



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 03:38 AM UTC

PDB ID : 7OB9 / pdb_00007ob9
EMDB ID : EMD-12795
Title : Cryo-EM structure of human RNA Polymerase I in elongation state
Authors : Misiaszek, A.D.; Girbig, M.; Mueller, C.W.
Deposited on : 2021-04-21
Resolution : 2.70 Å (reported)
Based on initial model : 7AEI

This is a Full wwPDB EM Validation 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:

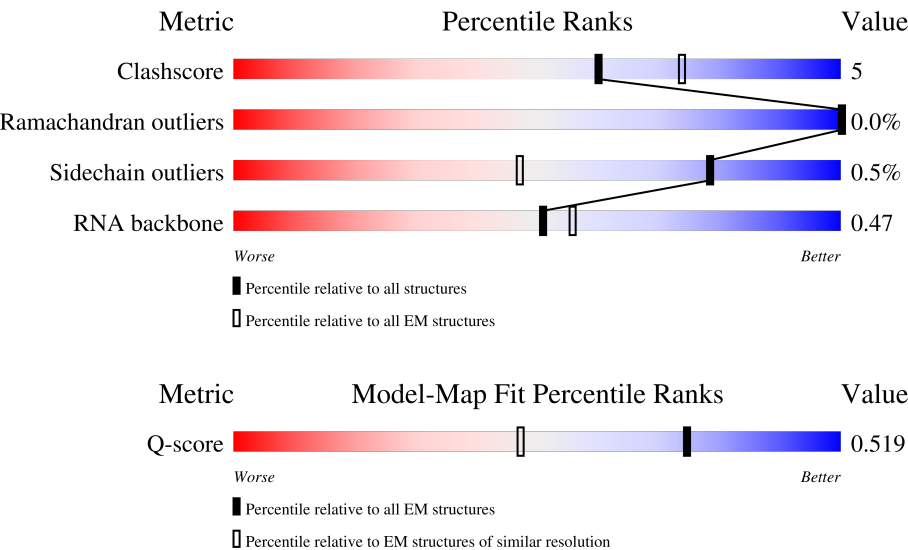
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.70 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	10327 (2.20 - 3.20)

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	1720	78% 11% 11%
2	B	1135	88% 11%
3	C	346	79% 10% 11%

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Mol	Chain	Length	Quality of chain
4	E	210	
5	F	127	
6	G	338	
7	H	150	
8	I	126	
9	J	67	
10	K	133	
11	L	58	
12	N	510	
13	M	419	
14	R	29	
15	S	43	
16	T	43	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 36345 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 I subunit RPA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1535	Total	C	N	O	S	0	0
			12222	7768	2140	2233	81		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1129	Total	C	N	O	S	0	0
			8957	5737	1526	1622	72		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	307	Total	C	N	O	S	0	0
			2458	1552	438	458	10		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	PHE	SER	conflict	UNP P19388

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	79	Total	C	N	O	S	0	0
			636	407	108	116	5		

- Molecule 6 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	176	Total	C	N	O	S	0	0
			1369	865	237	257	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	149	Total	C	N	O	S	0	0
			1197	759	195	238	5		

- Molecule 8 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	55	Total	C	N	O	S	0	0
			414	259	70	81	4		

- 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 polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	107	Total	C	N	O	S	0	0
			856	531	153	165	7		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	47	Total	C	N	O	S	0	0
			397	246	77	68	6		

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	149	Total	C	N	O	S	0	0
			1083	684	193	201	5		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	388	Total	C	N	O	S	0	0
			3062	1917	550	577	18		

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	21	Total	C	N	O	P	0	0
			449	201	84	143	21		

- Molecule 15 is a DNA chain called DNA non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	19	Total	C	N	O	P	0	0
			390	187	68	116	19		

- Molecule 16 is a DNA chain called DNA template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	29	Total	C	N	O	P	0	0
			595	284	106	176	29		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

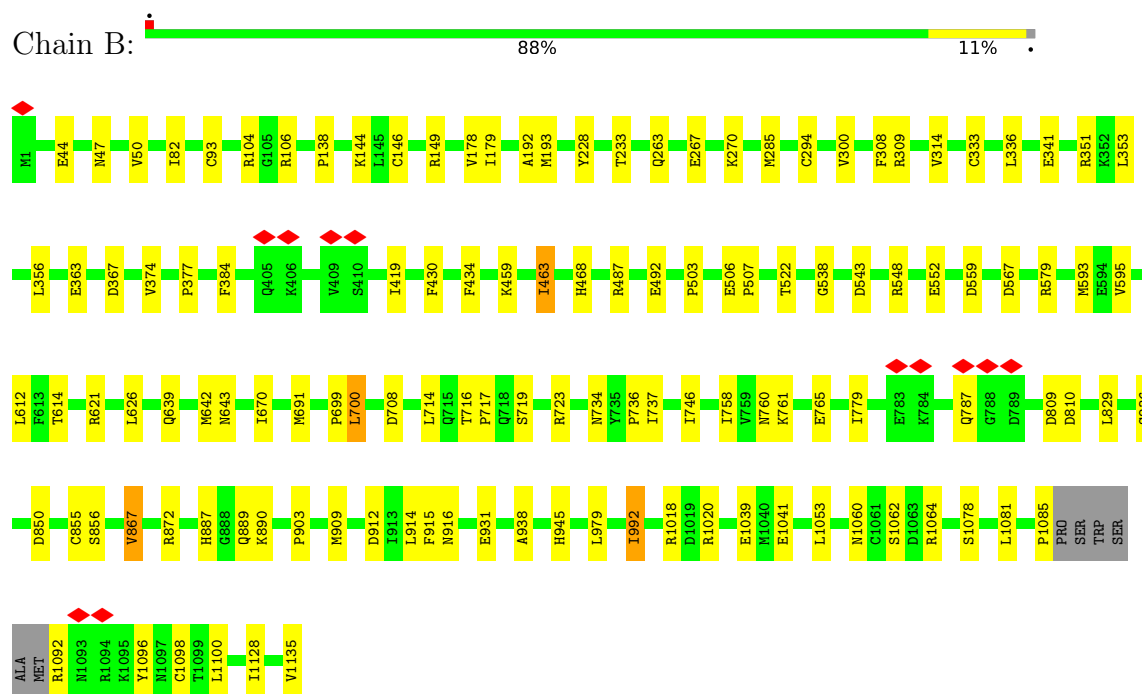
Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Zn	0
			2	2	
17	B	1	Total	Zn	0
			1	1	
17	I	1	Total	Zn	0
			1	1	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

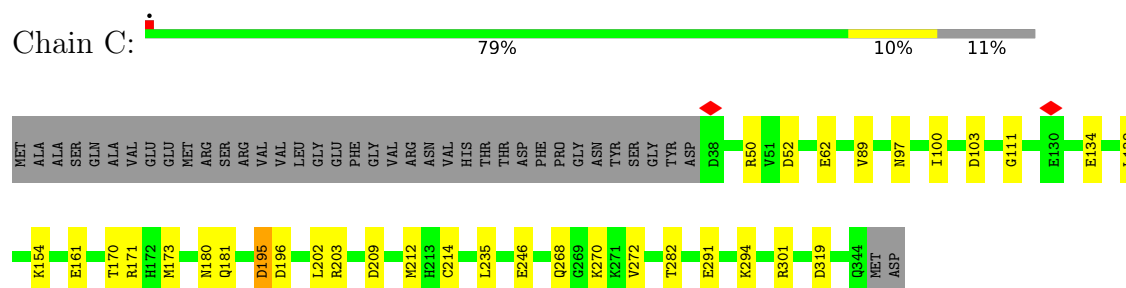
Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	



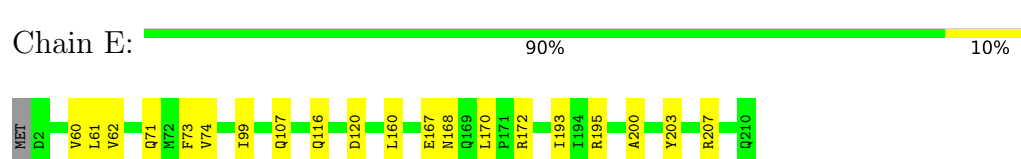
• Molecule 2: DNA-directed RNA polymerase I subunit RPA2



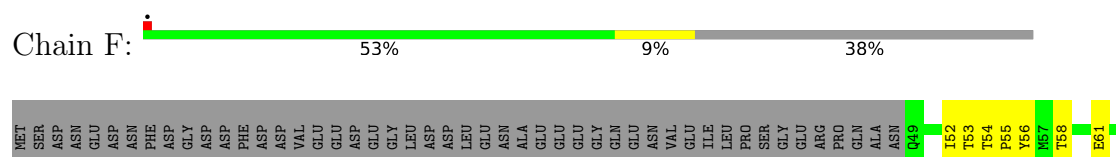
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

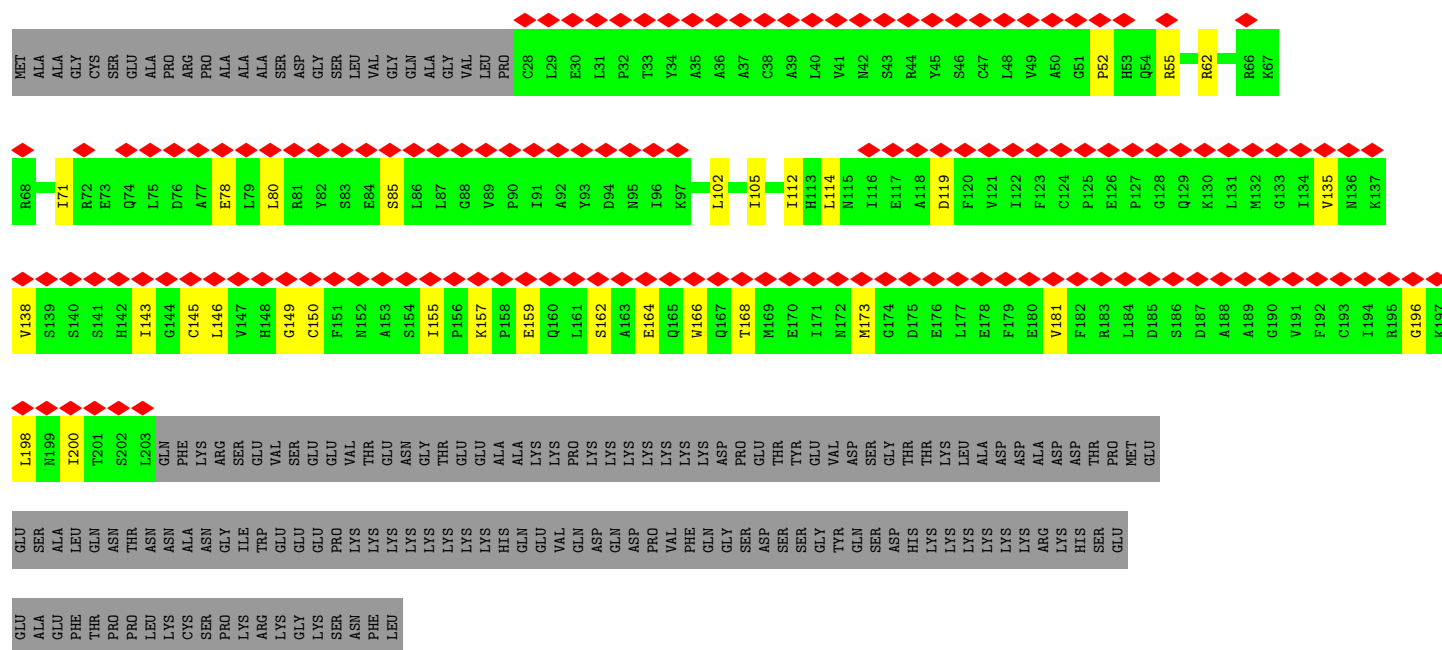
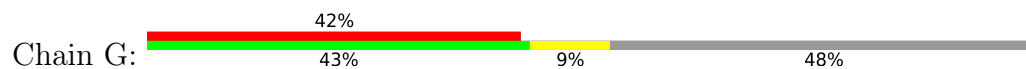


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

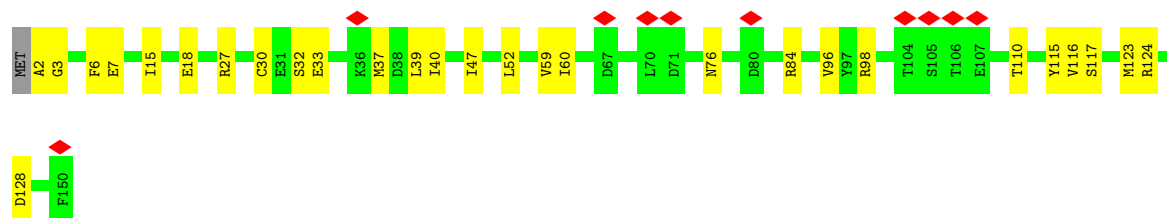
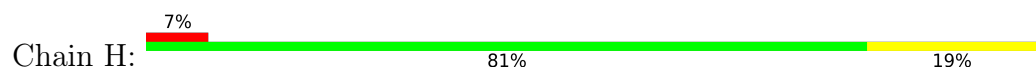




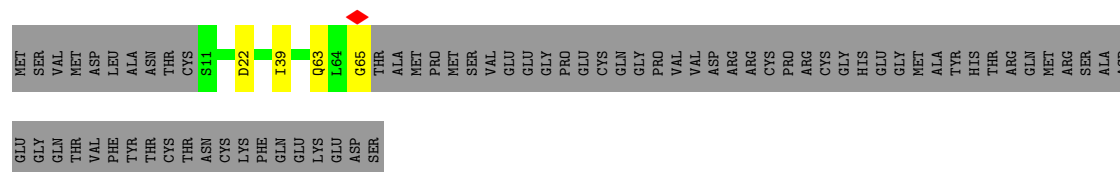
- Molecule 6: DNA-directed RNA polymerase I subunit RPA43



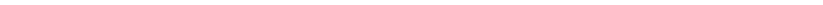
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC3

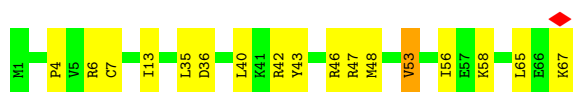


- Molecule 8: DNA-directed RNA polymerase I subunit RPA12

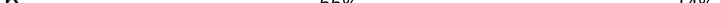


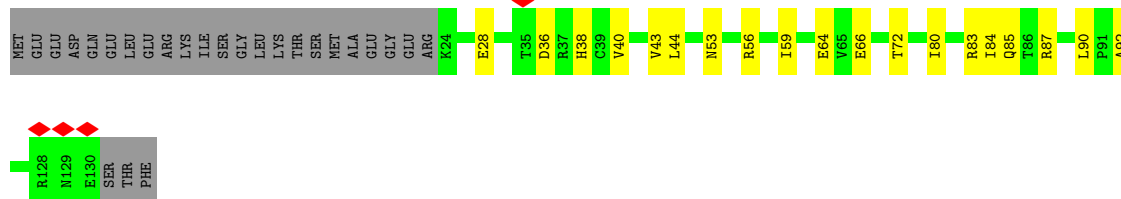
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  75% 24%

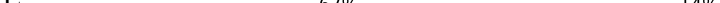


- Molecule 10: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:  66% 14% 20%

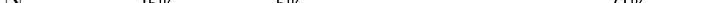


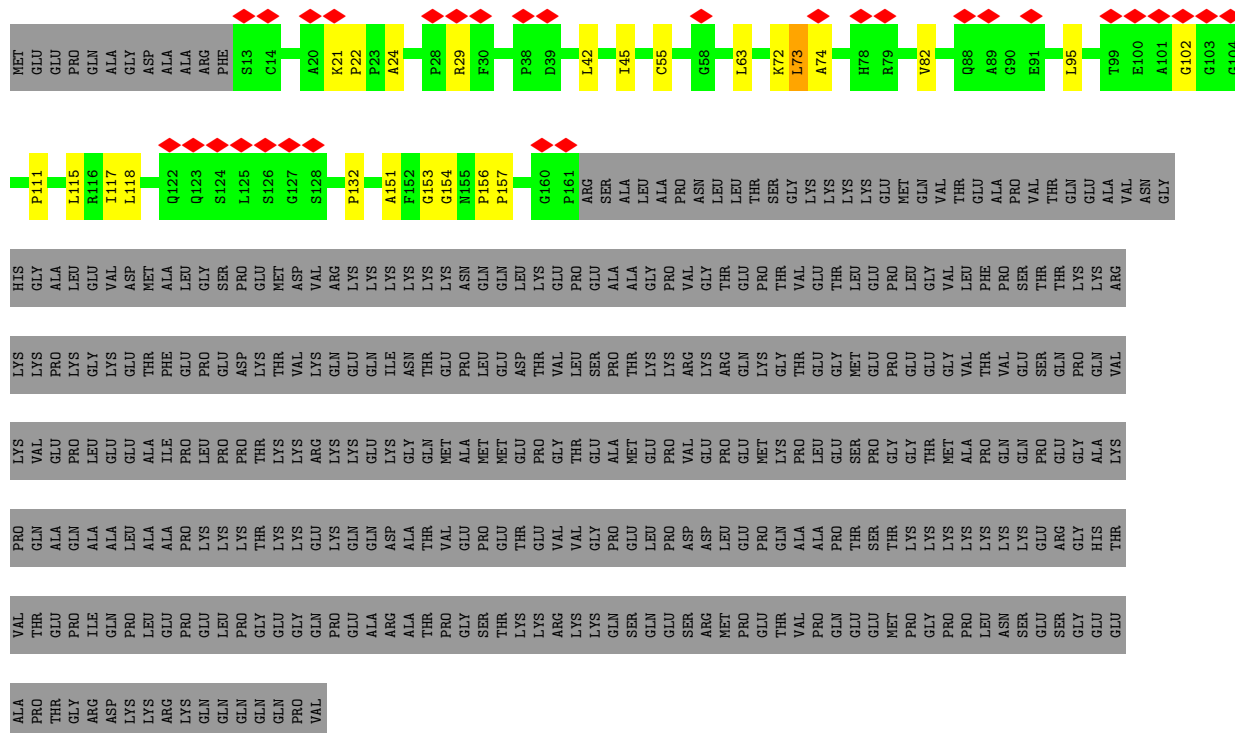
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC4

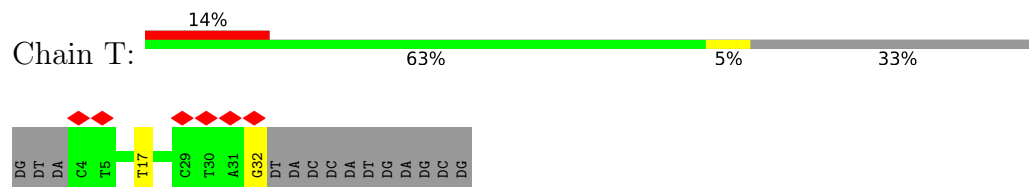
Chain L:  67% 14% 19%



- Molecule 12: DNA-directed RNA polymerase I subunit RPA34

Chain N:  6% 25% 5% 71%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	198822	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 ($e^-/\text{\AA}^2$)	50.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.057	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00839	Depositor
Map size ($\text{\AA}$)	230.16, 230.16, 230.16	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	0/12480	0.64	0/16858
2	B	0.62	0/9174	0.65	1/12414 (0.0%)
3	C	0.55	0/2506	0.63	2/3397 (0.1%)
4	E	0.46	0/1751	0.58	0/2366
5	F	0.51	0/646	0.64	0/873
6	G	0.29	0/1396	0.65	2/1891 (0.1%)
7	H	0.50	0/1219	0.62	0/1644
8	I	0.32	0/421	0.48	0/569
9	J	0.72	0/542	0.77	0/730
10	K	0.54	0/871	0.54	0/1174
11	L	0.59	0/403	0.66	0/536
12	N	0.37	1/1118 (0.1%)	0.60	0/1532
13	M	0.27	0/3112	0.63	0/4197
14	R	0.46	0/501	0.48	0/776
15	S	0.27	0/435	0.50	0/667
16	T	0.56	0/666	0.45	0/1026
All	All	0.52	1/37241 (0.0%)	0.63	5/50650 (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	4
2	B	0	1
4	E	0	1
6	G	0	1
12	N	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	22	PRO	C-N	6.94	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	309	ARG	N-CA-C	-7.30	106.30	114.62
3	C	195	ASP	CA-C-N	6.45	133.87	121.54
3	C	195	ASP	C-N-CA	6.45	133.87	121.54
6	G	159	GLU	CA-C-N	5.16	131.40	121.54
6	G	159	GLU	C-N-CA	5.16	131.40	121.54

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1003	TYR	Peptide
1	A	422	GLU	Peptide
1	A	423	LYS	Peptide
1	A	631	ILE	Peptide
2	B	708	ASP	Peptide
4	E	107	GLN	Peptide
6	G	168	THR	Peptide
12	N	154	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	A	12222	0	12336	121	0
2	B	8957	0	8942	79	0
3	C	2458	0	2456	21	0
4	E	1720	0	1737	14	0
5	F	636	0	667	10	0
6	G	1369	0	1355	17	0
7	H	1197	0	1156	17	0
8	I	414	0	395	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	533	0	553	13	0
10	K	856	0	840	12	0
11	L	397	0	401	7	0
12	N	1083	0	1079	15	0
13	M	3062	0	3094	46	0
14	R	449	0	229	5	0
15	S	390	0	218	8	0
16	T	595	0	329	6	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	I	1	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	36345	0	35787	326	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 5.

All (326) 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)
15:S:13:DC:C2	16:T:32:DG:N2	2.53	0.75
1:A:24:GLU:HG3	2:B:1100:LEU:HD11	1.71	0.71
15:S:27:DG:H1	16:T:17:DT:H3	1.39	0.71
1:A:678:PRO:HD2	7:H:47:ILE:HD12	1.79	0.65
15:S:13:DC:O2	16:T:32:DG:N2	2.30	0.64
1:A:381:GLN:HB3	1:A:386:LYS:HG2	1.80	0.63
1:A:119:LEU:HB2	1:A:142:LEU:HD13	1.80	0.63
1:A:668:VAL:H	10:K:85:GLN:HE22	1.47	0.62
1:A:951:VAL:HG12	1:A:953:GLY:H	1.63	0.62
1:A:659:ARG:NH1	1:A:790:GLN:OE1	2.33	0.62
2:B:463:ILE:HG23	2:B:670:ILE:HD12	1.81	0.62
2:B:459:LYS:HD2	2:B:700:LEU:HD23	1.82	0.62
1:A:74:CYS:O	1:A:308:ARG:NH1	2.33	0.61
7:H:7:GLU:HG3	7:H:59:VAL:HG22	1.81	0.61
13:M:257:ILE:HG12	13:M:348:HIS:HD2	1.66	0.60
15:S:13:DC:O2	16:T:32:DG:C2	2.54	0.60
2:B:93:CYS:SG	11:L:42:ARG:NH1	2.74	0.60
7:H:30:CYS:HB2	7:H:39:LEU:HB3	1.83	0.60
5:F:54:THR:HG22	5:F:56:TYR:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:35:LEU:HD13	9:J:46:ARG:HG3	1.82	0.60
1:A:181:VAL:HG21	4:E:168:ASN:HB3	1.84	0.59
1:A:346:ALA:HB1	13:M:181:VAL:HG23	1.84	0.59
2:B:178:VAL:HG11	2:B:468:HIS:HB3	1.84	0.59
13:M:161:ASN:HB3	13:M:163:SER:H	1.68	0.59
1:A:933:LYS:NZ	2:B:642:MET:O	2.35	0.59
1:A:442:ARG:HH11	1:A:595:ASN:HD21	1.49	0.58
2:B:367:ASP:OD1	15:S:26:DA:N6	2.34	0.58
2:B:734:ASN:OD1	9:J:58:LYS:NZ	2.37	0.58
3:C:50:ARG:NH1	3:C:52:ASP:OD2	2.36	0.58
13:M:345:LEU:HD11	13:M:399:LEU:HD13	1.86	0.58
1:A:1151:ARG:NH2	5:F:52:ILE:O	2.36	0.58
3:C:291:GLU:HA	3:C:294:LYS:HE3	1.86	0.58
13:M:310:LEU:HA	13:M:314:PHE:HD2	1.67	0.58
1:A:745:LEU:HD12	7:H:117:SER:HB3	1.86	0.58
2:B:106:ARG:HB2	11:L:43:ILE:HD11	1.85	0.58
2:B:1020:ARG:NH2	14:R:9:A:O2'	2.37	0.58
3:C:138:LEU:HB2	3:C:214:CYS:HB2	1.86	0.58
1:A:215:VAL:HG22	1:A:225:ILE:HG22	1.86	0.57
1:A:550:LEU:HD12	1:A:594:MET:HE3	1.85	0.57
2:B:1018:ARG:NH2	2:B:1062:SER:O	2.34	0.57
13:M:160:GLY:HA3	13:M:164:LEU:HD23	1.86	0.57
1:A:216:ARG:HD3	13:M:158:ARG:HE	1.68	0.57
1:A:1301:GLU:OE2	1:A:1313:GLN:NE2	2.37	0.57
15:S:13:DC:C2	16:T:32:DG:C2	2.92	0.57
2:B:333:CYS:HB3	2:B:336:LEU:HD12	1.85	0.57
6:G:52:PRO:HA	6:G:119:ASP:HA	1.87	0.57
6:G:143:ILE:HB	6:G:155:ILE:HB	1.86	0.57
1:A:549:LEU:HD11	2:B:1053:LEU:HD21	1.87	0.57
1:A:1239:MET:HE3	1:A:1581:GLU:HG2	1.87	0.56
7:H:15:ILE:HD12	7:H:52:LEU:HD22	1.87	0.56
9:J:43:TYR:HA	9:J:46:ARG:HB3	1.87	0.56
13:M:39:MET:HG2	13:M:64:THR:HG22	1.88	0.56
3:C:209:ASP:OD2	11:L:50:LYS:NZ	2.39	0.56
2:B:487:ARG:NH2	2:B:506:GLU:O	2.39	0.56
2:B:193:MET:HA	2:B:363:GLU:HG3	1.87	0.56
1:A:1119:GLU:OE1	1:A:1122:ARG:NH2	2.39	0.56
1:A:921:LEU:HD21	1:A:969:MET:HB3	1.89	0.55
2:B:887:HIS:NE2	2:B:931:GLU:OE1	2.37	0.55
2:B:1081:LEU:HD12	2:B:1096:TYR:HE1	1.70	0.55
1:A:1124:TRP:O	1:A:1132:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:621:ARG:HH21	2:B:639:GLN:HE21	1.54	0.55
7:H:60:ILE:HD11	7:H:123:MET:HE1	1.88	0.55
13:M:348:HIS:ND1	13:M:351:GLN:O	2.40	0.55
1:A:1097:GLN:NE2	1:A:1123:MET:SD	2.79	0.55
1:A:284:ASP:HB3	1:A:291:ARG:HD2	1.89	0.55
1:A:1187:LEU:HD21	1:A:1192:LEU:HD13	1.88	0.55
1:A:1059:ARG:NH2	1:A:1154:ILE:O	2.40	0.55
3:C:246:GLU:HG2	3:C:272:VAL:HG12	1.89	0.55
1:A:635:MET:HE3	1:A:902:ALA:HA	1.88	0.54
12:N:29:ARG:HE	12:N:102:GLY:HA3	1.72	0.54
2:B:810:ASP:OD2	11:L:17:TYR:OH	2.24	0.54
3:C:97:ASN:ND2	3:C:103:ASP:OD1	2.41	0.54
1:A:535:THR:HG23	6:G:62:ARG:HH22	1.72	0.54
13:M:10:ARG:NH2	13:M:96:SER:O	2.40	0.54
4:E:116:GLN:O	4:E:120:ASP:HB2	2.08	0.54
2:B:106:ARG:HG3	2:B:855:CYS:HB3	1.88	0.54
2:B:548:ARG:NH2	2:B:567:ASP:OD1	2.35	0.54
2:B:1078:SER:OG	2:B:1098:CYS:SG	2.62	0.54
4:E:170:LEU:O	4:E:172:ARG:NH1	2.41	0.54
2:B:192:ALA:HB1	2:B:356:LEU:HD22	1.89	0.54
2:B:233:THR:HG23	2:B:285:MET:HG2	1.90	0.54
13:M:152:ASN:HD22	13:M:155:ARG:HH21	1.56	0.54
1:A:1151:ARG:NH1	1:A:1153:ASP:OD2	2.42	0.53
2:B:856:SER:OG	11:L:34:ILE:O	2.23	0.53
12:N:95:LEU:HB2	13:M:24:VAL:HG23	1.89	0.53
13:M:22:ARG:NH1	13:M:105:GLU:OE2	2.41	0.53
2:B:719:SER:OG	2:B:723:ARG:NH2	2.41	0.53
13:M:277:ILE:HG13	13:M:347:ILE:HD13	1.89	0.53
13:M:129:LYS:HB2	13:M:132:ARG:HB3	1.91	0.53
1:A:622:LYS:HD2	1:A:1222:PRO:HG3	1.91	0.53
13:M:143:GLY:HA3	13:M:149:ARG:HD3	1.89	0.53
12:N:21:LYS:HB3	12:N:24:ALA:HB3	1.91	0.52
2:B:146:CYS:O	2:B:149:ARG:NH2	2.37	0.52
3:C:170:THR:HB	3:C:195:ASP:HA	1.91	0.52
1:A:379:PRO:HB2	1:A:386:LYS:HD2	1.92	0.52
1:A:457:GLY:HA3	1:A:576:ARG:HB2	1.91	0.52
1:A:701:ILE:HB	1:A:1046:VAL:HG22	1.90	0.52
13:M:368:MET:HE1	13:M:396:LEU:HD23	1.91	0.52
9:J:36:ASP:OD1	9:J:46:ARG:NH2	2.43	0.52
13:M:317:LEU:HB2	13:M:324:LEU:HD21	1.92	0.52
1:A:387:LEU:HA	1:A:390:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:32:SER:OG	7:H:33:GLU:N	2.42	0.52
1:A:95:LYS:HE2	1:A:1686:MET:HE1	1.92	0.52
1:A:481:ARG:HG3	1:A:519:ALA:HB1	1.91	0.52
2:B:384:PHE:HE2	2:B:430:PHE:HA	1.75	0.52
12:N:45:ILE:HB	13:M:88:PHE:HB2	1.92	0.52
2:B:691:MET:HE1	2:B:890:LYS:HE3	1.91	0.52
3:C:134:GLU:HG2	3:C:181:GLN:HG3	1.90	0.52
3:C:282:THR:HG22	12:N:151:ALA:HB2	1.92	0.52
2:B:138:PRO:HG2	2:B:434:PHE:HD2	1.75	0.51
13:M:89:VAL:HG23	13:M:104:ALA:HB2	1.91	0.51
1:A:718:LYS:NZ	1:A:889:PHE:O	2.42	0.51
2:B:761:LYS:NZ	2:B:765:GLU:OE2	2.38	0.51
1:A:860:MET:SD	1:A:864:LYS:NZ	2.83	0.51
1:A:1564:LEU:HB3	1:A:1578:LEU:HD23	1.93	0.51
2:B:50:VAL:HG13	2:B:82:ILE:HD12	1.92	0.51
1:A:126:VAL:HG11	1:A:134:ALA:HB3	1.91	0.51
1:A:1266:VAL:HG22	1:A:1600:LEU:HG	1.92	0.51
1:A:451:ILE:HG22	1:A:567:ARG:HD3	1.93	0.51
2:B:903:PRO:HB2	2:B:979:LEU:HD23	1.92	0.51
13:M:250:ASN:HD21	13:M:254:THR:HB	1.75	0.51
14:R:-9:U:H2'	14:R:-8:A:C8	2.46	0.51
6:G:105:ILE:HG12	6:G:112:ILE:HG22	1.91	0.51
6:G:162:SER:HB3	6:G:164:GLU:HG3	1.93	0.50
13:M:22:ARG:HG2	13:M:103:ASP:HB3	1.92	0.50
1:A:1112:GLY:HA3	4:E:60:VAL:HG12	1.92	0.50
12:N:45:ILE:HG12	12:N:115:LEU:HB2	1.93	0.50
1:A:1173:GLU:O	1:A:1177:GLN:NE2	2.44	0.50
2:B:758:ILE:HB	2:B:914:LEU:HB2	1.94	0.50
2:B:909:MET:HE2	9:J:42:ARG:HB3	1.92	0.50
6:G:80:LEU:HD21	6:G:150:CYS:HB3	1.92	0.50
1:A:1022:ASP:HB3	4:E:200:ALA:HB2	1.93	0.50
7:H:18:GLU:OE2	7:H:27:ARG:NH1	2.45	0.50
1:A:631:ILE:HA	1:A:635:MET:HE2	1.94	0.50
4:E:61:LEU:HD21	4:E:71:GLN:HG3	1.93	0.50
1:A:1602:SER:HB3	1:A:1608:ILE:HD11	1.93	0.50
6:G:143:ILE:O	6:G:155:ILE:N	2.44	0.50
2:B:593:MET:HE2	2:B:612:LEU:HD22	1.94	0.49
3:C:268:GLN:HB3	3:C:270:LYS:HG2	1.94	0.49
7:H:96:VAL:HG22	7:H:116:VAL:HG22	1.94	0.49
8:I:22:ASP:O	13:M:30:ASN:ND2	2.41	0.49
10:K:44:LEU:HD12	10:K:80:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:235:LEU:HB2	3:C:301:ARG:HD3	1.94	0.49
3:C:154:LYS:NZ	3:C:161:GLU:OE2	2.45	0.49
14:R:-9:U:H2'	14:R:-8:A:H8	1.77	0.49
1:A:1053:LEU:HD23	1:A:1056:VAL:HG11	1.93	0.49
2:B:787:GLN:O	13:M:364:SER:OG	2.30	0.49
6:G:71:ILE:HD11	6:G:114:LEU:HD11	1.93	0.49
13:M:265:SER:HB3	13:M:269:SER:HA	1.94	0.49
6:G:55:ARG:NH1	6:G:85:SER:OG	2.43	0.49
13:M:381:LYS:HE2	13:M:396:LEU:HG	1.95	0.49
1:A:64:CYS:SG	1:A:65:SER:N	2.86	0.49
2:B:938:ALA:HB2	2:B:945:HIS:HD1	1.78	0.49
13:M:352:ILE:O	13:M:395:LYS:NZ	2.45	0.49
10:K:40:VAL:HG12	10:K:92:ALA:HB3	1.93	0.49
3:C:134:GLU:HG3	3:C:180:ASN:H	1.78	0.48
1:A:1298:ASP:HB2	1:A:1318:ARG:HB3	1.94	0.48
2:B:267:GLU:HA	2:B:270:LYS:HE2	1.95	0.48
15:S:13:DC:N3	16:T:32:DG:N1	2.61	0.48
1:A:981:LYS:HD3	1:A:1227:THR:HA	1.95	0.48
2:B:267:GLU:O	2:B:351:ARG:NH1	2.47	0.48
1:A:44:ASN:ND2	13:M:330:ASP:OD2	2.47	0.48
1:A:564:HIS:NE2	1:A:585:TYR:OH	2.42	0.48
1:A:1715:LEU:HD23	5:F:104:ILE:HG21	1.96	0.48
2:B:559:ASP:OD2	2:B:614:THR:OG1	2.28	0.48
2:B:699:PRO:HB2	2:B:700:LEU:HG	1.96	0.48
9:J:6:ARG:HG2	9:J:13:ILE:HD13	1.96	0.48
1:A:13:GLN:HG3	2:B:1135:VAL:HB	1.96	0.47
1:A:691:LEU:HD22	1:A:784:LEU:HD22	1.96	0.47
1:A:1672:MET:HE2	1:A:1681:LEU:HA	1.95	0.47
2:B:47:ASN:HB3	2:B:144:LYS:HE2	1.96	0.47
1:A:142:LEU:HD12	1:A:161:LEU:HD11	1.95	0.47
10:K:53:ASN:OD1	10:K:56:ARG:NH2	2.47	0.47
1:A:929:MET:HG2	2:B:492:GLU:HG3	1.97	0.47
10:K:72:THR:HG22	10:K:80:ILE:HG22	1.96	0.47
1:A:1649:CYS:O	4:E:207:ARG:NH2	2.36	0.47
2:B:548:ARG:NE	2:B:552:GLU:OE1	2.47	0.47
3:C:100:ILE:HD11	9:J:56:ILE:HG13	1.96	0.47
1:A:990:ARG:NH1	2:B:1039:GLU:OE1	2.48	0.47
1:A:1564:LEU:HD13	1:A:1576:LEU:HD11	1.97	0.47
1:A:84:PRO:HD3	1:A:335:VAL:HG13	1.97	0.46
1:A:1113:ARG:HH11	4:E:62:VAL:HA	1.79	0.46
1:A:425:GLU:HA	1:A:430:LYS:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ASP:HB2	1:A:576:ARG:HD2	1.98	0.46
3:C:62:GLU:HG2	12:N:153:GLY:H	1.80	0.46
13:M:147:GLN:O	13:M:151:LEU:HB2	2.15	0.46
13:M:317:LEU:HD12	13:M:324:LEU:HD11	1.96	0.46
2:B:503:PRO:HB2	2:B:507:PRO:HG2	1.98	0.46
6:G:157:LYS:HE2	6:G:166:TRP:HA	1.97	0.46
1:A:639:ALA:O	1:A:643:THR:OG1	2.30	0.46
10:K:83:ARG:HH11	10:K:85:GLN:HE21	1.62	0.46
13:M:355:THR:HB	13:M:394:HIS:HB2	1.98	0.46
7:H:110:THR:OG1	7:H:128:ASP:OD1	2.33	0.46
1:A:1053:LEU:HD21	5:F:124:ILE:HD13	1.97	0.46
1:A:1287:ARG:HG3	1:A:1555:ALA:HB2	1.98	0.46
1:A:552:ARG:HB2	1:A:594:MET:SD	2.57	0.46
1:A:1264:MET:HE2	1:A:1583:ILE:HA	1.96	0.46
4:E:195:ARG:HD2	4:E:203:TYR:HD2	1.81	0.46
2:B:1060:ASN:HD22	2:B:1064:ARG:HD2	1.80	0.45
3:C:173:MET:HG2	3:C:212:MET:HE1	1.98	0.45
3:C:319:ASP:OD1	3:C:319:ASP:N	2.47	0.45
1:A:866:LYS:NZ	1:A:923:GLY:O	2.50	0.45
1:A:1693:LEU:HD13	1:A:1702:VAL:HG21	1.98	0.45
1:A:850:HIS:HD1	1:A:941:TYR:HH	1.63	0.45
1:A:1262:PRO:HB3	1:A:1583:ILE:HD12	1.98	0.45
2:B:543:ASP:HB3	13:M:79:LEU:HD12	1.98	0.45
1:A:407:ASP:O	1:A:413:LYS:NZ	2.33	0.45
1:A:557:HIS:ND1	1:A:559:PRO:HD2	2.31	0.45
3:C:202:LEU:O	3:C:203:ARG:NH1	2.48	0.45
1:A:1300:GLN:HB3	1:A:1316:GLN:HG2	1.97	0.45
2:B:336:LEU:HD22	2:B:341:GLU:HB3	1.97	0.45
2:B:714:LEU:HD23	2:B:717:PRO:HB3	1.98	0.45
2:B:736:PRO:HG3	9:J:53:VAL:HG11	1.99	0.45
4:E:160:LEU:HD21	4:E:167:GLU:HG3	1.97	0.45
1:A:42:LEU:HD12	13:M:334:ALA:HB1	1.97	0.45
1:A:1241:VAL:HA	1:A:1261:THR:HG21	1.99	0.45
13:M:48:ASP:OD1	13:M:48:ASP:N	2.50	0.44
1:A:167:GLU:O	1:A:171:ASN:HB2	2.17	0.44
2:B:179:ILE:HD12	2:B:377:PRO:HB3	1.99	0.44
2:B:760:ASN:HB2	2:B:912:ASP:HA	1.99	0.44
1:A:313:SER:HB2	14:R:10:C:H1'	1.99	0.44
1:A:1239:MET:HE1	1:A:1263:MET:HG3	1.99	0.44
1:A:1314:VAL:HG22	1:A:1530:LYS:HG3	1.99	0.44
9:J:47:ARG:NH1	9:J:48:MET:SD	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:288:ALA:HA	13:M:290:ARG:HH21	1.81	0.44
1:A:850:HIS:ND1	1:A:941:TYR:OH	2.51	0.44
12:N:73:LEU:HD13	12:N:74:ALA:H	1.82	0.44
11:L:17:TYR:HD1	11:L:46:LYS:HA	1.83	0.44
1:A:70:ASP:OD1	1:A:70:ASP:N	2.50	0.44
1:A:448:ASP:HB2	1:A:576:ARG:HB3	1.99	0.44
10:K:28:GLU:HB2	10:K:43:VAL:HB	1.99	0.44
12:N:55:CYS:HB3	12:N:72:LYS:HB3	1.99	0.44
1:A:449:MET:HE3	1:A:449:MET:HB2	1.74	0.44
1:A:1059:ARG:HH11	5:F:55:PRO:HG3	1.82	0.44
1:A:1615:GLU:HG3	4:E:193:ILE:HD13	1.99	0.44
6:G:138:VAL:HG21	6:G:173:MET:HE2	2.00	0.44
1:A:632:GLN:H	1:A:632:GLN:HG3	1.48	0.43
1:A:933:LYS:HE2	1:A:936:PRO:HA	2.00	0.43
12:N:63:LEU:HB2	13:M:7:PRO:HB2	2.01	0.43
1:A:94:ASP:OD1	1:A:217:LYS:NZ	2.52	0.43
4:E:73:PHE:HE2	4:E:99:ILE:HG13	1.83	0.43
9:J:65:LEU:HB3	9:J:67:LYS:HG2	2.00	0.43
1:A:1668:PRO:HD2	1:A:1691:ASP:HB2	2.00	0.43
7:H:76:ASN:OD1	10:K:87:ARG:NH2	2.52	0.43
10:K:36:ASP:HB2	10:K:38:HIS:HD2	1.83	0.43
2:B:579:ARG:NH2	2:B:595:VAL:O	2.51	0.43
8:I:63:GLN:NE2	8:I:65:GLY:O	2.51	0.43
10:K:64:GLU:HB3	10:K:90:LEU:HD21	2.01	0.43
1:A:1000:VAL:HG12	1:A:1210:ALA:HA	1.99	0.43
1:A:1713:PHE:O	5:F:64:ARG:NH1	2.51	0.43
6:G:55:ARG:NE	6:G:78:GLU:OE2	2.52	0.43
13:M:14:CYS:SG	13:M:15:GLY:N	2.92	0.43
13:M:387:ALA:H	13:M:393:ASP:HB3	1.84	0.43
1:A:477:VAL:HG11	1:A:523:LEU:HD22	2.01	0.43
1:A:1044:TYR:HD1	1:A:1195:LEU:HD22	1.82	0.43
2:B:716:THR:HG21	9:J:4:PRO:HG3	2.00	0.43
5:F:107:ARG:HH22	6:G:102:LEU:HD22	1.84	0.43
2:B:308:PHE:HB2	13:M:142:PHE:CD2	2.54	0.43
1:A:1162:THR:HG22	1:A:1166:LYS:HE3	2.01	0.43
1:A:445:ILE:HG21	1:A:594:MET:HG3	2.01	0.42
1:A:881:MET:HG3	1:A:910:MET:HG2	2.01	0.42
2:B:463:ILE:HD13	2:B:737:ILE:HD13	2.00	0.42
1:A:1499:GLU:HG2	1:A:1500:ARG:HD2	2.00	0.42
2:B:294:CYS:HB3	2:B:300:VAL:HG22	2.01	0.42
10:K:66:GLU:N	10:K:85:GLN:O	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:VAL:HG11	1:A:1278:VAL:HG21	2.02	0.42
2:B:809:ASP:HB2	11:L:15:MET:HE3	2.00	0.42
6:G:181:VAL:HA	6:G:196:GLY:HA3	2.01	0.42
13:M:199:TYR:CZ	13:M:206:ASP:HB3	2.54	0.42
2:B:779:ILE:HB	2:B:867:VAL:HG12	2.01	0.42
13:M:134:LYS:HE2	13:M:134:LYS:HB3	1.92	0.42
7:H:40:ILE:HD13	7:H:124:ARG:HD3	2.01	0.42
1:A:855:GLN:O	1:A:859:ASN:ND2	2.53	0.42
2:B:263:GLN:HE22	13:M:108:ASN:HD21	1.67	0.42
6:G:135:VAL:HA	6:G:145:CYS:HA	2.00	0.42
6:G:198:LEU:HD22	6:G:200:ILE:HG13	2.00	0.42
1:A:731:SER:HB3	7:H:115:TYR:HE2	1.85	0.42
2:B:228:TYR:HB2	2:B:353:LEU:HD11	2.01	0.42
2:B:746:ILE:HD12	2:B:992:ILE:HG12	2.02	0.42
1:A:750:ASP:OD1	1:A:750:ASP:N	2.53	0.42
3:C:203:ARG:HD3	3:C:203:ARG:HA	1.85	0.42
13:M:46:ASN:ND2	13:M:54:LYS:O	2.42	0.42
2:B:538:GLY:HA2	12:N:118:LEU:HD22	2.02	0.42
1:A:391:TRP:HD1	1:A:391:TRP:HA	1.77	0.42
1:A:551:ASN:HD21	2:B:1041:GLU:HG2	1.85	0.42
1:A:1003:TYR:OH	5:F:61:GLU:OE2	2.37	0.42
2:B:829:LEU:HA	2:B:836:SER:HA	2.01	0.42
9:J:7:CYS:HA	9:J:48:MET:HE2	2.02	0.42
1:A:1288:VAL:HG13	1:A:1553:ILE:HB	2.00	0.41
1:A:1685:THR:HG21	2:B:1128:ILE:HG12	2.01	0.41
3:C:89:VAL:HB	3:C:111:GLY:HA2	2.02	0.41
13:M:204:TYR:HD2	13:M:404:PRO:HA	1.85	0.41
2:B:691:MET:HE2	2:B:691:MET:HB3	1.94	0.41
9:J:40:LEU:HD23	9:J:46:ARG:HA	2.02	0.41
15:S:33:DT:H2"	15:S:34:DA:C8	2.55	0.41
1:A:475:TRP:HH2	5:F:89:PRO:HG3	1.85	0.41
2:B:419:ILE:H	2:B:419:ILE:HG13	1.64	0.41
2:B:1085:PRO:HG2	2:B:1092:ARG:HD2	2.01	0.41
2:B:889:GLN:HE21	2:B:915:PHE:HZ	1.68	0.41
4:E:60:VAL:HG22	4:E:74:VAL:HB	2.02	0.41
4:E:73:PHE:CE2	4:E:99:ILE:HG13	2.55	0.41
13:M:214:TYR:HH	13:M:278:TRP:CD1	2.38	0.41
1:A:310:ARG:HA	1:A:322:ASN:HD21	1.86	0.41
1:A:933:LYS:NZ	2:B:643:ASN:OD1	2.44	0.41
6:G:146:LEU:HD23	6:G:149:GLY:HA2	2.03	0.41
2:B:626:LEU:HD22	12:N:132:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ALA:HA	1:A:65:SER:HB2	2.03	0.41
2:B:104:ARG:HH11	2:B:104:ARG:HD2	1.77	0.41
2:B:308:PHE:HB2	13:M:142:PHE:CE2	2.55	0.41
12:N:156:PRO:HA	12:N:157:PRO:HD3	1.93	0.41
1:A:461:VAL:HG21	1:A:573:LYS:HG2	2.03	0.41
1:A:689:SER:HB3	1:A:743:GLU:HA	2.02	0.41
7:H:3:GLY:H	7:H:84:ARG:NH2	2.19	0.41
1:A:1655:LYS:HE2	1:A:1655:LYS:HB3	1.95	0.40
7:H:6:PHE:CZ	7:H:37:MET:HG3	2.56	0.40
10:K:59:ILE:HD13	10:K:84:ILE:HD11	2.02	0.40
12:N:42:LEU:HB2	12:N:111:PRO:HA	2.02	0.40
14:R:-8:A:H2'	14:R:-7:U:C6	2.56	0.40
2:B:850:ASP:OD1	2:B:872:ARG:NH1	2.55	0.40
3:C:171:ARG:HB3	3:C:195:ASP:HB2	2.04	0.40
1:A:314:ARG:HE	1:A:319:MET:HE1	1.86	0.40
12:N:82:VAL:HG22	12:N:117:ILE:HG12	2.03	0.40
1:A:1207:PRO:HD2	5:F:58:THR:HG21	2.02	0.40
2:B:44:GLU:OE1	2:B:522:THR:OG1	2.40	0.40
7:H:2:ALA:HA	7:H:84:ARG:HH22	1.86	0.40
7:H:98:ARG:HG2	7:H:115:TYR:HB2	2.03	0.40

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	1527/1720 (89%)	1455 (95%)	71 (5%)	1 (0%)	48	73
2	B	1125/1135 (99%)	1062 (94%)	63 (6%)	0	100	100
3	C	305/346 (88%)	297 (97%)	7 (2%)	1 (0%)	36	60
4	E	207/210 (99%)	199 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	77/127 (61%)	74 (96%)	3 (4%)	0	100	100
6	G	174/338 (52%)	159 (91%)	15 (9%)	0	100	100
7	H	147/150 (98%)	142 (97%)	5 (3%)	0	100	100
8	I	53/126 (42%)	51 (96%)	2 (4%)	0	100	100
9	J	65/67 (97%)	60 (92%)	5 (8%)	0	100	100
10	K	105/133 (79%)	101 (96%)	4 (4%)	0	100	100
11	L	45/58 (78%)	41 (91%)	4 (9%)	0	100	100
12	N	147/510 (29%)	137 (93%)	10 (7%)	0	100	100
13	M	384/419 (92%)	342 (89%)	42 (11%)	0	100	100
All	All	4361/5339 (82%)	4120 (94%)	239 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	LYS
3	C	196	ASP

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	1349/1504 (90%)	1340 (99%)	9 (1%)	76	90
2	B	987/992 (100%)	980 (99%)	7 (1%)	76	90
3	C	270/302 (89%)	270 (100%)	0	100	100
4	E	191/192 (100%)	191 (100%)	0	100	100
5	F	69/111 (62%)	68 (99%)	1 (1%)	59	82
6	G	150/288 (52%)	150 (100%)	0	100	100
7	H	130/131 (99%)	130 (100%)	0	100	100
8	I	49/111 (44%)	48 (98%)	1 (2%)	48	76
9	J	56/56 (100%)	55 (98%)	1 (2%)	51	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	K	96/119 (81%)	96 (100%)	0	100	100
11	L	44/55 (80%)	43 (98%)	1 (2%)	44	73
12	N	118/427 (28%)	117 (99%)	1 (1%)	73	88
13	M	338/366 (92%)	338 (100%)	0	100	100
All	All	3847/4654 (83%)	3826 (100%)	21 (0%)	78	92

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	96	LEU
1	A	120	LEU
1	A	132	LEU
1	A	391	TRP
1	A	631	ILE
1	A	744	LEU
1	A	778	LEU
1	A	1704	LYS
2	B	314	VAL
2	B	374	VAL
2	B	463	ILE
2	B	700	LEU
2	B	867	VAL
2	B	916	ASN
2	B	992	ILE
5	F	53	THR
8	I	39	ILE
9	J	53	VAL
11	L	28	ILE
12	N	73	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	143	ASN
1	A	264	HIS
1	A	349	GLN
1	A	482	GLN
1	A	595	ASN

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Mol	Chain	Res	Type
1	A	597	HIS
1	A	617	GLN
1	A	821	HIS
1	A	825	GLN
1	A	895	GLN
1	A	1109	ASN
1	A	1328	GLN
1	A	1537	ASN
1	A	1690	HIS
2	B	154	GLN
2	B	160	HIS
2	B	188	ASN
2	B	501	HIS
2	B	513	HIS
2	B	580	HIS
2	B	715	GLN
2	B	876	ASN
2	B	889	GLN
2	B	916	ASN
2	B	1060	ASN
3	C	48	ASN
3	C	160	ASN
4	E	35	GLN
6	G	56	HIS
6	G	113	HIS
6	G	129	GLN
6	G	167	GLN
10	K	31	GLN
10	K	85	GLN
12	N	78	HIS
13	M	56	ASN
13	M	98	GLN
13	M	108	ASN
13	M	147	GLN
13	M	152	ASN
13	M	307	ASN
13	M	358	GLN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	R	19/29 (65%)	3 (15%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	R	6	A
14	R	9	A
14	R	10	C

There are no RNA pucker outliers to report.

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 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

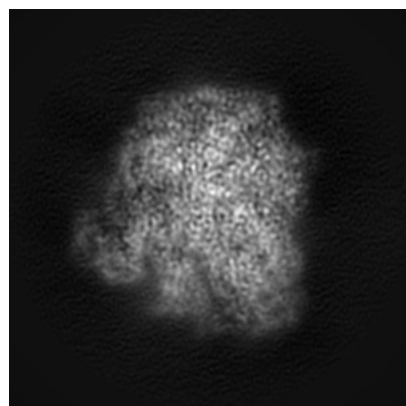
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12795. These allow visual inspection of the internal detail of the map and identification of artifacts.

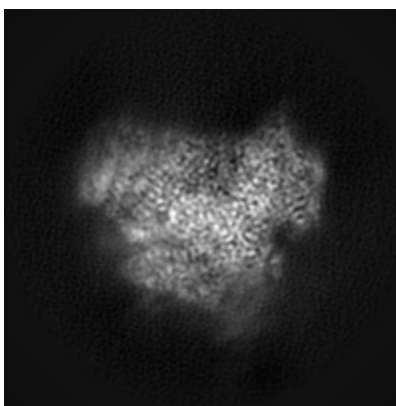
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

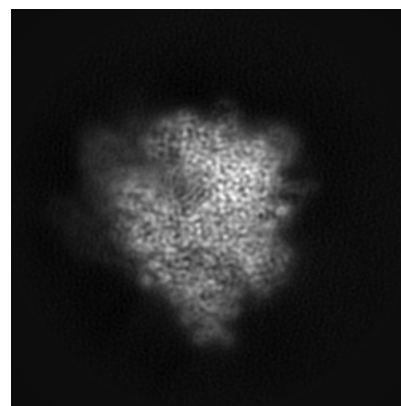
6.1.1 Primary map



X

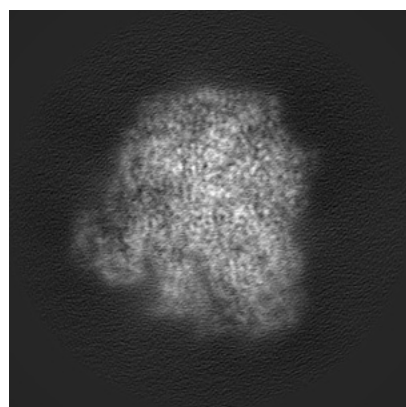


Y

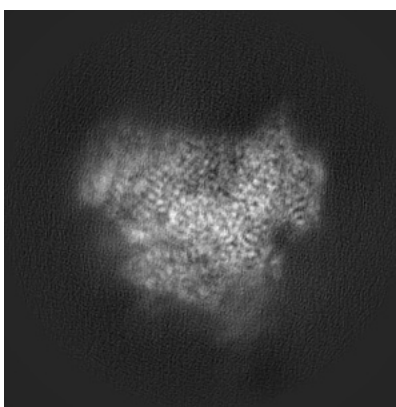


Z

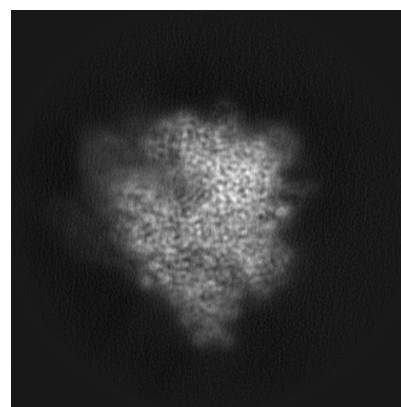
6.1.2 Raw map



X



Y

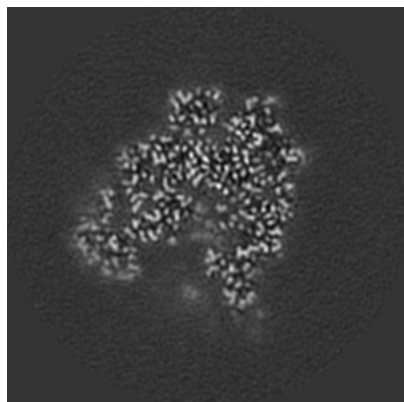


Z

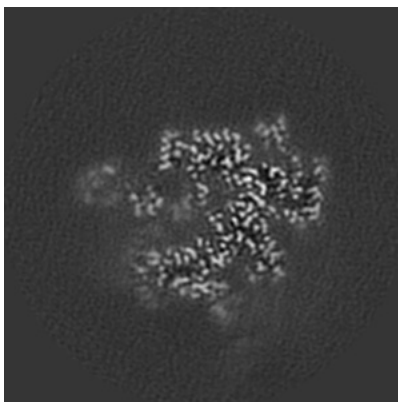
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

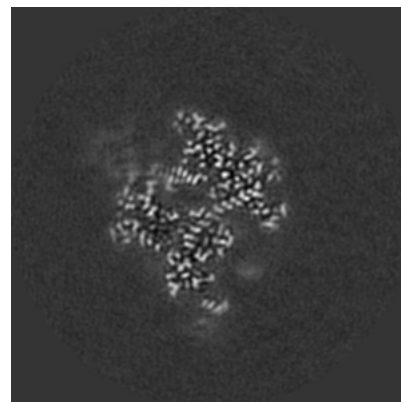
6.2.1 Primary map



X Index: 140

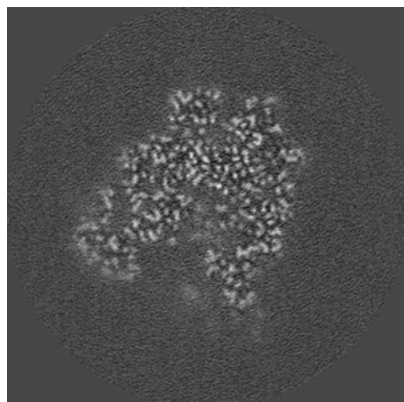


Y Index: 140

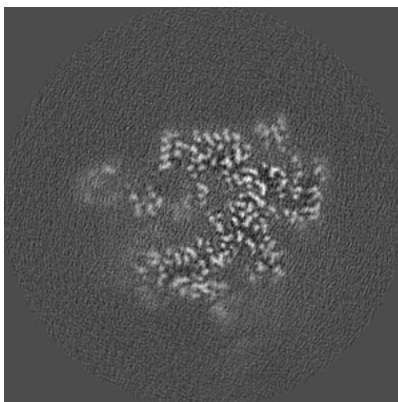


Z Index: 140

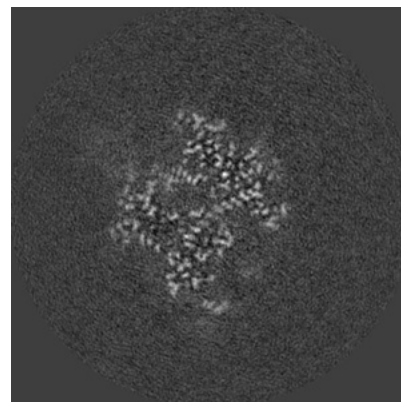
6.2.2 Raw map



X Index: 140



Y Index: 140

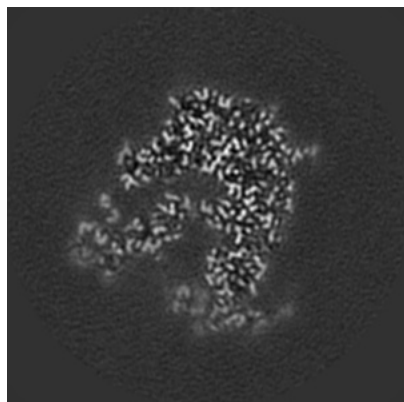


Z Index: 140

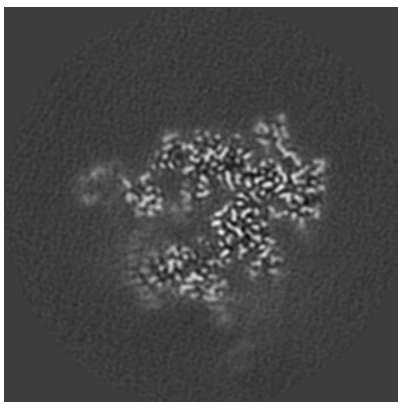
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

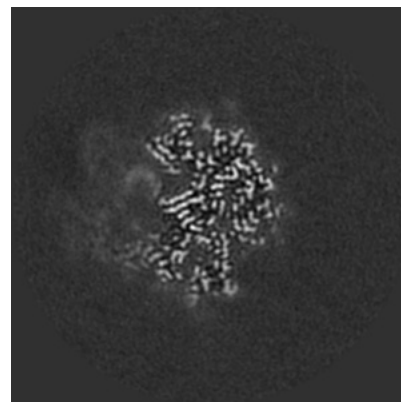
6.3.1 Primary map



X Index: 147

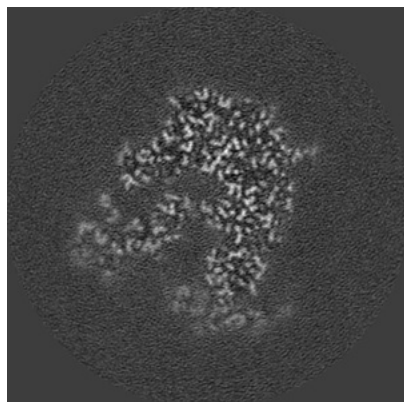


Y Index: 142

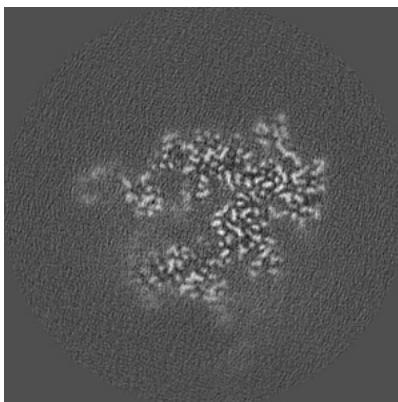


Z Index: 165

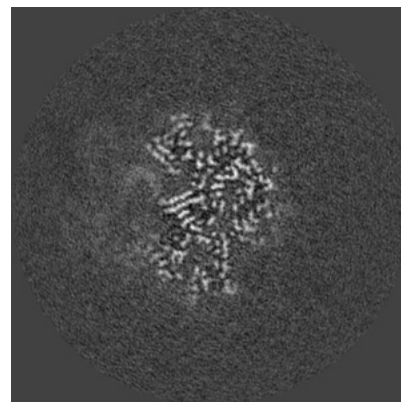
6.3.2 Raw map



X Index: 147



Y Index: 142

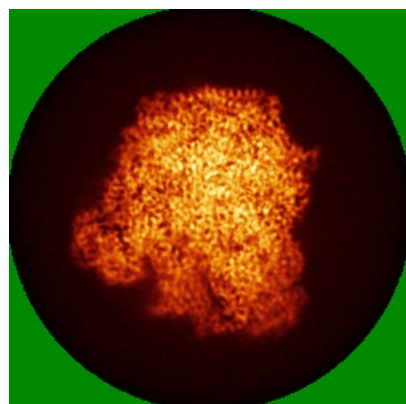


Z Index: 165

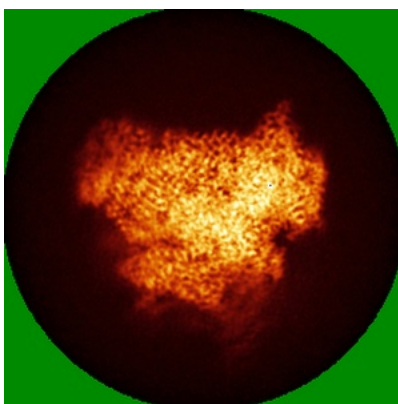
The images above show the largest variance slices of the map in three orthogonal directions.

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

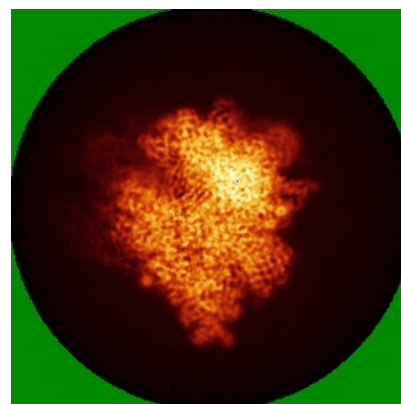
6.4.1 Primary map



X

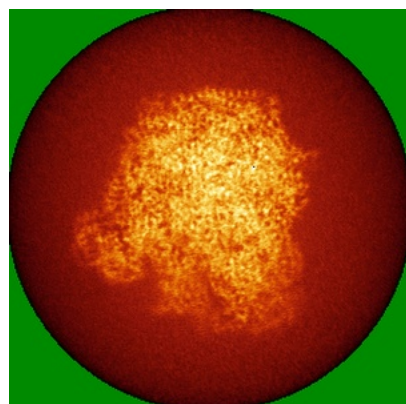


Y

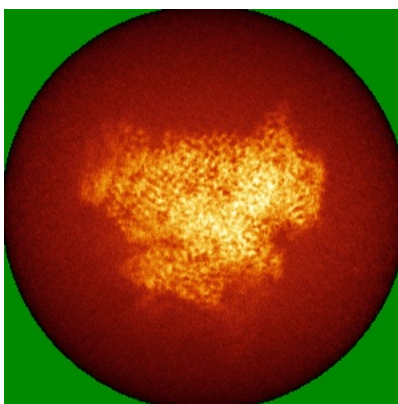


Z

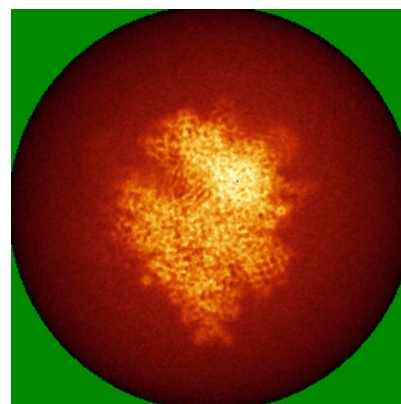
6.4.2 Raw map



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



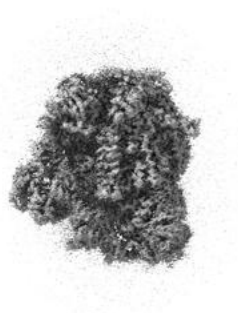
Y



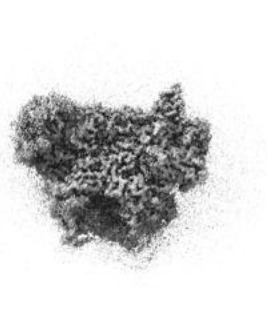
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00839. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

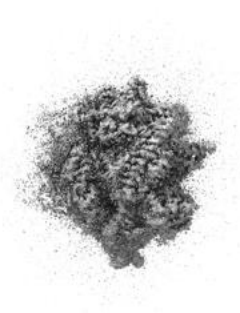
6.5.2 Raw map



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.

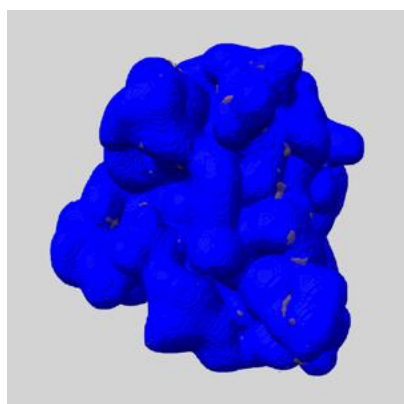
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

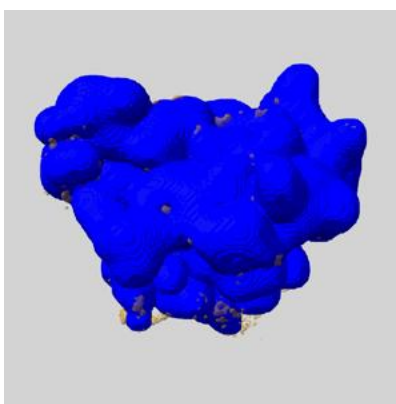
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

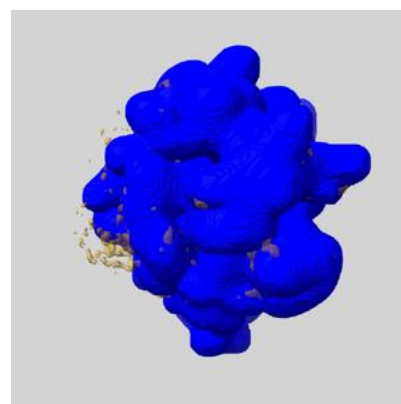
6.6.1 emd_12795_msk_3.map [i](#)



X

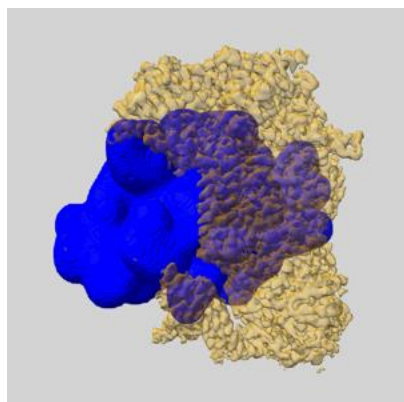


Y

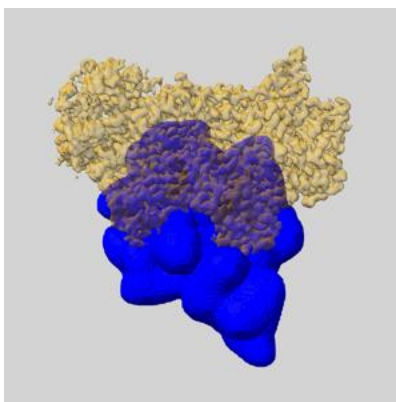


Z

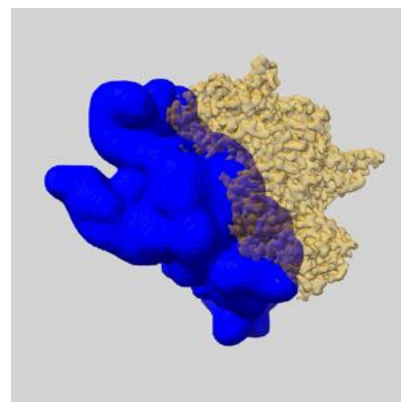
6.6.2 emd_12795_msk_1.map [i](#)



X

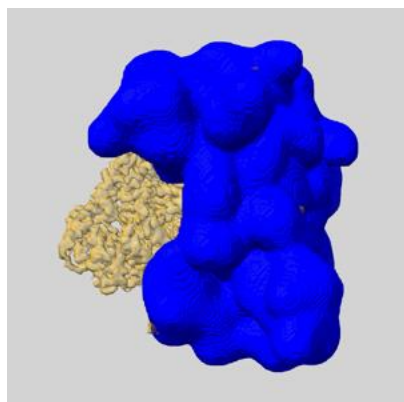


Y

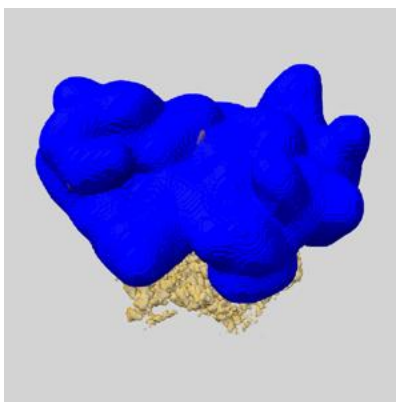


Z

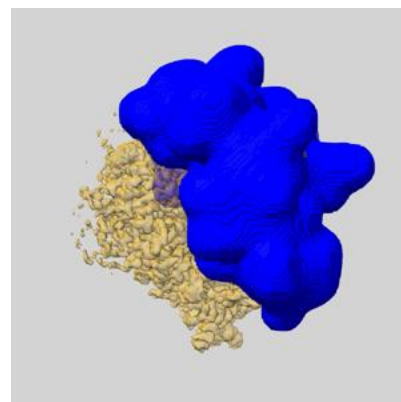
6.6.3 emd_12795_msk_2.map [i](#)



X



Y

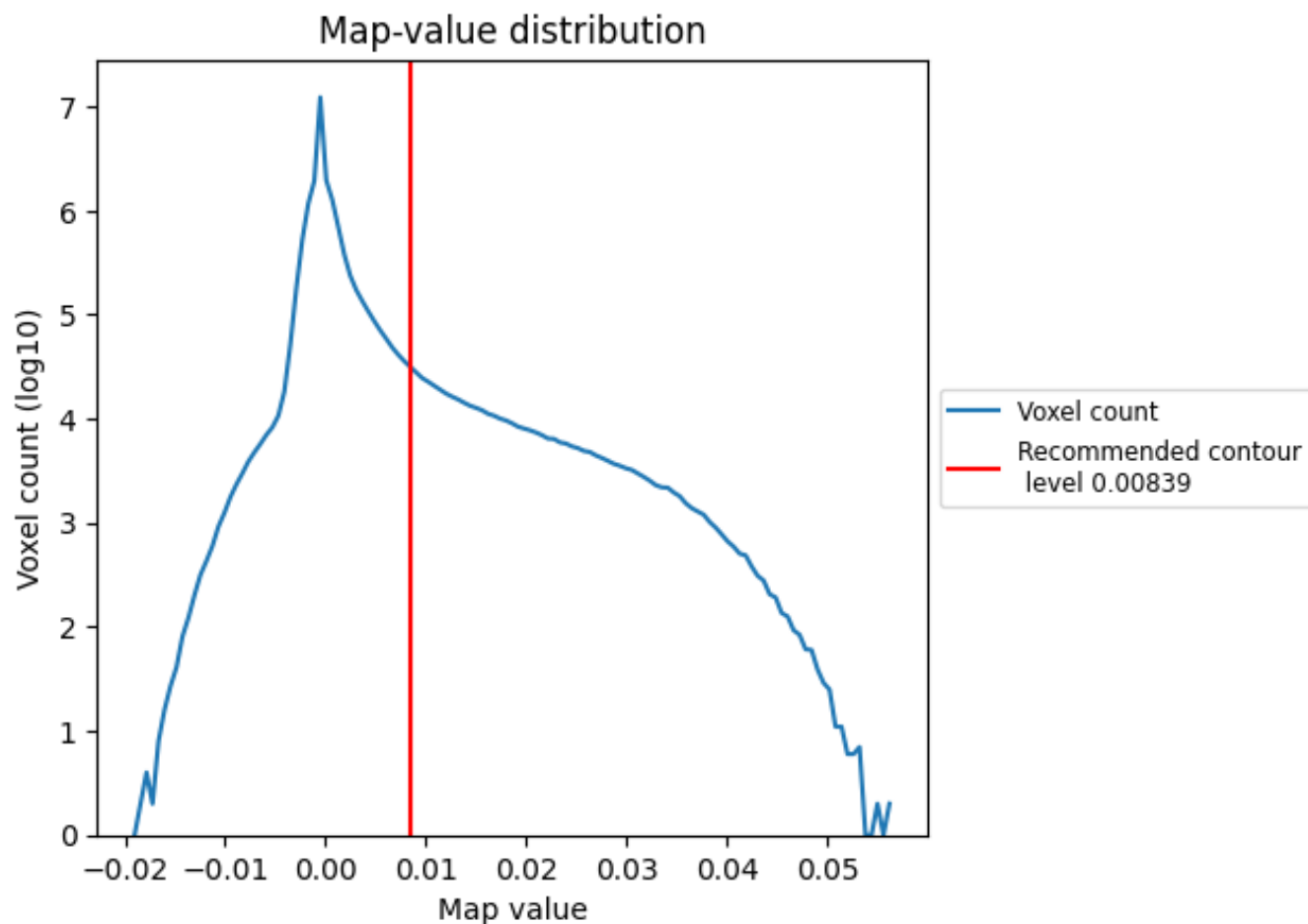


Z

7 Map analysis [i](#)

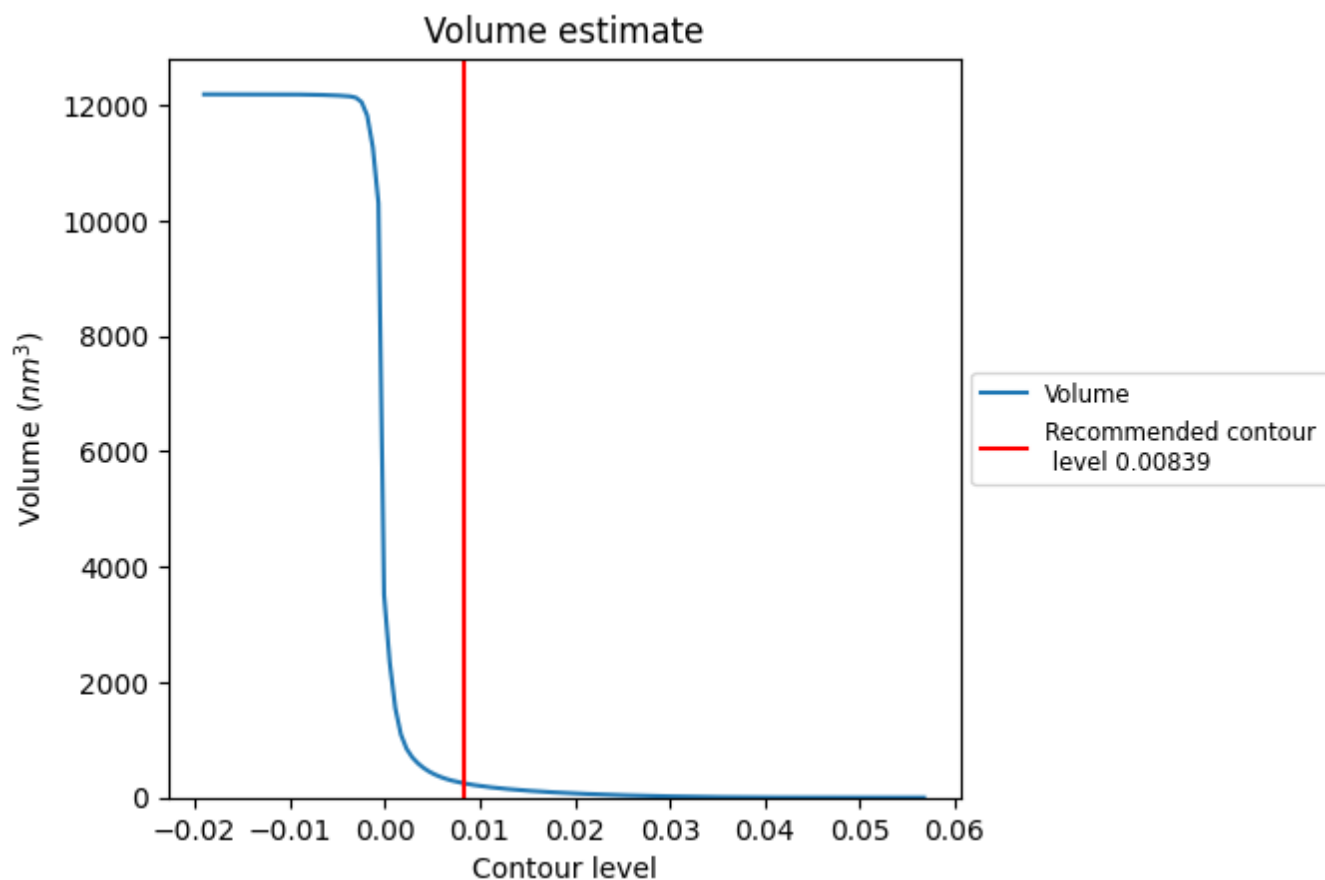
This section contains the results of statistical analysis of the map.

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.

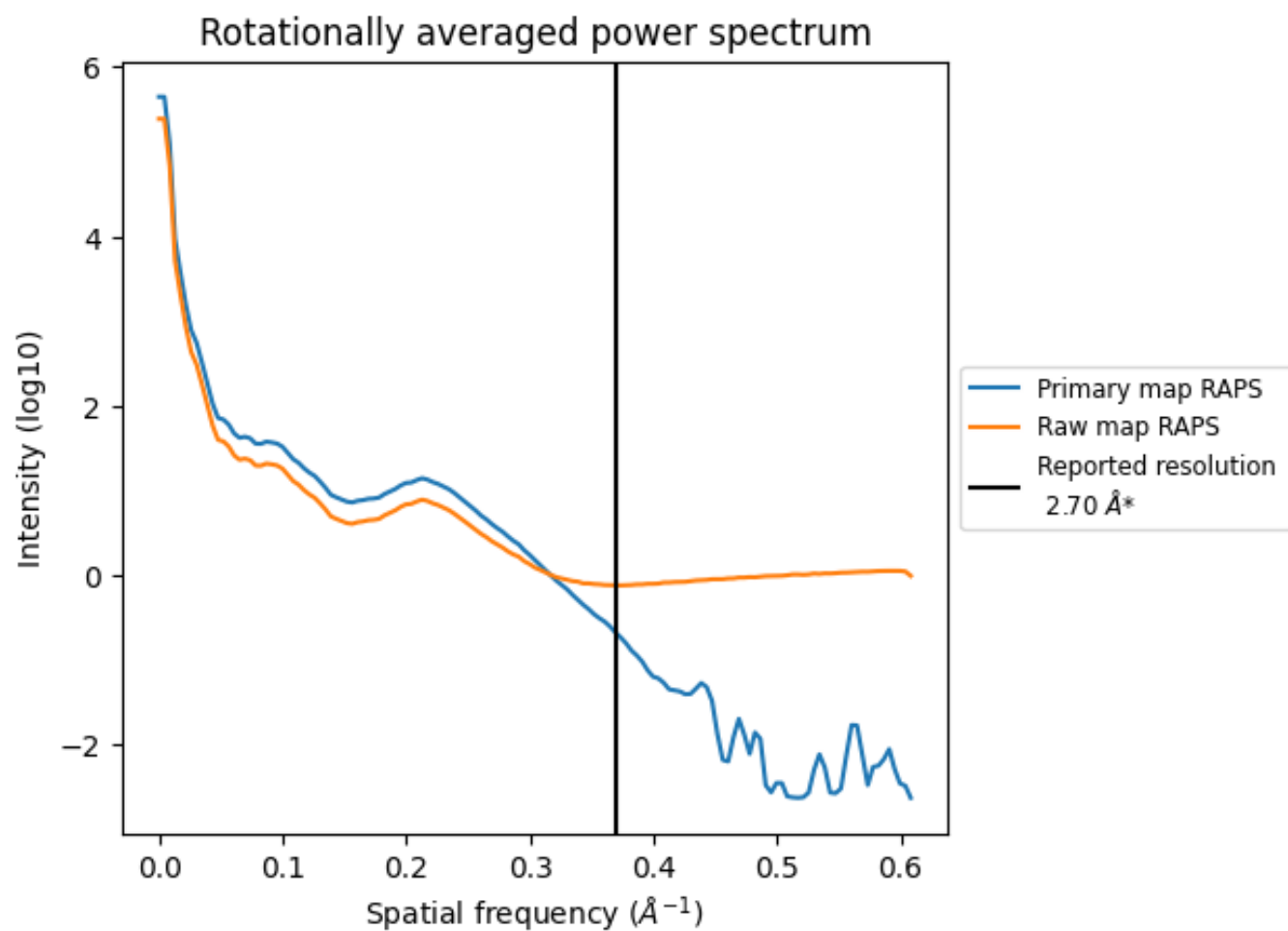
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 246 nm^3 ; this corresponds to an approximate mass of 222 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 ⓘ

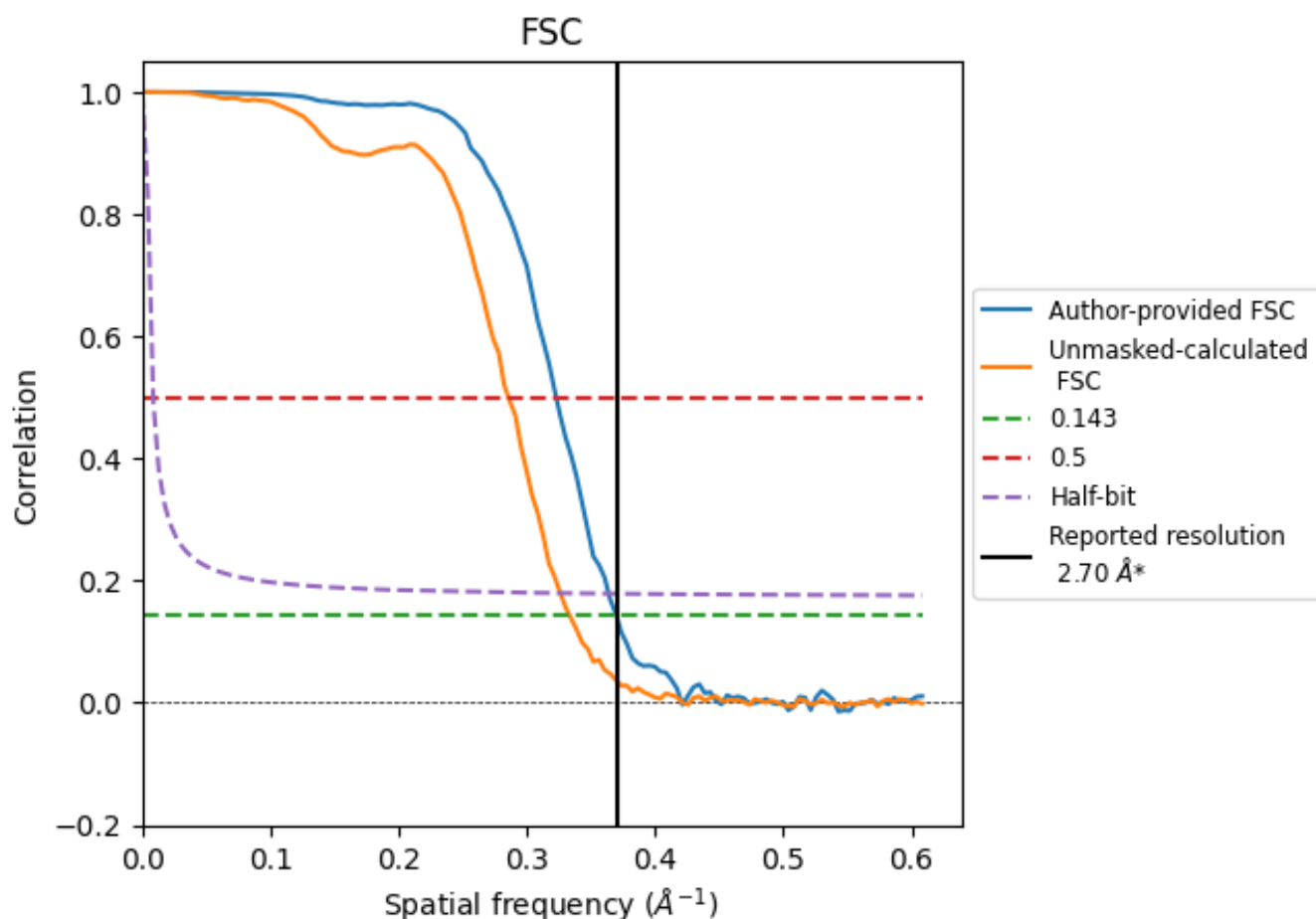


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

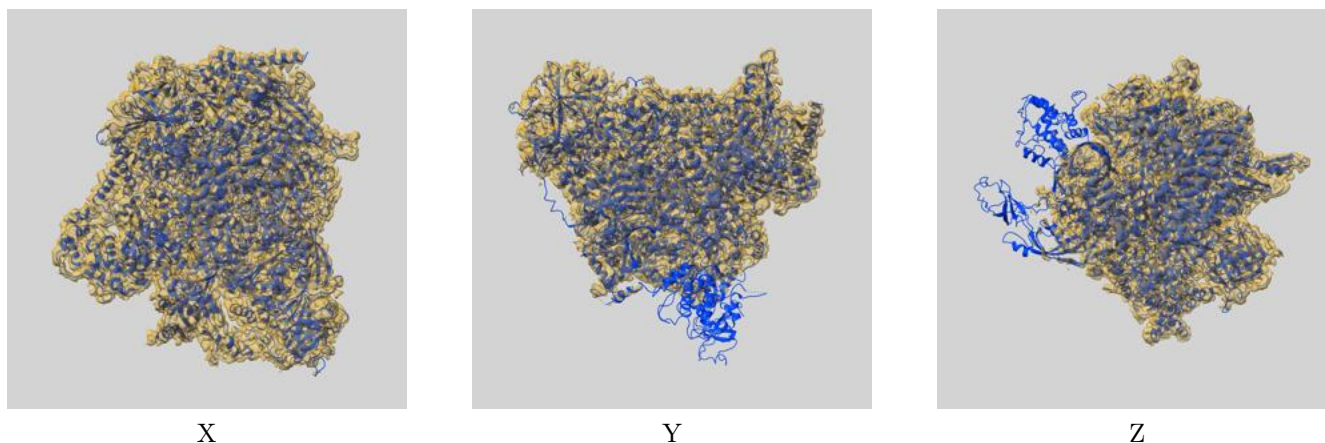
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.10	2.75
Unmasked-calculated*	3.00	3.50	3.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.00 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

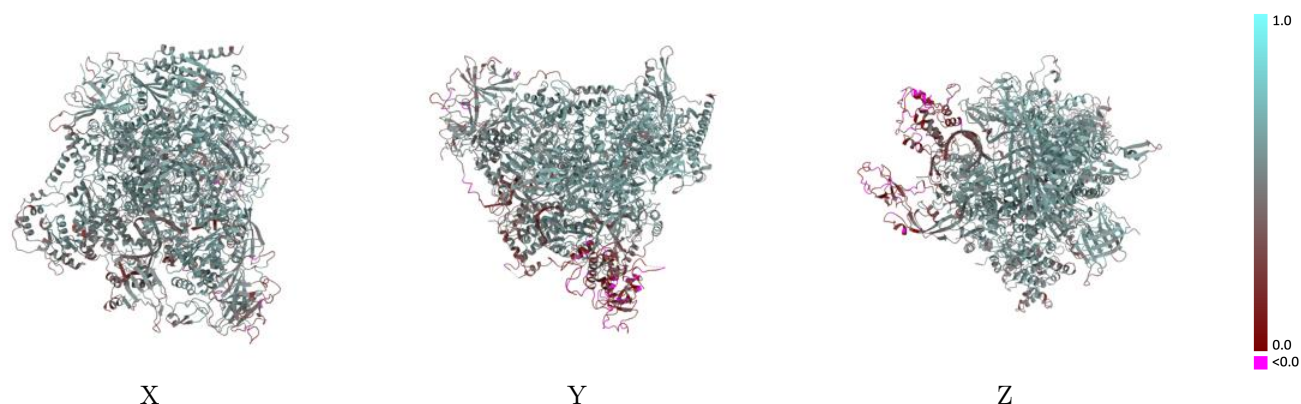
This section contains information regarding the fit between EMDB map EMD-12795 and PDB model 7OB9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



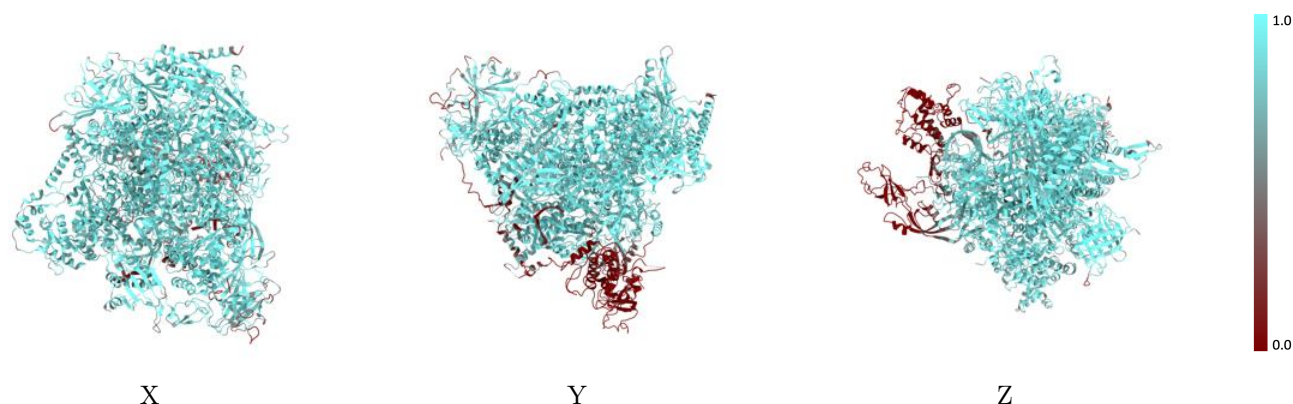
The images above show the 3D surface view of the map at the recommended contour level 0.00839 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



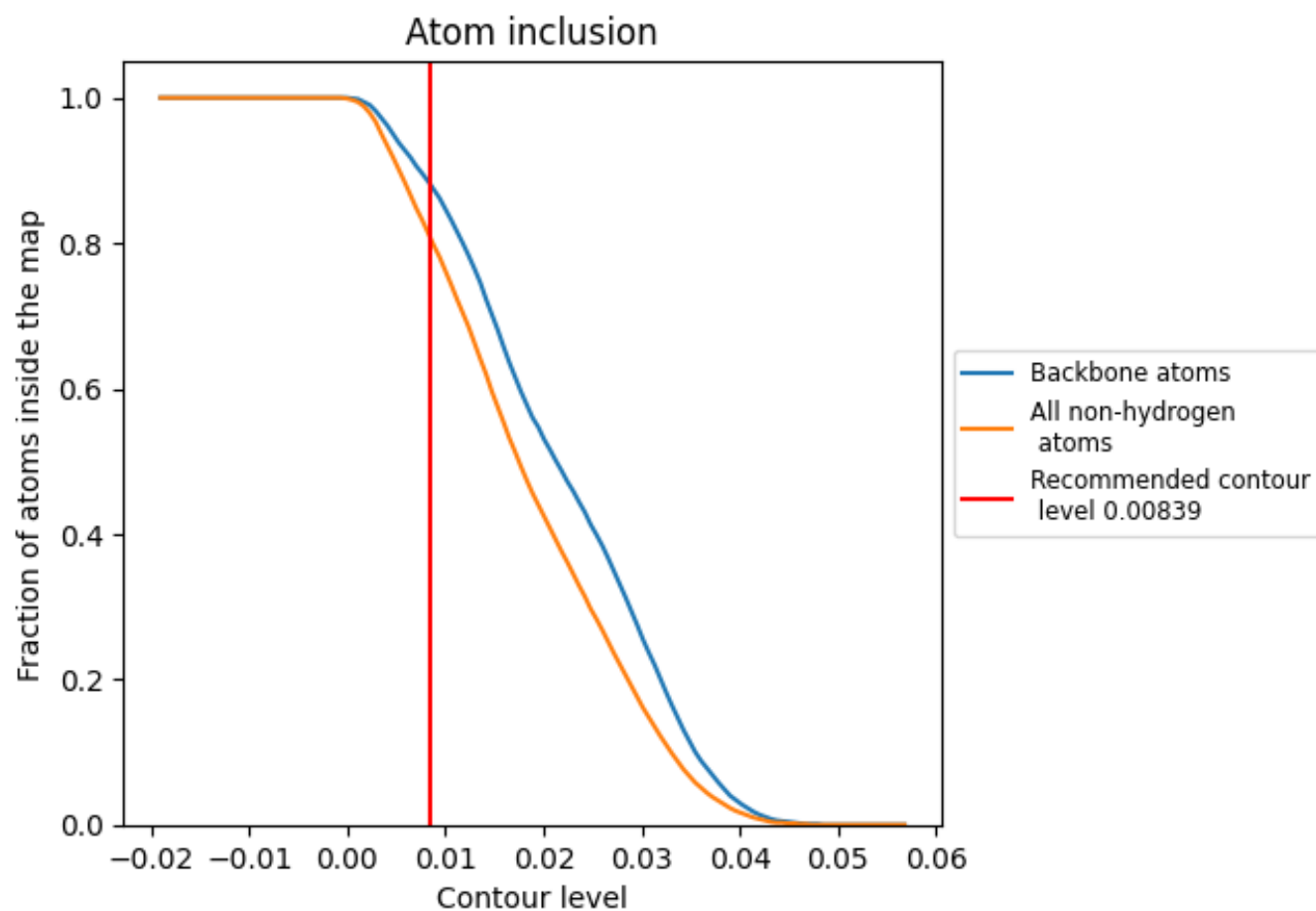
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00839).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (0.00839) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8090	 0.5190
A	 0.8860	 0.5460
B	 0.9330	 0.5890
C	 0.9170	 0.5770
E	 0.8950	 0.5370
F	 0.8960	 0.5730
G	 0.1780	 0.2850
H	 0.8660	 0.5350
I	 0.8440	 0.5110
J	 0.9290	 0.5980
K	 0.8970	 0.5720
L	 0.8950	 0.5670
M	 0.2690	 0.2800
N	 0.6620	 0.4300
R	 0.8660	 0.4620
S	 0.5770	 0.3440
T	 0.7730	 0.4520

