Full wwPDB EM Validation Report (i)

Jul 3, 2024 – 04:42 am BST

PDB ID	:	7OB9
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

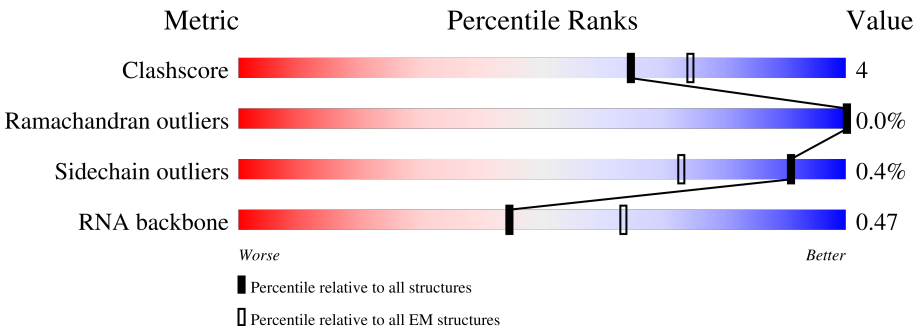
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	89% 10%
3	C	346	79% 9% 11%
4	E	210	89% 10%
5	F	127	53% 9% 38%
6	G	338	42% 43% 9% 48%
7	H	150	7% 82% 17%

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Mol	Chain	Length	Quality of chain
8	I	126	41% 56%
9	J	67	78% 22%
10	K	133	65% 15% 20%
11	L	58	71% 10% 19%
12	N	510	6% 25% 71%
13	M	419	64% 76% 17% 7%
14	R	29	48% 14% 10% 28%
15	S	43	16% 33% 12% 56%
16	T	43	14% 58% 9% 33%

2 Entry composition (i)

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
			Total	C	N	O	S		
1	A	1535	12222	7768	2140	2233	81	0	0

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

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

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

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

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

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

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
			Total	C	N	O	S		
5	F	79	636	407	108	116	5	0	0

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

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

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

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

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

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

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

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

- Molecule 14 is a RNA chain called RNA.

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

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

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

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

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

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

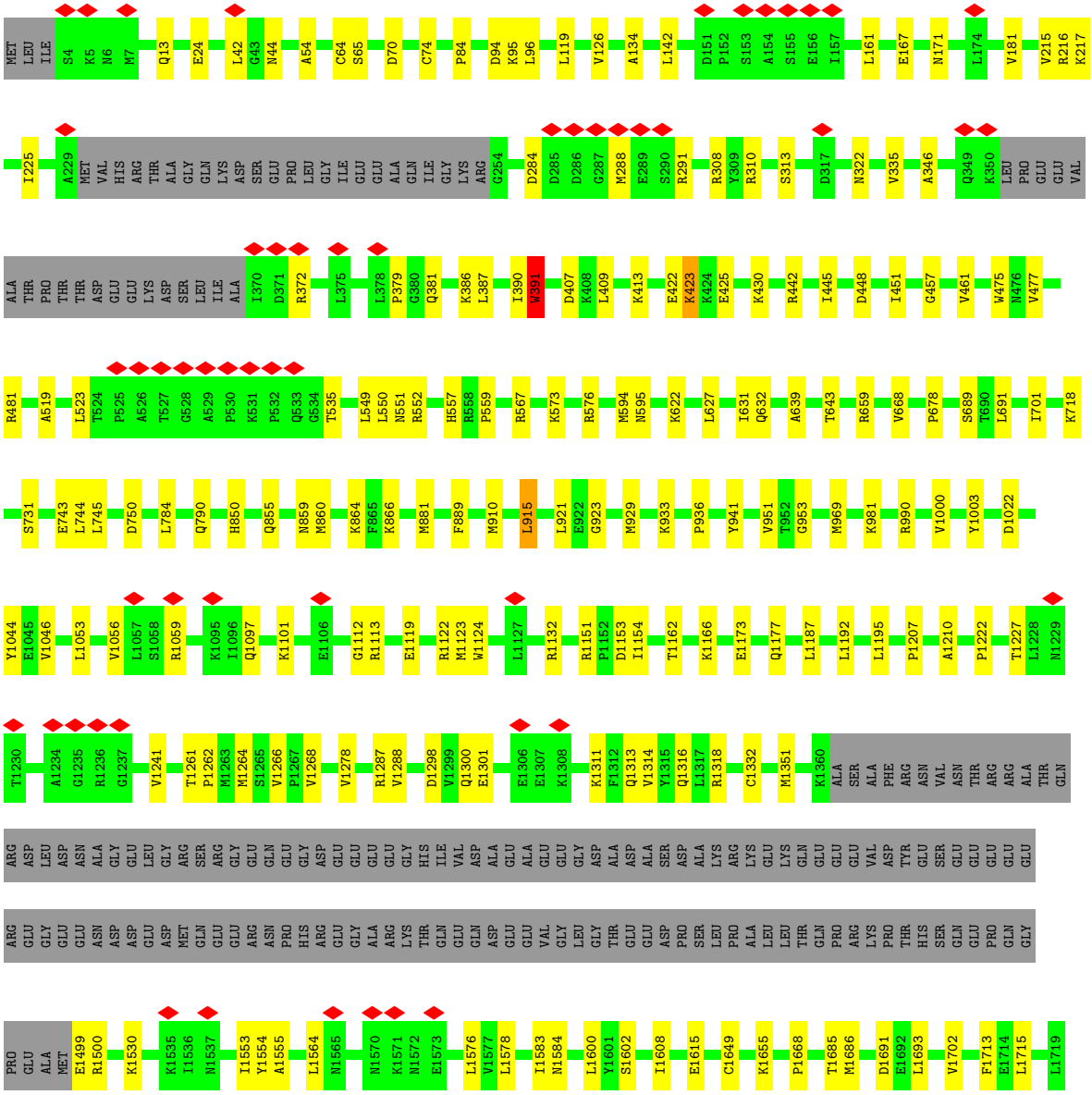
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
18	A	1	1	1	0

3 Residue-property plots (i)

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

- Molecule 1: DNA-directed RNA polymerase I subunit RPA1

Chain A:



ARG

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

Chain B:

M1 N47 V50 I82 C93 R104 G105 R106 P138 K144 L145 C146 R149 V178 I179 A192 M193 V215 Y228 T233 Q263 E267 K270 M285 C294 V300 F308 V314 C333 L336 E341 R351 K352 L353

L356 E363 D367 P377 F384 Q405 K406 V409 S410 I419 F430 F434 K459 I463 H468 R487 R488 L489 E492 P503 E506 P507 G538 D543 R548 E552 D559 V566 D567 R579 M593 E594 V595 L612 F613

T614 R621 L626 Q639 M642 N643 I670 P699 L700 D708 L714 Q715 T716 P717 Q718 S719 R723 N734 Y735 P736 I737 I746 I758 V759 N760 K761 E765 I779 E783 K784 Q787 G788 D789 D810 L829 S836 D850 C855 S856

V867 R872 H887 G888 Q889 P903 D912 I913 L914 F915 N916 E931 L979 I992 R1018 D1019 R1020 E1039 M1040 E1041 L1053 N1060 C1061 S1062 D1063 R1064 S1078 L1081 P1085 PRO SER TRP SER ALA MET R1092 N1093 R1094 K1095 Y1096 N1097 C1098 T1099 L1100

I1128 V1135

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

Chain C:

MET ALA ALA SER GLN ALA VAL GLU GLU MET ARG SER ARG VAL VAL LEU GLY GLU PHE GLY VAL ARG ASN VAL HIS THR THR ASP PHE PRO GLY ASN TYR SER GLY TYR ASP D38 R50 V51 D52 E62 V89 N97 I100 D103 G111 E130 E134 L138

K154 E161 T170 R171 N180 Q181 D195 D196 L202 R203 D209 C214 L235 E246 Q268 C269 K270 K271 V272 T282 E291 K294 R301 D319 Q344 MET ASP

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

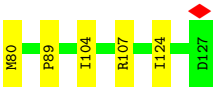
Chain E:

MET D2 V60 L61 V62 Q71 M72 F73 V74 I99 Q107 Q116 D120 M121 L160 L165 R166 E167 N168 Q169 L170 P171 R172 I193 I194 R195 A200 Y203 R207 Q210

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

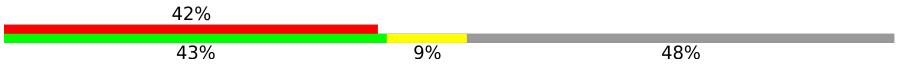
Chain F:

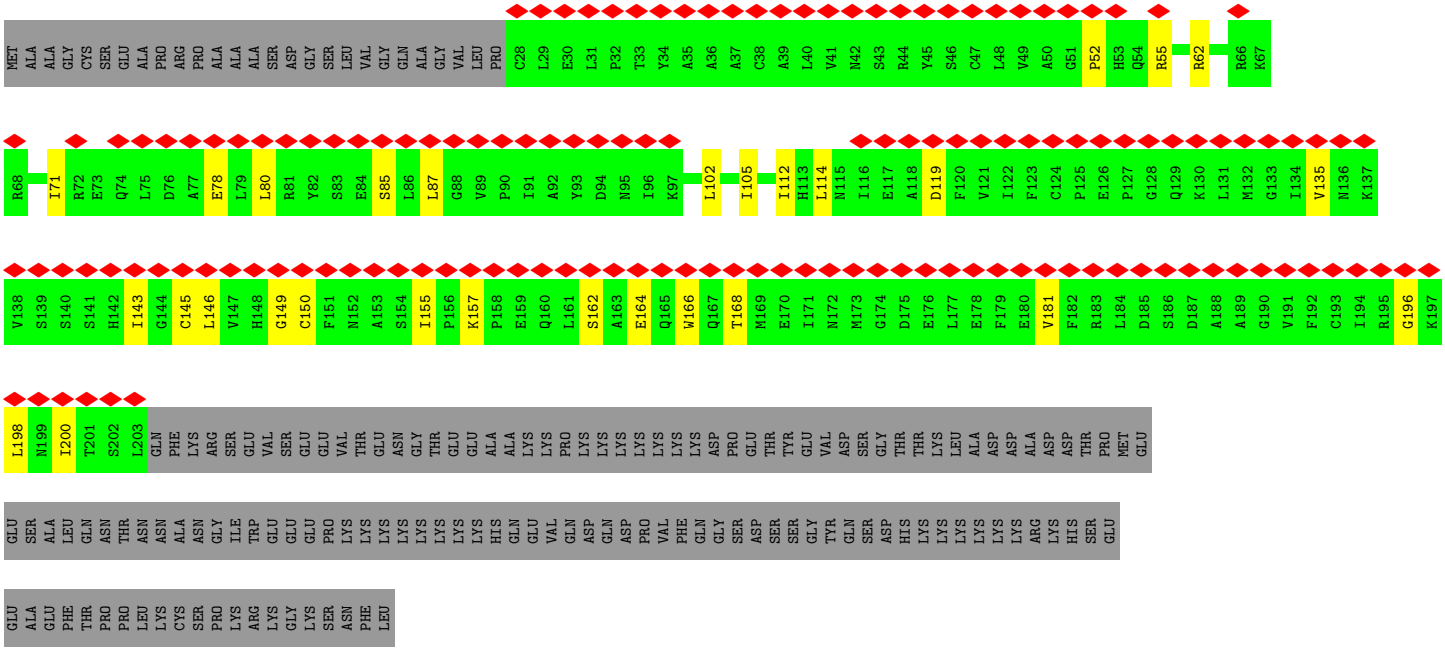
MET SER ASP ASN GLU ASP ASN PHE ASP GLY ASP ASP PHE ASP ASP VAL GLU GLU ASP GLU GLY LEU ASP ASP LEU GLU ASN ALA GLU GLU GLU GLY GLN GLU ASN VAL GLU ILE LEU PRO SER GLY GLU ARG PRO GLN ALA ASN Q49 I52 T53 T54 P55 Y56 M57 T58 R64



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

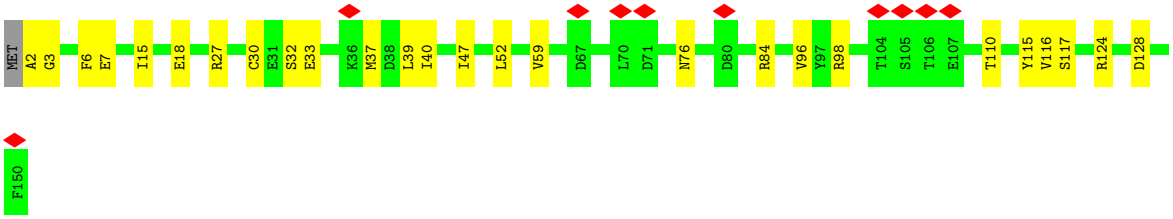
Chain G:





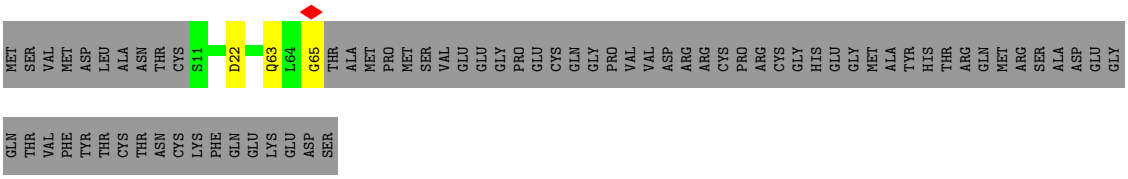
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



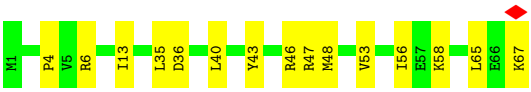
• Molecule 8: DNA-directed RNA polymerase I subunit RPA12

Chain I:



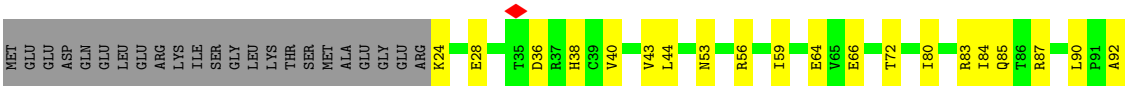
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC5

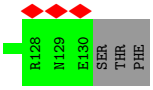
Chain J:



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

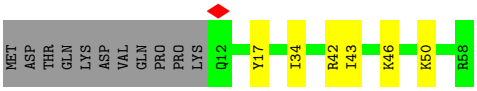
Chain K:





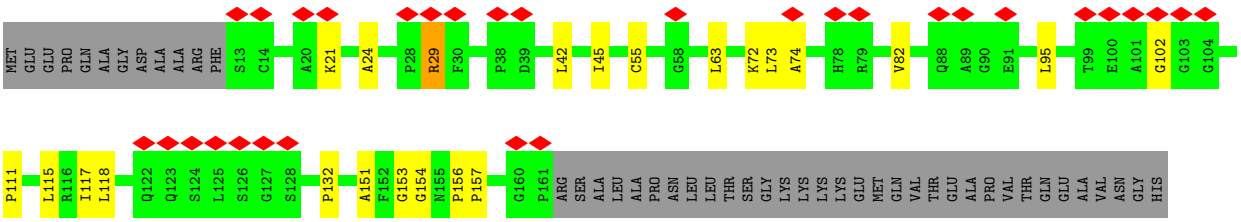
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC4

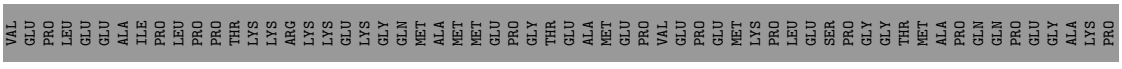
Chain L:



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

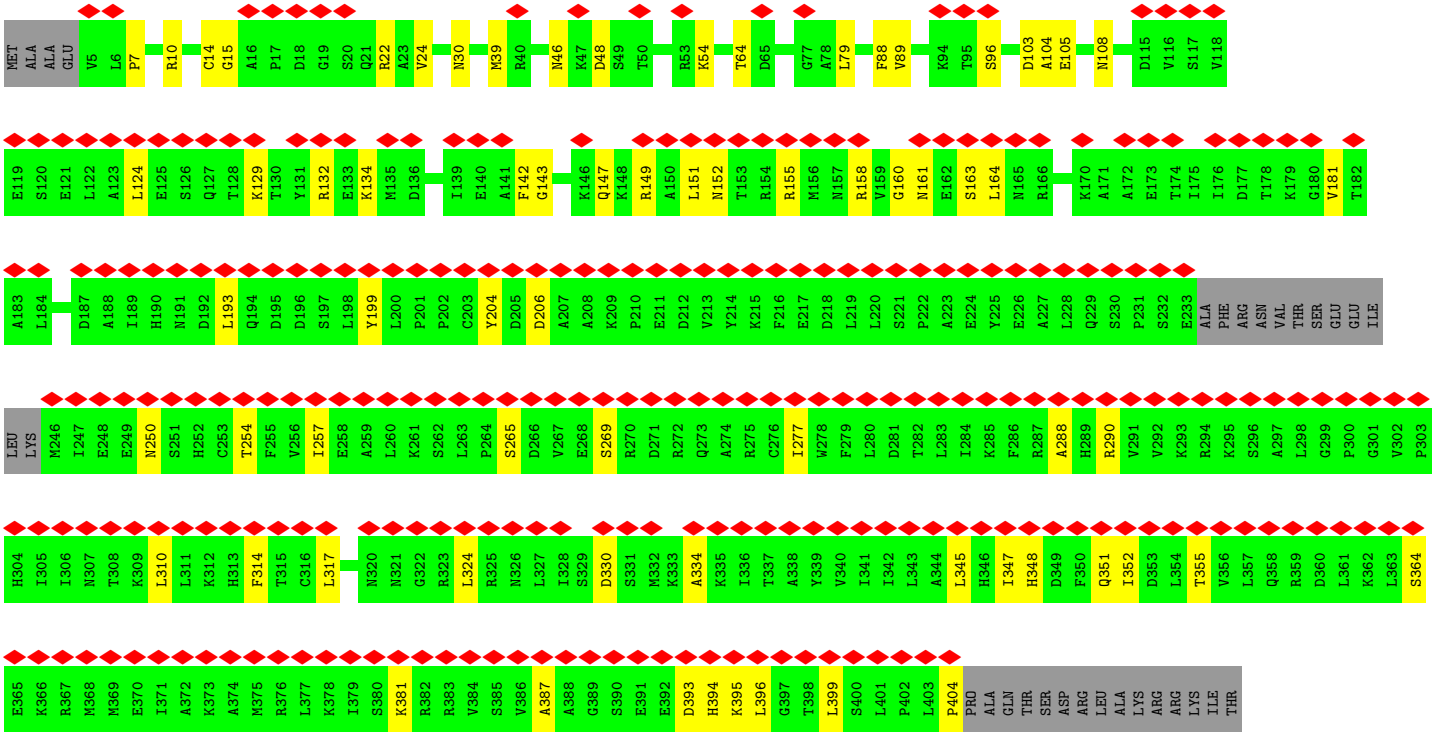
Chain N:





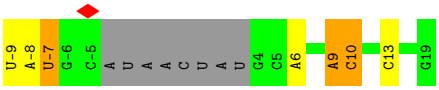
- Molecule 13: DNA-directed RNA polymerase I subunit RPA49

Chain M:



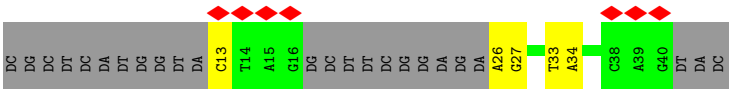
- Molecule 14: RNA

Chain R:



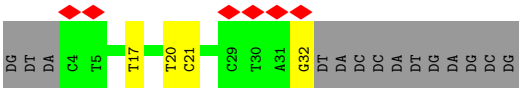
- Molecule 15: DNA non-template strand

Chain S:



- Molecule 16: DNA template strand

Chain T:



4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	230.16, 230.16, 230.16	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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: 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	0.58	1/12480 (0.0%)	0.65	5/16858 (0.0%)
2	B	0.69	3/9174 (0.0%)	0.66	0/12414
3	C	0.60	0/2506	0.63	1/3397 (0.0%)
4	E	0.52	0/1751	0.62	1/2366 (0.0%)
5	F	0.59	0/646	0.67	0/873
6	G	0.33	0/1396	0.60	1/1891 (0.1%)
7	H	0.59	0/1219	0.66	0/1644
8	I	0.44	0/421	0.58	0/569
9	J	0.75	0/542	0.73	0/730
10	K	0.60	0/871	0.59	0/1174
11	L	0.67	0/403	0.64	0/536
12	N	0.37	0/1118	0.60	0/1532
13	M	0.32	0/3112	0.61	2/4197 (0.0%)
14	R	0.93	0/501	1.28	2/776 (0.3%)
15	S	0.66	0/435	1.03	0/667
16	T	1.20	0/666	1.00	2/1026 (0.2%)
All	All	0.61	4/37241 (0.0%)	0.67	14/50650 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	566	VAL	CB-CG2	-5.75	1.40	1.52
1	A	391	TRP	CB-CG	-5.13	1.41	1.50
2	B	215	VAL	CB-CG2	-5.08	1.42	1.52
2	B	489	LEU	C-N	-5.01	1.22	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	409	LEU	CA-CB-CG	6.55	130.38	115.30
1	A	96	LEU	CA-CB-CG	6.07	129.25	115.30
16	T	21	DC	O4'-C4'-C3'	-6.01	102.09	104.50
6	G	87	LEU	CA-CB-CG	5.92	128.92	115.30
14	R	-7	U	C5-C6-N1	5.85	125.62	122.70
1	A	915	LEU	CB-CG-CD2	-5.74	101.25	111.00
13	M	193	LEU	CA-CB-CG	5.64	128.27	115.30
16	T	20	DT	O4'-C4'-C3'	-5.42	102.33	104.50
1	A	744	LEU	CA-CB-CG	5.32	127.54	115.30
3	C	196	ASP	CB-CG-OD1	5.30	123.07	118.30
4	E	165	LEU	CA-CB-CG	5.25	127.39	115.30
1	A	627	LEU	CA-CB-CG	5.24	127.35	115.30
14	R	13	C	C2-N1-C1'	5.17	124.49	118.80
13	M	124	LEU	CA-CB-CG	5.08	126.99	115.30

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 (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	12222	0	12336	112	0
2	B	8957	0	8942	73	0
3	C	2458	0	2456	20	0
4	E	1720	0	1737	14	0
5	F	636	0	667	9	0
6	G	1369	0	1355	16	0
7	H	1197	0	1156	16	0
8	I	414	0	395	2	0
9	J	533	0	553	11	0
10	K	856	0	840	12	0
11	L	397	0	401	6	0
12	N	1083	0	1079	15	0
13	M	3062	0	3094	44	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	305	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 4.

All (305) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:95:LYS:HE2	1:A:1686:MET:HE1	1.83	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:621:ARG:HH21	2:B:639:GLN:HE21	1.54	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:H:32:SER:OG	7:H:33:GLU:N	2.42	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
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:850:HIS:HD1	1:A:941:TYR:HH	1.59	0.50
1:A:1112:GLY:HA3	4:E:60:VAL:HG12	1.92	0.50
1:A:1332:CYS:HG	1:A:1554:TYR:HH	1.53	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
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
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
3:C:268:GLN:HB3	3:C:270:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:559:ASP:OD2	2:B:614:THR:OG1	2.28	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
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:1715:LEU:HD23	5:F:104:ILE:HG21	1.96	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
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
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: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
2:B:593:MET:HE2	2:B:612:LEU:HB3	1.97	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:N	13:M:48:ASP:OD1	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: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
13:M:288:ALA:HA	13:M:290:ARG:HH21	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:550:LEU:HB3	1:A:594:MET:HE3	2.00	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
1:A:1268:VAL:HG11	1:A:1278:VAL:HG21	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:829:LEU:HA	2:B:836:SER:HA	2.01	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
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
1:A:1264:MET:HE1	1:A:1584:ASN:H	1.86	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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%)	51 78
2	B	1125/1135 (99%)	1062 (94%)	63 (6%)	0	100 100
3	C	305/346 (88%)	297 (97%)	7 (2%)	1 (0%)	41 66
4	E	207/210 (99%)	199 (96%)	8 (4%)	0	100 100
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1349/1504 (90%)	1342 (100%)	7 (0%)	88	96
2	B	987/992 (100%)	983 (100%)	4 (0%)	91	97
3	C	270/302 (89%)	270 (100%)	0	100	100
4	E	191/192 (100%)	190 (100%)	1 (0%)	88	96
5	F	69/111 (62%)	67 (97%)	2 (3%)	42	71
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%)	49 (100%)	0	100	100
9	J	56/56 (100%)	56 (100%)	0	100	100
10	K	96/119 (81%)	95 (99%)	1 (1%)	76	91
11	L	44/55 (80%)	44 (100%)	0	100	100
12	N	118/427 (28%)	117 (99%)	1 (1%)	81	93
13	M	338/366 (92%)	338 (100%)	0	100	100
All	All	3847/4654 (83%)	3831 (100%)	16 (0%)	91	97

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	MET

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Mol	Chain	Res	Type
1	A	372	ARG
1	A	391	TRP
1	A	915	LEU
1	A	1101	LYS
1	A	1311	LYS
1	A	1351	MET
2	B	314	VAL
2	B	723	ARG
2	B	867	VAL
2	B	916	ASN
4	E	121	MET
5	F	53	THR
5	F	80	MET
10	K	24	LYS
12	N	29	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	HIS
1	A	595	ASN
1	A	895	GLN
1	A	1109	ASN
1	A	1690	HIS
2	B	580	HIS
2	B	916	ASN
2	B	1060	ASN
10	K	85	GLN
12	N	78	HIS
13	M	108	ASN
13	M	152	ASN

5.3.3 RNA (i)

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 monosaccharides 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 (i)

There are no chain breaks in this entry.

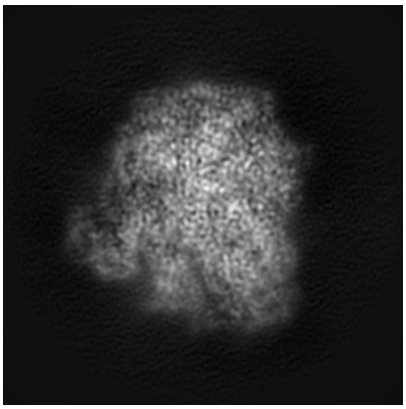
6 Map visualisation (i)

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.

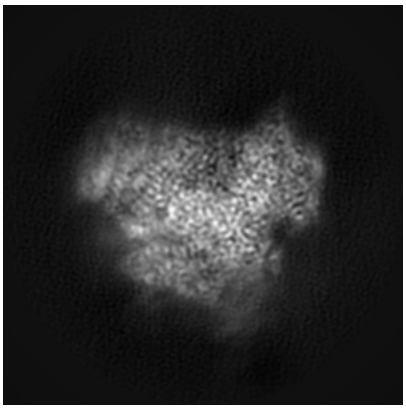
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

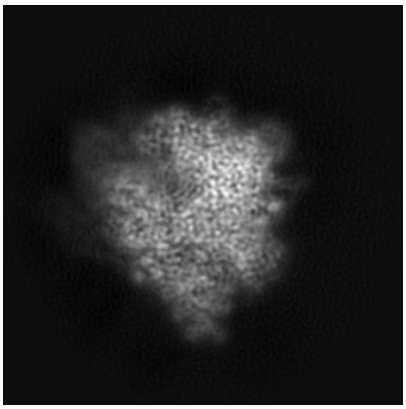
6.1.1 Primary map



X

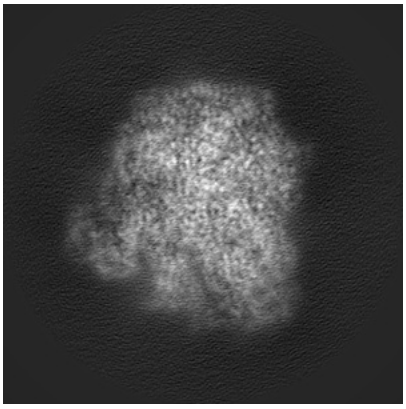


Y

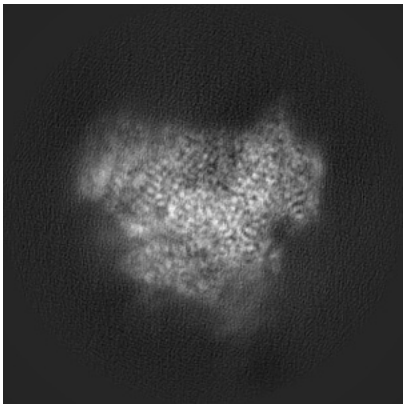


Z

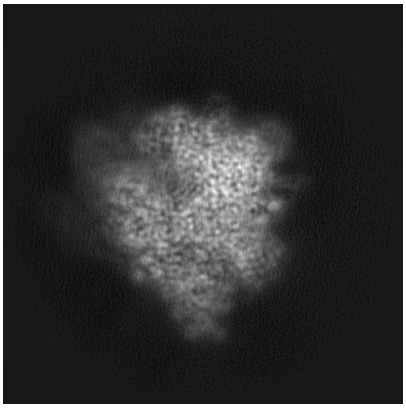
6.1.2 Raw map



X



Y

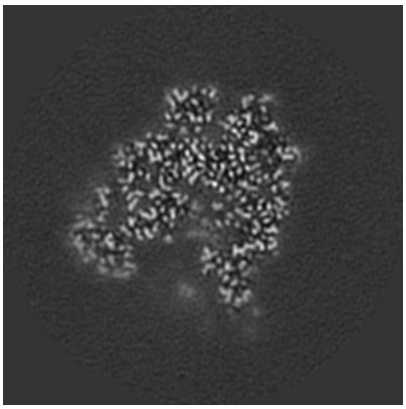


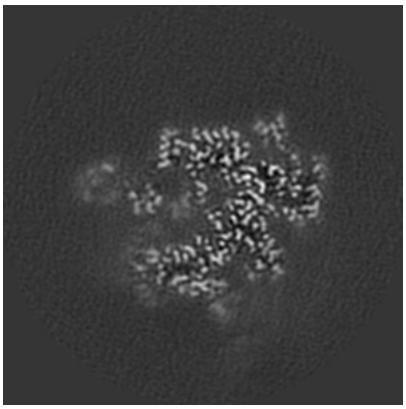
Z

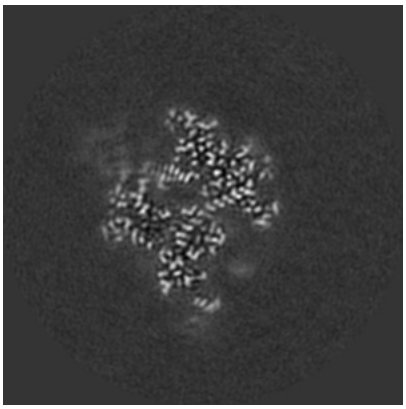
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

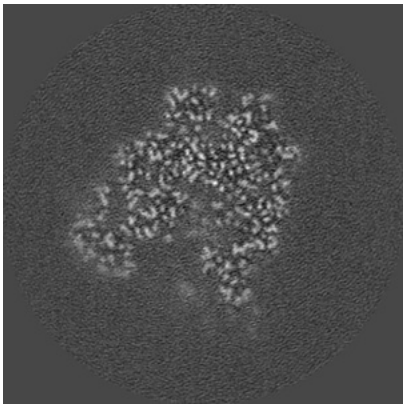
6.2.1 Primary map

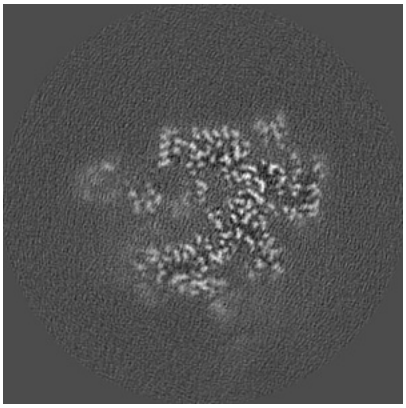

X Index: 140

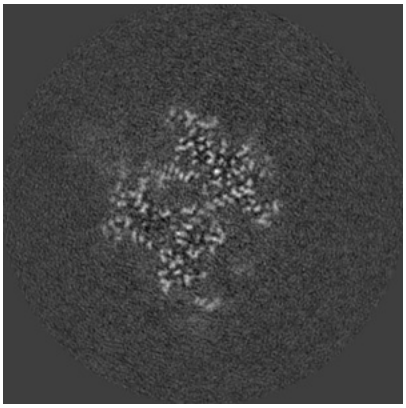

Y Index: 140


Z Index: 140

6.2.2 Raw map


X Index: 140

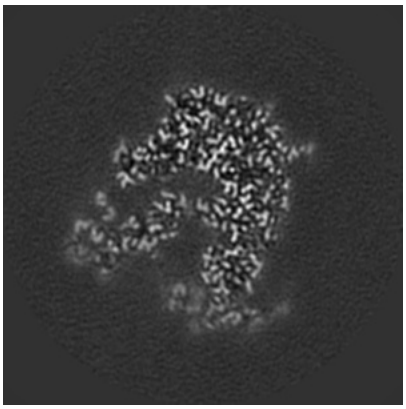

Y Index: 140

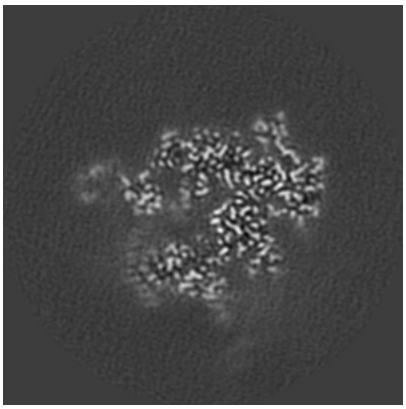

Z Index: 140

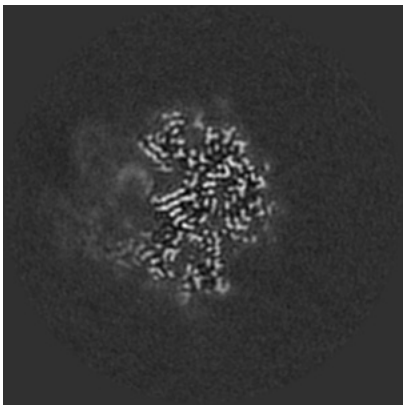
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

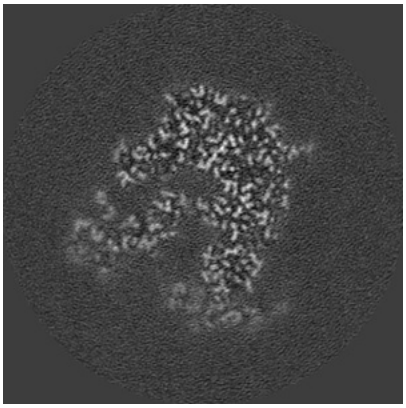
6.3.1 Primary map

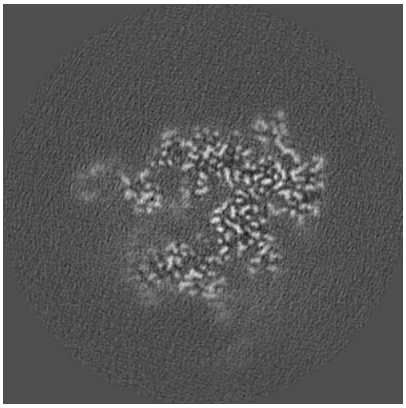

X Index: 147

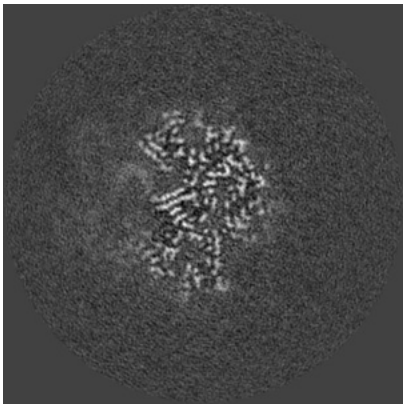

Y Index: 142


Z Index: 165

6.3.2 Raw map


X Index: 147

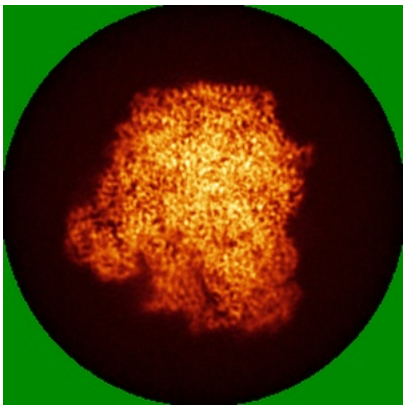

Y Index: 142

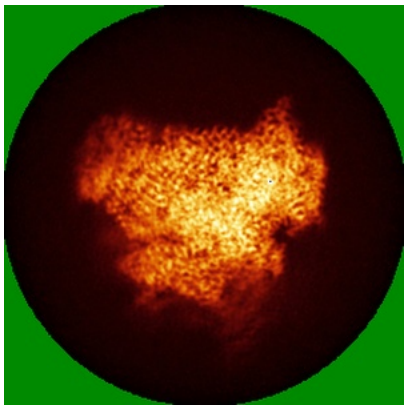

Z Index: 165

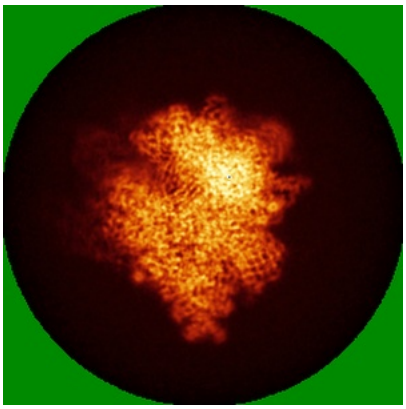
The images above show the largest variance slices of the map in three orthogonal directions.

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

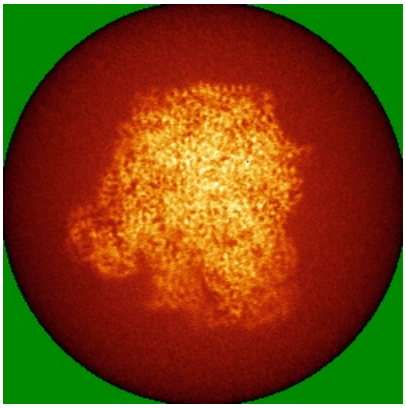
6.4.1 Primary map

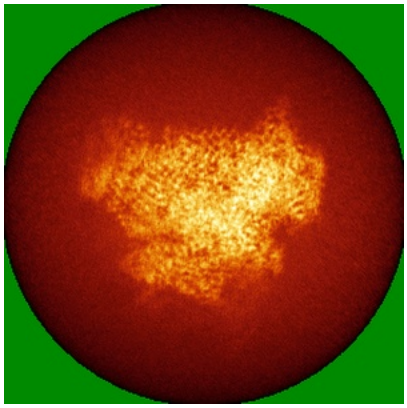

X

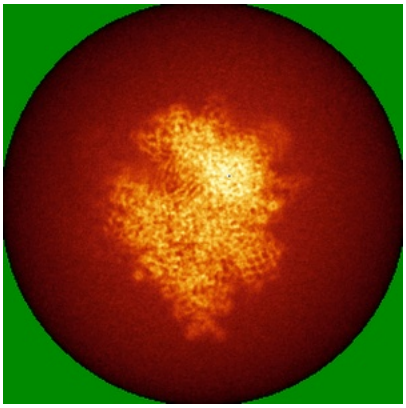

Y


Z

6.4.2 Raw map


X

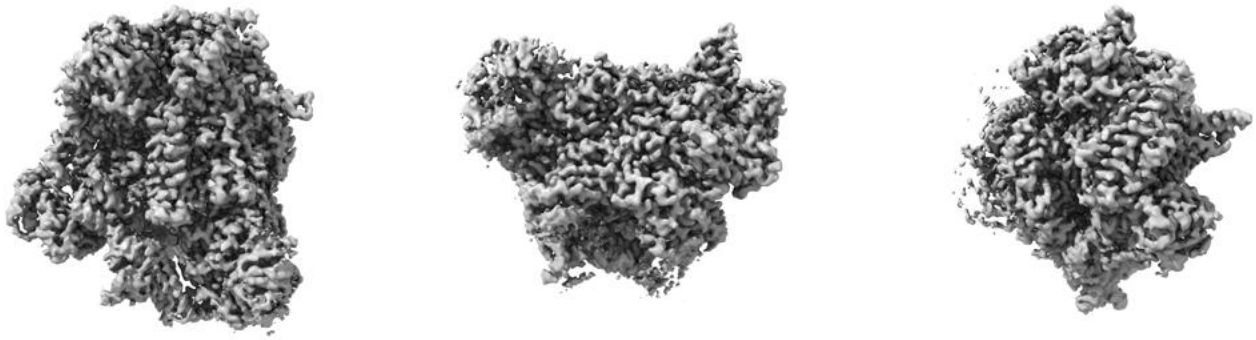

Y


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)

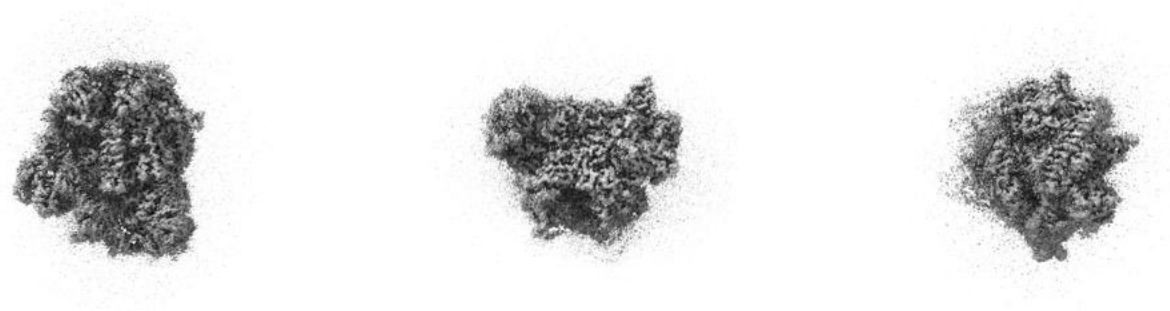
6.5.1 Primary map



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.

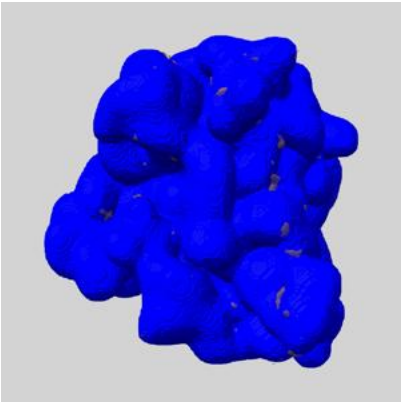
6.6 Mask visualisation (i)

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

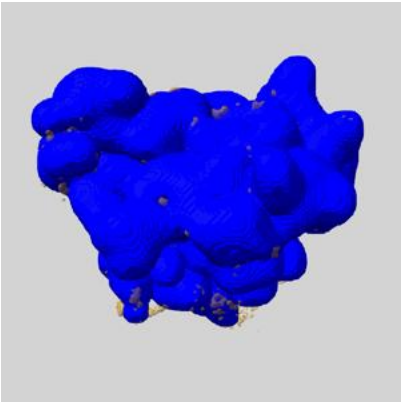
A mask typically either:

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

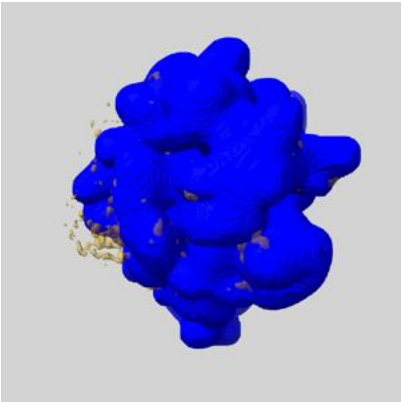
6.6.1 emd_12795_msk_3.map (i)



X

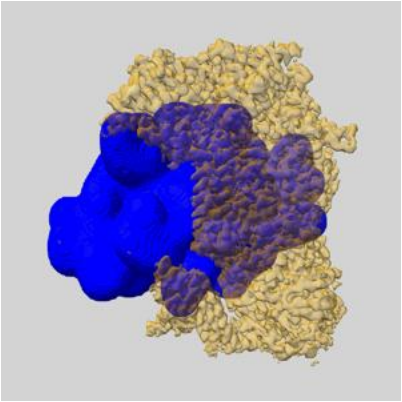


Y

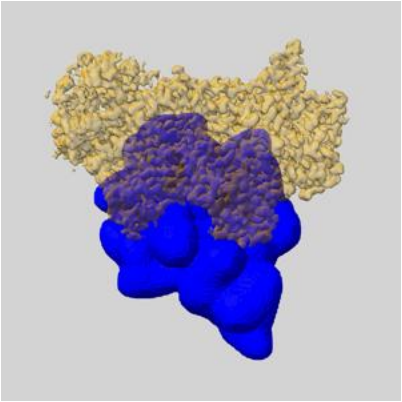


Z

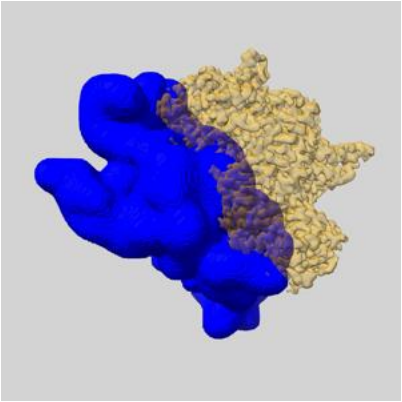
6.6.2 emd_12795_msk_1.map (i)



X

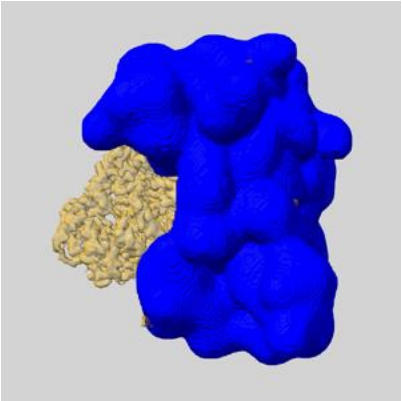


Y

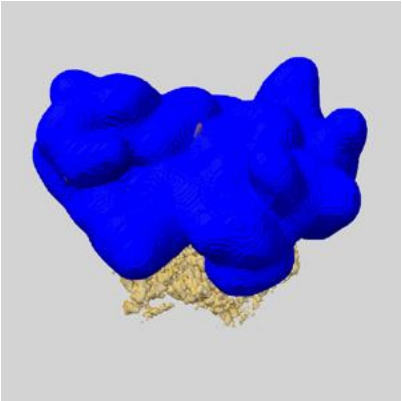


Z

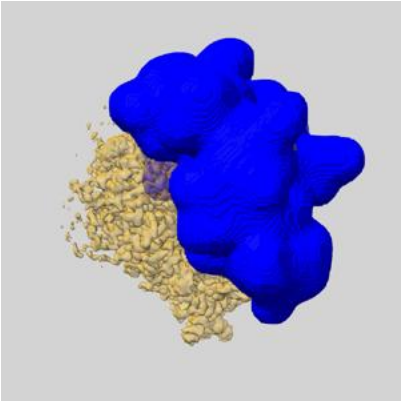
6.6.3 emd_12795_msk_2.map ⓘ



X



Y

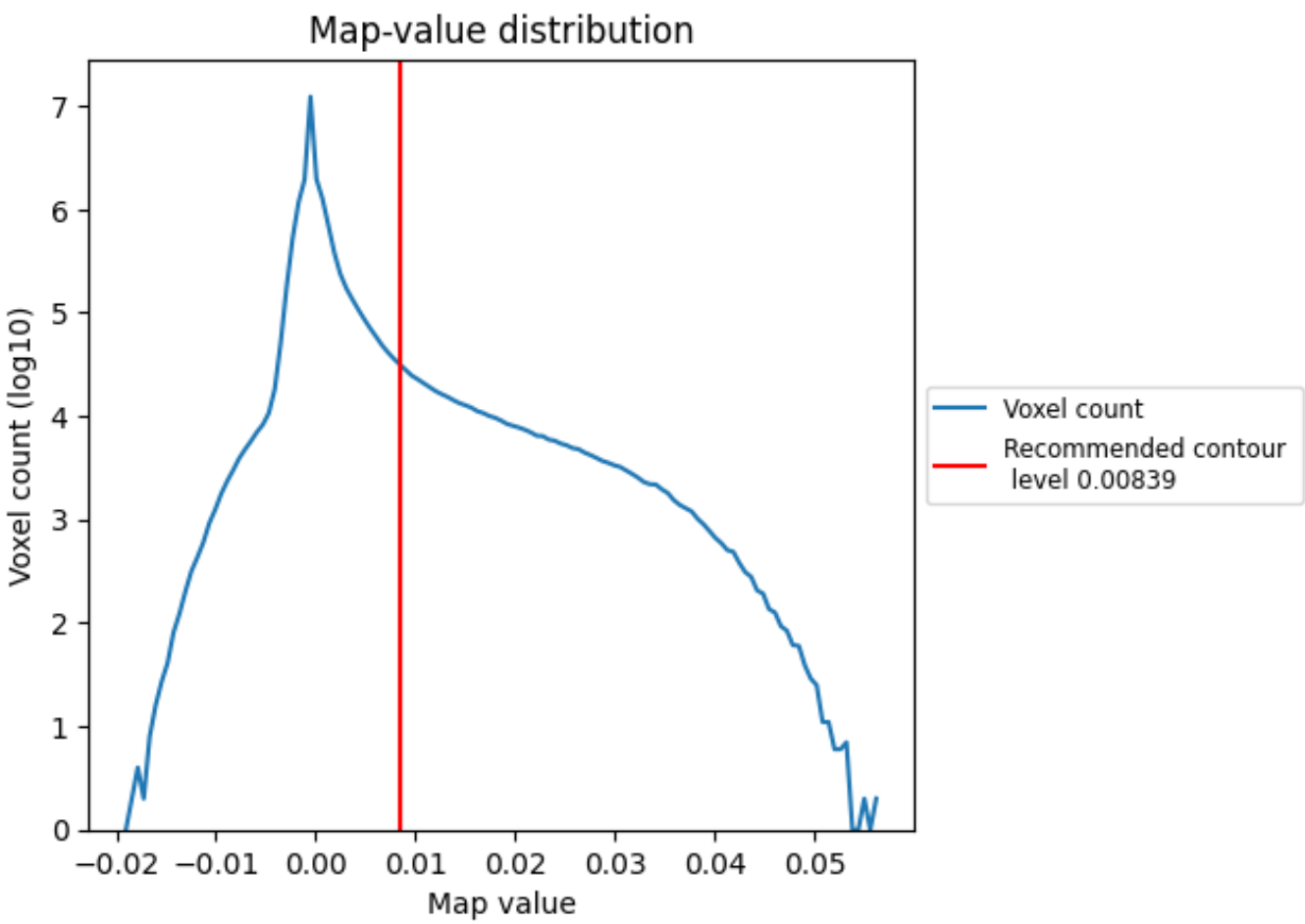


Z

7 Map analysis (i)

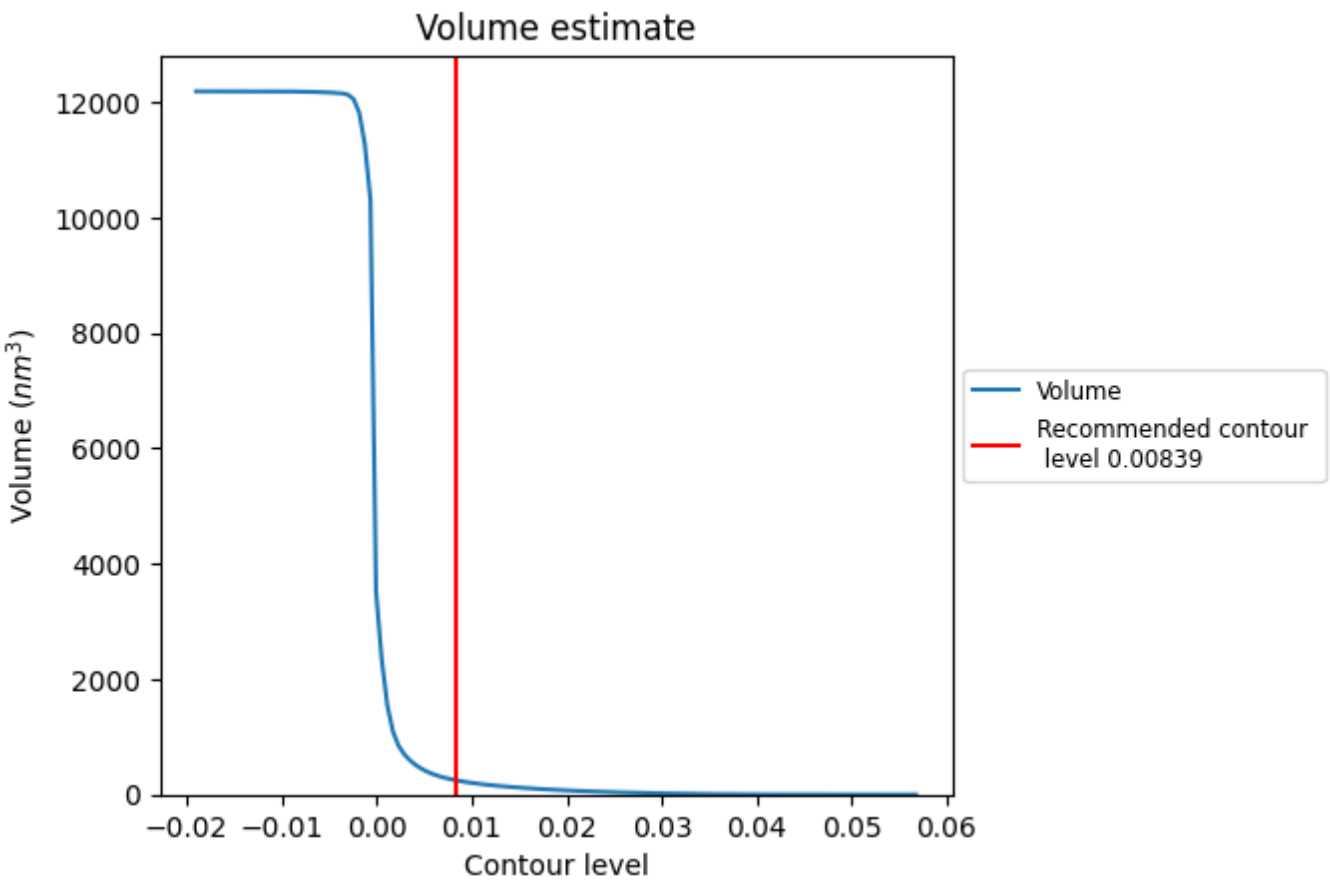
This section contains the results of statistical analysis of the map.

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.

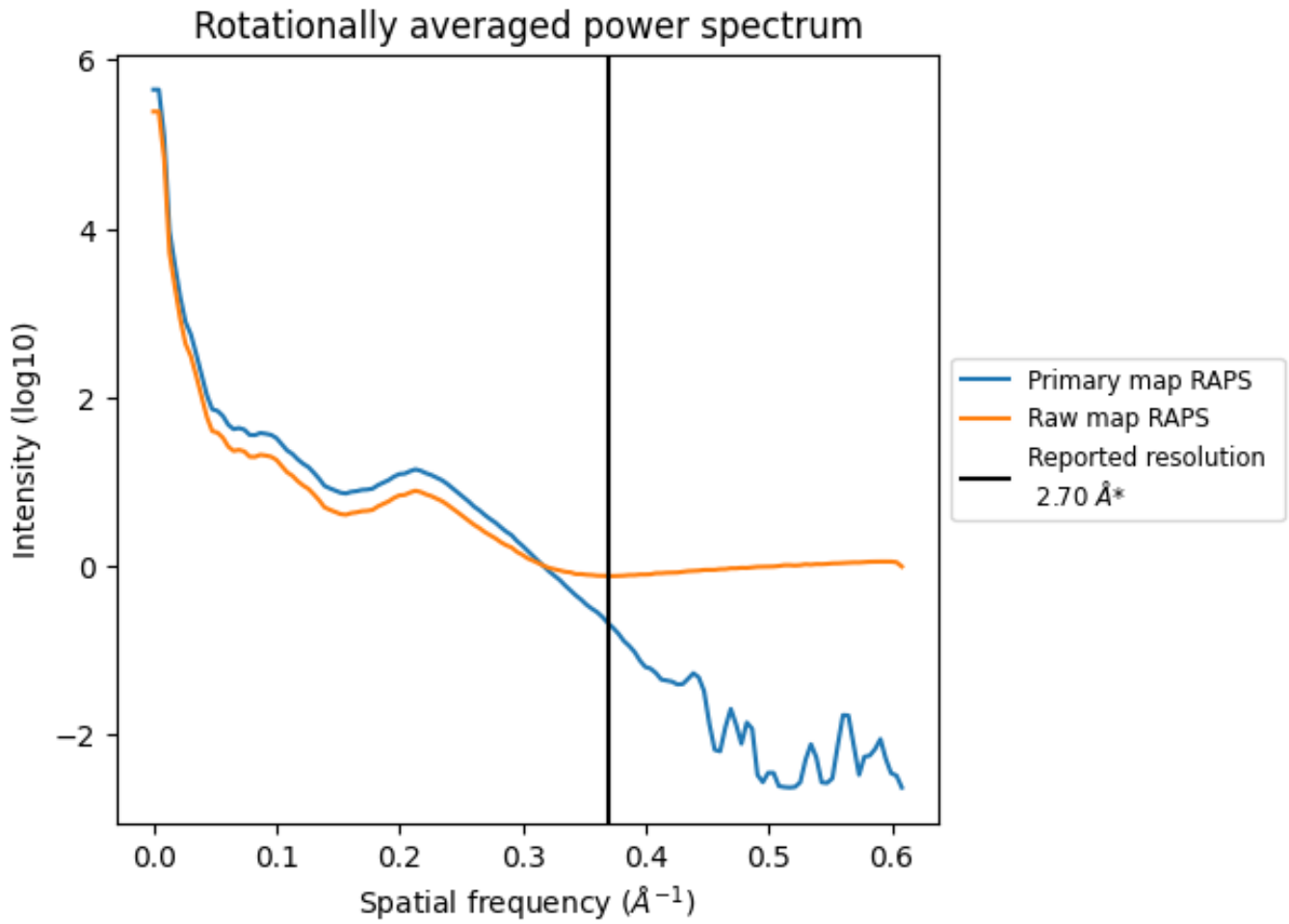
7.2 Volume estimate (i)



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 (i)

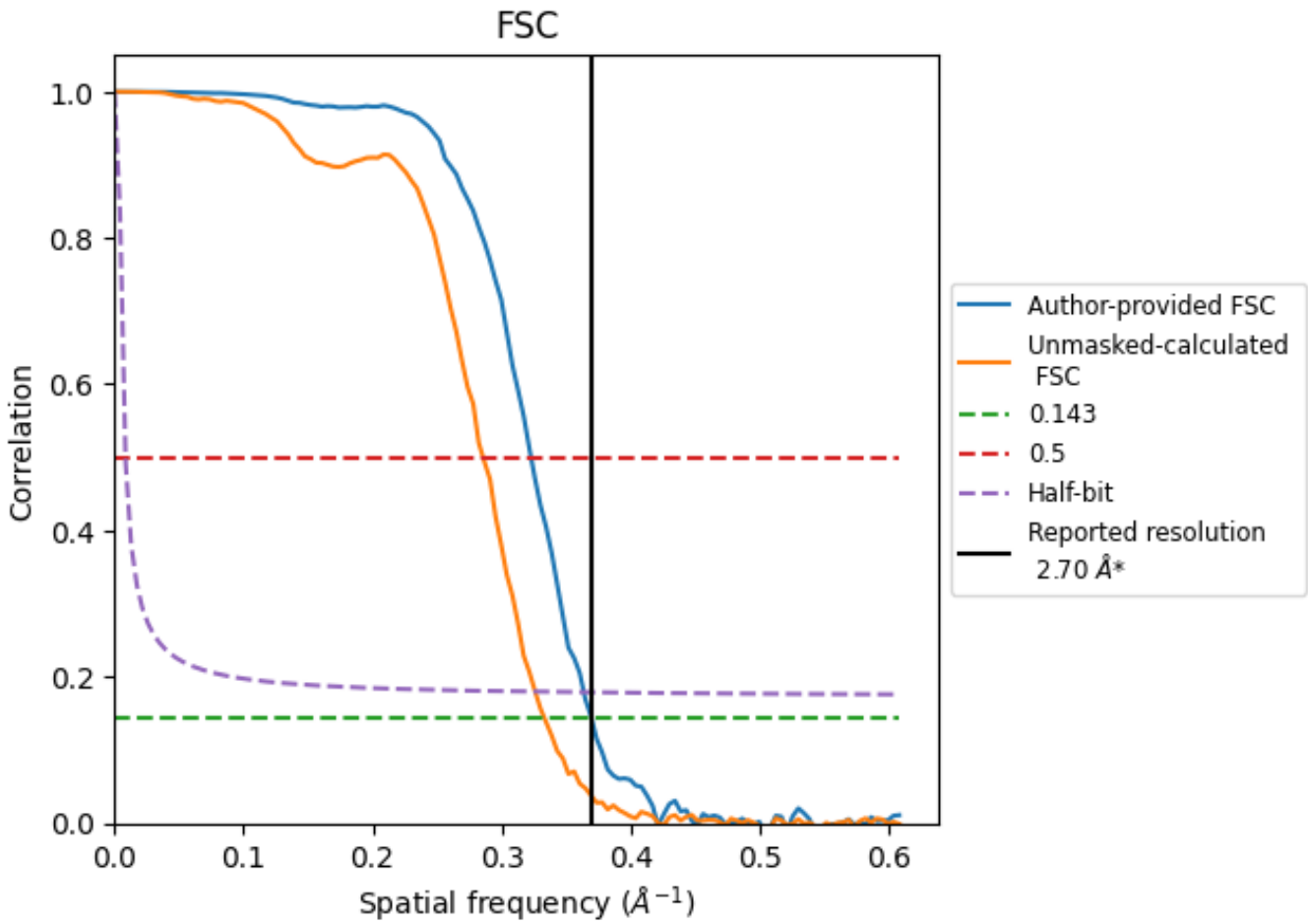


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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 Å^{-1}

8.2 Resolution estimates (i)

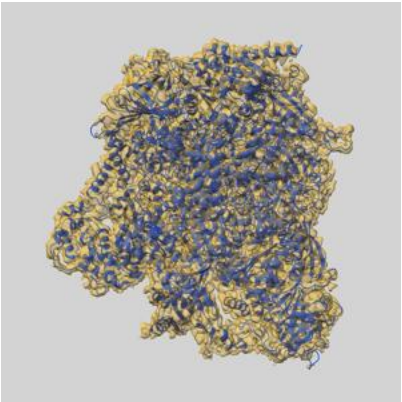
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.10	2.75
Unmasked-calculated*	3.00	3.50	3.07

*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 %

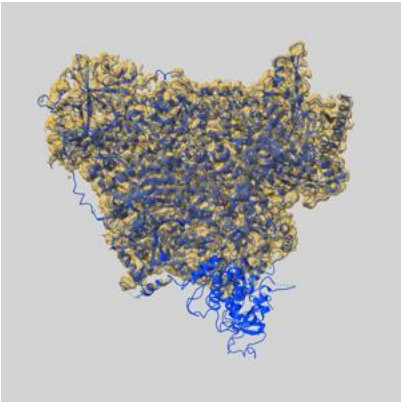
9 Map-model fit (i)

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.

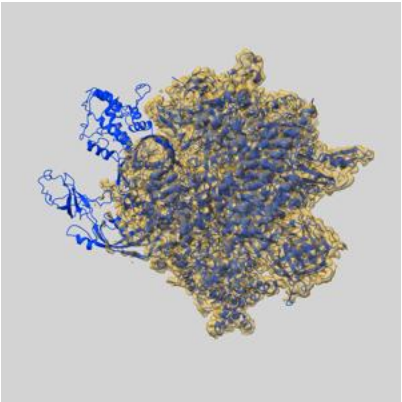
9.1 Map-model overlay (i)



X



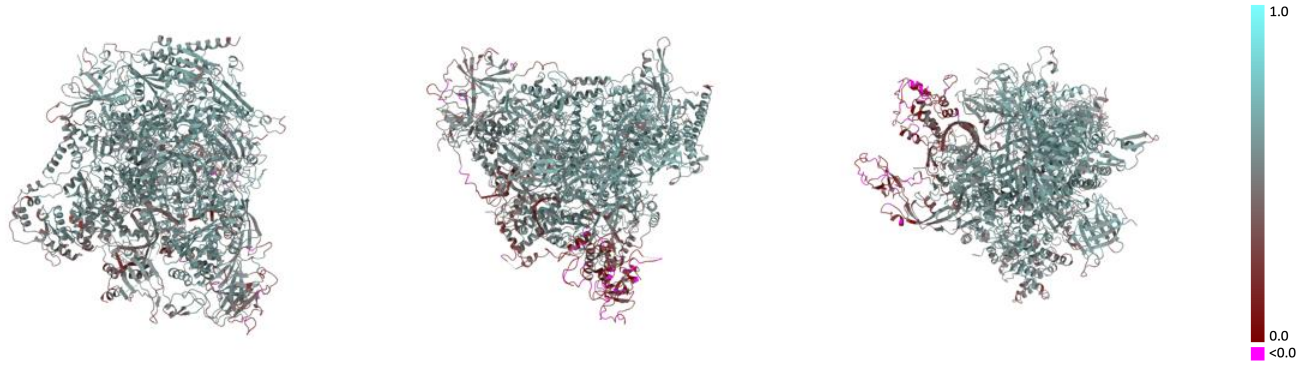
Y



Z

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.

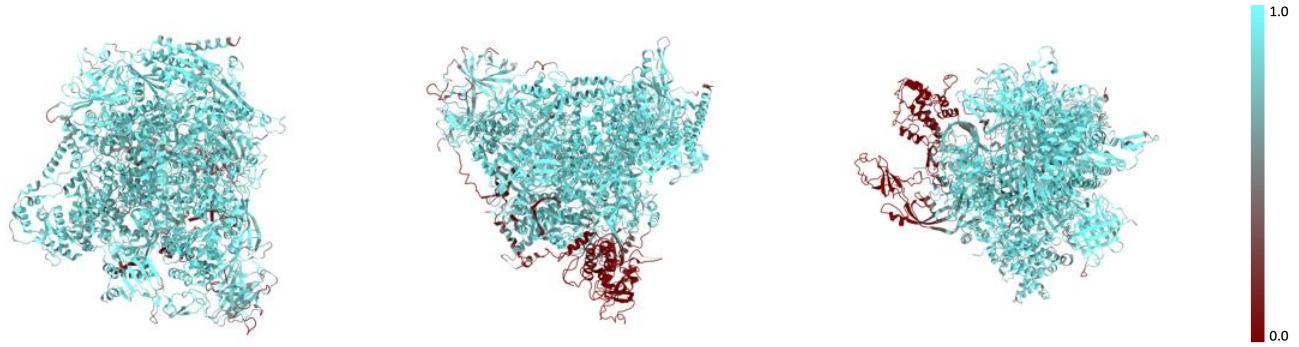
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

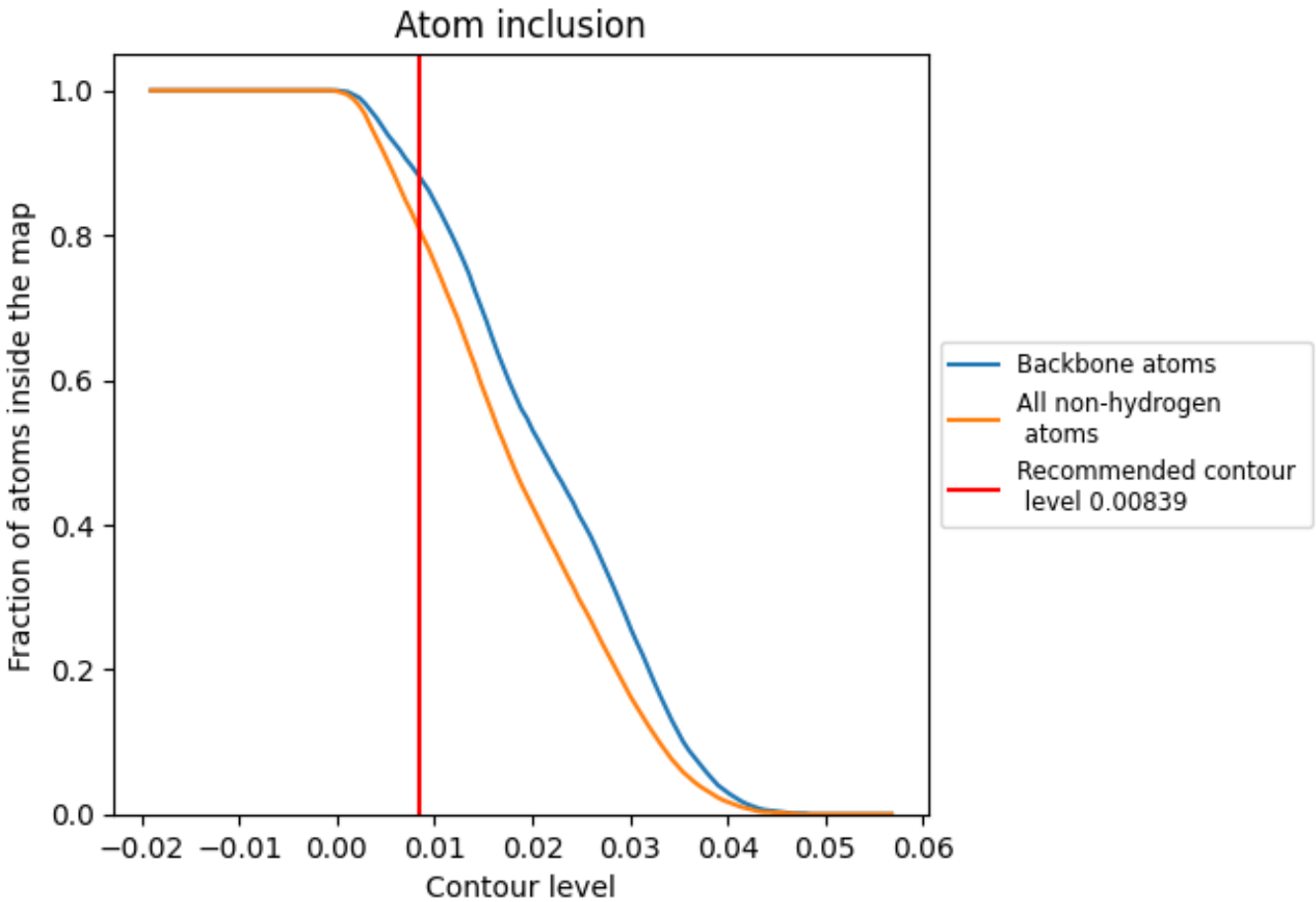
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00839).

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 (i)

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