



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 09:20 am BST

PDB ID : 5FJ8
EMDB ID : EMD-3178
Title : Cryo-EM structure of yeast RNA polymerase III elongation complex at 3.9 Å
Authors : Hoffmann, N.A.; Jakobi, A.J.; Moreno-Morcillo, M.; Glatt, S.; Kosinski, J.; Hagen, W.J.; Sachse, C.; Muller, C.W.
Deposited on : 2015-10-06
Resolution : 3.90 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:

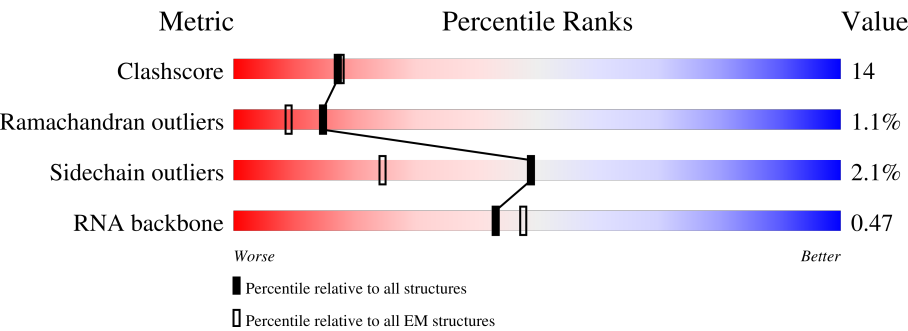
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





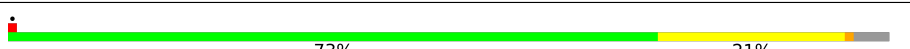

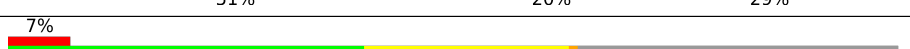
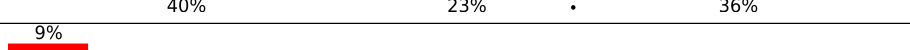
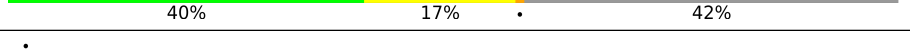

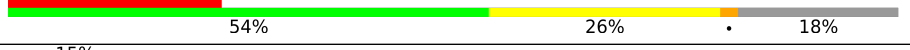




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1460	<div><div>6%</div><div>69%</div><div>27%</div><div>..</div></div>
2	B	1149	<div><div>68%</div><div>28%</div><div>..</div></div>
3	C	335	<div><div>70%</div><div>28%</div><div>.</div></div>
4	D	161	<div><div>6%</div><div>46%</div><div>27%</div><div>.</div><div>26%</div></div>
5	E	215	<div><div>9%</div><div>62%</div><div>35%</div><div>.</div></div>
6	F	155	<div><div>44%</div><div>8%</div><div>.</div><div>46%</div></div>
7	G	212	<div><div>8%</div><div>50%</div><div>37%</div><div>.</div><div>10%</div></div>

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Mol	Chain	Length	Quality of chain
8	H	146	
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	104	
18	R	23	
19	S	15	
20	T	9	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 39284 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 III SUBUNIT RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1422	Total	C	N	O	S	0	0
			11130	7013	1966	2092	59		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	60		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			977	628	156	187	6		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	191	Total	C	N	O	S	0	0
			1544	1007	250	281	6		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	42	Total	C	N	O	S	0	0
			321	204	47	64	6		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	164	Total	C	N	O	S	0	0
			1338	857	227	253	1		

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	110	Total	C	N	O	S	0	0
			845	536	152	154	3		

- Molecule 15 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	539	Total	C	N	O	S	0	0
			4329	2756	741	813	19		

- Molecule 16 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	89	Total	C	N	O	S	0	0
			738	474	115	146	3		

- Molecule 17 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	63	Total	C	N	O	0	0
			390	243	73	74		

- Molecule 18 is a DNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	23	Total	C	N	O	P	0	0
			470	224	85	138	23		

- Molecule 19 is a DNA chain called NON-TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	15	Total	C	N	O	P	0	0
			309	148	56	90	15		

- Molecule 20 is a RNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	9	Total	C	N	O	P	0	0
			195	87	39	60	9		

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

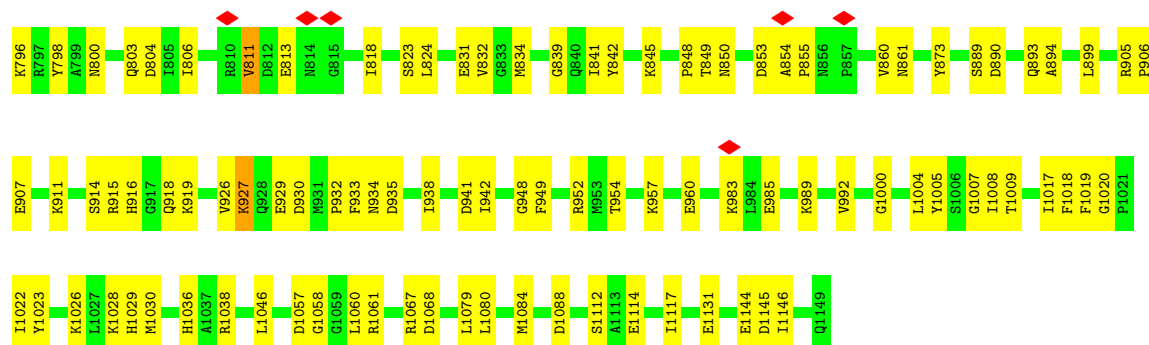
Mol	Chain	Residues	Atoms		AltConf
21	A	2	Total	Zn	0
			2	2	
21	B	1	Total	Zn	0
			1	1	
21	I	1	Total	Zn	0
			1	1	
21	J	1	Total	Zn	0
			1	1	
21	L	1	Total	Zn	0
			1	1	

3 Residue-property plots

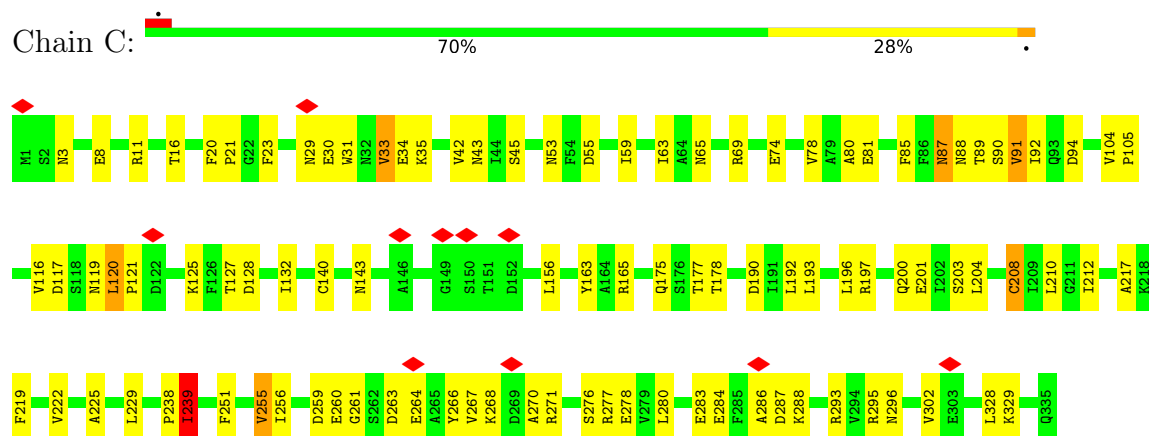
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC1

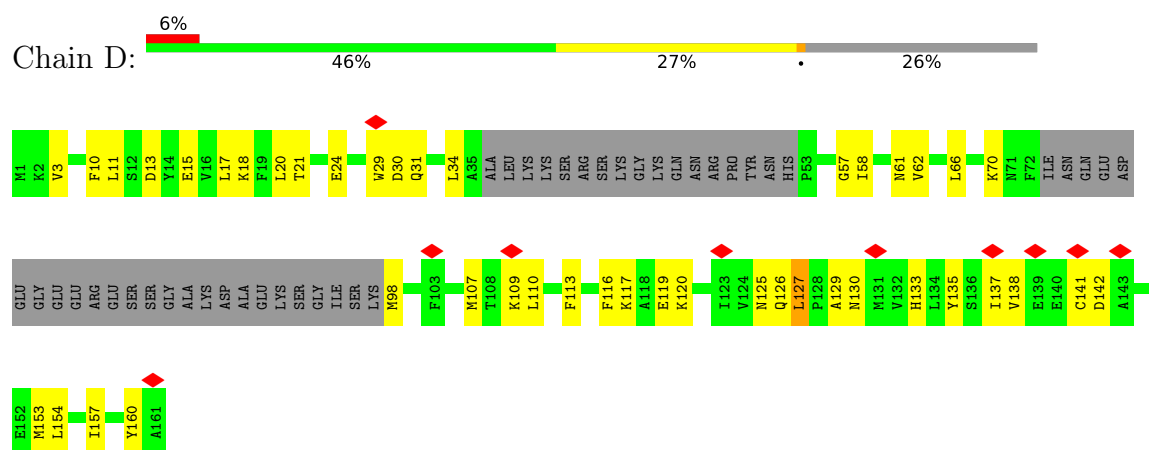




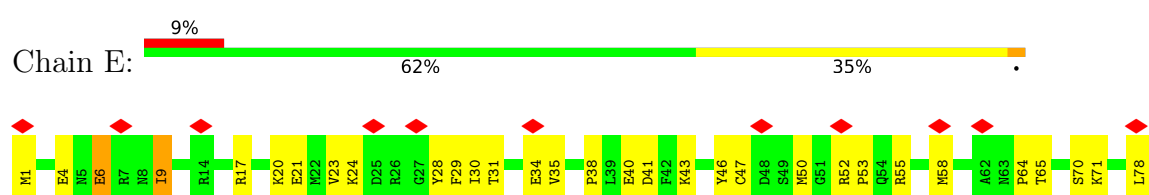
• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

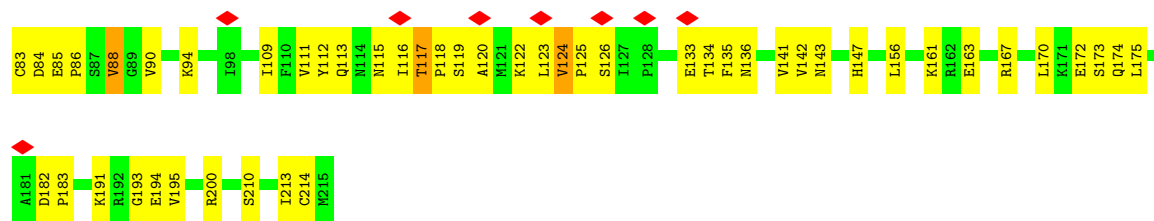


• Molecule 4: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC9



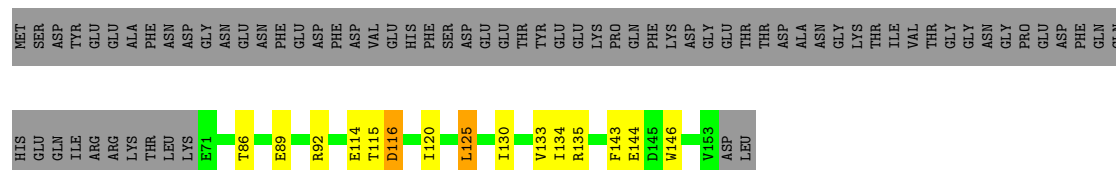
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1





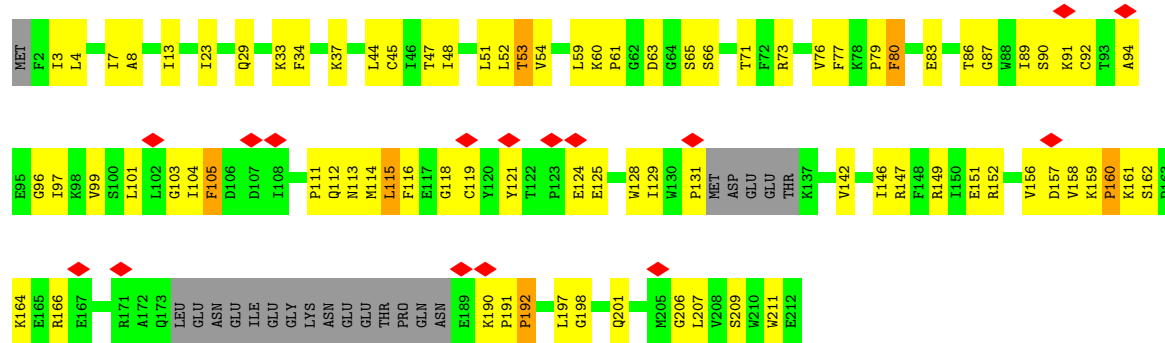
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2

Chain F: 44% 8% 46%



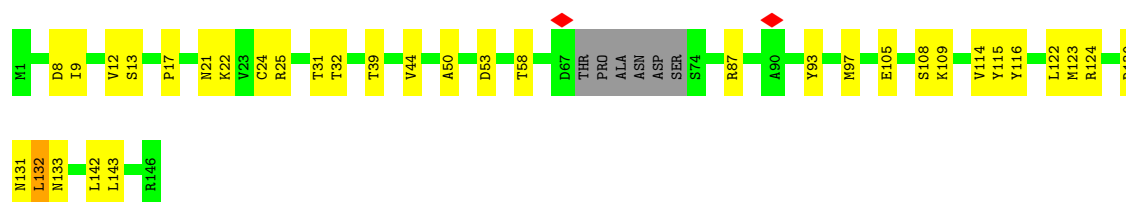
• Molecule 7: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC8

Chain G: 8% 50% 37% 10%



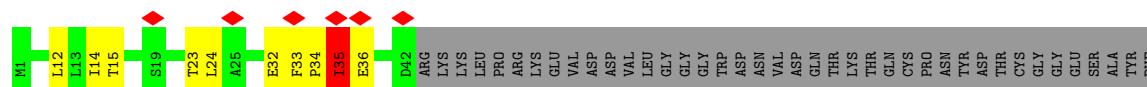
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H: 73% 23% 4%



• Molecule 9: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC10

Chain I: 5% 29% 8% 62%



PHE GLN LEU GLN ILE ARG SER ALA ASP GLU PRO MET THR THR PHE TYR LYS CYS VAL ASN CYS GLY HIS ARG TRP LYS GLU ASN

- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:  73% 21% . .

W R6 C7 G11 K12 V13 D16 K17 V18 E19 E29 L30 D31 L39 K42 R43 R48 L61 P65 L66 E67 LYS ARG ASP

- Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2

Chain K:  51% 20% 29%

MET THR GLU ASP ILE GLU LYS LYS THR ALA THR VAL THR PRO GLN GLU PRO LYS HIS ILE GLN GLU VAL ASP ASP MET THR GLY ASP GLU GLU GLN GLU GLU P42 P43 R44 I47 D57 S60 F63 R64 I65 R77 I80 R81 R82

R83 R84 D85 V86 E87 F88 P94 S97 E98 L101 R104 I105 Q106 T107 Y108 G109 E110 T111 A113 L121 L122 D123 L127 K138 R142

- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:  7% 40% 23% 36%

MET SER ARG GLU GLY PHE GLN ILE THR VAL THR ASN LEU ASP ALA ALA ALA GLY THR SER GLN ALA ARG THR ALA T26 T27 K28 Y29 I30 C34 L40 S41 R42 T43 D44 C48 K49 D50 C51 R54 L57 K58 A59 R60 T61 R70

- Molecule 13: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC5

Chain M:  9% 40% 17% 42%

MET SER ILE ASP ASN LYS PHE VAL PRO THR GLU GLU ASP GLU ASP GLU ASP THR ARG ALA ASP VAL GLU ASP THR ASP MET ILE ALA ALA ASN GLU GLN GLU GLU LYS SER GLU VAL LYS ALA GLU ASP ASP

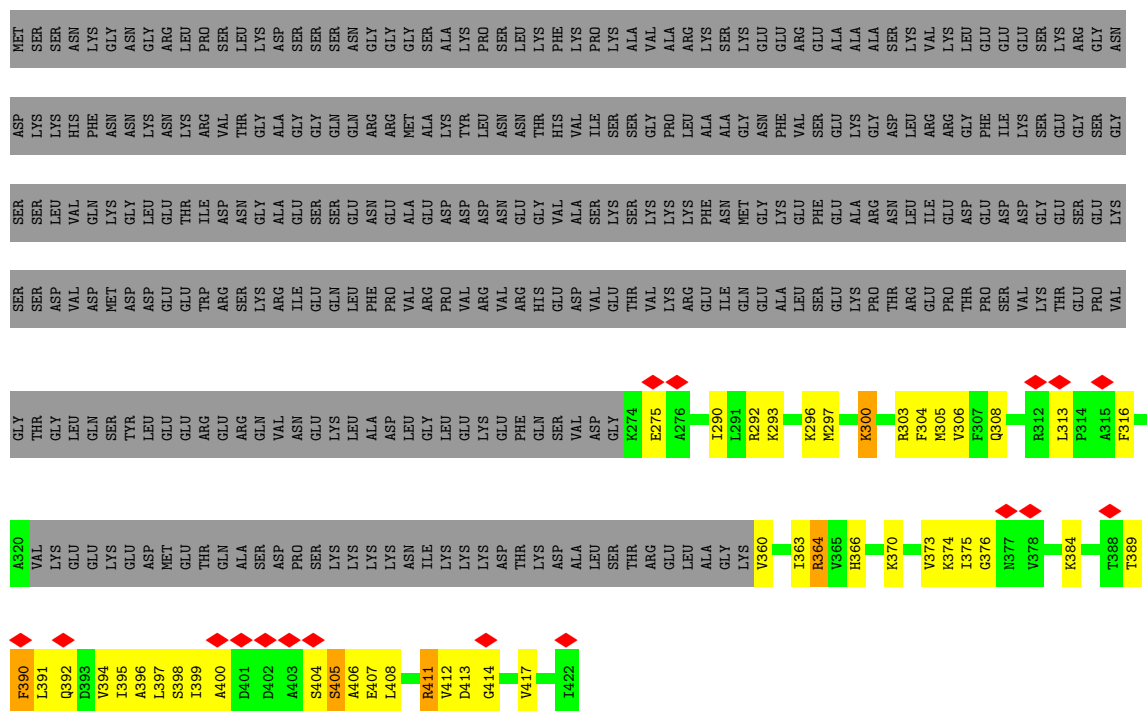
THR GLY GLU GLU V143 N144 V145 L148 G152 A160 K164 L170 V176 L179 K180 P181 Y185 I186 D187 N190 E196 G98 R99 K100 P101 A102 I107 S108 A109 K113 P114 K115 S116 H117 L118 W119 E120 I121 D122 D126 E127 Q128 N132 E137

S138 G142 V143 N144 V145 L148 G152 A160 K164 L170 V176 L179 K180 P181 Y185 I186 D187 N190 E196 G98 R99 K100 P101 A102 I107 S108 A109 K113 P114 K115 S116 H117 L118 W119 E120 I121 D122 D126 E127 Q128 N132 E137

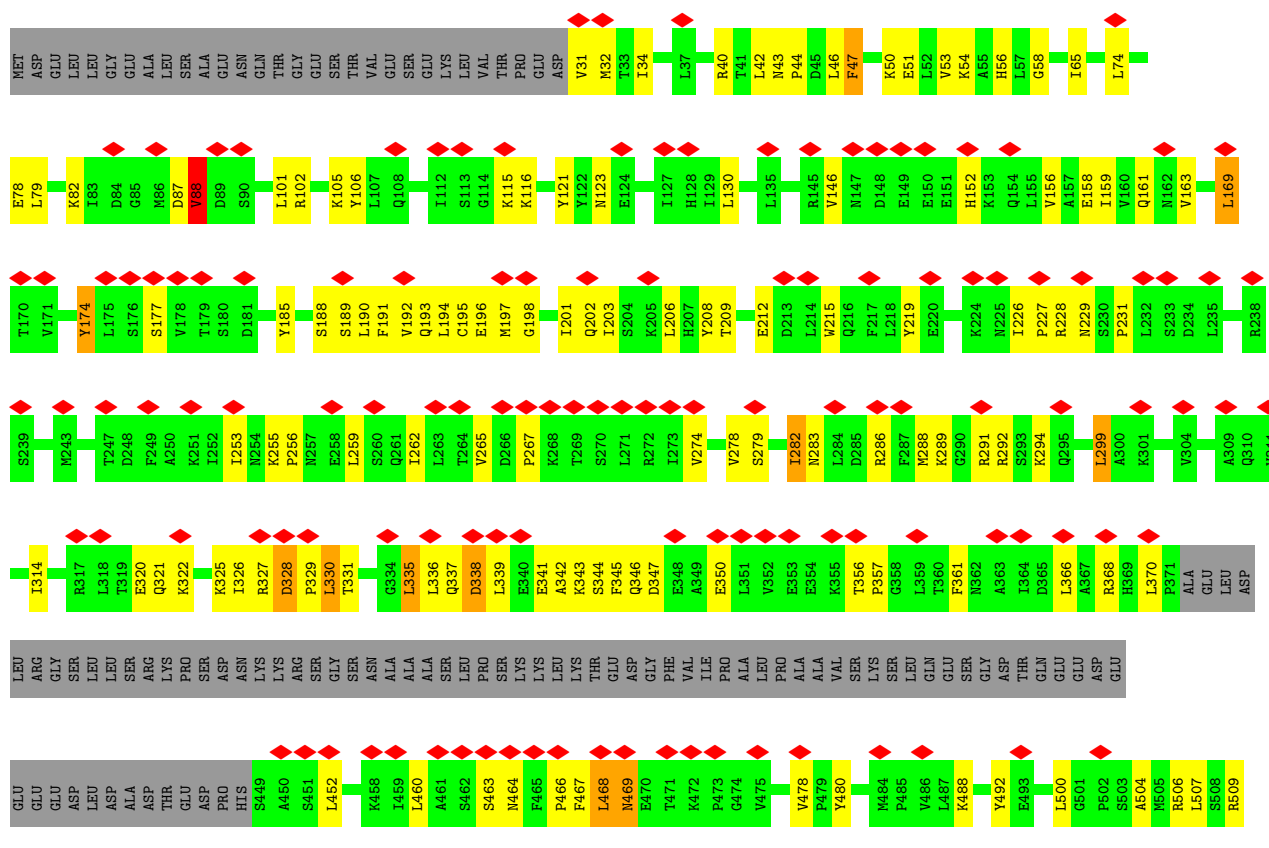
L227 T228 G229 S230 L231 A237 D238 E239 E240 A241 N242 T246 N247 F252 F255 T259 V260 K261 E262 ALA GLU ASP LYS THR LEU VAL ALA LEU GLU LYS GLN GLU ASP TYR THR ASP ASN LEU VAL

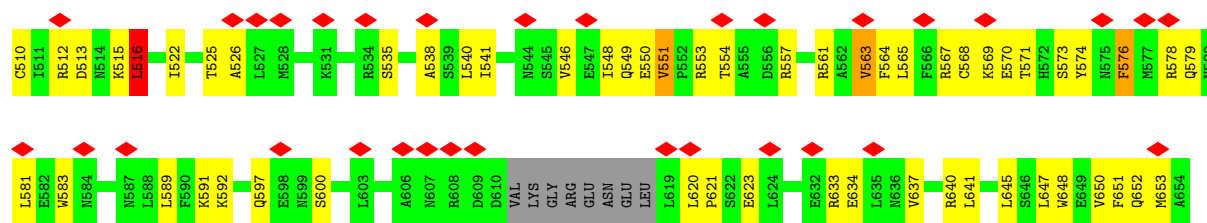
- Molecule 14: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC4

Chain N:  15% 9% 74%

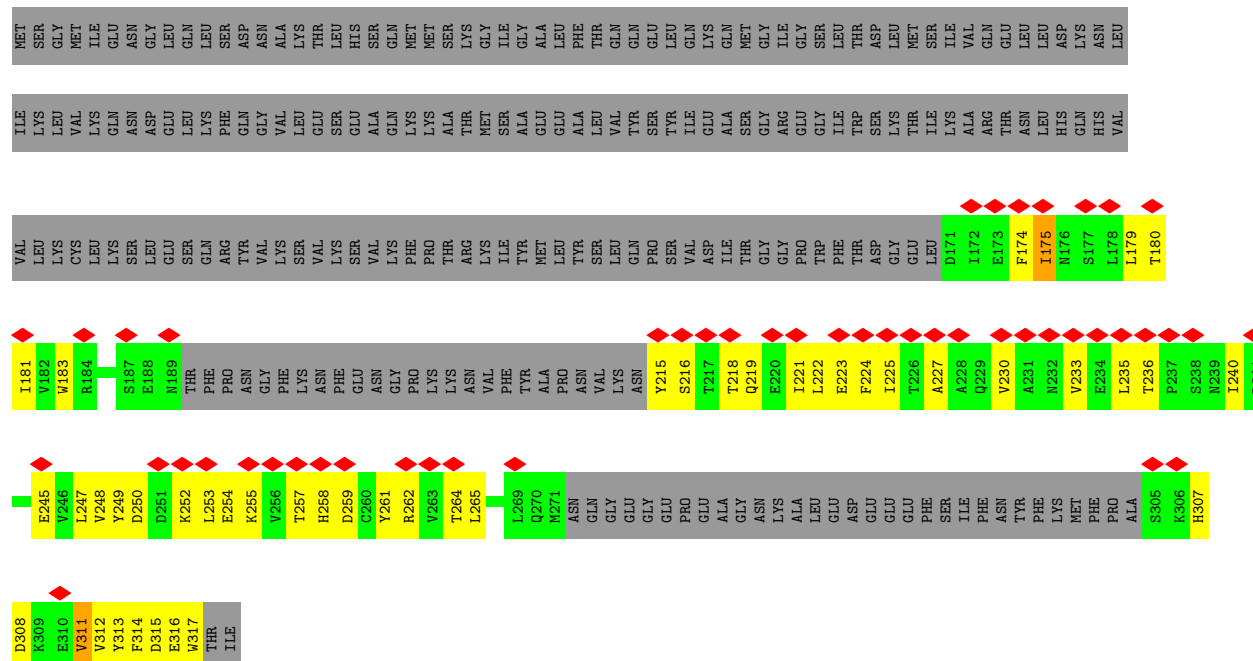


• Molecule 15: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3

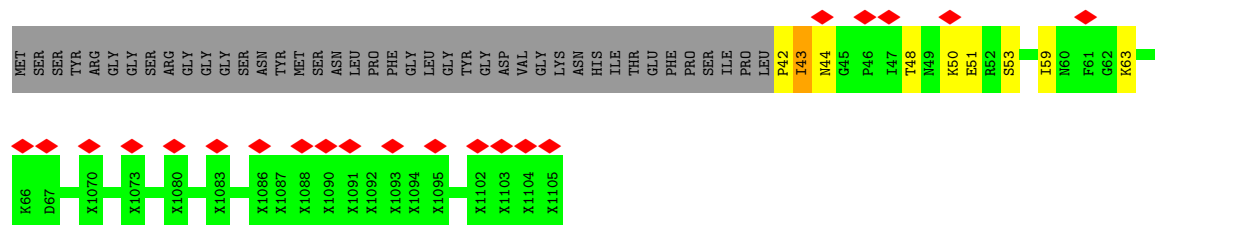




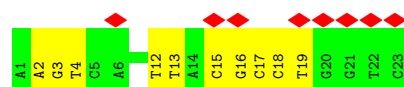
• Molecule 16: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC6



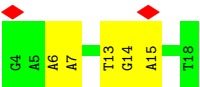
• Molecule 17: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC7



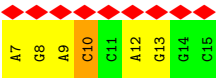
• Molecule 18: RNA



• Molecule 19: NON-TEMPLATE DNA



• Molecule 20: TEMPLATE DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49543	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	4200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.536	Depositor
Minimum map value	-0.327	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	320.86398, 320.86398, 320.86398	wwPDB
Map dimensions	296, 296, 296	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.084, 1.084, 1.084	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

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	0.22	0/11328	0.47	0/15303
2	B	0.22	0/8943	0.45	0/12068
3	C	0.23	0/2711	0.46	1/3676 (0.0%)
4	D	0.23	0/991	0.51	0/1328
5	E	0.23	0/1795	0.45	0/2416
6	F	0.21	0/683	0.42	0/923
7	G	0.23	0/1583	0.49	0/2146
8	H	0.21	0/1138	0.45	0/1540
9	I	0.30	0/328	0.48	0/445
10	J	0.21	0/558	0.45	0/750
11	K	0.22	0/803	0.43	0/1083
12	L	0.24	0/360	0.49	0/478
13	M	0.23	0/1369	0.46	0/1851
14	N	0.26	0/855	0.56	0/1149
15	O	0.23	0/4394	0.50	1/5928 (0.0%)
16	P	0.28	0/750	0.53	0/1017
17	Q	0.27	0/219	0.44	0/294
18	R	0.47	0/526	0.89	0/809
19	S	0.51	0/346	0.94	0/532
20	T	0.13	0/218	0.69	0/338
All	All	0.23	0/39898	0.49	2/54074 (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	A	0	3
2	B	0	2
11	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	N	0	2
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	120	LEU	CA-CB-CG	5.32	127.52	115.30
15	O	516	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	ASP	Peptide
1	A	599	LYS	Peptide
1	A	601	TYR	Peptide
2	B	319	ILE	Peptide
2	B	839	GLY	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	11130	0	11258	310	0
2	B	8788	0	8902	246	0
3	C	2655	0	2628	73	0
4	D	977	0	983	35	0
5	E	1759	0	1788	53	0
6	F	671	0	692	12	0
7	G	1544	0	1540	66	0
8	H	1120	0	1089	24	0
9	I	321	0	304	11	0
10	J	549	0	560	13	0
11	K	792	0	790	22	0
12	L	358	0	381	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1338	0	1307	41	0
14	N	845	0	891	36	0
15	O	4329	0	4497	168	0
16	P	738	0	719	41	0
17	Q	390	0	269	5	0
18	R	470	0	260	10	0
19	S	309	0	171	4	0
20	T	195	0	100	2	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	I	1	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
All	All	39284	0	39129	1051	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 14.

The worst 5 of 1051 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:1163:LYS:HZ1	1:A:1280:ARG:HA	1.36	0.91
1:A:829:ASP:OD2	1:A:838:ASN:ND2	2.03	0.91
1:A:615:LYS:NZ	1:A:620:SER:O	2.05	0.88
4:D:126:GLN:HG3	4:D:127:LEU:HG	1.56	0.88
3:C:16:THR:O	3:C:295:ARG:NH1	2.07	0.87

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	
1	A	1414/1460 (97%)	1166 (82%)	234 (16%)	14 (1%)	13	46
2	B	1112/1149 (97%)	943 (85%)	160 (14%)	9 (1%)	16	51
3	C	333/335 (99%)	284 (85%)	44 (13%)	5 (2%)	8	39
4	D	113/161 (70%)	83 (74%)	30 (26%)	0	100	100
5	E	213/215 (99%)	172 (81%)	39 (18%)	2 (1%)	14	48
6	F	81/155 (52%)	73 (90%)	8 (10%)	0	100	100
7	G	185/212 (87%)	155 (84%)	24 (13%)	6 (3%)	3	26
8	H	136/146 (93%)	115 (85%)	21 (15%)	0	100	100
9	I	40/110 (36%)	33 (82%)	6 (15%)	1 (2%)	4	30
10	J	65/70 (93%)	53 (82%)	11 (17%)	1 (2%)	8	39
11	K	99/142 (70%)	84 (85%)	15 (15%)	0	100	100
12	L	43/70 (61%)	34 (79%)	9 (21%)	0	100	100
13	M	160/282 (57%)	138 (86%)	20 (12%)	2 (1%)	10	41
14	N	106/422 (25%)	82 (77%)	23 (22%)	1 (1%)	14	48
15	O	533/654 (82%)	437 (82%)	89 (17%)	7 (1%)	10	41
16	P	83/317 (26%)	54 (65%)	24 (29%)	5 (6%)	1	16
17	Q	26/104 (25%)	23 (88%)	2 (8%)	1 (4%)	2	23
All	All	4742/6004 (79%)	3929 (83%)	759 (16%)	54 (1%)	15	45

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	587	ILE
1	A	1371	ILE
13	M	97	VAL
13	M	107	ILE
15	O	88	VAL

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	
1	A	1231/1257 (98%)	1213 (98%)	18 (2%)	60	74
2	B	975/1006 (97%)	960 (98%)	15 (2%)	60	74
3	C	296/296 (100%)	289 (98%)	7 (2%)	44	63
4	D	110/145 (76%)	107 (97%)	3 (3%)	40	60
5	E	197/197 (100%)	192 (98%)	5 (2%)	42	62
6	F	73/137 (53%)	70 (96%)	3 (4%)	26	50
7	G	170/190 (90%)	167 (98%)	3 (2%)	54	71
8	H	123/128 (96%)	121 (98%)	2 (2%)	58	73
9	I	38/98 (39%)	37 (97%)	1 (3%)	41	61
10	J	62/65 (95%)	60 (97%)	2 (3%)	34	56
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	40/57 (70%)	38 (95%)	2 (5%)	20	45
13	M	142/249 (57%)	136 (96%)	6 (4%)	25	49
14	N	92/360 (26%)	88 (96%)	4 (4%)	25	49
15	O	495/593 (84%)	477 (96%)	18 (4%)	30	54
16	P	86/285 (30%)	85 (99%)	1 (1%)	67	78
17	Q	24/56 (43%)	24 (100%)	0	100	100
All	All	4245/5249 (81%)	4155 (98%)	90 (2%)	49	67

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	13	VAL
15	O	42	LEU
12	L	34	CYS
13	M	242	ASN
15	O	169	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	117	HIS
13	M	190	ASN
16	P	219	GLN
15	O	580	ASN
1	A	431	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	T	9/9 (100%)	2 (22%)	1 (11%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	T	8	G
20	T	10	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	T	7	A

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	Q	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	1088:UNK	C	1090:UNK	N	14.86
1	Q	69:PRO	C	1070:UNK	N	8.26

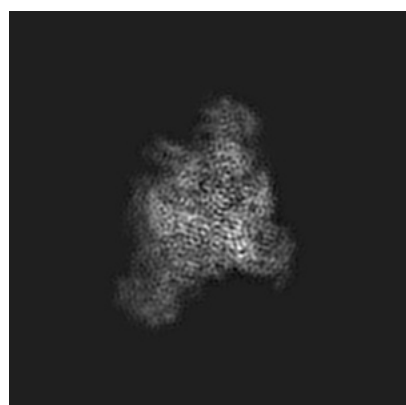
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3178. These allow visual inspection of the internal detail of the map and identification of artifacts.

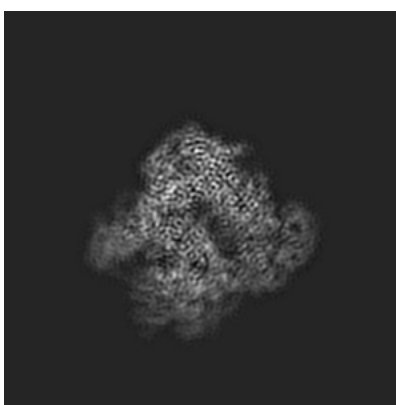
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

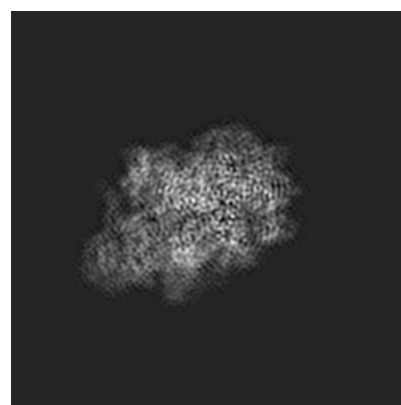
6.1.1 Primary map



X



Y

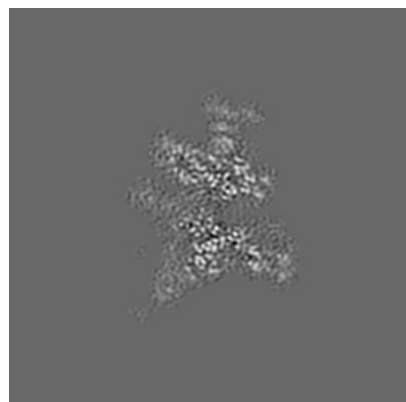


Z

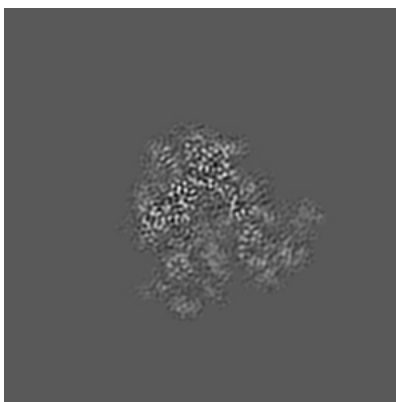
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

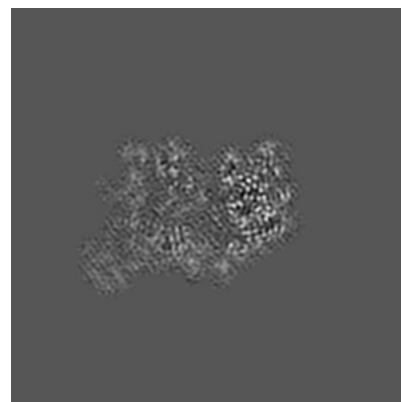
6.2.1 Primary map



X Index: 148



Y Index: 148

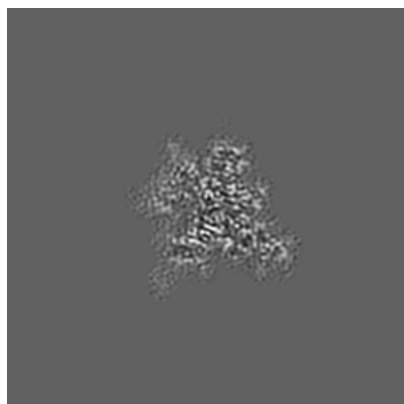


Z Index: 148

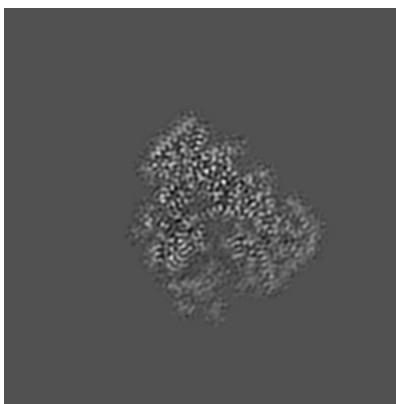
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

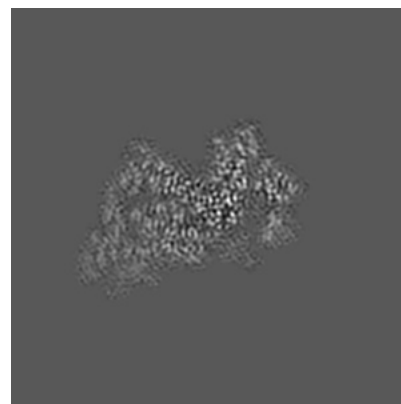
6.3.1 Primary map



X Index: 161



Y Index: 161

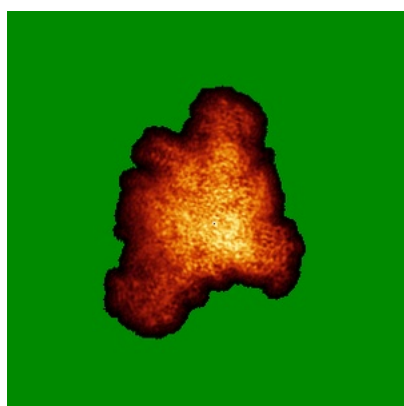


Z Index: 132

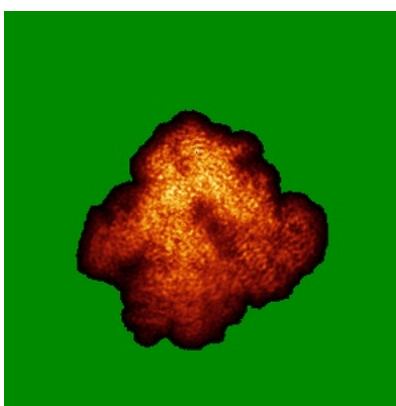
The images above show the largest variance slices of the map in three orthogonal directions.

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

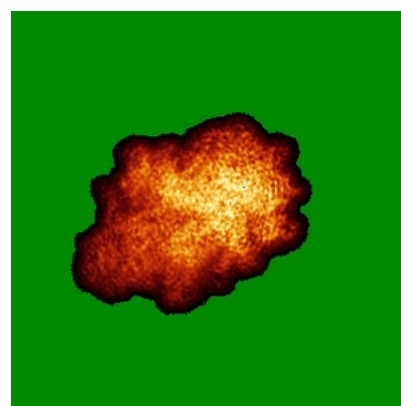
6.4.1 Primary map



X



Y

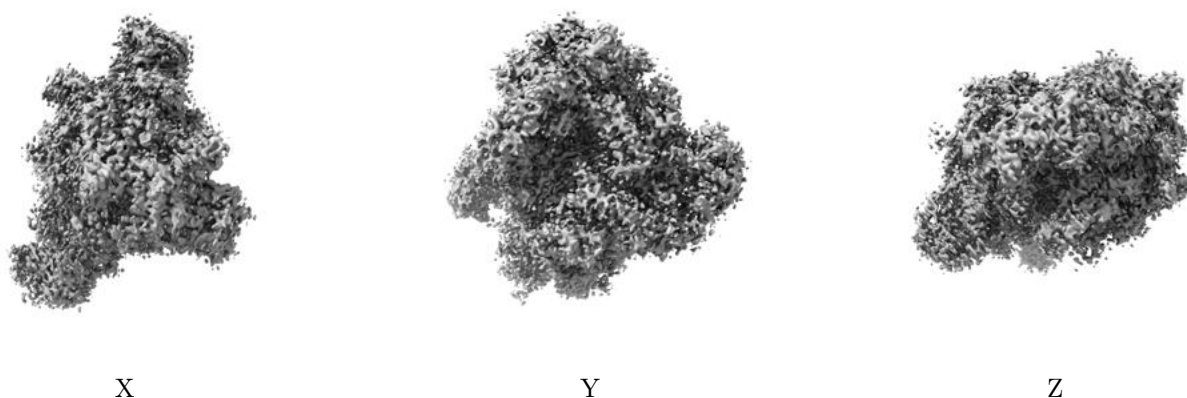


Z

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

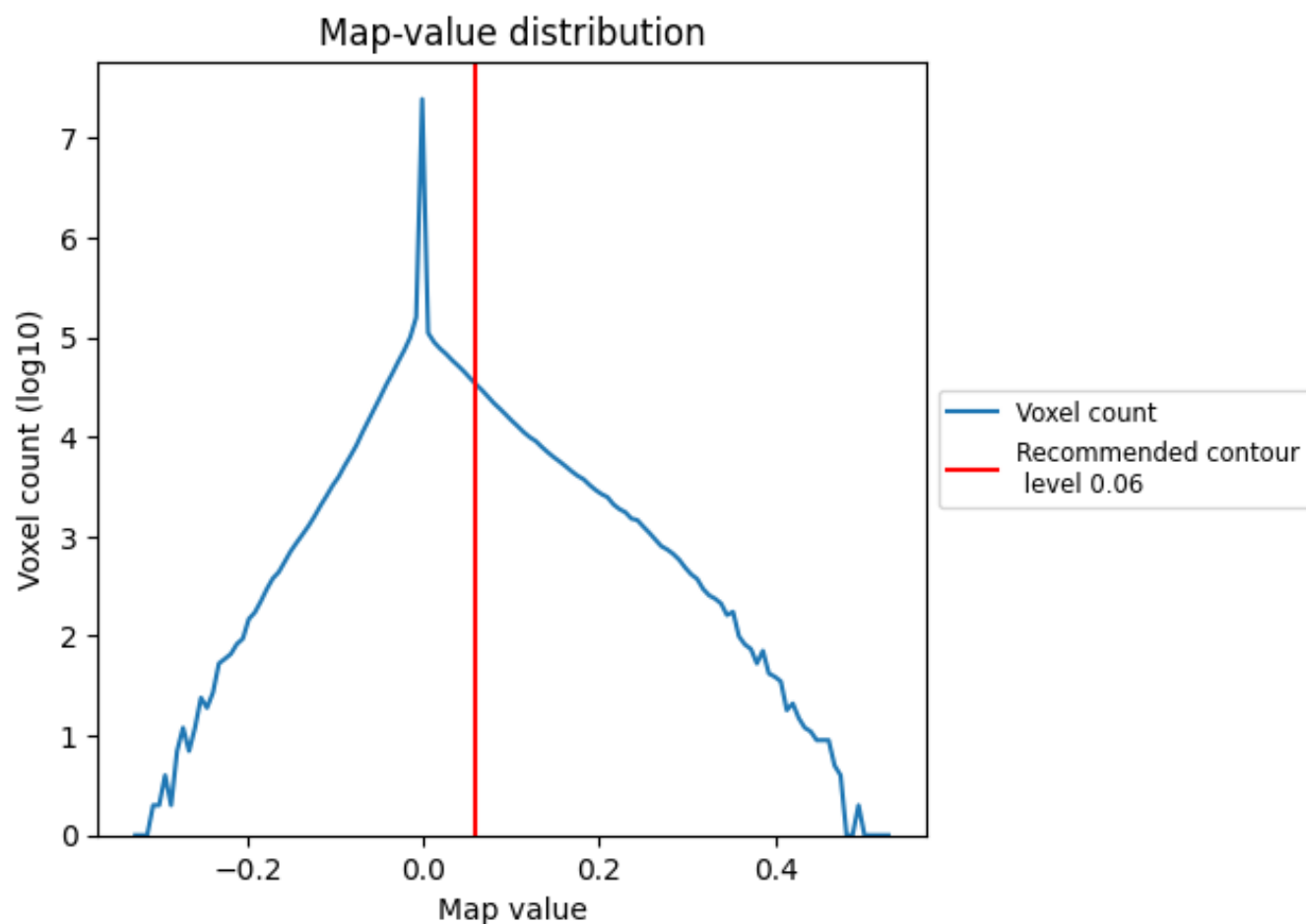
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

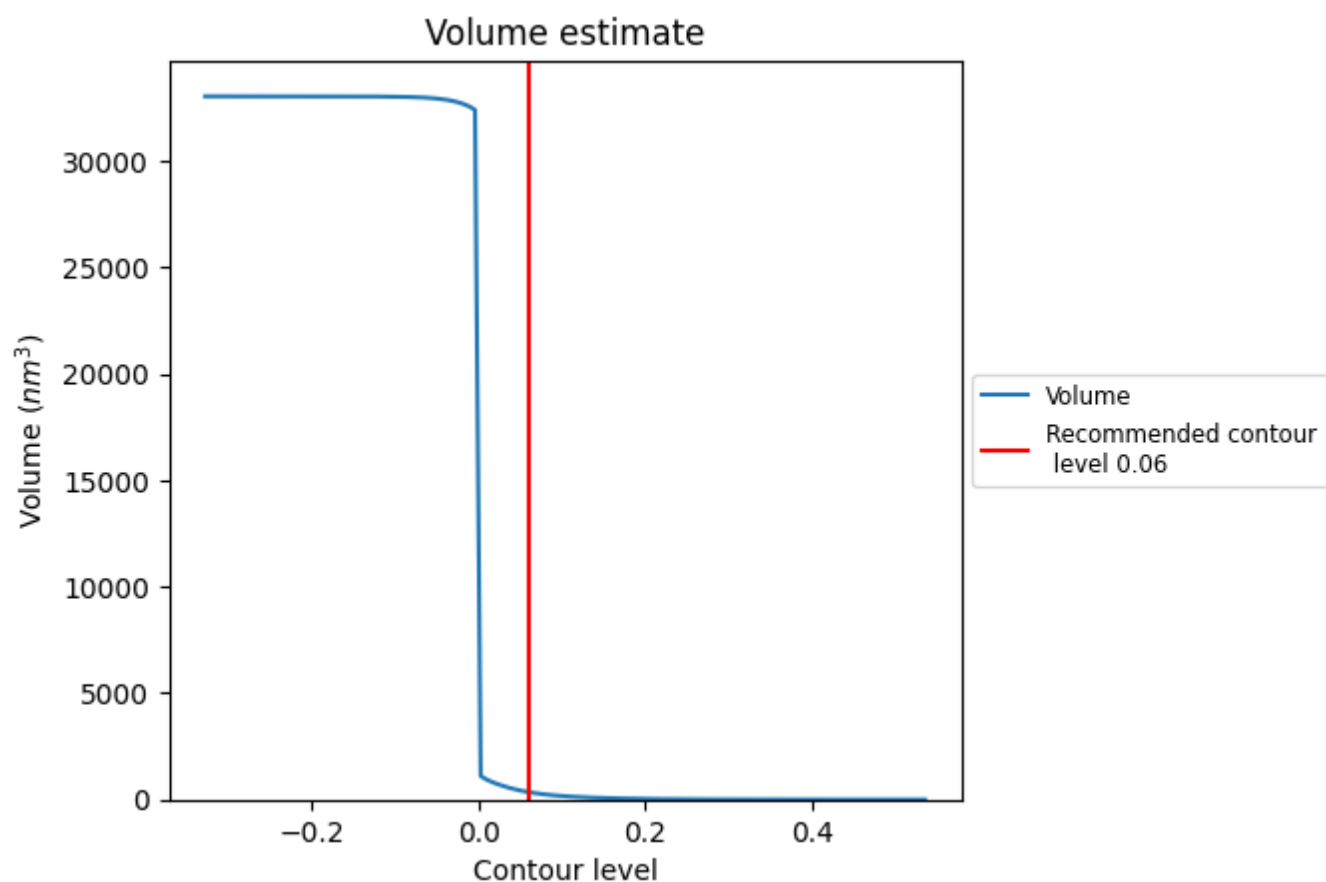
This section contains the results of statistical analysis of the map.

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.

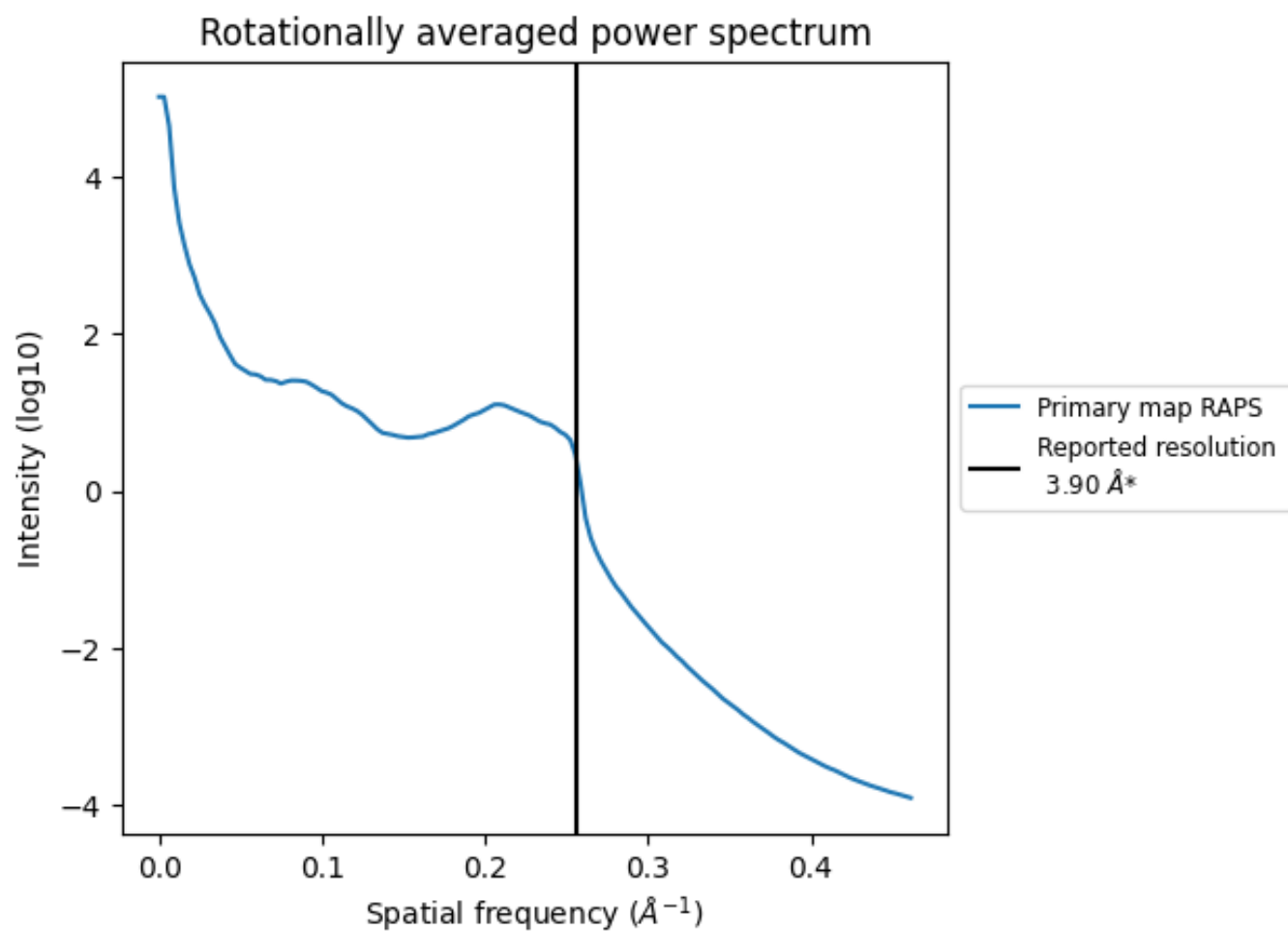
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 352 nm³; this corresponds to an approximate mass of 318 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 ⓘ

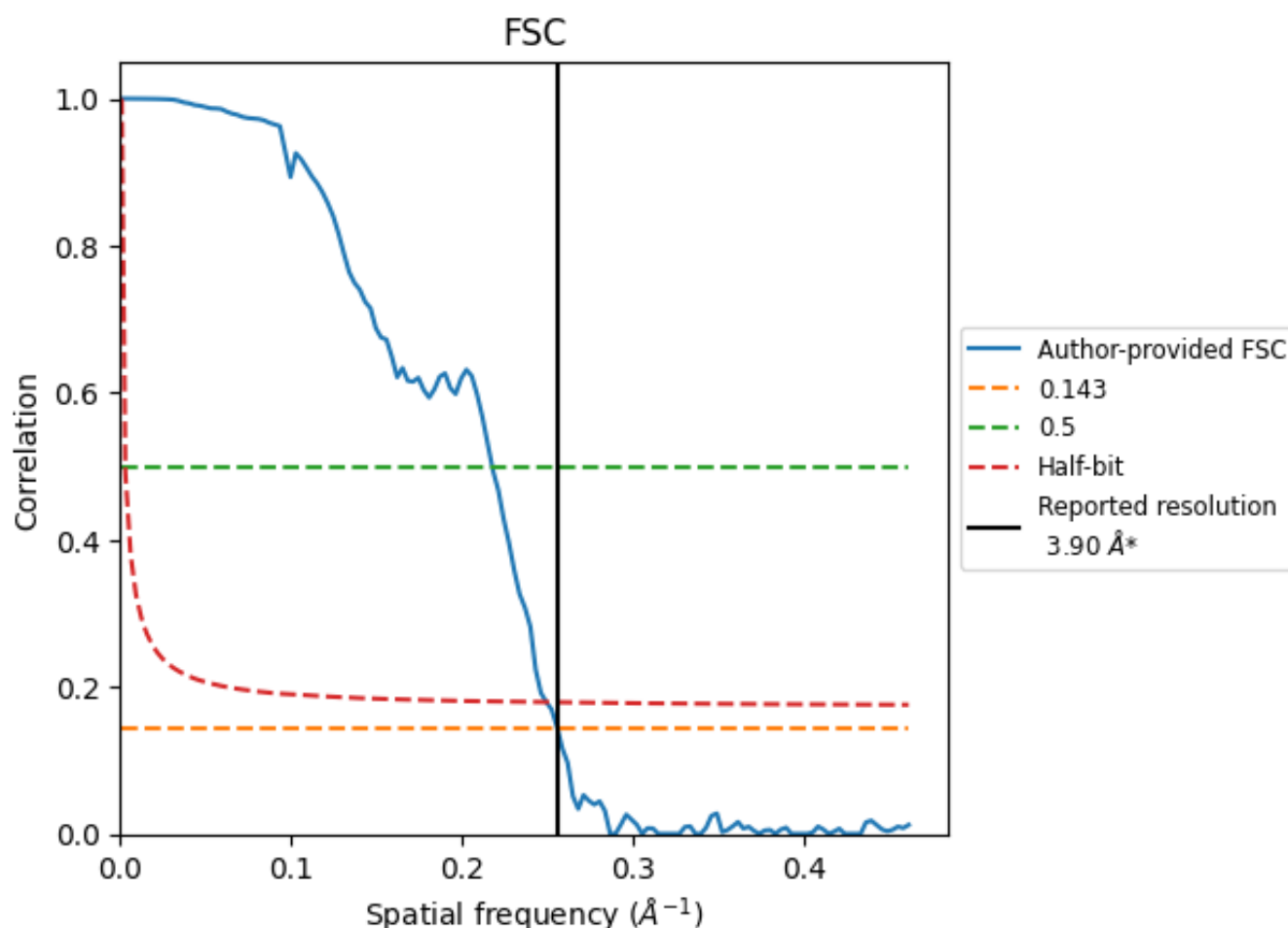


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

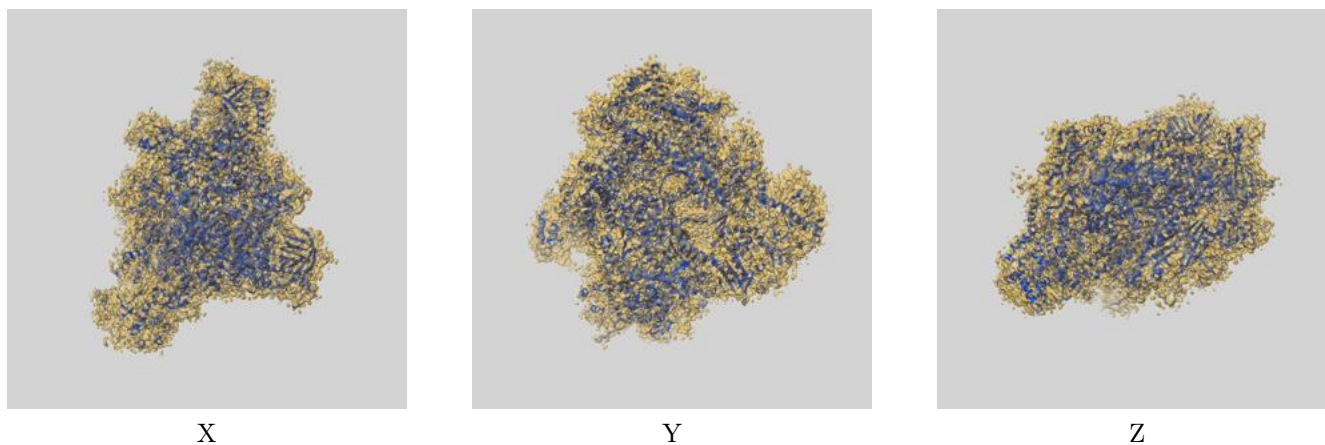
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.91	4.60	4.01
Unmasked-calculated*	-	-	-

*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-3178 and PDB model 5FJ8. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



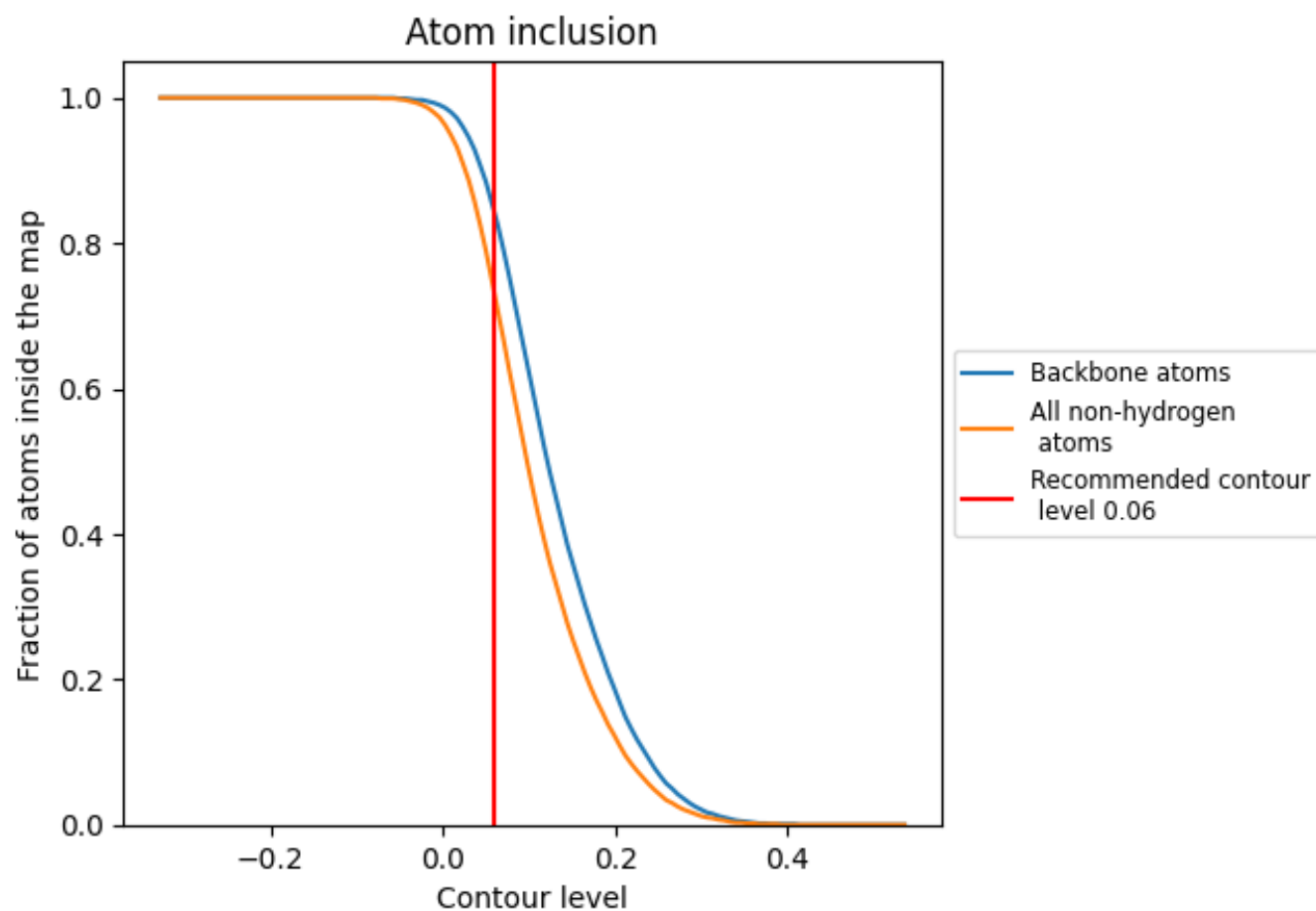
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7300	 0.3450
A	 0.7720	 0.3750
B	 0.8050	 0.3940
C	 0.8330	 0.3950
D	 0.7090	 0.2710
E	 0.7440	 0.3350
F	 0.8520	 0.4190
G	 0.6950	 0.3020
H	 0.8260	 0.3960
I	 0.6660	 0.2970
J	 0.8430	 0.4180
K	 0.8260	 0.4020
L	 0.7280	 0.3370
M	 0.6250	 0.2580
N	 0.6930	 0.2990
O	 0.5380	 0.2430
P	 0.3620	 0.1680
Q	 0.5760	 0.1970
R	 0.4300	 0.2000
S	 0.5400	 0.1870
T	 0.2310	 0.1480

