Full wwPDB EM Validation Report (i)

Jul 3, 2024 – 07:41 am BST

PDB ID	:	7ODE
EMDB ID	:	EMD-12826
Title	:	E. coli 50S ribosome LiCl core particle
Authors	:	Larsson, D.S.D.; Selmer, M.
Deposited on	:	2021-04-29
Resolution	:	2.84 Å(reported)
Based on initial model	:	4YBB

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:

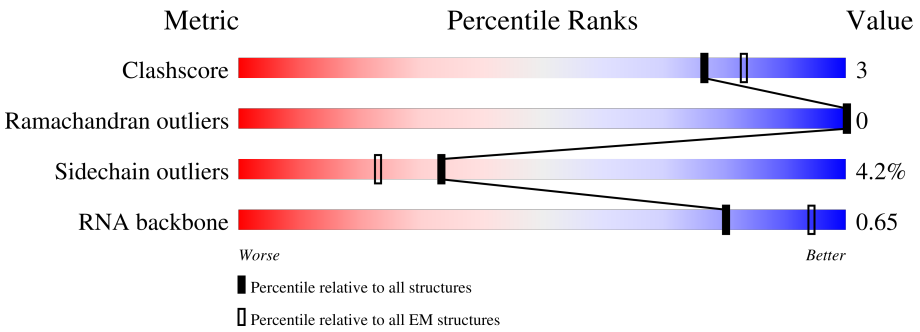
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.84 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	I	2904	55% 12% • 31%
2	K	273	68% 14% • 17%
3	L	209	78% 10% 12%
4	M	201	19% 63% 18% • 18%
5	R	142	87% 13%
6	S	123	50% 87% 12% •
7	V	127	82% 12% • 6%

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Mol	Chain	Length	Quality of chain
8	X	115	30% 90% 9%
9	Y	118	86% 12%
10	Z	103	86% 14%
11	a	110	97%
12	b	100	90% 7%
13	c	104	64% 94%
14	g	63	98%
15	i	57	58% 89% 9%
16	k	46	98%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 92569 atoms, of which 36041 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	I	1990	64256	19077	21509	7915	13771	1984	0	0

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	K	226	3509	1066	1788	344	304	7	0	0

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	L	183	2813	869	1438	247	255	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	M	165	2619	809	1337	225	243	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	R	142	2291	714	1162	212	199	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	S	122	1950	587	1012	180	165	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	V	120	1960	593	1000	196	166	5	0	0

- Molecule 8 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	X	114	1879	574	962	179	163	1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
9	Y	117	1967	604	1020	192	151	0	0

- Molecule 10 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	Z	103	1655	516	839	153	145	2	0	0

- Molecule 11 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	a	110	1779	532	922	166	156	3	0	0

- Molecule 12 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	b	93	1545	466	807	139	131	2	0	0

- Molecule 13 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
13	c	102	1612	492	833	146	141	0	0

- Molecule 14 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
14	g	62	1032	308	531	98	94	1	0	0

- Molecule 15 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
15	i	56	907	269	463	94	80	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L34.

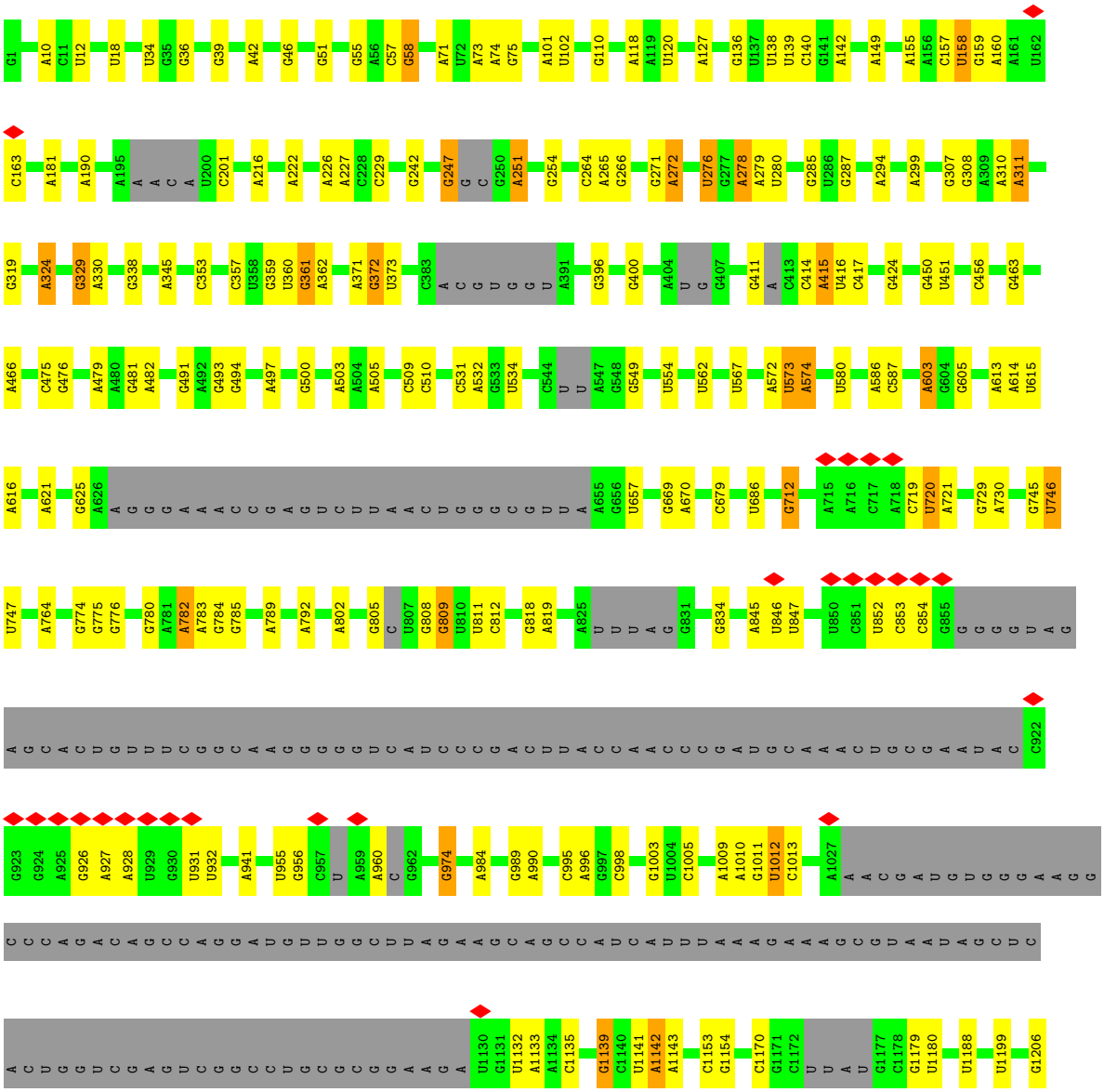
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
16	k	46	795	228	418	90	57	2	0	0

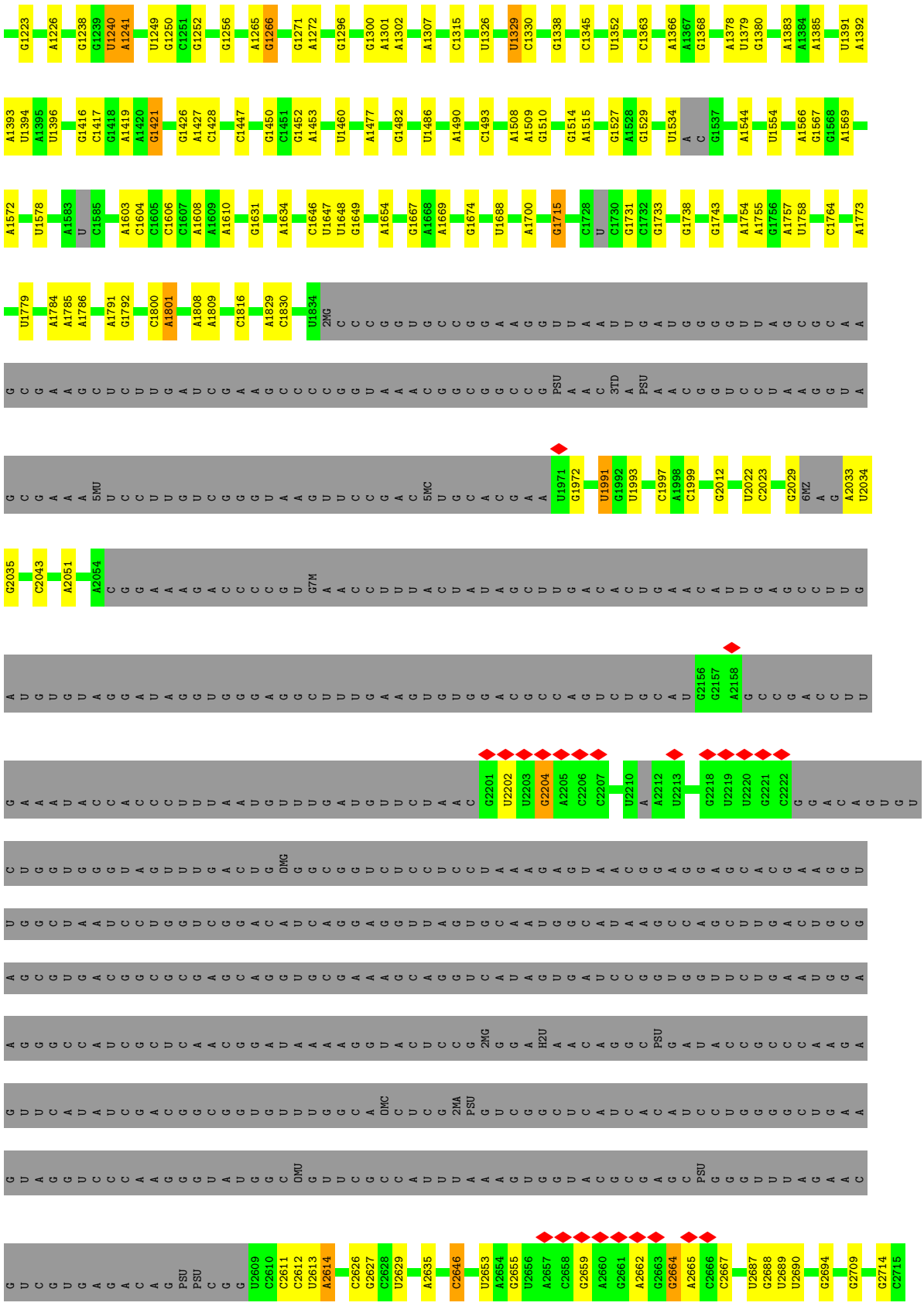
3 Residue-property plots (i)

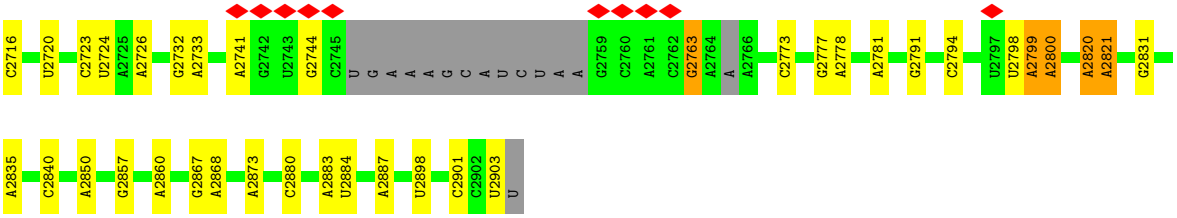
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S rRNA

Chain I:

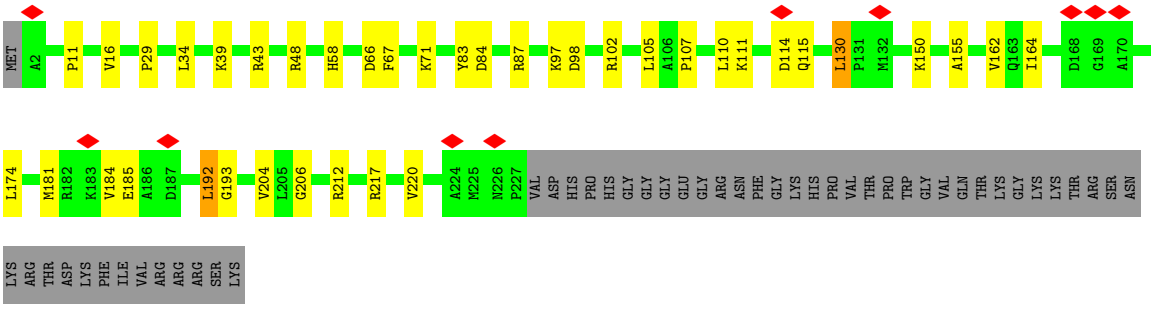



G1223 A1226 G1238 G1239 U1240 A1241 U1249 G1250 C1251 G1252 G1256 A1265 G1266 G1271 A1272 G1296 G1300 A1301 A1302 A1307 C1315 U1326 U1329 C1330 G1338 C1345 U1352 C1363 A1366 A1367 G1368 A1378 U1379 G1380 A1383 A1384 A1385 U1391 A1392
A1393 U1394 A1395 U1396 G1416 C1417 G1418 A1419 A1420 G1421 G1426 A1427 C1428 C1447 G1450 C1451 G1452 A1453 U1460 A1477 G1482 U1486 A1490 C1493 A1508 A1509 G1510 G1514 A1515 G1527 A1528 G1529 U1534 A C G1537 A1544 U1554 A1566 G1567 G1568 A1569
A1572 U1578 A1583 U C1585 A1603 C1604 C1605 C1606 C1607 A1608 A1609 A1610 G1631 A1634 C1646 U1647 U1648 G1649 A1654 G1667 A1668 A1669 G1674 U1688 A1700 G1715 C1728 U C1730 G1731 C1732 G1733 G1738 G1743 A1754 A1755 G1756 A1757 U1758 C1764 A1773
U1779 A1784 A1785 A1786 A1791 G1792 C1800 A1801 A1808 A1809 C1816 A1829 C1830 U1834 2MG
G C G A A G C U U C U U G A U C G A A G C C C G U U C G G C C G A A G G U A A C 3TD A PSU A A C U U G A U G G G G U U C C G A U
G C G A A A 5MU U C C U U G U C U G C C C G A C 5MC U G G C A C G A U G U A A G C U U C C C G A C U G C U A U G U U U G A A G U U G U U U U A A G G G G A G G C C U U U A A G G G C C C C C G U G A A C A C C U U G A U U G U U G A A C U U G U U G U U U U U A U A G G G U U U U U A A G G G U U U U U A A G G G U U U U U A



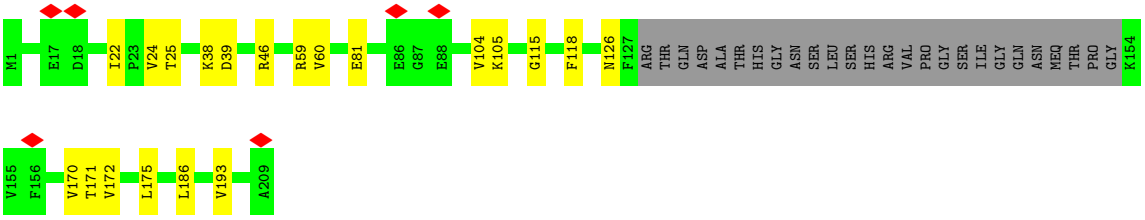
- Molecule 2: 50S ribosomal protein L2

Chain K:



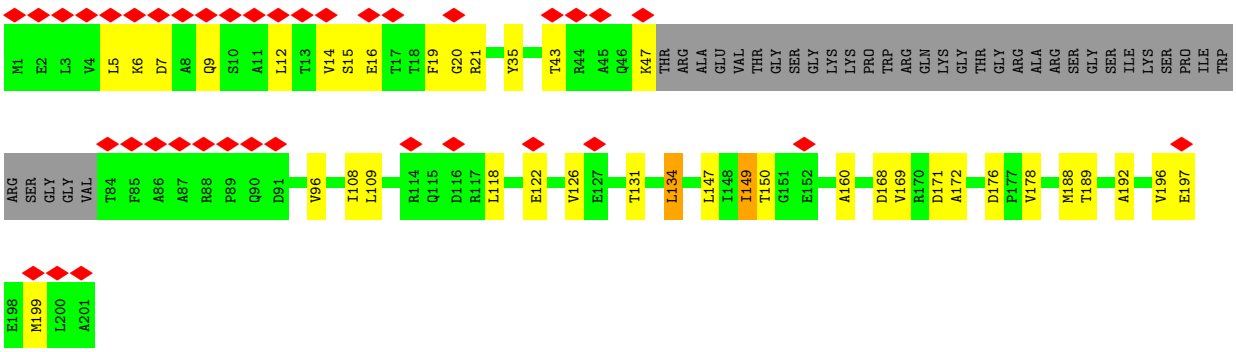
- Molecule 3: 50S ribosomal protein L3

Chain L:



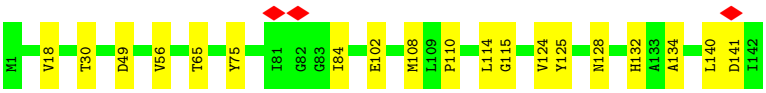
- Molecule 4: 50S ribosomal protein L4

Chain M:



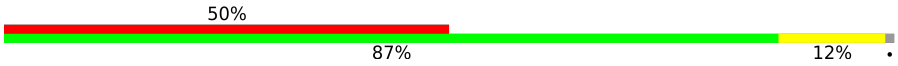
- Molecule 5: 50S ribosomal protein L13

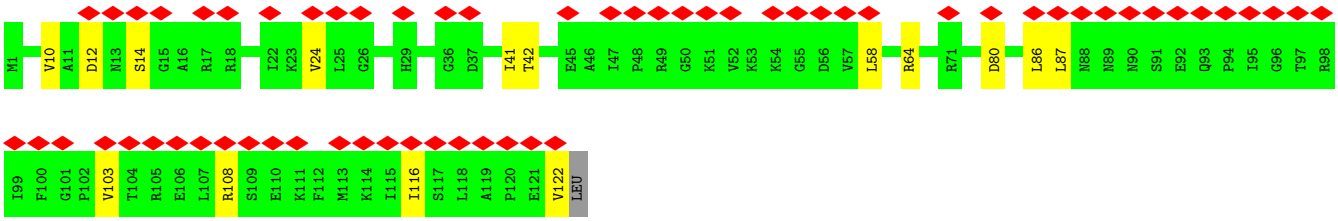
Chain R:



• Molecule 6: 50S ribosomal protein L14

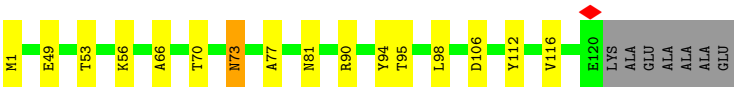
Chain S:





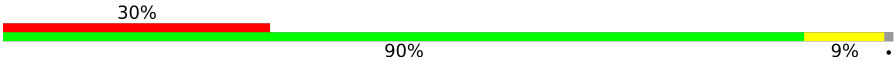
• Molecule 7: 50S ribosomal protein L17

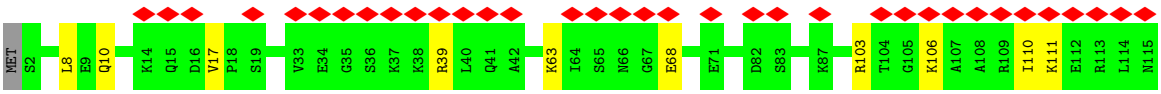
Chain V:



• Molecule 8: 50S ribosomal protein L19

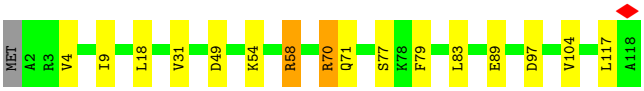
Chain X:





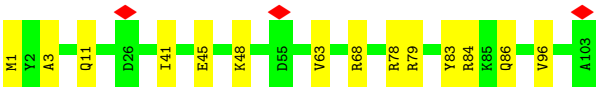
• Molecule 9: 50S ribosomal protein L20

Chain Y:



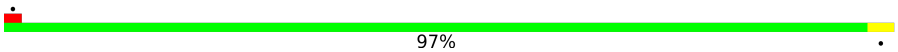
• Molecule 10: 50S ribosomal protein L21

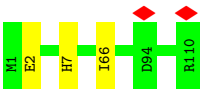
Chain Z:



• Molecule 11: 50S ribosomal protein L22

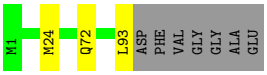
Chain a:





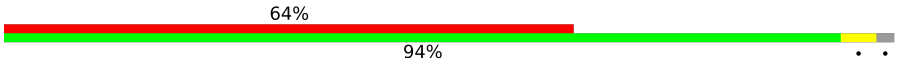
• Molecule 12: 50S ribosomal protein L23

Chain b:



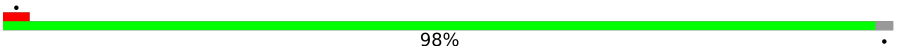
• Molecule 13: 50S ribosomal protein L24

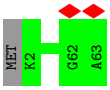
Chain c:



• Molecule 14: 50S ribosomal protein L29

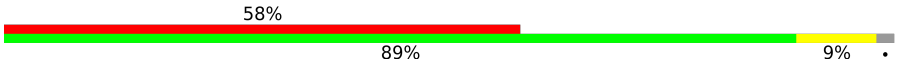
Chain g:

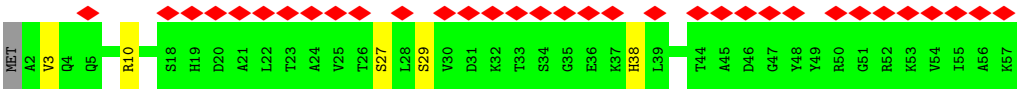




• Molecule 15: 50S ribosomal protein L32

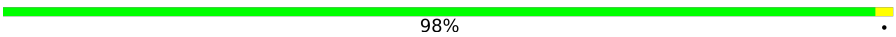
Chain i:





• Molecule 16: 50S ribosomal protein L34

Chain k:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	384374	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 ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.178	Depositor
Minimum map value	-0.499	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	479.36002, 479.36002, 479.36002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: PSU, 5MU, 1MG

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	I	0.26	0/47771	0.67	0/74478
2	K	0.25	0/1750	0.56	0/2356
3	L	0.26	0/1391	0.51	0/1867
4	M	0.24	0/1294	0.46	0/1741
5	R	0.25	0/1152	0.49	0/1551
6	S	0.25	0/947	0.55	0/1268
7	V	0.25	0/973	0.56	0/1301
8	X	0.24	0/929	0.54	0/1242
9	Y	0.26	0/960	0.52	0/1278
10	Z	0.26	0/829	0.54	0/1107
11	a	0.25	0/864	0.54	0/1156
12	b	0.25	0/744	0.50	0/994
13	c	0.25	0/787	0.51	0/1051
14	g	0.22	0/502	0.50	0/667
15	i	0.24	0/450	0.57	0/599
16	k	0.26	0/380	0.66	0/498
All	All	0.26	0/61723	0.64	0/93154

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	I	42747	21509	21541	127	0
2	K	1721	1788	1788	25	0
3	L	1375	1438	1437	14	0
4	M	1282	1337	1336	25	0
5	R	1129	1162	1162	10	0
6	S	938	1012	1012	8	0
7	V	960	1000	1000	11	0
8	X	917	962	962	5	0
9	Y	947	1020	1019	13	0
10	Z	816	839	839	6	0
11	a	857	922	922	0	0
12	b	738	807	807	0	0
13	c	779	833	831	0	0
14	g	501	531	531	0	0
15	i	444	463	458	0	0
16	k	377	418	418	0	0
All	All	56528	36041	36063	210	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 3.

All (210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1667:G:O2'	1:I:1991:U:O4	1.95	0.85
1:I:1567:G:OP2	2:K:83:TYR:OH	1.98	0.82
1:I:1649:G:O2'	7:V:106:ASP:OD2	1.99	0.81
1:I:1296:G:OP1	1:I:2709:G:O2'	2.04	0.75
1:I:1715:G:O2'	1:I:1743:G:O6	2.04	0.74
2:K:29:PRO:HG2	2:K:34:LEU:HD11	1.70	0.74
1:I:1779:U:OP2	1:I:1784:A:N6	2.21	0.74
2:K:185:GLU:OE1	2:K:185:GLU:N	2.22	0.73
1:I:1154:G:OP2	9:Y:58:ARG:NH1	2.22	0.73
4:M:149:ILE:HD11	4:M:172:ALA:HA	1.72	0.72
1:I:1419:A:O2'	1:I:1421:G:N7	2.21	0.71
1:I:476:G:N1	1:I:479:A:OP2	2.25	0.70
1:I:276:U:O2'	1:I:278:A:N7	2.26	0.69
1:I:1450:G:N2	1:I:1452:G:O6	2.26	0.68
1:I:2659:G:N2	1:I:2662:A:OP2	2.25	0.68
8:X:110:ILE:HD12	8:X:110:ILE:O	1.93	0.68
1:I:1801:A:OP2	2:K:150:LYS:NZ	2.29	0.66
5:R:18:VAL:HG22	5:R:140:LEU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:G:H1'	4:M:43:THR:HG21	1.80	0.64
1:I:974:G:O2'	1:I:989:G:N2	2.32	0.63
1:I:1688:U:O2'	1:I:1700:A:N7	2.30	0.63
4:M:171:ASP:OD1	4:M:172:ALA:N	2.31	0.63
1:I:956:G:N2	1:I:960:A:OP2	2.32	0.63
1:I:1250:G:H4'	9:Y:9:ILE:HD11	1.80	0.62
7:V:56:LYS:NZ	7:V:90:ARG:O	2.33	0.62
1:I:1754:A:O3'	8:X:103:ARG:NH2	2.33	0.62
5:R:75:TYR:HB3	5:R:84:ILE:HD11	1.81	0.62
1:I:1447:C:O2'	1:I:1544:A:N3	2.32	0.61
1:I:1654:A:O2'	3:L:118:PHE:O	2.18	0.61
1:I:2840:C:H5"	7:V:53:THR:HG21	1.82	0.61
4:M:131:THR:HG22	4:M:160:ALA:O	2.01	0.61
1:I:1426:G:O2'	1:I:1572:A:N6	2.31	0.60
4:M:118:LEU:HD11	4:M:188:MET:SD	2.40	0.60
1:I:1527:G:N1	1:I:1544:A:OP2	2.34	0.60
1:I:1250:G:C4'	9:Y:9:ILE:HD11	2.32	0.59
4:M:126:VAL:HG21	4:M:134:LEU:HD22	1.84	0.59
4:M:14:VAL:HG13	4:M:197:GLU:OE1	2.03	0.59
1:I:500:G:N1	1:I:503:A:OP2	2.36	0.58
2:K:67:PHE:CE1	2:K:105:LEU:HD21	2.38	0.58
1:I:324:A:N6	1:I:338:G:O2'	2.36	0.58
1:I:1785:A:HO2'	1:I:1786:A:H8	1.51	0.58
5:R:128:ASN:O	5:R:128:ASN:ND2	2.37	0.58
1:I:780:G:OP1	2:K:217:ARG:NH2	2.37	0.57
1:I:534:U:O2'	9:Y:49:ASP:OD2	2.14	0.57
1:I:586:A:N1	1:I:809:G:O2'	2.33	0.56
2:K:174:LEU:HD11	2:K:184:VAL:HG11	1.87	0.56
1:I:247:G:N2	1:I:251:A:OP2	2.39	0.56
9:Y:117:LEU:O	9:Y:117:LEU:HD23	2.05	0.56
1:I:475:C:O2	1:I:479:A:N6	2.32	0.55
2:K:192:LEU:HD13	2:K:193:GLY:N	2.22	0.54
1:I:190:A:N3	1:I:679:C:O2'	2.38	0.54
1:I:307:G:N1	1:I:310:A:OP2	2.40	0.53
2:K:67:PHE:HE1	2:K:105:LEU:HD21	1.73	0.53
1:I:998:C:OP2	9:Y:58:ARG:NH2	2.40	0.53
6:S:10:VAL:HG12	6:S:12:ASP:H	1.72	0.53
1:I:2627:G:O2'	1:I:2781:A:N1	2.32	0.53
7:V:73:ASN:OD1	7:V:73:ASN:N	2.35	0.53
1:I:242:G:O2'	1:I:254:G:O6	2.19	0.53
1:I:247:G:O2'	1:I:251:A:N6	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1009:A:N3	1:I:1153:C:O2'	2.41	0.52
7:V:49:GLU:OE2	7:V:95:THR:HG22	2.09	0.52
6:S:64:ARG:NH1	8:X:68:GLU:OE1	2.43	0.52
1:I:852:U:O2	1:I:926:G:N1	2.44	0.51
1:I:2688:G:N1	1:I:2720:U:OP2	2.34	0.51
1:I:1631:G:N2	1:I:1634:A:OP2	2.39	0.51
10:Z:63:VAL:HA	10:Z:96:VAL:HG12	1.91	0.51
1:I:55:G:O2'	1:I:127:A:N1	2.36	0.51
1:I:2857:G:N2	1:I:2860:A:OP2	2.33	0.51
4:M:176:ASP:OD2	4:M:178:VAL:HG12	2.11	0.51
1:I:712:G:N2	1:I:720:U:O2'	2.43	0.51
1:I:271:G:O2'	1:I:272:A:P	2.69	0.51
7:V:66:ALA:O	7:V:70:THR:HG22	2.11	0.51
1:I:780:G:O2'	1:I:783:A:N6	2.44	0.51
1:I:2773:C:OP1	3:L:171:THR:OG1	2.26	0.51
4:M:168:ASP:OD1	4:M:169:VAL:N	2.44	0.51
1:I:310:A:O2'	1:I:311:A:OP2	2.25	0.51
2:K:39:LYS:NZ	2:K:58:HIS:O	2.28	0.51
4:M:149:ILE:HD11	4:M:172:ALA:CA	2.39	0.50
1:I:1792:G:H5"	2:K:204:VAL:HG13	1.92	0.50
1:I:1477:A:N6	1:I:1514:G:O2'	2.41	0.50
2:K:130:LEU:N	2:K:130:LEU:HD23	2.26	0.50
10:Z:83:TYR:O	10:Z:83:TYR:CG	2.65	0.50
1:I:1385:A:O2'	1:I:1396:U:O2	2.29	0.50
2:K:114:ASP:OD1	2:K:115:GLN:N	2.45	0.50
6:S:108:ARG:HG2	6:S:116:ILE:HD13	1.94	0.50
1:I:1999:C:O2	1:I:2687:U:O2'	2.26	0.49
1:I:1754:A:N1	1:I:2716:C:O2'	2.30	0.49
1:I:1792:G:C5'	2:K:204:VAL:HG13	2.42	0.49
1:I:2033:A:O2'	1:I:2035:G:OP2	2.23	0.49
4:M:192:ALA:O	4:M:196:VAL:HG23	2.13	0.49
5:R:56:VAL:HB	5:R:124:VAL:HG12	1.94	0.49
1:I:1378:A:O2'	1:I:1380:G:OP2	2.30	0.49
1:I:2635:A:O2'	3:L:81:GLU:OE2	2.25	0.49
3:L:186:LEU:HD21	8:X:8:LEU:HD21	1.93	0.49
1:I:2646:C:OP2	1:I:2732:G:O2'	2.30	0.49
3:L:22:ILE:O	3:L:24:VAL:HG13	2.12	0.49
4:M:14:VAL:HG11	4:M:19:PHE:CE1	2.47	0.49
1:I:2202:U:HO2'	1:I:2204:G:P	2.34	0.49
9:Y:89:GLU:O	10:Z:11:GLN:NE2	2.41	0.49
9:Y:79:PHE:CZ	9:Y:83:LEU:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:172:VAL:HG12	3:L:175:LEU:HD21	1.95	0.48
4:M:14:VAL:HG11	4:M:19:PHE:HE1	1.78	0.48
1:I:372:G:O2'	1:I:373:U:OP2	2.31	0.47
1:I:1141:U:OP2	5:R:65:THR:OG1	2.17	0.47
1:I:2821:A:OP2	3:L:115:GLY:N	2.47	0.47
1:I:1141:U:H4'	1:I:1142:A:O4'	2.14	0.47
1:I:2831:G:N7	3:L:59:ARG:NH2	2.62	0.47
5:R:102:GLU:HG3	5:R:124:VAL:HG21	1.97	0.47
1:I:280:U:O4	1:I:361:G:N2	2.47	0.47
1:I:927:A:H2'	1:I:928:A:O4'	2.15	0.47
1:I:1199:U:H1'	9:Y:4:VAL:HG22	1.97	0.47
1:I:1363:C:O2'	1:I:1809:A:N3	2.41	0.47
1:I:782:A:N7	2:K:220:VAL:HG21	2.30	0.47
3:L:38:LYS:NZ	3:L:81:GLU:OE2	2.43	0.47
1:I:39:G:C1'	4:M:43:THR:HG21	2.44	0.47
1:I:57:C:H2'	1:I:58:G:O4'	2.15	0.47
1:I:2655:G:HO2'	1:I:2664:G:H1	1.63	0.46
6:S:41:ILE:HD11	6:S:86:LEU:HD22	1.97	0.46
4:M:7:ASP:OD1	4:M:7:ASP:N	2.48	0.46
1:I:2820:A:O2'	1:I:2821:A:OP1	2.32	0.46
7:V:98:LEU:O	7:V:112:TYR:N	2.46	0.46
1:I:299:A:N3	1:I:319:G:O2'	2.47	0.46
1:I:1223:G:OP2	10:Z:68:ARG:NH2	2.48	0.46
1:I:974:G:O4'	1:I:990:A:N6	2.48	0.46
1:I:1011:G:P	9:Y:77:SER:HG	2.39	0.46
6:S:14:SER:OG	6:S:86:LEU:HD12	2.16	0.46
1:I:573:U:H1'	1:I:2033:A:C5	2.50	0.46
4:M:189:THR:HG23	4:M:192:ALA:H	1.81	0.46
1:I:493:G:H2'	1:I:494:G:O4'	2.17	0.45
2:K:71:LYS:NZ	2:K:98:ASP:OD2	2.49	0.45
10:Z:3:ALA:HB2	10:Z:41:ILE:HD13	1.97	0.45
2:K:105:LEU:H	2:K:105:LEU:HD22	1.82	0.45
4:M:126:VAL:HG21	4:M:134:LEU:CD2	2.45	0.45
1:I:226:A:O2'	1:I:229:C:N4	2.48	0.45
1:I:567:U:H3	1:I:574:A:H61	1.64	0.45
1:I:1266:G:O2'	1:I:2012:G:O6	2.16	0.45
1:I:1315:C:O2'	1:I:1392:A:N3	2.40	0.45
3:L:25:THR:HG21	3:L:193:VAL:HG22	1.99	0.45
4:M:5:LEU:HD23	4:M:122:GLU:HG3	1.99	0.45
1:I:1755:A:N6	1:I:2694:G:O2'	2.50	0.44
1:I:2051:A:H61	1:I:2614:A:H2'	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:107:PRO:HD2	2:K:110:LEU:HD22	1.99	0.44
1:I:58:G:O2'	1:I:73:A:N1	2.40	0.44
3:L:104:VAL:O	3:L:105:LYS:CG	2.66	0.44
6:S:116:ILE:HG23	6:S:122:VAL:HG21	1.98	0.44
1:I:482:A:O2'	1:I:497:A:N1	2.44	0.44
1:I:603:A:N1	1:I:625:G:O2'	2.46	0.44
3:L:60:VAL:O	3:L:60:VAL:HG13	2.17	0.44
3:L:104:VAL:O	3:L:105:LYS:HG2	2.18	0.44
1:I:1223:G:N2	1:I:1226:A:OP2	2.48	0.44
1:I:1307:A:N6	1:I:1606:C:O2'	2.51	0.44
7:V:90:ARG:NH2	7:V:116:VAL:HG11	2.33	0.44
1:I:1003:G:O2'	1:I:1010:A:N1	2.36	0.43
1:I:2850:A:N7	1:I:2868:A:O2'	2.36	0.43
1:I:414:C:H2'	1:I:415:A:O4'	2.18	0.43
5:R:49:ASP:HB3	5:R:114:LEU:HD11	2.00	0.43
1:I:12:U:O2	1:I:2626:C:H4'	2.19	0.43
1:I:2033:A:HO2'	1:I:2035:G:P	2.40	0.43
1:I:1394:U:H4'	1:I:1603:A:H4'	2.00	0.43
4:M:16:GLU:O	4:M:20:GLY:N	2.50	0.43
4:M:108:ILE:HD12	4:M:109:LEU:N	2.34	0.43
1:I:2723:C:H2'	1:I:2724:U:O4'	2.19	0.42
4:M:96:VAL:HG23	4:M:96:VAL:O	2.19	0.42
4:M:6:LYS:O	4:M:9:GLN:NE2	2.52	0.42
1:I:1240:U:O2'	1:I:1241:A:O5'	2.34	0.42
1:I:1329:U:OP2	1:I:1330:C:N4	2.49	0.42
2:K:164:ILE:HD12	2:K:164:ILE:N	2.34	0.42
1:I:1139:G:O2'	1:I:1143:A:N1	2.37	0.42
1:I:227:A:N6	1:I:411:G:HO2'	2.18	0.42
1:I:359:G:H2'	1:I:360:U:O4'	2.20	0.42
4:M:14:VAL:HG12	4:M:15:SER:N	2.35	0.42
4:M:149:ILE:C	4:M:149:ILE:HD13	2.40	0.42
1:I:271:G:O2'	1:I:272:A:O5'	2.30	0.41
1:I:1792:G:O2'	1:I:1830:C:OP1	2.37	0.41
1:I:463:G:N2	1:I:466:A:OP2	2.47	0.41
1:I:729:G:N2	2:K:11:PRO:O	2.53	0.41
1:I:1338:G:O2'	1:I:1393:A:N1	2.45	0.41
1:I:308:G:O2'	1:I:329:G:N2	2.54	0.41
1:I:372:G:O2'	1:I:400:G:O6	2.37	0.41
1:I:605:G:N3	1:I:657:U:O2'	2.54	0.41
1:I:818:G:N1	1:I:1188:U:OP2	2.41	0.41
9:Y:104:VAL:HG11	10:Z:45:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:416:U:H2'	1:I:417:C:O4'	2.21	0.41
2:K:16:VAL:HG22	2:K:206:GLY:HA3	2.03	0.41
2:K:66:ASP:OD2	2:K:102:ARG:NH1	2.53	0.41
1:I:157:C:H2'	1:I:158:U:O4'	2.21	0.41
1:I:1604:C:O2'	1:I:1610:A:N1	2.43	0.41
2:K:155:ALA:HB2	2:K:162:VAL:HG23	2.02	0.41
3:L:175:LEU:HD22	3:L:175:LEU:N	2.36	0.41
1:I:1757:A:O2'	1:I:1758:U:OP1	2.28	0.41
1:I:2799:A:O2'	1:I:2800:A:H5"	2.21	0.41
4:M:149:ILE:HD13	4:M:150:THR:N	2.35	0.41
1:I:580:U:O3'	9:Y:31:VAL:HG13	2.20	0.40
1:I:774:G:OP1	2:K:48:ARG:NH2	2.47	0.40
1:I:2898:U:O2'	5:R:134:ALA:O	2.31	0.40
5:R:125:TYR:OH	5:R:132:HIS:NE2	2.42	0.40
7:V:1:MET:SD	7:V:1:MET:N	2.87	0.40
7:V:53:THR:HG22	7:V:94:TYR:OH	2.20	0.40
7:V:77:ALA:O	7:V:81:ASN:ND2	2.54	0.40
8:X:17:VAL:O	8:X:17:VAL:HG23	2.20	0.40
1:I:18:U:O2'	1:I:554:U:OP1	2.33	0.40
1:I:669:G:H2'	1:I:670:A:C8	2.57	0.40
2:K:84:ASP:OD2	2:K:87:ARG:NE	2.47	0.40
6:S:42:THR:HG23	6:S:42:THR:O	2.21	0.40
5:R:110:PRO:O	5:R:115:GLY:HA3	2.22	0.40
1:I:1223:G:N1	1:I:1226:A:OP2	2.48	0.40
1:I:36:G:N3	1:I:450:G:O2'	2.52	0.40
1:I:1012:U:OP2	9:Y:70:ARG:NH2	2.51	0.40
1:I:2741:A:N6	1:I:2763:G:O2'	2.54	0.40
6:S:24:VAL:HG23	6:S:24:VAL:O	2.21	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	
2	K	224/273 (82%)	220 (98%)	4 (2%)	0	100	100
3	L	179/209 (86%)	174 (97%)	5 (3%)	0	100	100
4	M	161/201 (80%)	160 (99%)	1 (1%)	0	100	100
5	R	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
6	S	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
7	V	118/127 (93%)	116 (98%)	2 (2%)	0	100	100
8	X	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
9	Y	115/118 (98%)	115 (100%)	0	0	100	100
10	Z	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
11	a	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
12	b	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
13	c	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
14	g	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
15	i	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
16	k	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
All	All	1727/1891 (91%)	1692 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	178/218 (82%)	171 (96%)	7 (4%)	32	58
3	L	143/163 (88%)	139 (97%)	4 (3%)	43	68
4	M	138/165 (84%)	130 (94%)	8 (6%)	20	38
5	R	116/116 (100%)	113 (97%)	3 (3%)	46	70
6	S	103/104 (99%)	99 (96%)	4 (4%)	32	58
7	V	100/103 (97%)	99 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	X	99/100 (99%)	94 (95%)	5 (5%)	24	45
9	Y	89/90 (99%)	83 (93%)	6 (7%)	16	32
10	Z	84/84 (100%)	78 (93%)	6 (7%)	14	30
11	a	93/93 (100%)	90 (97%)	3 (3%)	39	63
12	b	80/84 (95%)	77 (96%)	3 (4%)	33	59
13	c	83/85 (98%)	79 (95%)	4 (5%)	25	49
14	g	54/55 (98%)	54 (100%)	0	100	100
15	i	47/48 (98%)	42 (89%)	5 (11%)	6	14
16	k	38/38 (100%)	37 (97%)	1 (3%)	46	70
All	All	1445/1546 (94%)	1385 (96%)	60 (4%)	33	54

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	43	ARG
2	K	97	LYS
2	K	111	LYS
2	K	130	LEU
2	K	181	MET
2	K	192	LEU
2	K	212	ARG
3	L	39	ASP
3	L	46	ARG
3	L	126	ASN
3	L	170	VAL
4	M	12	LEU
4	M	21	ARG
4	M	35	TYR
4	M	47	LYS
4	M	134	LEU
4	M	147	LEU
4	M	149	ILE
4	M	199	MET
5	R	30	THR
5	R	108	MET
5	R	141	ASP
6	S	58	LEU
6	S	80	ASP
6	S	87	LEU

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Mol	Chain	Res	Type
6	S	103	VAL
7	V	73	ASN
8	X	10	GLN
8	X	39	ARG
8	X	63	LYS
8	X	106	LYS
8	X	111	LYS
9	Y	18	LEU
9	Y	54	LYS
9	Y	58	ARG
9	Y	70	ARG
9	Y	71	GLN
9	Y	97	ASP
10	Z	1	MET
10	Z	48	LYS
10	Z	78	ARG
10	Z	79	ARG
10	Z	84	ARG
10	Z	86	GLN
11	a	2	GLU
11	a	7	HIS
11	a	66	ILE
12	b	24	MET
12	b	72	GLN
12	b	93	LEU
13	c	6	ARG
13	c	7	ARG
13	c	86	ARG
13	c	89	ASP
15	i	3	VAL
15	i	10	ARG
15	i	27	SER
15	i	29	SER
15	i	38	HIS
16	k	24	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	1964/2904 (67%)	229 (11%)	1 (0%)

All (229) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	10	A
1	I	34	U
1	I	42	A
1	I	46	G
1	I	51	G
1	I	58	G
1	I	71	A
1	I	74	A
1	I	75	G
1	I	101	A
1	I	102	U
1	I	110	G
1	I	118	A
1	I	120	U
1	I	136	G
1	I	138	U
1	I	139	U
1	I	140	C
1	I	142	A
1	I	149	A
1	I	155	A
1	I	158	U
1	I	159	G
1	I	160	A
1	I	163	C
1	I	181	A
1	I	201	C
1	I	216	A
1	I	222	A
1	I	247	G
1	I	251	A
1	I	264	C
1	I	265	A
1	I	266	G
1	I	272	A
1	I	276	U
1	I	278	A
1	I	279	A

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Mol	Chain	Res	Type
1	I	285	G
1	I	287	G
1	I	294	A
1	I	311	A
1	I	324	A
1	I	329	G
1	I	330	A
1	I	345	A
1	I	353	C
1	I	357	C
1	I	361	G
1	I	362	A
1	I	371	A
1	I	372	G
1	I	396	G
1	I	415	A
1	I	424	G
1	I	451	U
1	I	456	C
1	I	481	G
1	I	491	G
1	I	505	A
1	I	509	C
1	I	510	C
1	I	531	C
1	I	532	A
1	I	549	G
1	I	562	U
1	I	572	A
1	I	573	U
1	I	574	A
1	I	587	C
1	I	603	A
1	I	613	A
1	I	614	A
1	I	615	U
1	I	616	A
1	I	621	A
1	I	686	U
1	I	712	G
1	I	719	C
1	I	720	U

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Mol	Chain	Res	Type
1	I	721	A
1	I	730	A
1	I	746	PSU
1	I	747	5MU
1	I	764	A
1	I	775	G
1	I	776	G
1	I	782	A
1	I	784	G
1	I	785	G
1	I	789	A
1	I	792	A
1	I	802	A
1	I	805	G
1	I	808	G
1	I	809	G
1	I	811	U
1	I	812	C
1	I	819	A
1	I	834	G
1	I	845	A
1	I	846	U
1	I	847	U
1	I	853	C
1	I	854	C
1	I	931	U
1	I	932	U
1	I	941	A
1	I	974	G
1	I	984	A
1	I	995	C
1	I	996	A
1	I	1005	C
1	I	1012	U
1	I	1013	C
1	I	1132	U
1	I	1133	A
1	I	1135	C
1	I	1139	G
1	I	1142	A
1	I	1170	C
1	I	1179	G

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Mol	Chain	Res	Type
1	I	1180	U
1	I	1206	G
1	I	1238	G
1	I	1241	A
1	I	1249	U
1	I	1252	G
1	I	1256	G
1	I	1265	A
1	I	1266	G
1	I	1271	G
1	I	1272	A
1	I	1300	G
1	I	1301	A
1	I	1302	A
1	I	1326	U
1	I	1329	U
1	I	1345	C
1	I	1352	U
1	I	1366	A
1	I	1368	G
1	I	1379	U
1	I	1383	A
1	I	1391	U
1	I	1416	G
1	I	1417	C
1	I	1421	G
1	I	1427	A
1	I	1428	C
1	I	1453	A
1	I	1460	U
1	I	1482	G
1	I	1486	U
1	I	1490	A
1	I	1493	C
1	I	1508	A
1	I	1509	A
1	I	1510	G
1	I	1515	A
1	I	1529	G
1	I	1534	U
1	I	1554	U
1	I	1566	A

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Mol	Chain	Res	Type
1	I	1569	A
1	I	1578	U
1	I	1608	A
1	I	1646	C
1	I	1647	U
1	I	1648	U
1	I	1669	A
1	I	1674	G
1	I	1715	G
1	I	1731	G
1	I	1733	G
1	I	1738	G
1	I	1764	C
1	I	1773	A
1	I	1791	A
1	I	1800	C
1	I	1801	A
1	I	1808	A
1	I	1816	C
1	I	1829	A
1	I	1972	G
1	I	1991	U
1	I	1993	U
1	I	1997	C
1	I	2022	U
1	I	2023	C
1	I	2029	G
1	I	2034	U
1	I	2043	C
1	I	2204	G
1	I	2611	C
1	I	2612	C
1	I	2613	U
1	I	2614	A
1	I	2629	U
1	I	2646	C
1	I	2653	U
1	I	2664	G
1	I	2665	A
1	I	2667	C
1	I	2689	U
1	I	2690	U

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Mol	Chain	Res	Type
1	I	2714	G
1	I	2726	A
1	I	2733	A
1	I	2744	G
1	I	2763	G
1	I	2777	G
1	I	2778	A
1	I	2791	G
1	I	2794	C
1	I	2798	U
1	I	2799	A
1	I	2800	A
1	I	2820	A
1	I	2821	A
1	I	2835	A
1	I	2867	G
1	I	2873	A
1	I	2880	C
1	I	2883	A
1	I	2884	U
1	I	2887	A
1	I	2901	C
1	I	2903	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	1240	U

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	I	746	1	18,21,22	1.07	2 (11%)	22,30,33	1.46	2 (9%)
1	PSU	I	955	1	18,21,22	0.82	1 (5%)	22,30,33	1.45	2 (9%)
1	1MG	I	745	1	18,26,27	1.01	1 (5%)	19,39,42	0.72	0
1	5MU	I	747	1	19,22,23	0.44	0	28,32,35	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	I	746	1	-	2/7/25/26	0/2/2/2
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	1MG	I	745	1	-	0/3/25/26	0/3/3/3
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	746	PSU	O4'-C1'	-3.08	1.39	1.43
1	I	955	PSU	C6-N1	-2.32	1.32	1.36
1	I	746	PSU	C6-N1	-2.31	1.32	1.36
1	I	745	1MG	C5-C4	-2.30	1.37	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	955	PSU	C6-N1-C2	4.94	127.74	122.68
1	I	746	PSU	C6-N1-C2	4.76	127.55	122.68
1	I	955	PSU	N1-C2-N3	-2.75	112.02	115.13
1	I	746	PSU	N1-C2-N3	-2.73	112.03	115.13

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	746	PSU	O4'-C4'-C5'-O5'
1	I	746	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

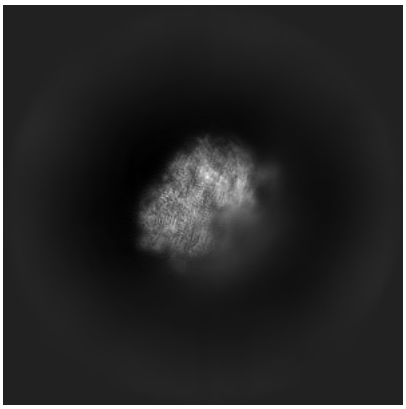
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12826. These allow visual inspection of the internal detail of the map and identification of artifacts.

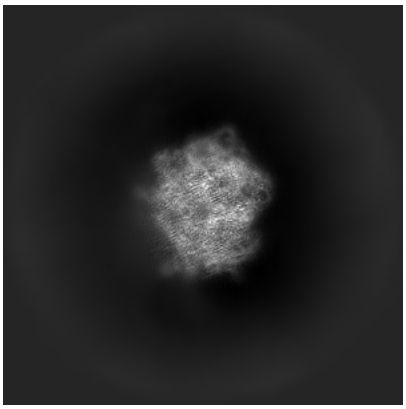
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

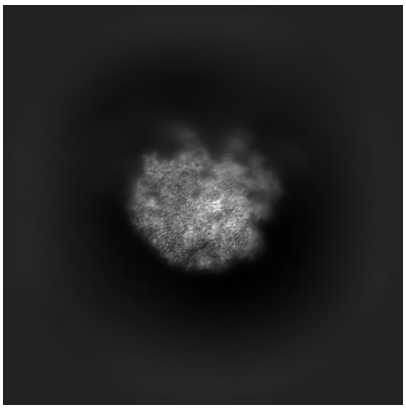
6.1.1 Primary map



X

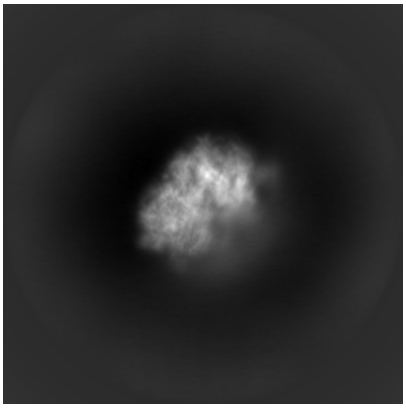


Y

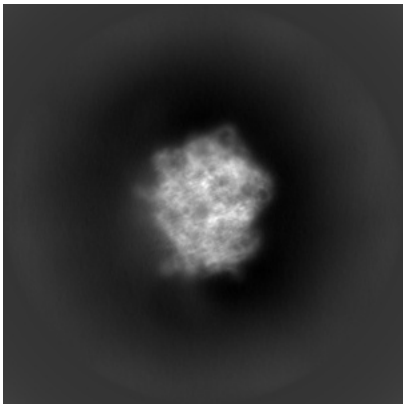


Z

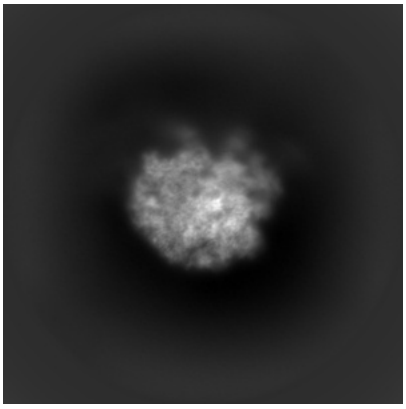
6.1.2 Raw map



X



Y

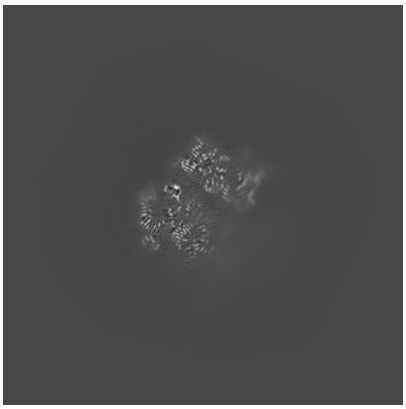


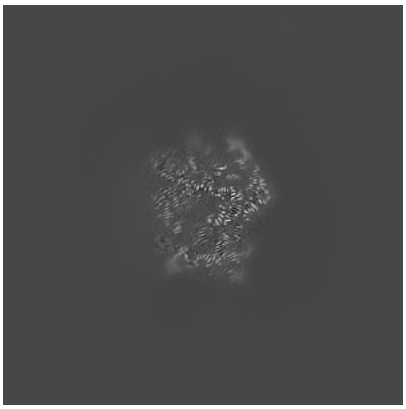
Z

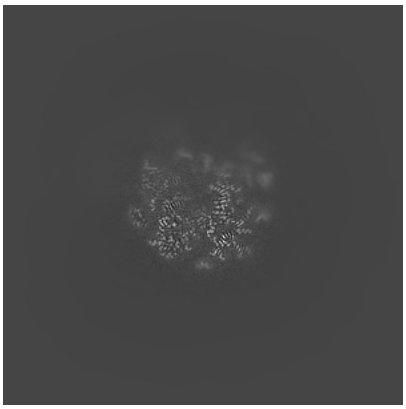
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

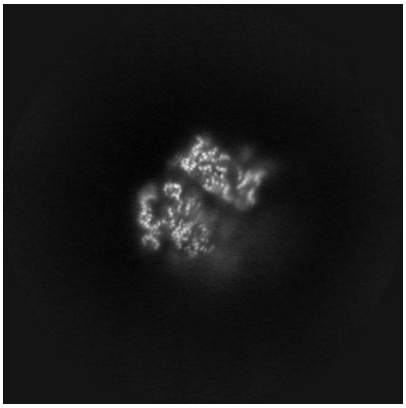
6.2.1 Primary map

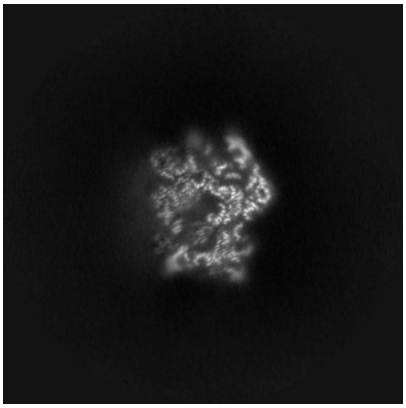

X Index: 224

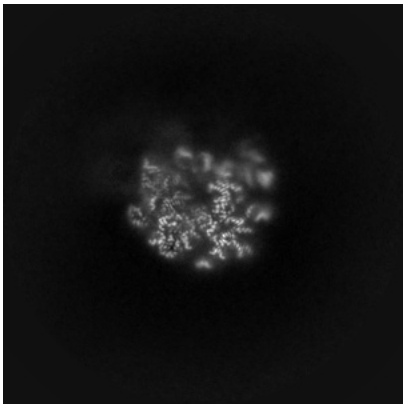

Y Index: 224


Z Index: 224

6.2.2 Raw map


X Index: 224

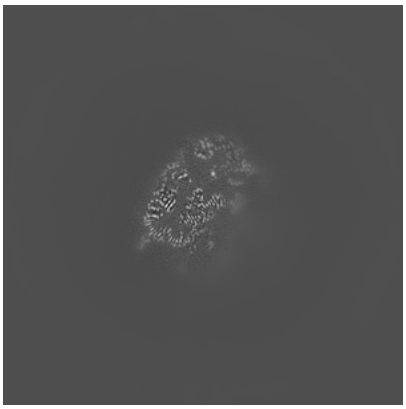

Y Index: 224

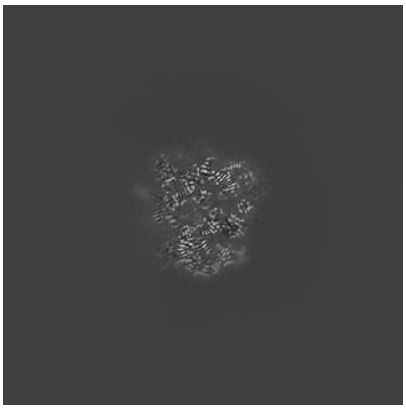

Z Index: 224

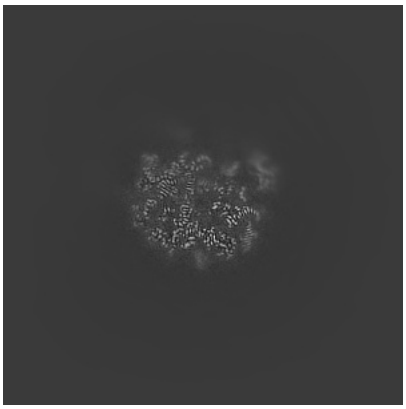
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

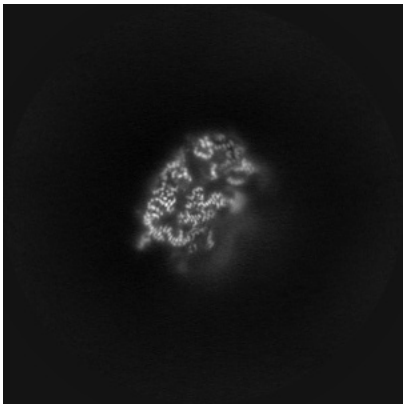
6.3.1 Primary map

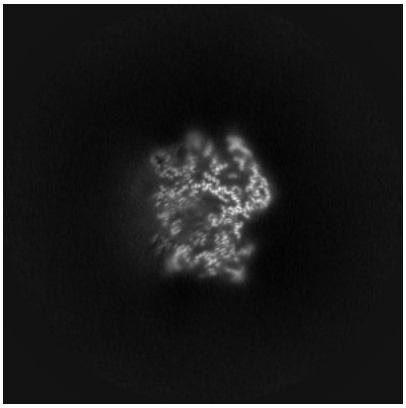

X Index: 246

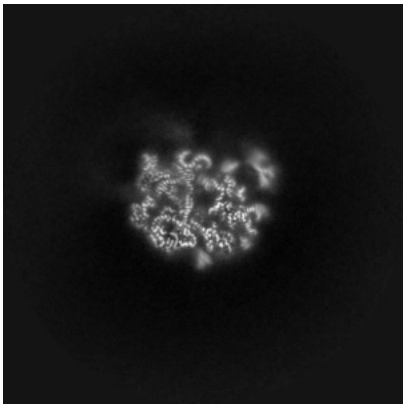

Y Index: 203


Z Index: 235

6.3.2 Raw map


X Index: 246

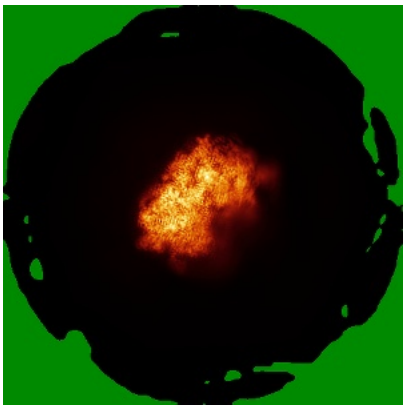

Y Index: 222


Z Index: 232

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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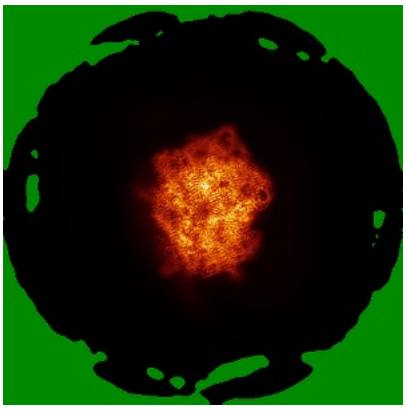
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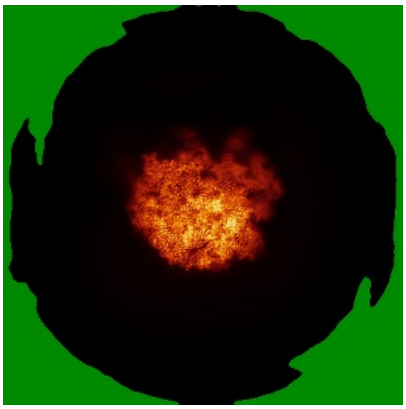
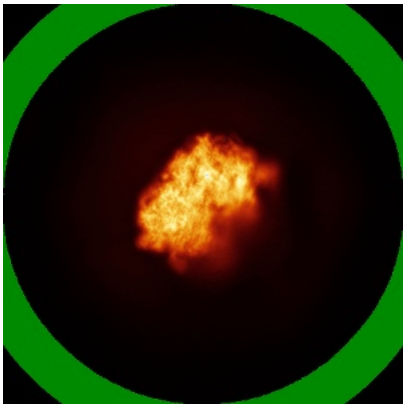
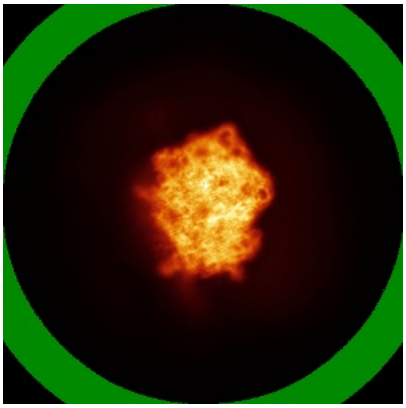

Z

6.4.2 Raw map


X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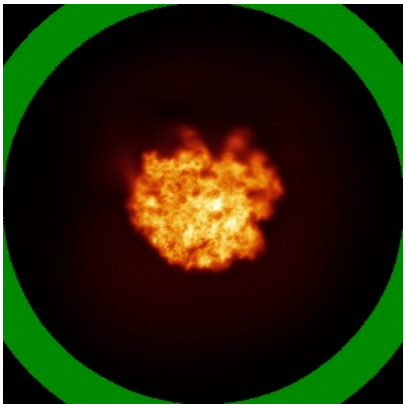
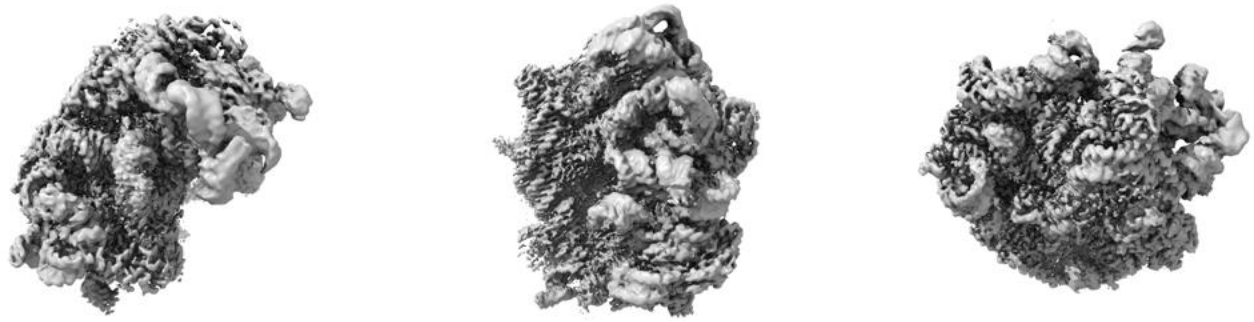

Z

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)

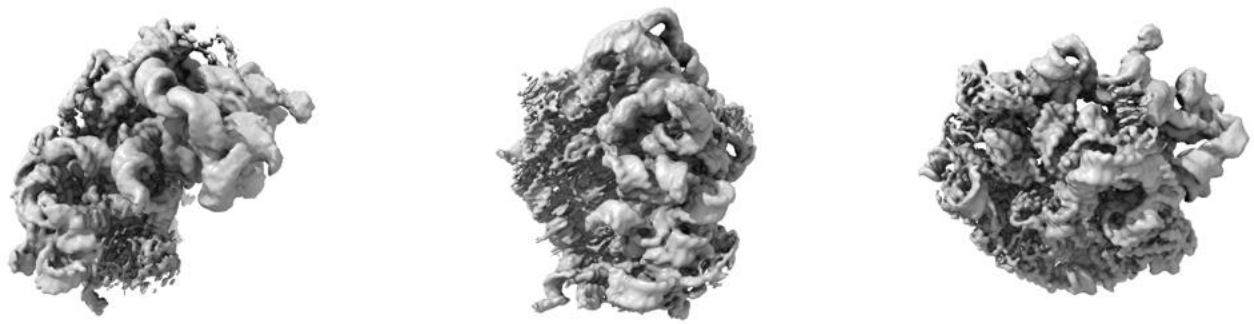
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

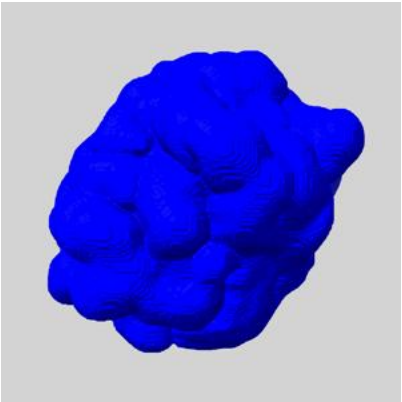
6.6 Mask visualisation (i)

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

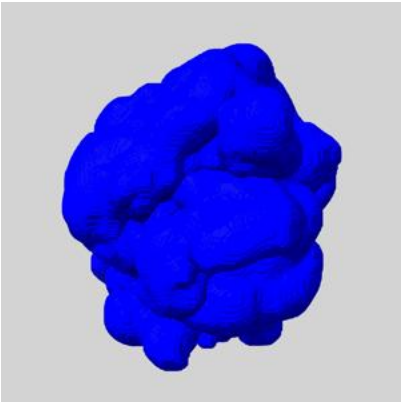
A mask typically either:

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

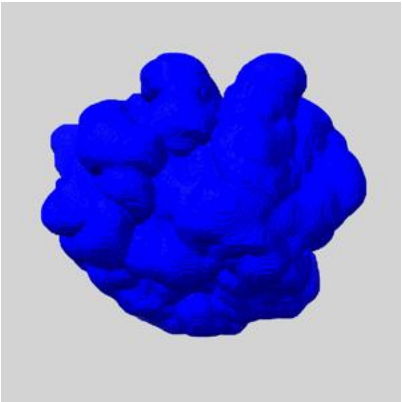
6.6.1 emd_12826_msk_1.map (i)



X



Y

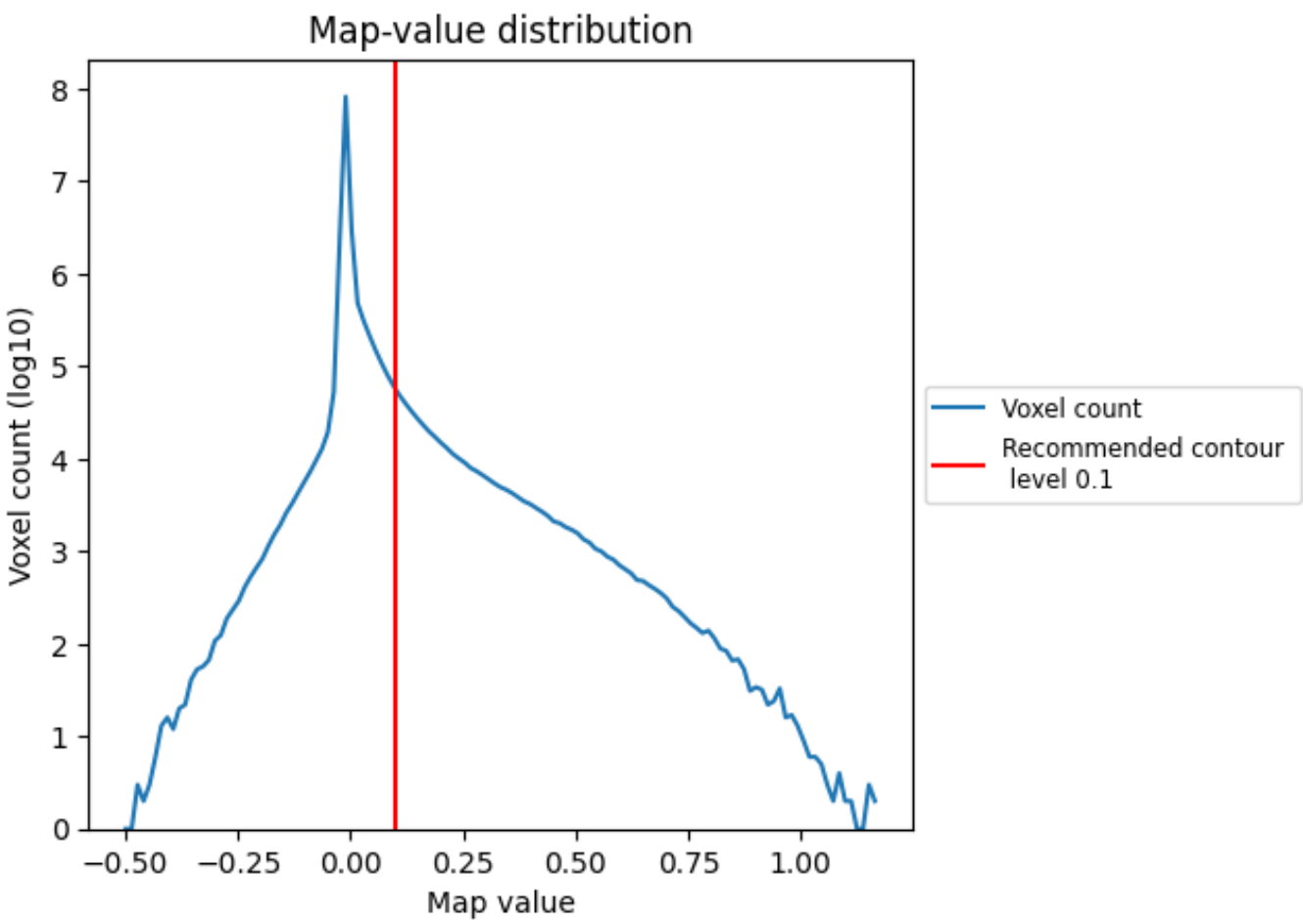


Z

7 Map analysis (i)

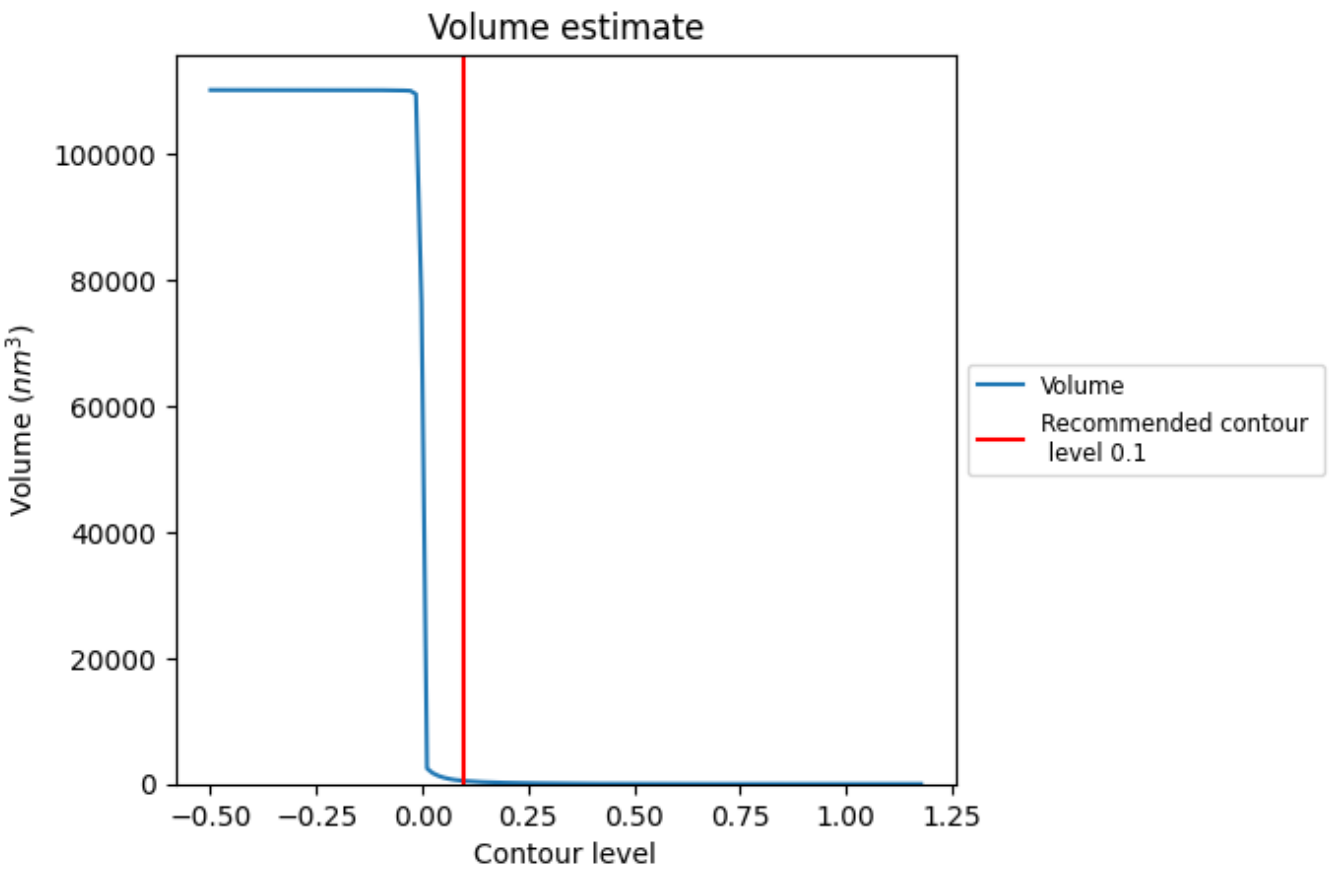
This section contains the results of statistical analysis of the map.

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.

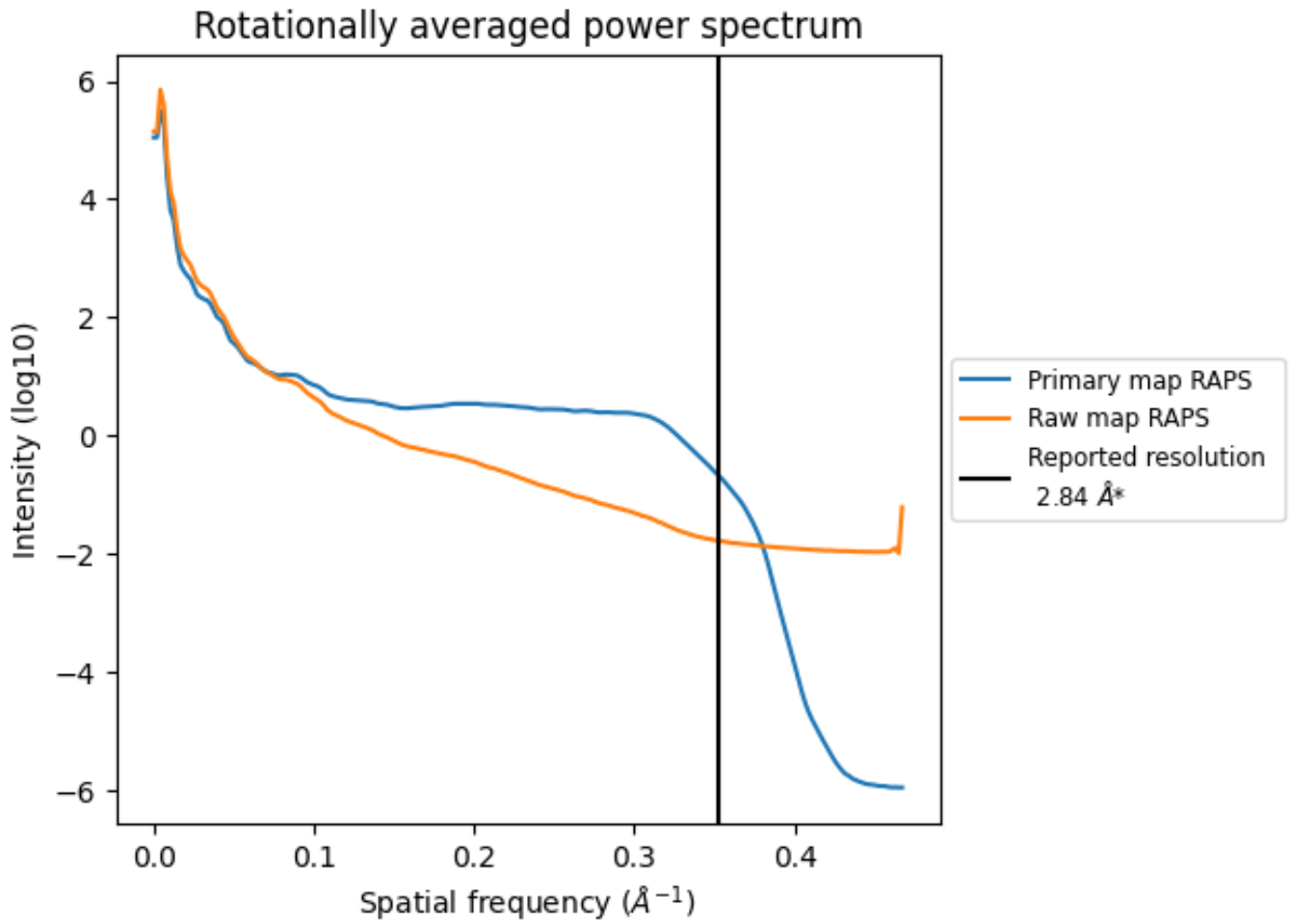
7.2 Volume estimate (i)



The volume at the recommended contour level is 484 nm^3; this corresponds to an approximate mass of 437 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)

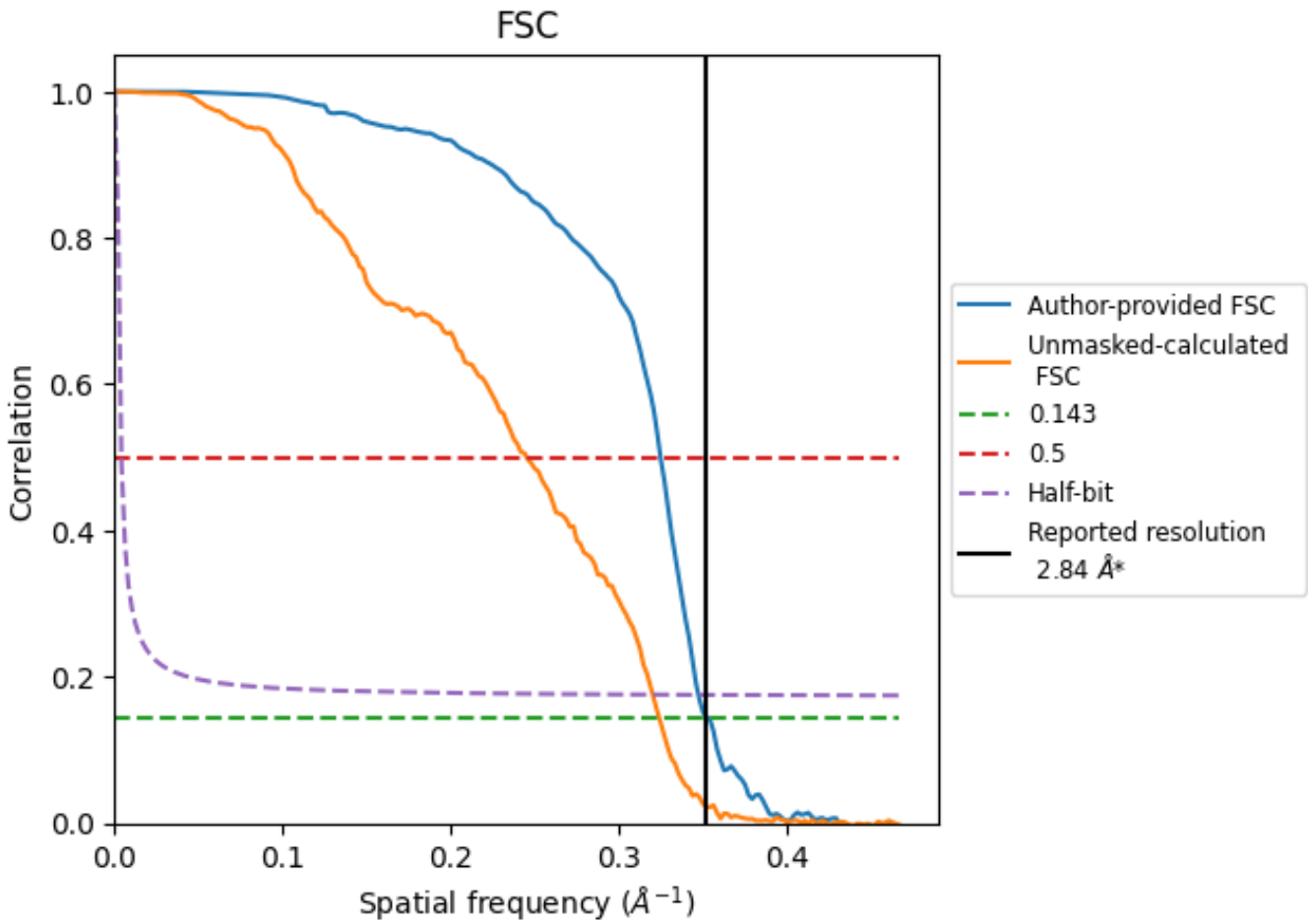


*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

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 0.352 Å^{-1}

8.2 Resolution estimates (i)

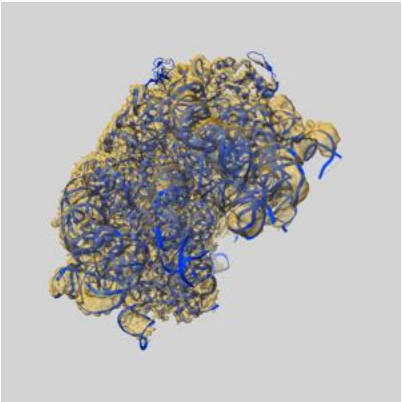
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.83	3.08	2.88
Unmasked-calculated*	3.08	4.07	3.12

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

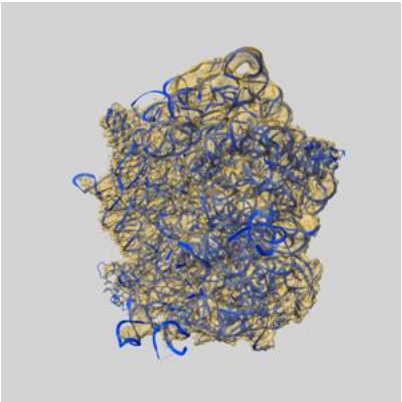
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12826 and PDB model 7ODE. Per-residue inclusion information can be found in section 3 on page 7.

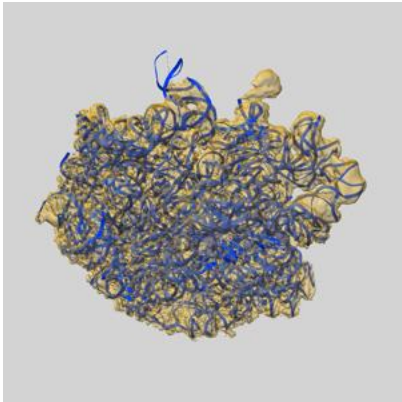
9.1 Map-model overlay (i)



X



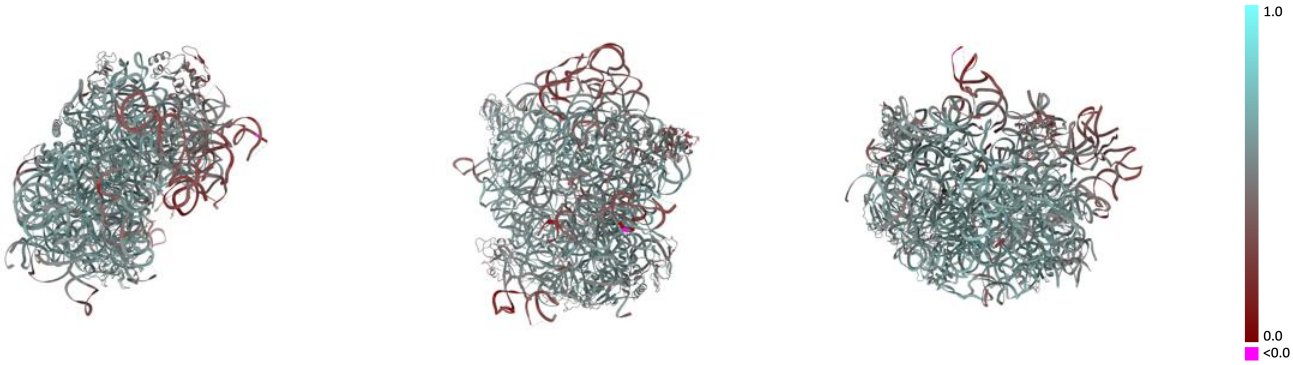
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

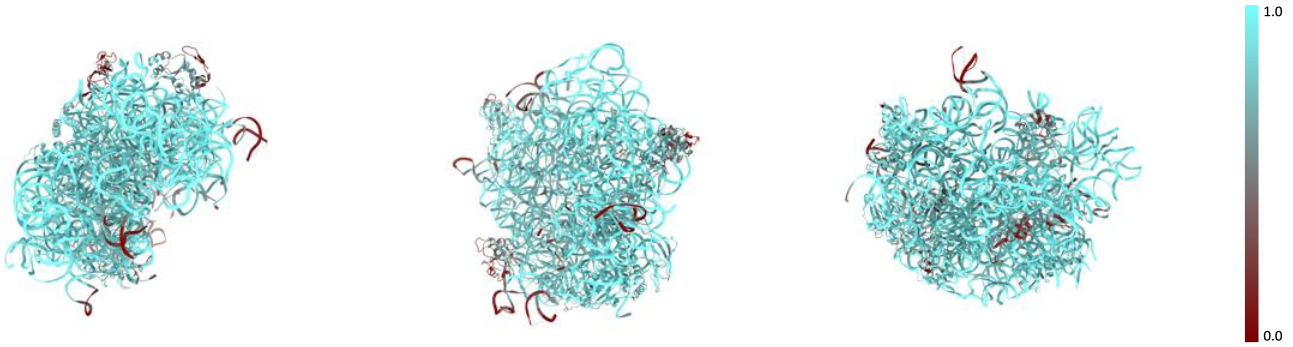
9.2 Q-score mapped to coordinate model (i)



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.

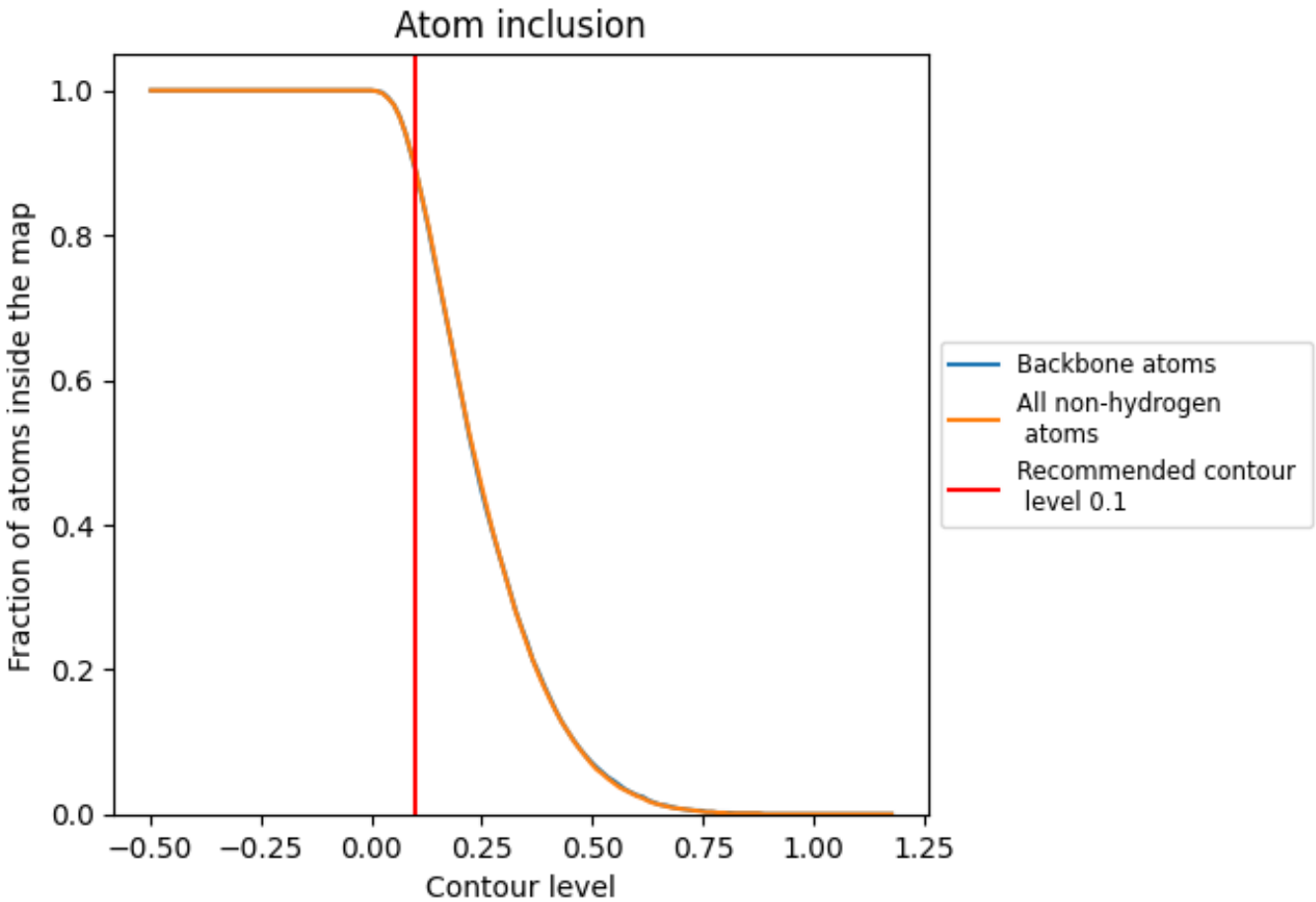
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8910	0.5400
I	0.9370	0.5440
K	0.8190	0.5590
L	0.8690	0.5510
M	0.5860	0.4250
R	0.8610	0.5360
S	0.4150	0.4690
V	0.9590	0.6060
X	0.5950	0.5100
Y	0.9140	0.5490
Z	0.8360	0.4930
a	0.9030	0.5720
b	0.9180	0.5870
c	0.3000	0.4640
g	0.8710	0.5460
i	0.3460	0.4460
k	0.9520	0.5950