A20	A21	A22	A23	A24	A25	A26	A27	A28	A29	A30	A31	A32	A33	A34	A35	A36	A37	A38	A39	A40	A41	A42	A43	A44	A45	A46	A47	A48	A49	A50	A51	A52	A53	A54	A55	A56	A57	A58	A59	A60
A61	A62	A63	A64	A65	A66	A67	A68	A69	A70	A71	A72	A73	A74	A75	A76	A77	A78	A79	A80	A81	A82	A83	A84	A85	A86	A87	A88	A89	A90	A91	A92	A93	A94	A95	A96	A97	A98	A99	A100	A101	A102	A103	A104	A105	A106	A107	A108	A109	A110	A111	A112	A113	A114	A115	A116	A117			

- Chain Z: 

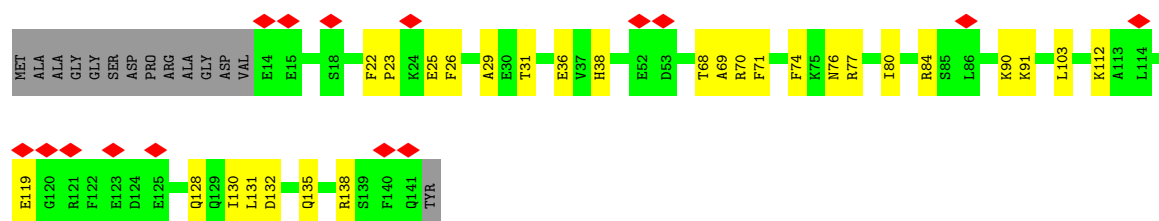
[illegible]



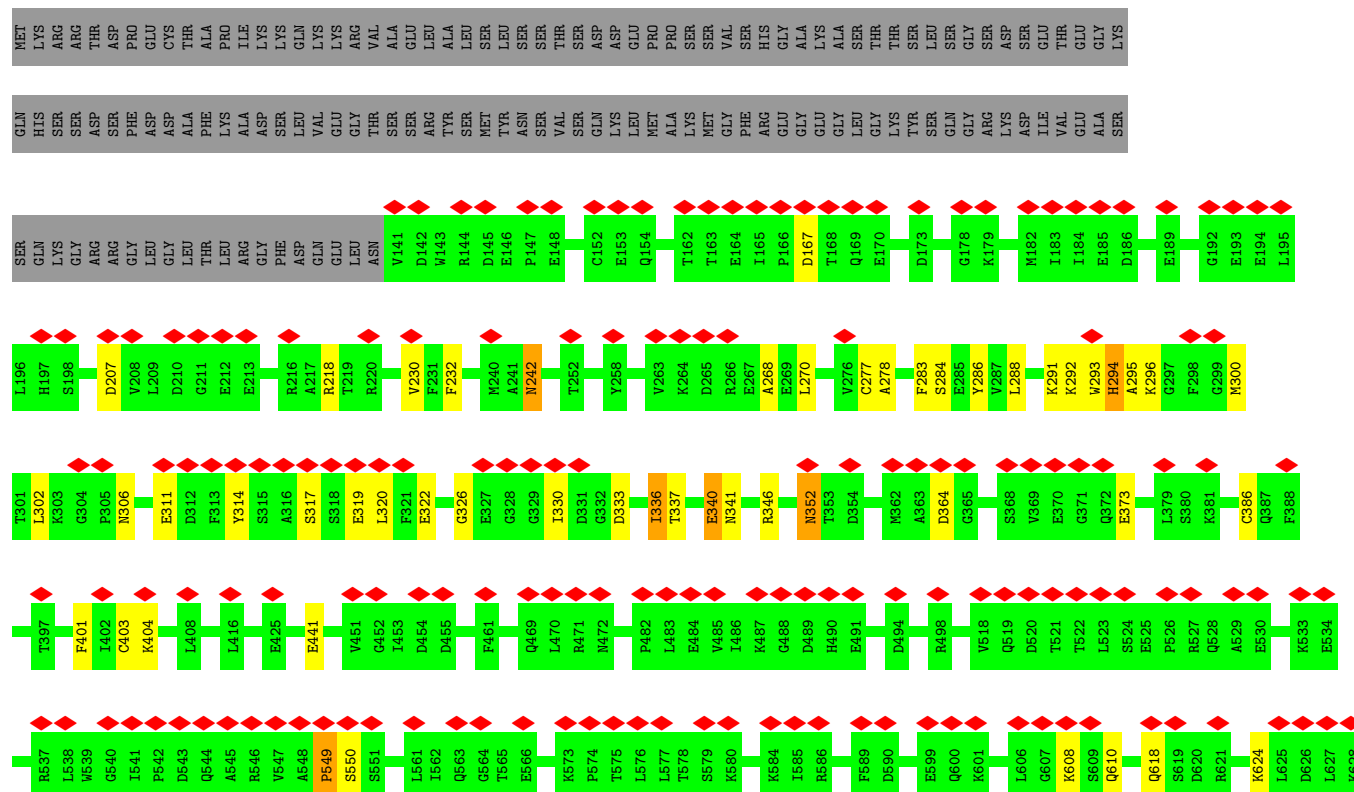
- Molecule 16: DNA-directed RNA polymerase II subunit RPB7

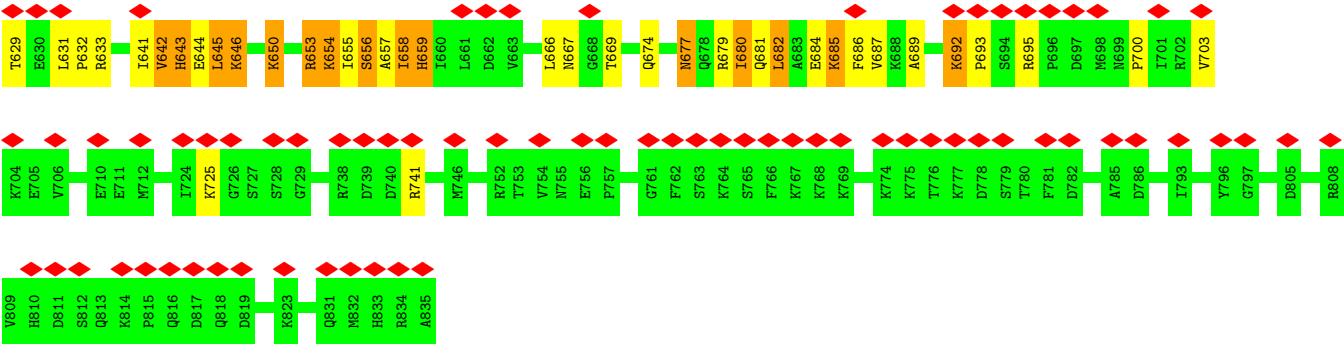


Chain D: 11% 70% 20% 10%



Chain O: 29% 72% 8% 17%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31423	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.021	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0193	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: MGT, ZN, SAM, 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	P	0.48	0/699	1.30	8/1088 (0.7%)
2	A	0.47	0/11467	0.57	1/15479 (0.0%)
3	B	0.53	0/9325	0.61	0/12589
4	C	0.56	0/2122	0.60	0/2883
5	E	0.43	0/1742	0.57	1/2353 (0.0%)
6	F	0.48	0/668	0.59	0/903
7	H	0.50	0/1207	0.56	0/1628
8	I	0.35	0/968	0.57	0/1311
9	J	0.61	0/542	0.63	0/730
10	K	0.51	0/939	0.55	0/1271
11	L	0.50	0/385	0.56	0/511
12	N	0.31	0/674	0.81	0/1037
13	T	0.43	0/866	0.79	1/1333 (0.1%)
14	Y	0.73	1/927 (0.1%)	0.84	2/1250 (0.2%)
15	Z	0.80	2/3963 (0.1%)	0.91	14/5339 (0.3%)
16	G	0.42	0/1372	0.92	2/1861 (0.1%)
17	D	0.21	0/1022	0.61	0/1377
18	O	2.30	4/5775 (0.1%)	1.47	10/7785 (0.1%)
All	All	0.96	7/44663 (0.0%)	0.83	39/60728 (0.1%)

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	P	2	0
2	A	0	1
14	Y	0	1
18	O	0	1
All	All	2	3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	O	659	HIS	CE1-NE2	120.64	2.53	1.32
18	O	659	HIS	ND1-CE1	83.26	2.15	1.32
18	O	659	HIS	CD2-NE2	69.81	2.14	1.37
18	O	549	PRO	C-N	24.00	1.66	1.33
14	Y	105	GLY	CA-C	12.37	1.69	1.51

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	O	549	PRO	O-C-N	39.16	165.67	122.98
18	O	549	PRO	CA-C-N	-30.39	76.04	121.31
18	O	549	PRO	C-N-CA	-30.39	76.04	121.31
18	O	659	HIS	ND1-CE1-NE2	-23.44	84.96	108.40
18	O	659	HIS	CG-CD2-NE2	21.61	128.81	107.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	P	31	G	C1'
1	P	33	C	C1'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	910	LYS	Peptide
18	O	314	TYR	Sidechain
14	Y	105	GLY	Mainchain

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	P	622	0	316	58	0
2	A	11261	0	11390	327	0
3	B	9142	0	9157	301	0
4	C	2079	0	2032	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1711	0	1729	41	0
6	F	658	0	686	22	0
7	H	1186	0	1147	33	0
8	I	946	0	881	25	0
9	J	533	0	553	15	0
10	K	920	0	942	18	0
11	L	379	0	386	18	0
12	N	610	0	330	9	0
13	T	774	0	431	12	0
14	Y	911	0	904	5	0
15	Z	3894	0	3957	91	0
16	G	1341	0	1348	95	0
17	D	1008	0	970	19	0
18	O	5643	0	5592	153	0
19	P	32	0	16	5	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
20	Y	1	0	0	0	0
21	A	1	0	0	0	0
22	O	27	0	22	12	0
All	All	43686	0	42789	1097	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 13.

The worst 5 of 1097 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)
16:G:170:LEU:HD11	18:O:725:LYS:CE	1.55	1.32
16:G:170:LEU:CD1	18:O:725:LYS:HE3	1.59	1.29
3:B:327:LYS:NZ	15:Z:250:TRP:CE3	2.09	1.19
18:O:330:ILE:HG12	18:O:695:ARG:HD3	1.27	1.16
16:G:141:ASP:OD2	18:O:725:LYS:NZ	1.78	1.16

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	1411/1970 (72%)	1353 (96%)	57 (4%)	1 (0%)	48	81
3	B	1143/1174 (97%)	1088 (95%)	55 (5%)	0	100	100
4	C	255/275 (93%)	238 (93%)	17 (7%)	0	100	100
5	E	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
6	F	80/127 (63%)	78 (98%)	2 (2%)	0	100	100
7	H	146/150 (97%)	140 (96%)	6 (4%)	0	100	100
8	I	115/125 (92%)	105 (91%)	9 (8%)	1 (1%)	14	48
9	J	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
10	K	113/117 (97%)	113 (100%)	0	0	100	100
11	L	43/58 (74%)	40 (93%)	3 (7%)	0	100	100
14	Y	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
15	Z	480/1087 (44%)	463 (96%)	13 (3%)	4 (1%)	16	52
16	G	169/172 (98%)	158 (94%)	5 (3%)	6 (4%)	2	23
17	D	126/142 (89%)	113 (90%)	12 (10%)	1 (1%)	16	52
18	O	693/835 (83%)	666 (96%)	25 (4%)	2 (0%)	36	70
All	All	5160/6626 (78%)	4926 (96%)	219 (4%)	15 (0%)	37	70

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	G	18	PHE
16	G	124	ASN
16	G	133	GLU
8	I	12	VAL
15	Z	362	GLU

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	A	1252/1749 (72%)	1252 (100%)	0	100	100
3	B	996/1027 (97%)	995 (100%)	1 (0%)	88	89
4	C	236/252 (94%)	236 (100%)	0	100	100
5	E	189/192 (98%)	189 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	H	129/131 (98%)	128 (99%)	1 (1%)	73	77
8	I	105/112 (94%)	104 (99%)	1 (1%)	68	76
9	J	56/56 (100%)	56 (100%)	0	100	100
10	K	104/106 (98%)	104 (100%)	0	100	100
11	L	42/55 (76%)	42 (100%)	0	100	100
14	Y	102/103 (99%)	101 (99%)	1 (1%)	68	76
15	Z	429/940 (46%)	429 (100%)	0	100	100
16	G	149/153 (97%)	132 (89%)	17 (11%)	5	22
17	D	107/126 (85%)	105 (98%)	2 (2%)	50	67
18	O	623/741 (84%)	598 (96%)	25 (4%)	28	50
All	All	4590/5854 (78%)	4542 (99%)	48 (1%)	65	76

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	O	340	GLU
18	O	646	LYS
18	O	346	ARG
18	O	642	VAL
18	O	653	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
15	Z	591	GLN
18	O	515	HIS
15	Z	625	HIS
17	D	66	ASN
18	O	681	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	P	28/29 (96%)	18 (64%)	7 (25%)

5 of 18 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	P	26	A
1	P	27	A
1	P	28	A
1	P	29	A
1	P	30	A

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	P	35	U
1	P	36	A
1	P	42	A
1	P	40	A
1	P	33	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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$
22	SAM	O	901	-	27,29,29	1.90	7 (25%)	34,42,42	2.19	10 (29%)
19	MGT	P	101	1	30,34,35	4.01	6 (20%)	39,53,56	1.88	10 (25%)

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
22	SAM	O	901	-	-	2/17/33/33	0/3/3/3
19	MGT	P	101	1	-	6/19/49/50	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	101	MGT	C8-N9	-17.77	1.34	1.45
19	P	101	MGT	O6-C6	9.32	1.41	1.23
19	P	101	MGT	C2-N2	5.71	1.47	1.34
22	O	901	SAM	C6-N6	4.96	1.46	1.34
22	O	901	SAM	C3'-C4'	-3.45	1.44	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	901	SAM	C5-C4-N3	-4.74	120.19	126.72
22	O	901	SAM	N3-C2-N1	-4.71	121.45	128.58
19	P	101	MGT	C5-C6-N1	4.55	118.95	110.94
19	P	101	MGT	C2-N3-C4	4.42	119.92	112.30
19	P	101	MGT	N9-C8-N7	4.30	109.46	103.37

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

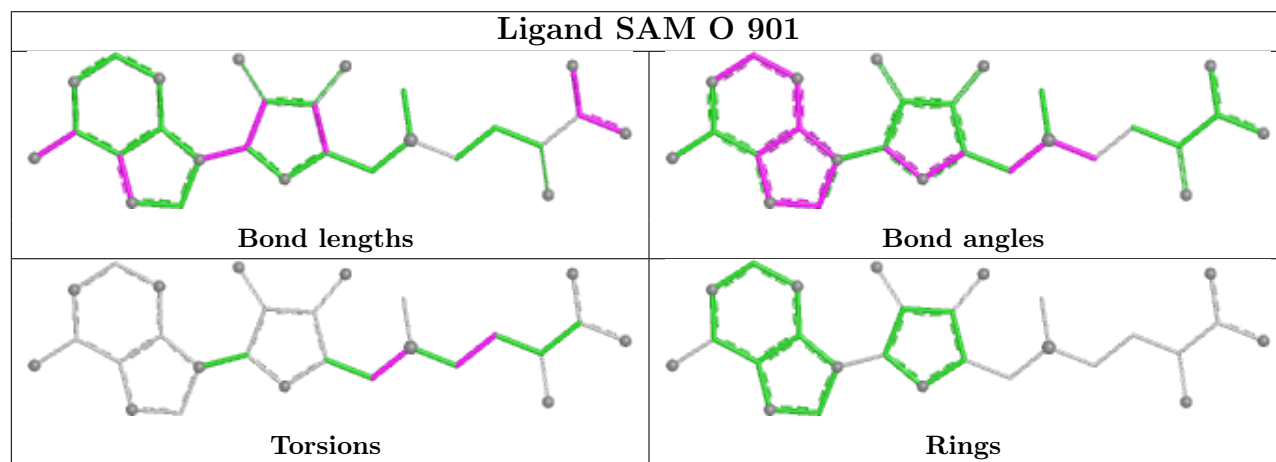
Mol	Chain	Res	Type	Atoms
19	P	101	MGT	C5'-O5'-PA-O2A
22	O	901	SAM	C4'-C5'-SD-CE
19	P	101	MGT	O4'-C4'-C5'-O5'
19	P	101	MGT	C3'-C4'-C5'-O5'
22	O	901	SAM	CA-CB-CG-SD

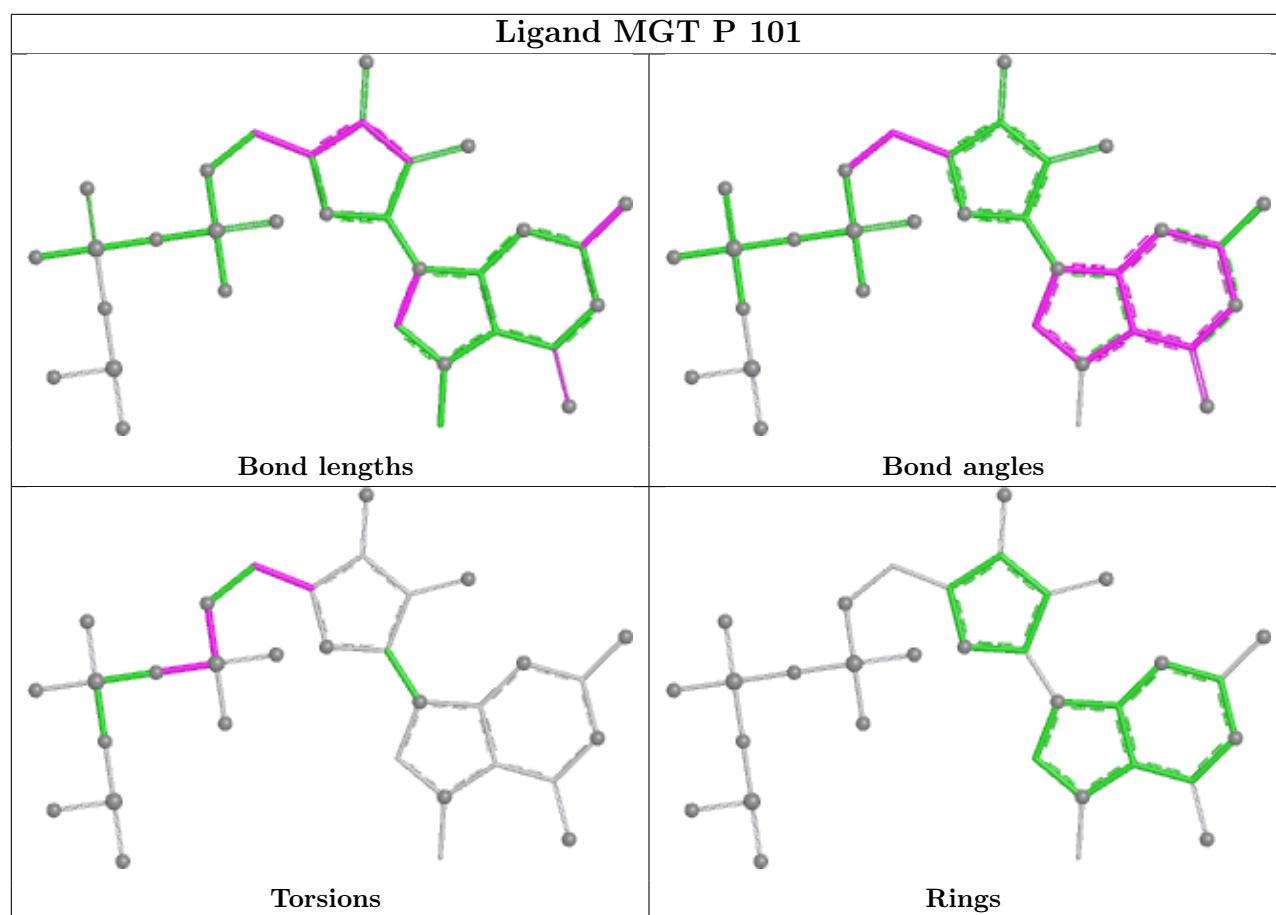
There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	O	901	SAM	12	0
19	P	101	MGT	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	N	1
18	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	14:DT	O3'	15:DT	P	3.16
1	O	549:PRO	C	550:SER	N	1.66

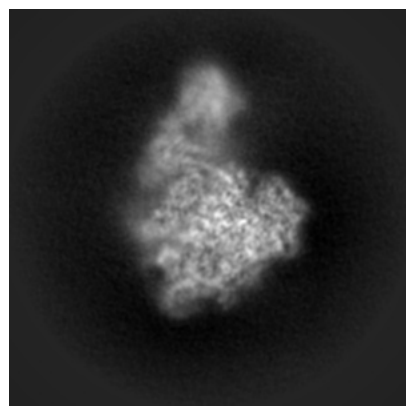
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17408. These allow visual inspection of the internal detail of the map and identification of artifacts.

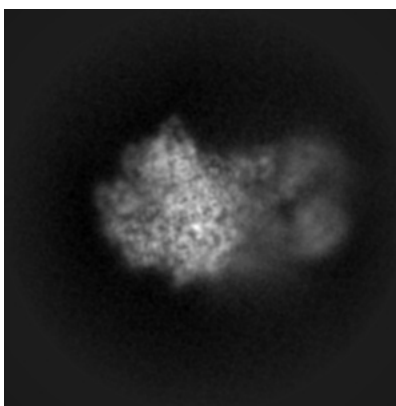
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

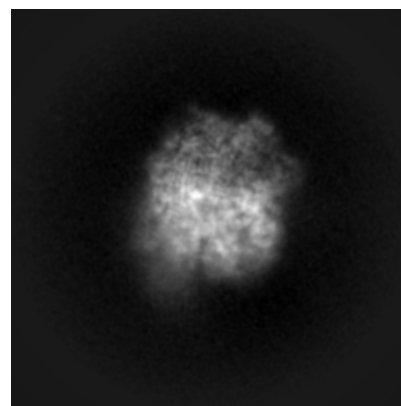
6.1.1 Primary map



X

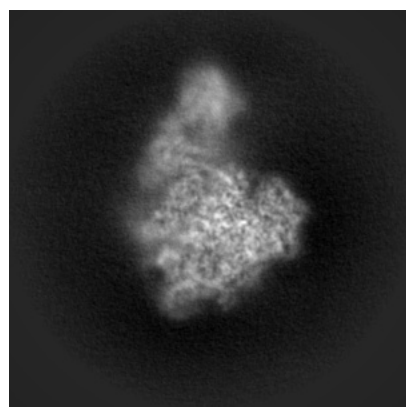


Y

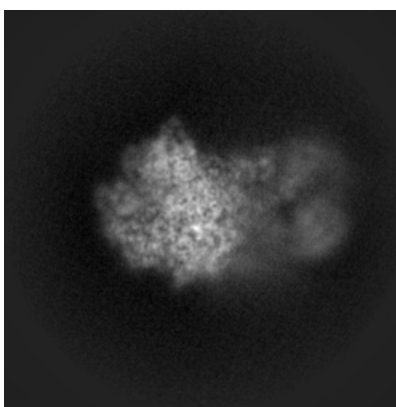


Z

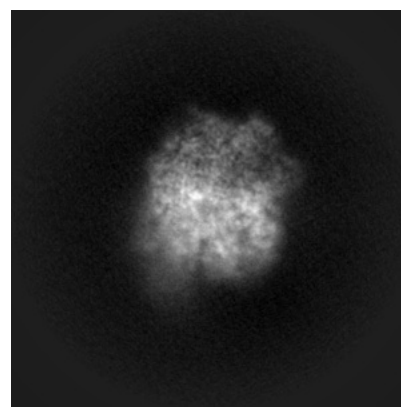
6.1.2 Raw map



X



Y

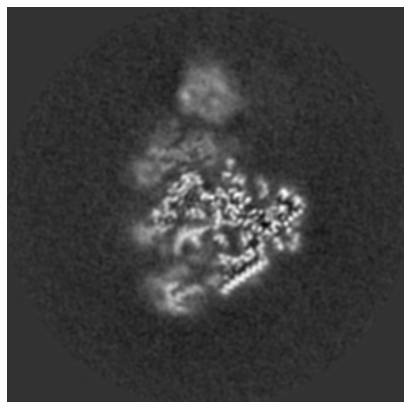


Z

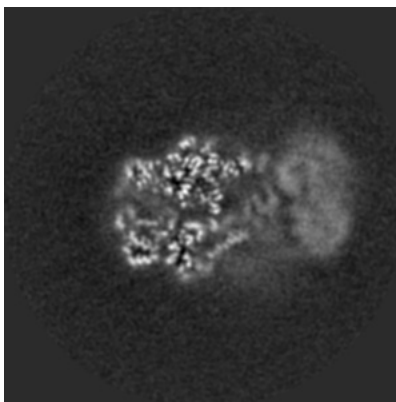
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

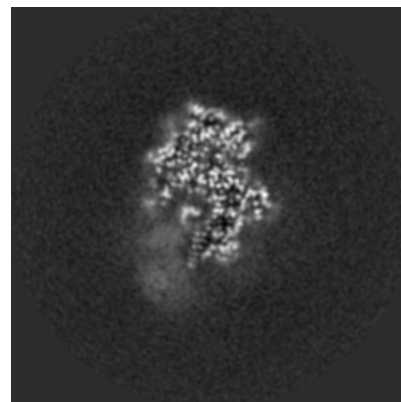
6.2.1 Primary map



X Index: 150

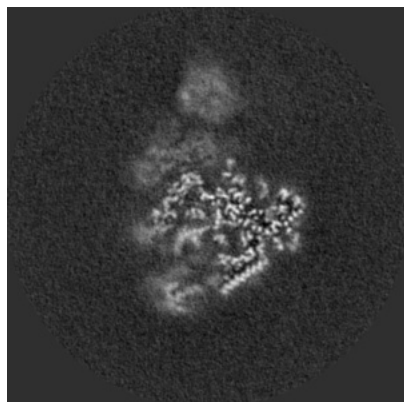


Y Index: 150

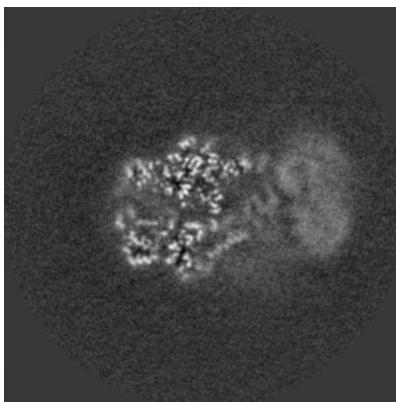


Z Index: 150

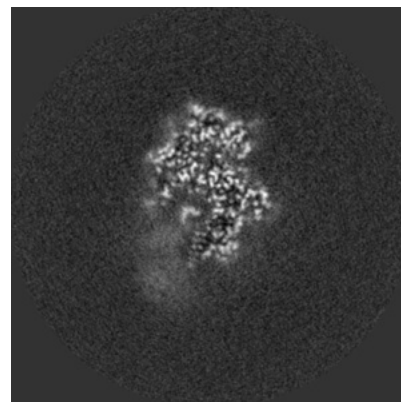
6.2.2 Raw map



X Index: 150



Y Index: 150

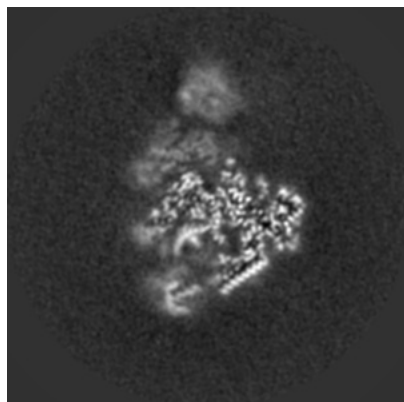


Z Index: 150

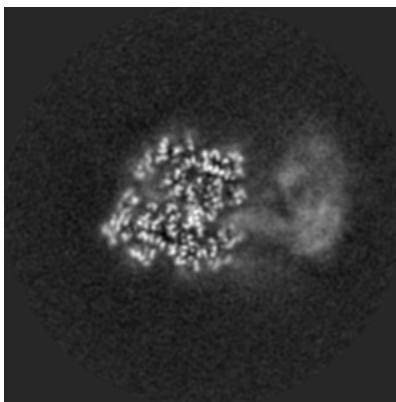
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

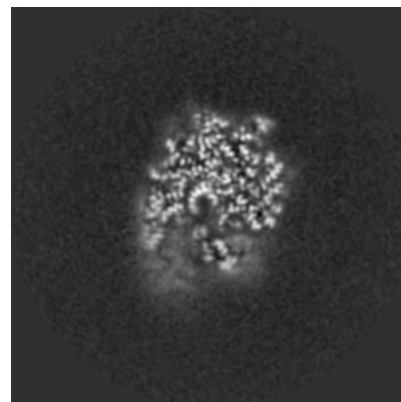
6.3.1 Primary map



X Index: 151

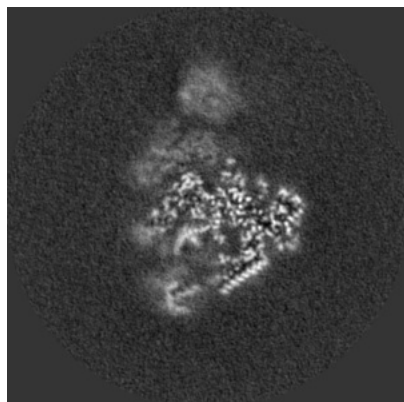


Y Index: 160

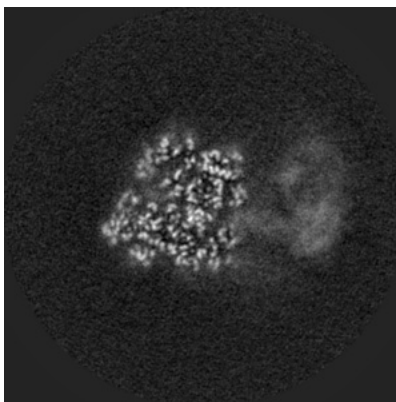


Z Index: 139

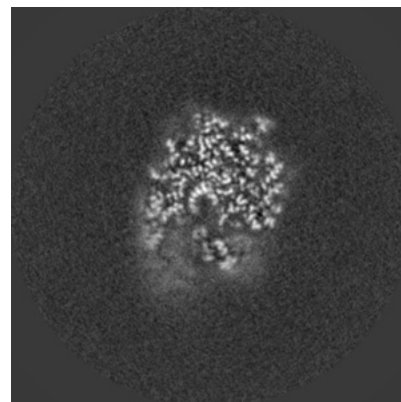
6.3.2 Raw map



X Index: 151



Y Index: 161

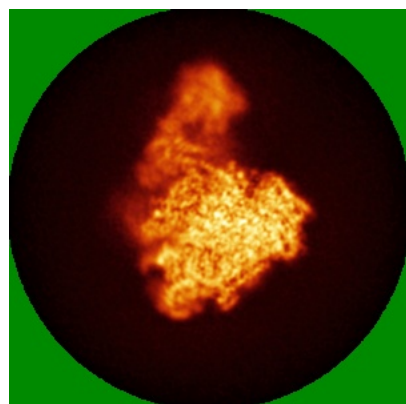


Z Index: 139

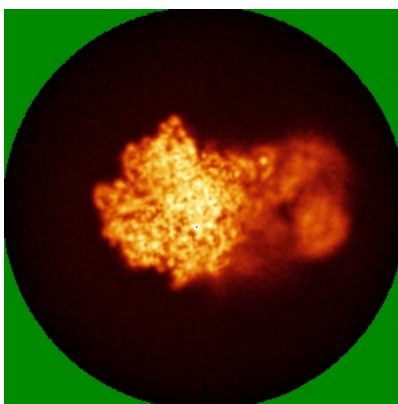
The images above show the largest variance slices of the map in three orthogonal directions.

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

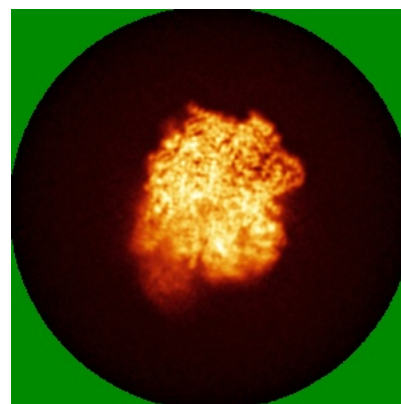
6.4.1 Primary map



X



Y

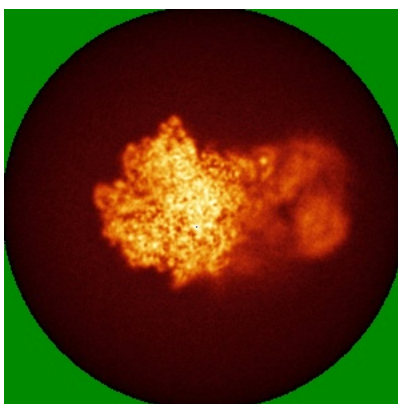


Z

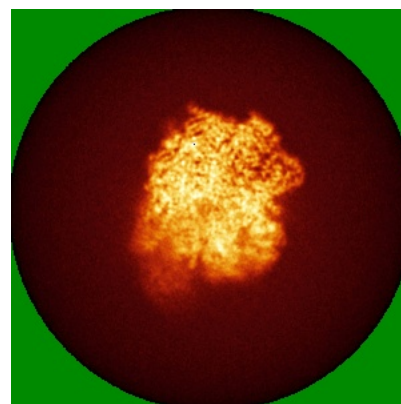
6.4.2 Raw map



X



Y

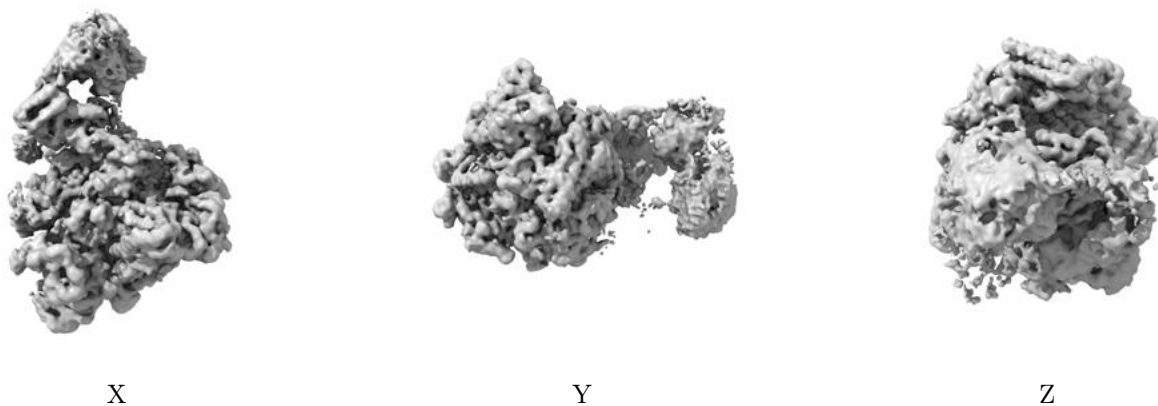


Z

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.

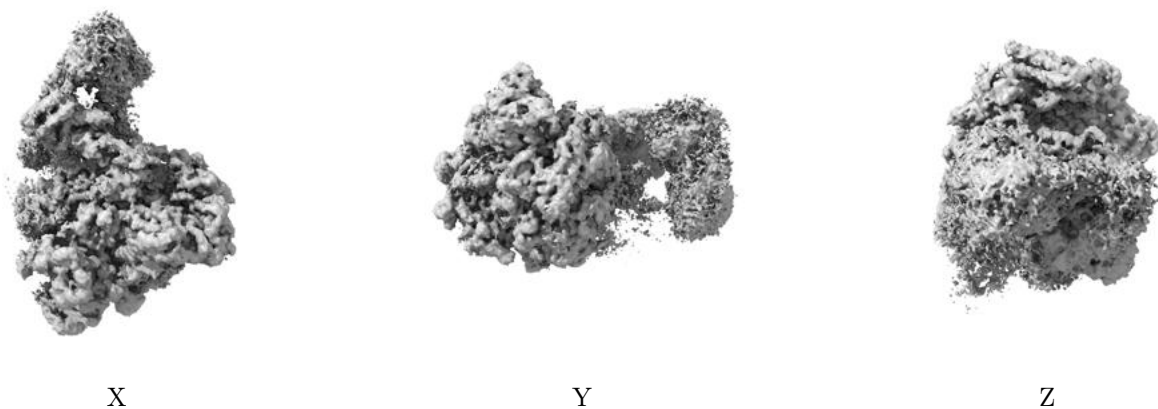
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0193. 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



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.

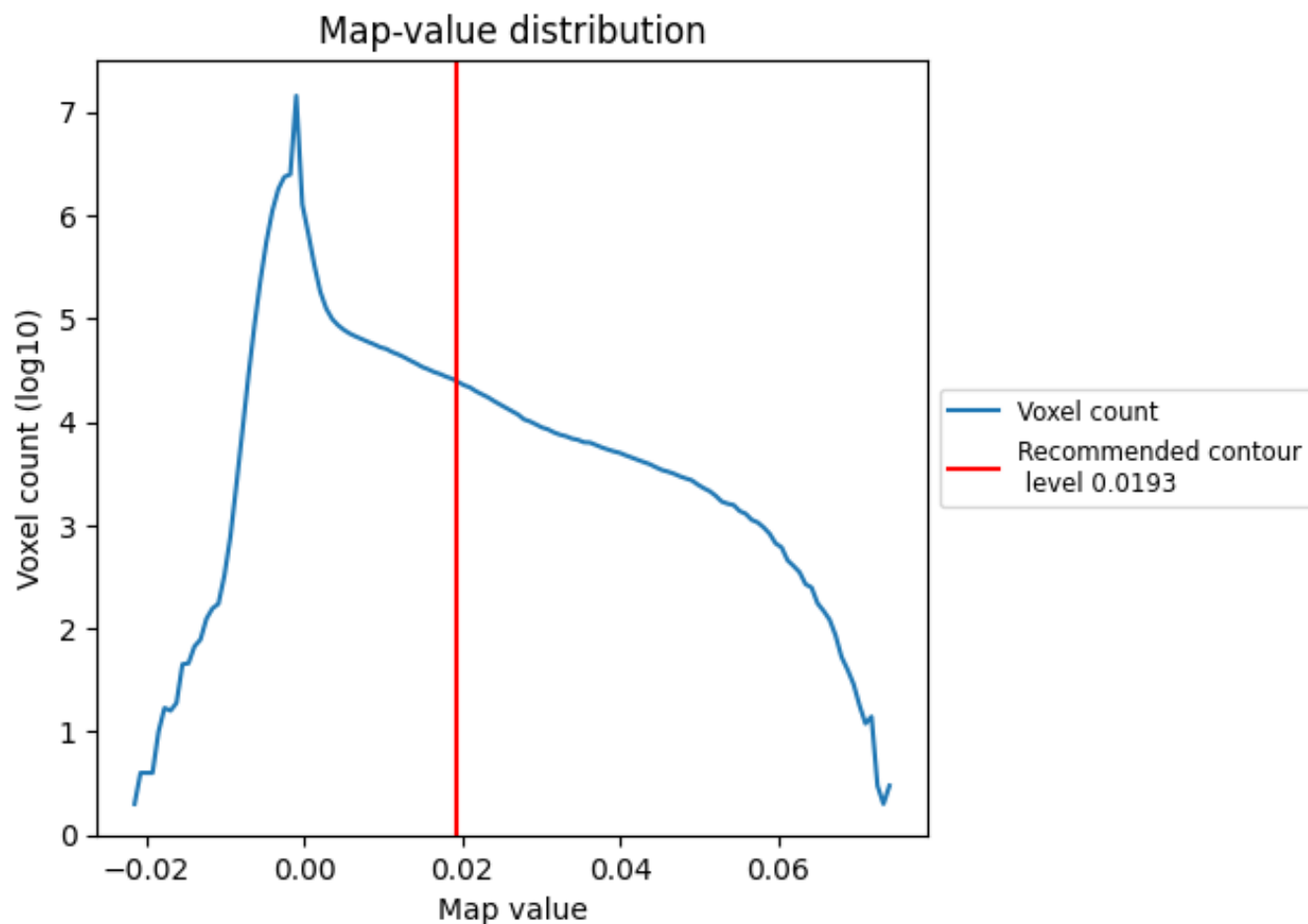
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

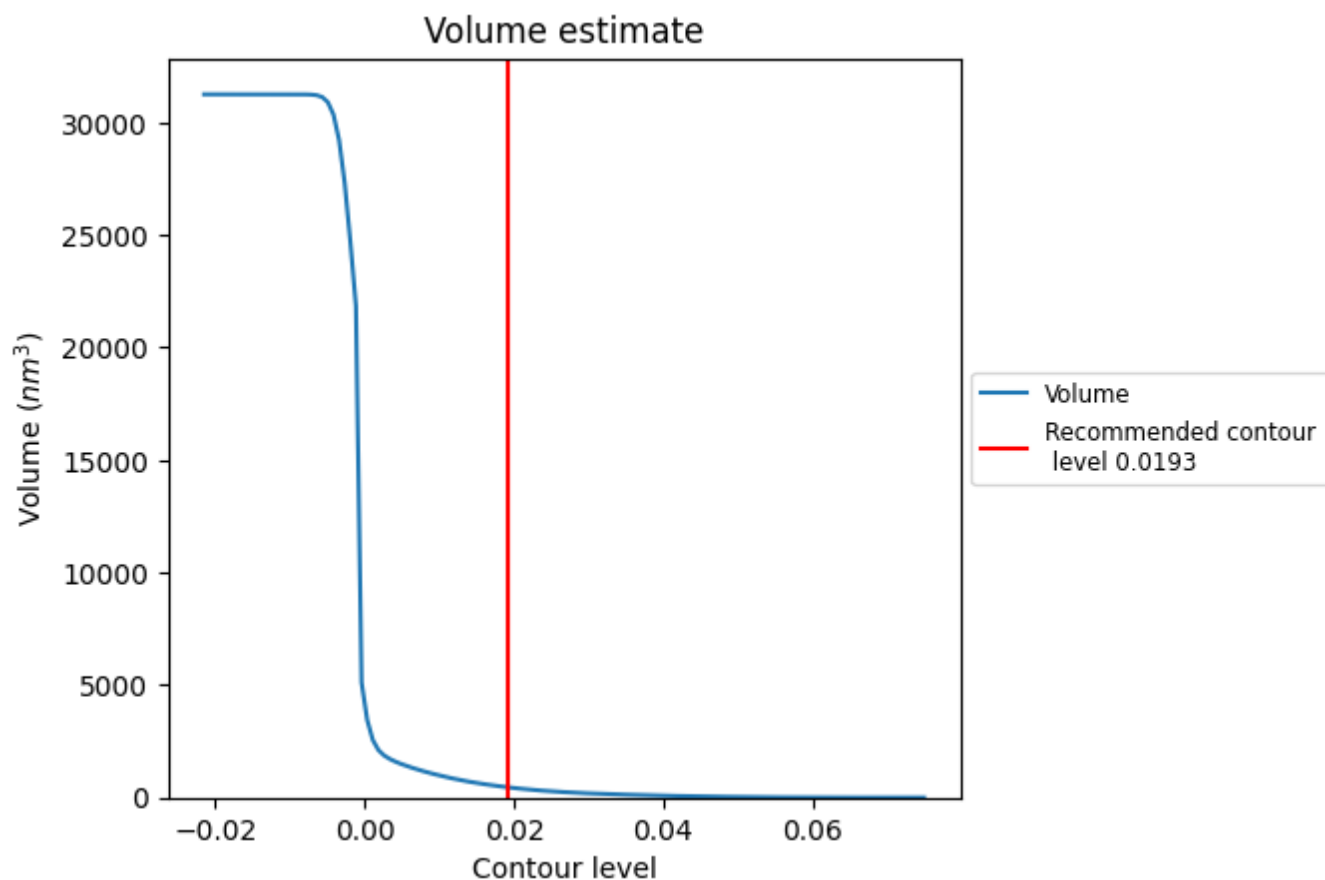
This section contains the results of statistical analysis of the map.

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.

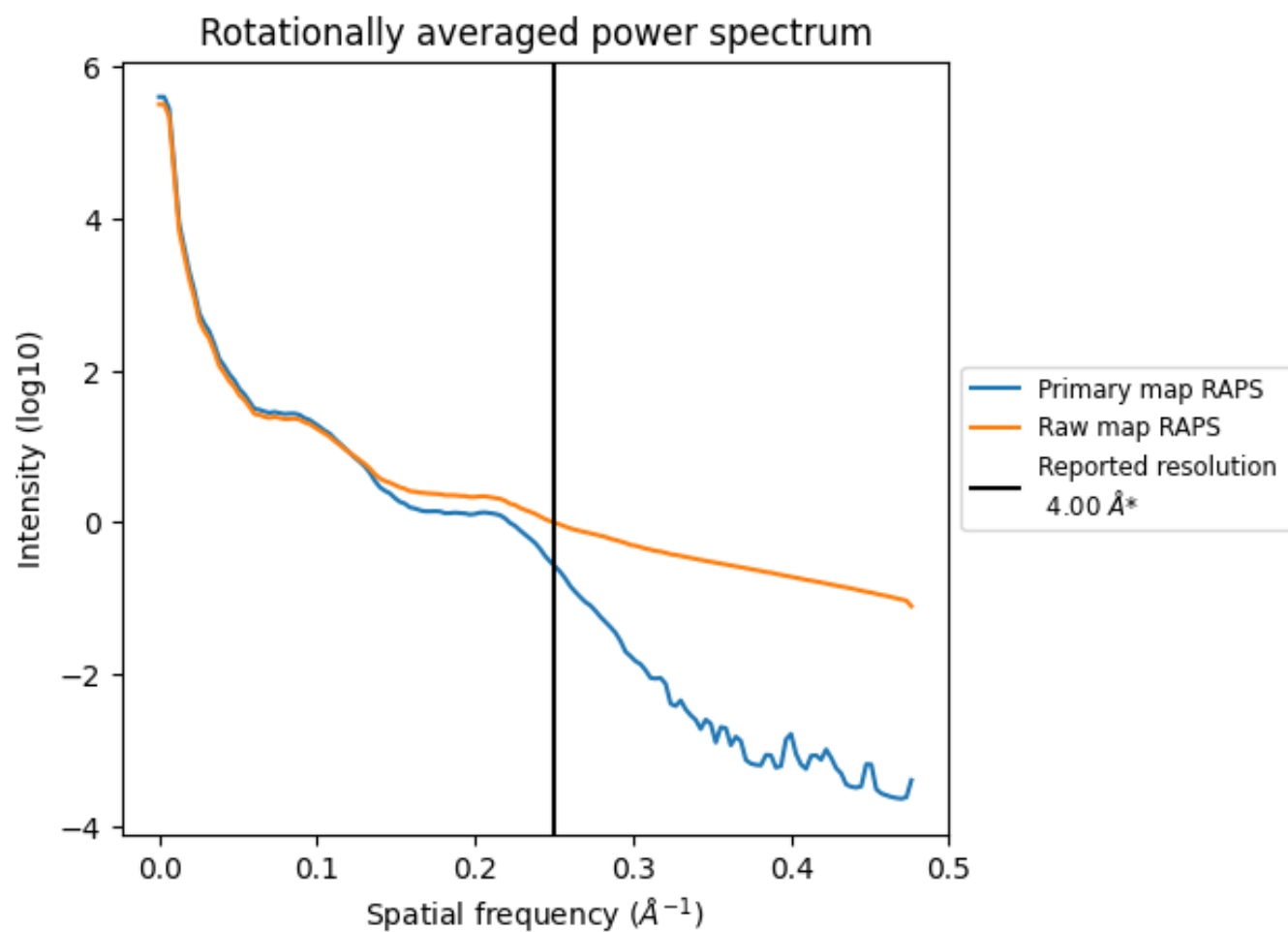
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 452 nm³; this corresponds to an approximate mass of 408 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 ⓘ

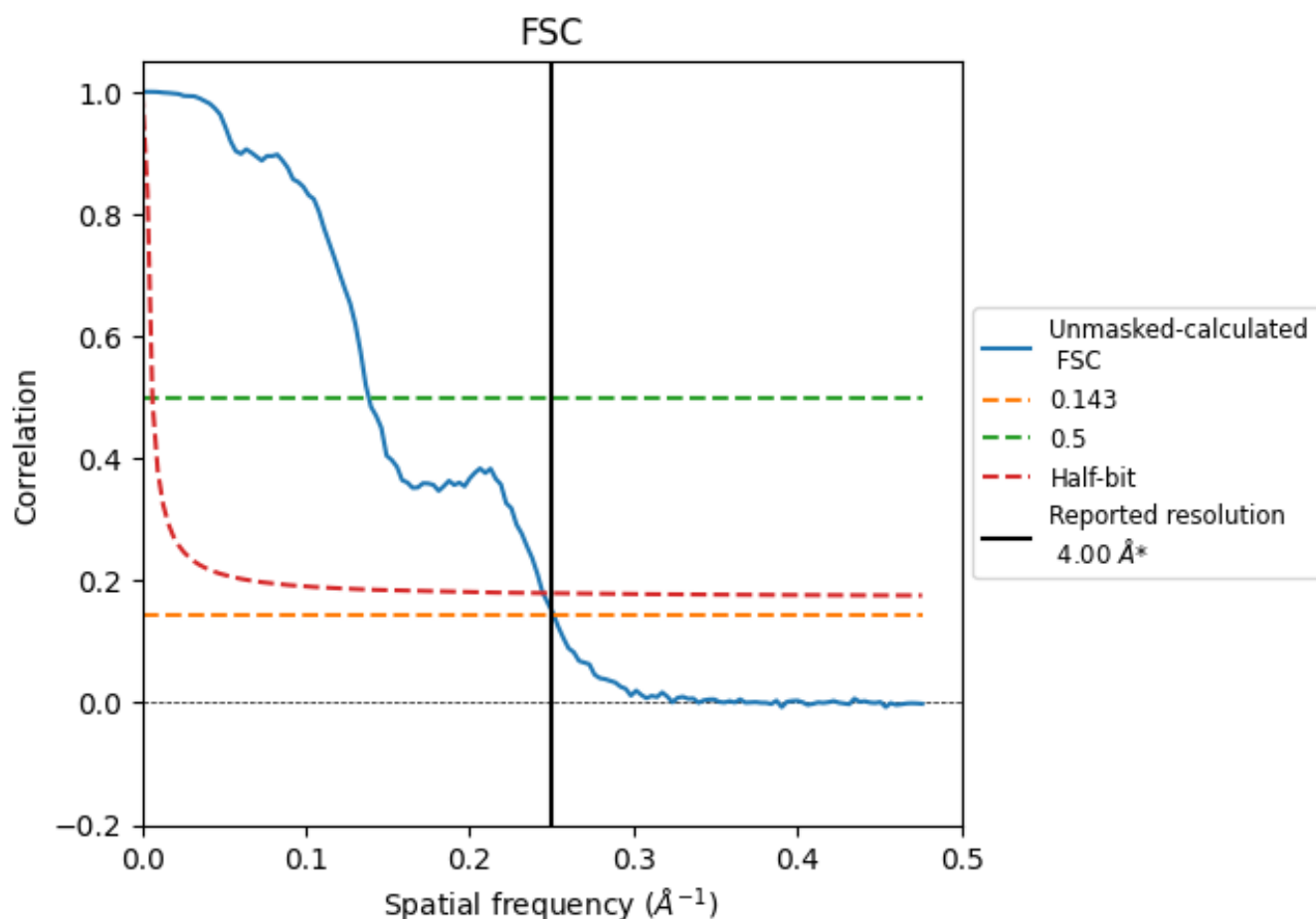


*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

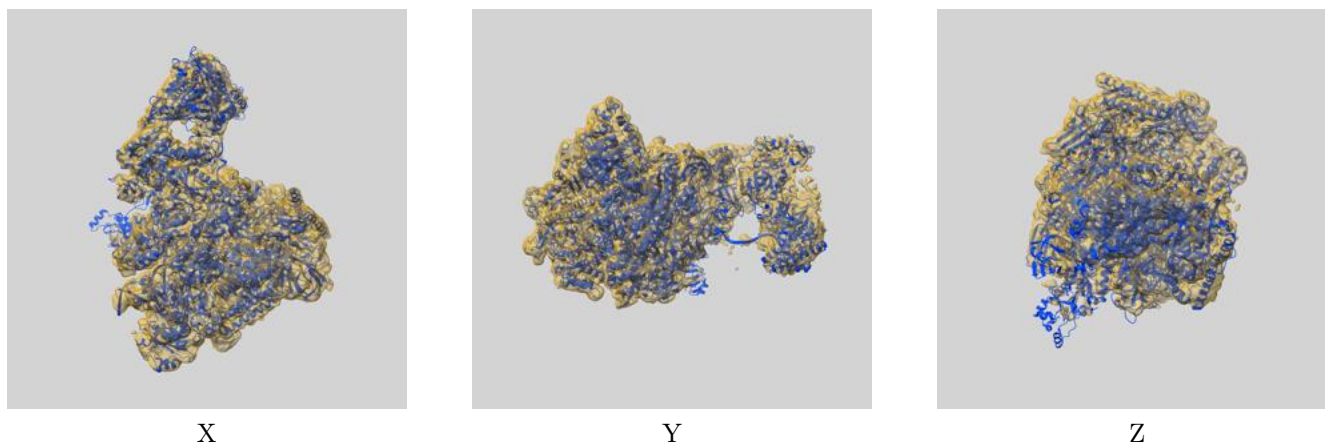
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.98	7.23	4.09

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

9 Map-model fit [i](#)

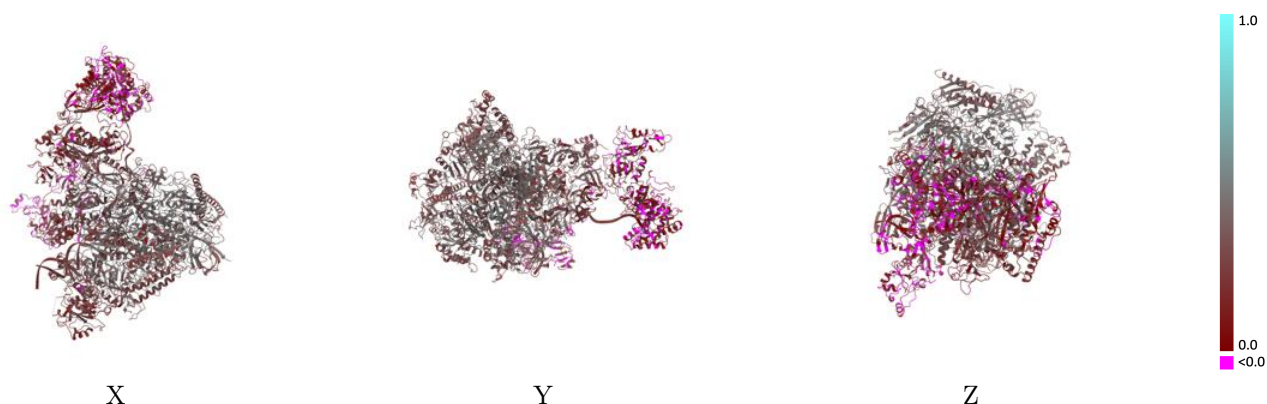
This section contains information regarding the fit between EMDB map EMD-17408 and PDB model 8P4F. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



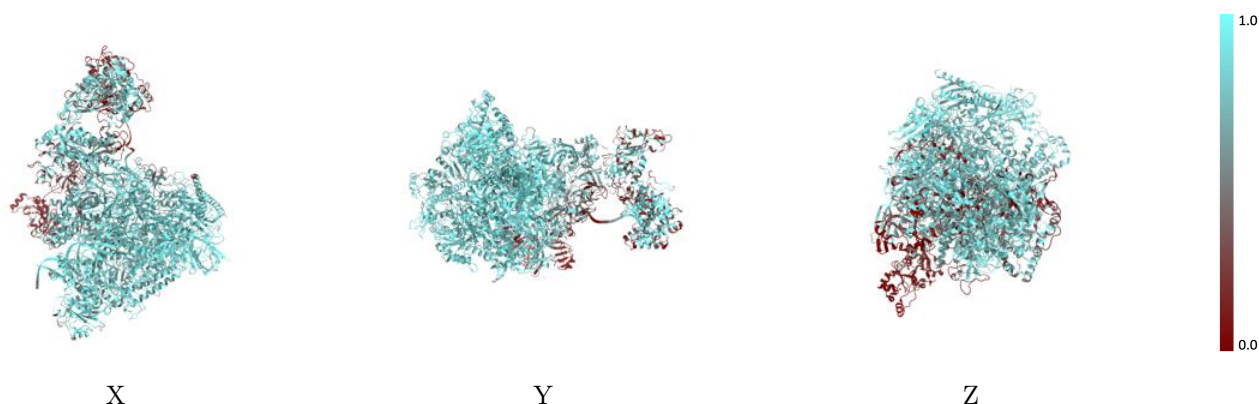
The images above show the 3D surface view of the map at the recommended contour level 0.0193 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



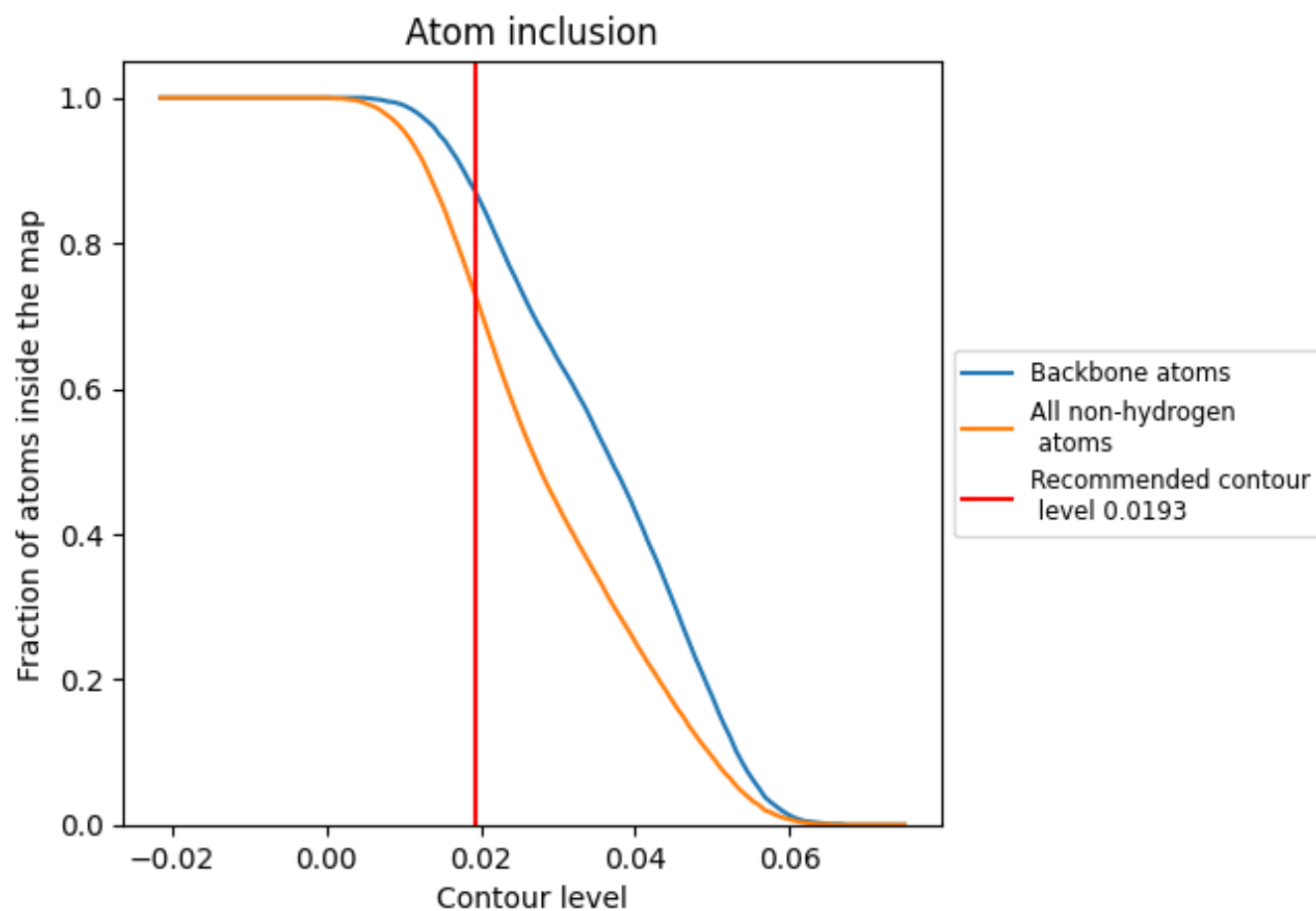
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0193).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 73% 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 (0.0193) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7290	 0.2900
A	 0.8350	 0.3530
B	 0.8340	 0.3700
C	 0.8570	 0.3820
D	 0.6920	 0.2230
E	 0.8400	 0.3240
F	 0.8330	 0.3670
G	 0.7810	 0.2920
H	 0.8510	 0.3670
I	 0.8430	 0.3040
J	 0.8620	 0.3950
K	 0.8610	 0.3890
L	 0.8380	 0.3560
N	 0.6660	 0.1740
O	 0.5780	 0.0970
P	 0.7890	 0.2460
T	 0.7600	 0.2460
Y	 0.0330	 0.0520
Z	 0.2920	 0.1620

