



## Full wwPDB EM Validation Report ⓘ

Mar 30, 2023 – 07:54 pm BST

PDB ID : 8C91  
EMDB ID : EMD-16498  
Title : Cryo-EM captures early ribosome assembly in action  
Authors : Lauer, S.; Nikolay, R.; Qin, B.  
Deposited on : 2023-01-21  
Resolution : 4.19 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

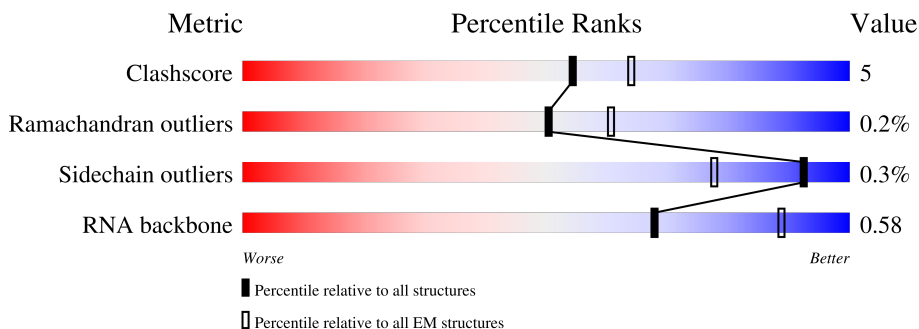
EMDB validation analysis : 0.0.1.dev50  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.2

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.19 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	273	
2	D	209	
3	E	201	
4	J	142	
5	K	123	
6	L	144	
7	N	127	

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Mol	Chain	Length	Quality of chain
8	P	115	
9	Q	118	
10	R	103	
11	S	110	
12	T	100	
13	U	104	
14	Y	63	
15	0	57	
16	2	46	
17	Z	59	
18	A	2904	

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 59110 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	156	1195	747	224	220	4	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	180	1348	849	243	252	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	190	1461	920	260	276	5	0	0

- Molecule 4 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	140	1121	710	210	197	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	121	929	581	178	164	6	0	0

- Molecule 6 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	L	108	769	477	147	145	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	N	120	960	593	196	166	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	P	114	917	574	179	163	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	Q	117	947	604	192	151	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	R	103	816	516	153	145	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	S	101	786	491	147	145	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	T	92	730	461	138	130	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	U	102	779	492	146	141	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	39	Total	C	N	O	S	0	0
			315	189	78	47	1		

- Molecule 17 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

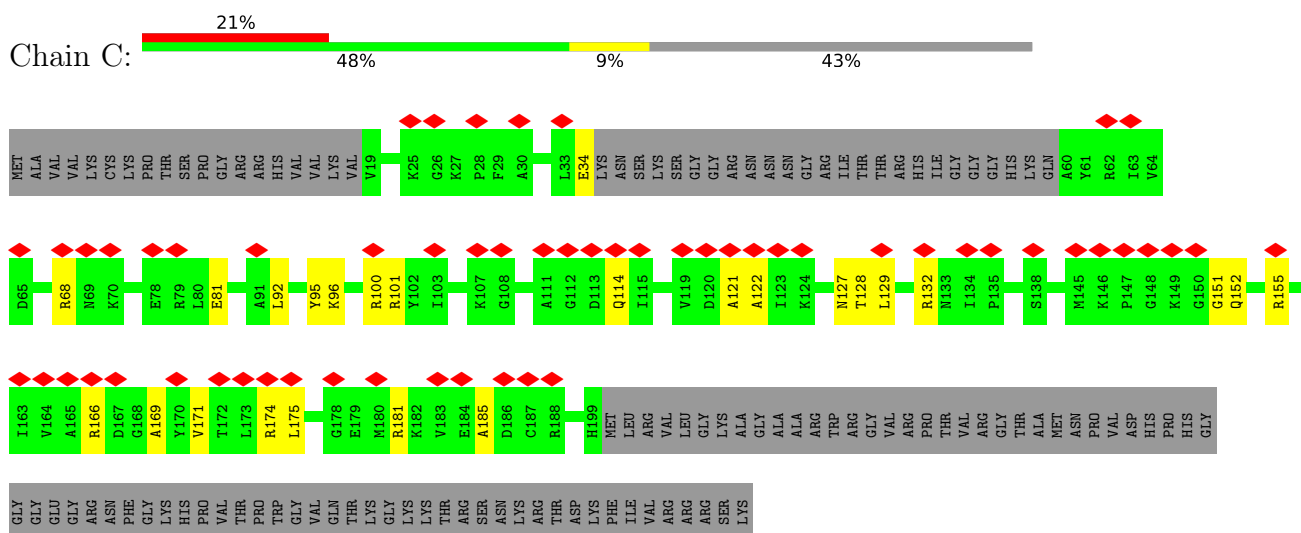
- Molecule 18 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A	2077	Total	C	N	O	P	0	0
			44635	19914	8271	14373	2077		

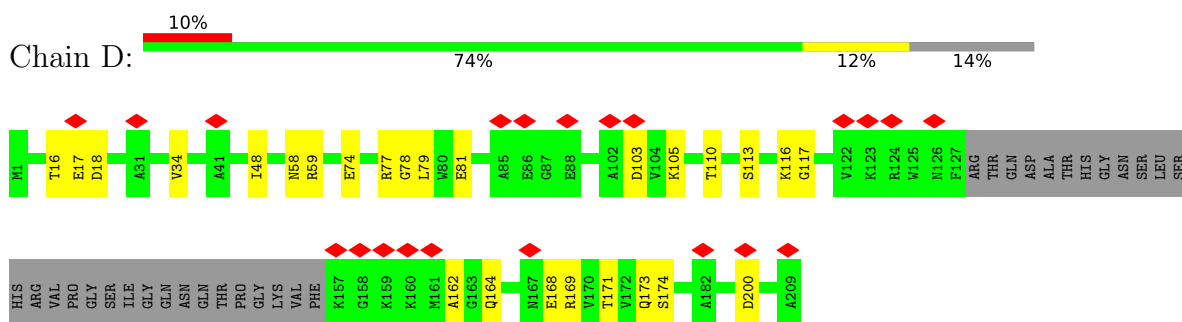
### 3 Residue-property plots [i](#)

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.

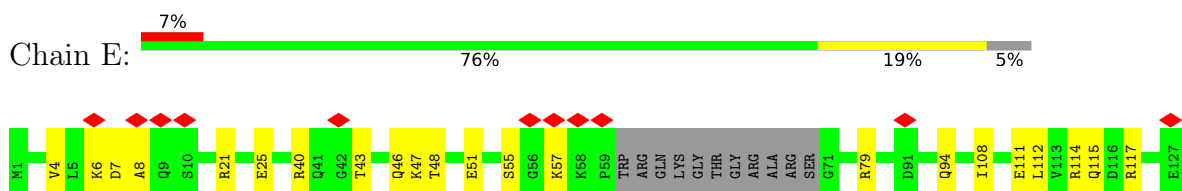
- Molecule 1: 50S ribosomal protein L2

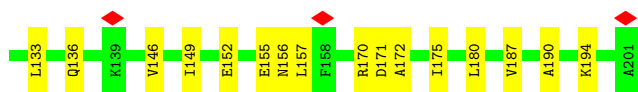


- Molecule 2: 50S ribosomal protein L3

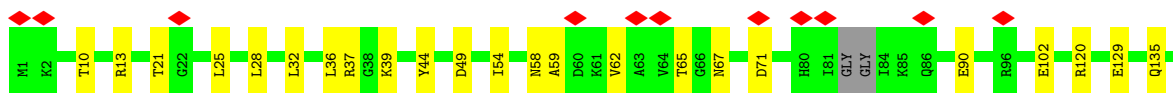
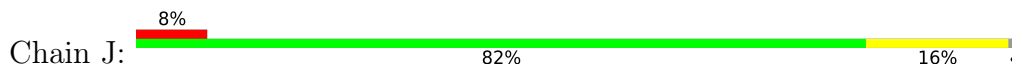


- Molecule 3: 50S ribosomal protein L4

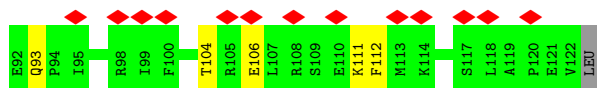
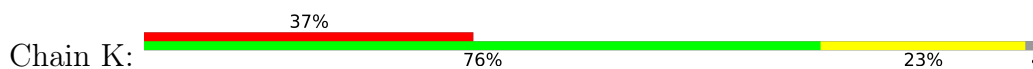




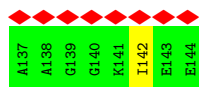
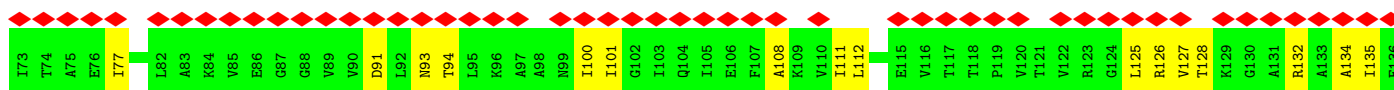
• Molecule 4: 50S ribosomal protein L13



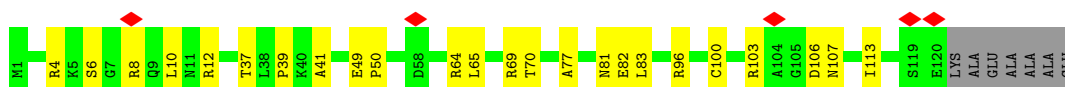
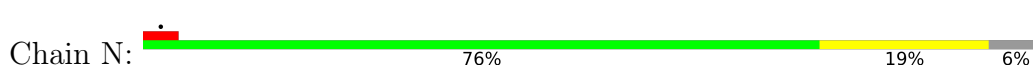
• Molecule 5: 50S ribosomal protein L14



• Molecule 6: 50S ribosomal protein L15

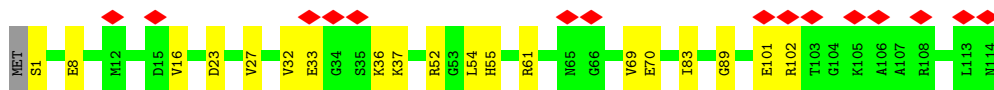
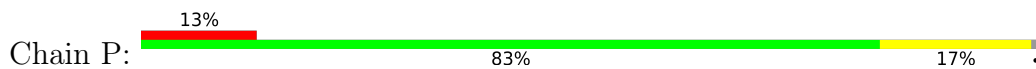


• Molecule 7: 50S ribosomal protein L17

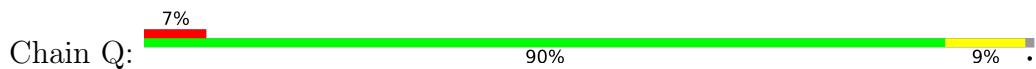


• Molecule 8: 50S ribosomal protein L19

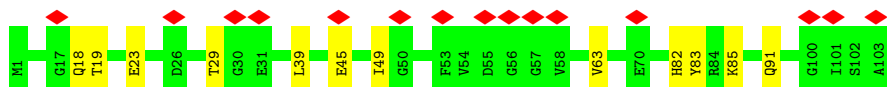
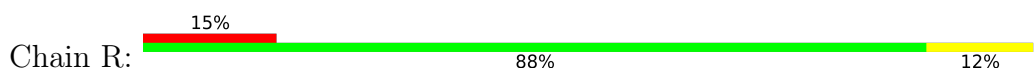




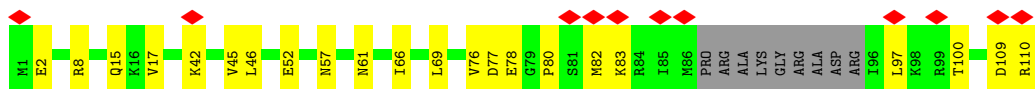
- Molecule 9: 50S ribosomal protein L20



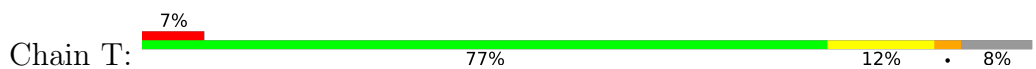
- Molecule 10: 50S ribosomal protein L21



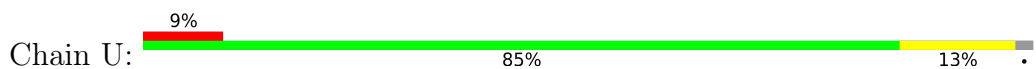
- Molecule 11: 50S ribosomal protein L22



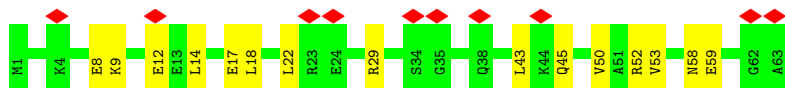
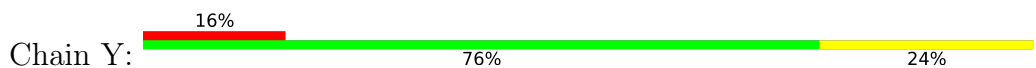
- Molecule 12: 50S ribosomal protein L23



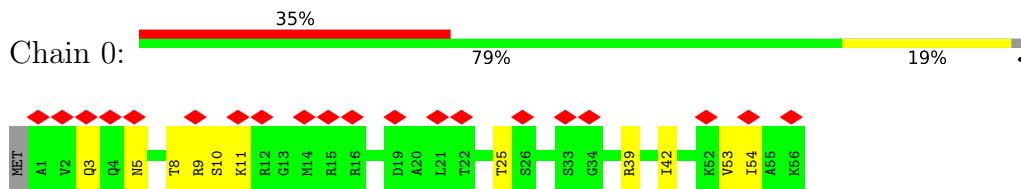
- Molecule 13: 50S ribosomal protein L24



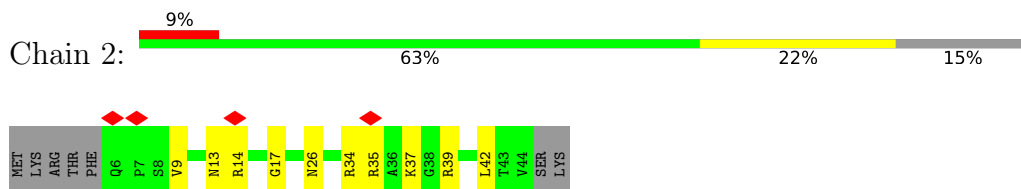
- Molecule 14: 50S ribosomal protein L29



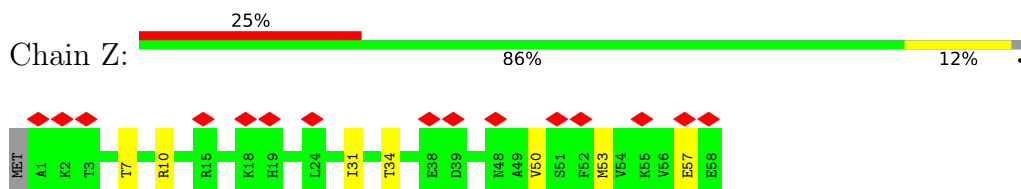
• Molecule 15: 50S ribosomal protein L32



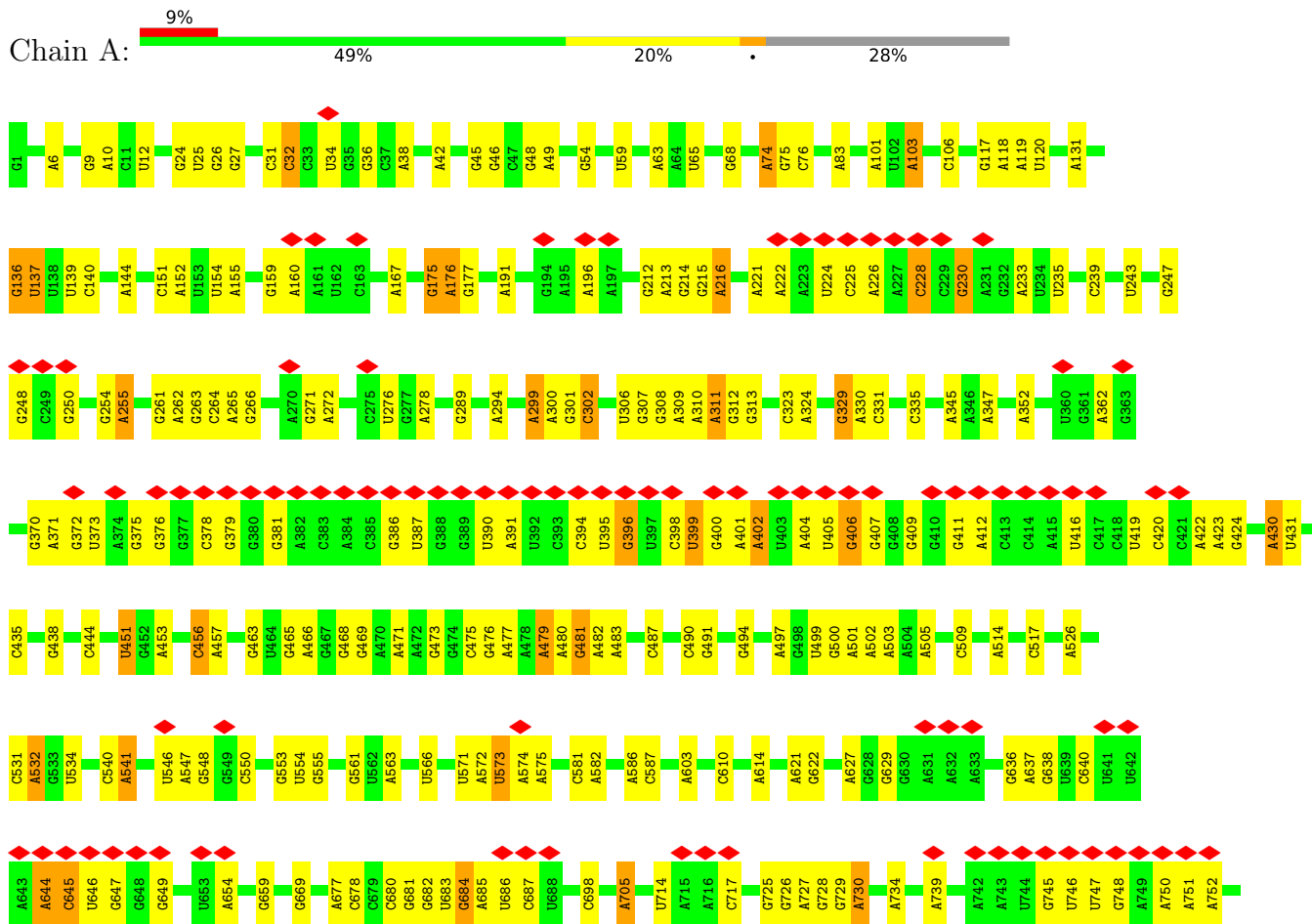
• Molecule 16: 50S ribosomal protein L34

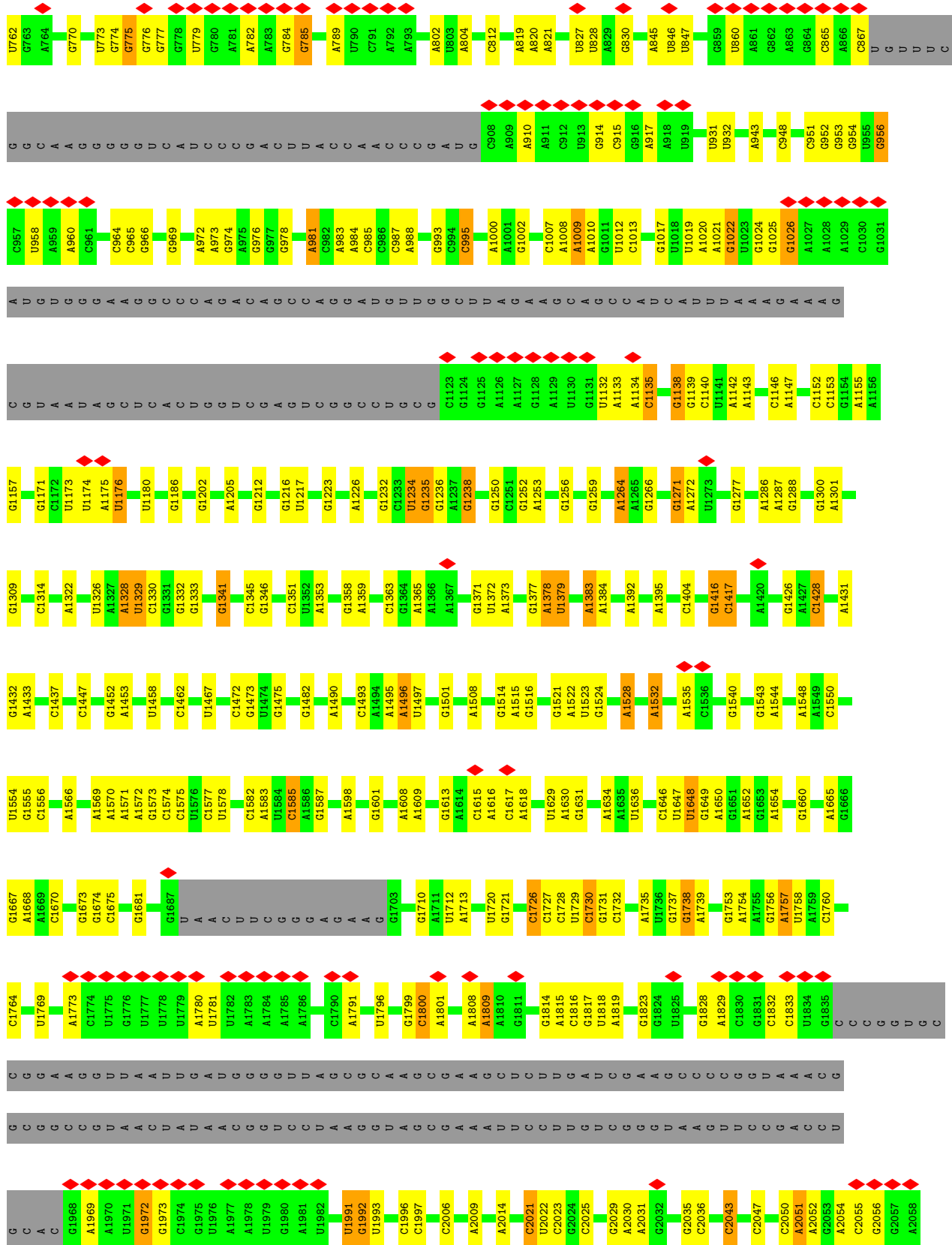


• Molecule 17: 50S ribosomal protein L30



• Molecule 18: 23S rRNA







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5001	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	62	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.518	Depositor
Minimum map value	-0.557	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	375.0, 375.0, 375.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.25, 1.25, 1.25	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	C	0.24	0/1214	0.52	0/1637
2	D	0.24	0/1363	0.50	0/1830
3	E	0.24	0/1477	0.46	0/1987
4	J	0.24	0/1143	0.50	0/1538
5	K	0.25	0/937	0.54	0/1254
6	L	0.25	0/771	0.55	0/1030
7	N	0.24	0/973	0.58	0/1301
8	P	0.24	0/929	0.54	0/1242
9	Q	0.24	0/960	0.51	0/1278
10	R	0.25	0/829	0.53	0/1107
11	S	0.23	0/791	0.49	0/1058
12	T	0.26	0/736	0.51	0/984
13	U	0.26	0/787	0.53	0/1051
14	Y	0.25	0/510	0.53	0/677
15	0	0.23	0/450	0.55	0/599
16	2	0.23	0/317	0.66	0/418
17	Z	0.24	0/453	0.56	0/605
18	A	0.14	0/50004	0.71	9/78005 (0.0%)
All	All	0.17	0/64644	0.67	9/97601 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	398	C	N3-C2-O2	-7.73	116.49	121.90
18	A	964	C	N3-C2-O2	-7.25	116.83	121.90
18	A	398	C	N1-C2-O2	6.94	123.06	118.90
18	A	1832	C	N1-C2-O2	6.88	123.03	118.90
18	A	964	C	N1-C2-O2	6.32	122.69	118.90
18	A	32	C	N3-C2-O2	-5.71	117.91	121.90
18	A	1973	G	N1-C6-O6	-5.43	116.64	119.90
18	A	1726	C	N1-C2-O2	5.22	122.03	118.90
18	A	1973	G	C5-C6-O6	5.07	131.64	128.60

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	C	1195	0	1222	18	0
2	D	1348	0	1406	19	0
3	E	1461	0	1525	26	0
4	J	1121	0	1155	17	0
5	K	929	0	998	18	0
6	L	769	0	828	19	0
7	N	960	0	1000	18	0
8	P	917	0	965	17	0
9	Q	947	0	1022	10	0
10	R	816	0	839	8	0
11	S	786	0	845	15	0
12	T	730	0	795	15	0
13	U	779	0	834	11	0
14	Y	509	0	543	14	0
15	0	444	0	461	9	0
16	2	315	0	346	9	0
17	Z	449	0	491	6	0
18	A	44635	0	22451	315	0
All	All	59110	0	37726	487	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (487) 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)
18:A:175:G:O2'	18:A:176:A:O5'	1.90	0.88
18:A:1462:C:O2'	18:A:2702:G:O2'	1.90	0.88
12:T:2:ILE:HG23	12:T:7:LEU:HD11	1.55	0.86
9:Q:83:LYS:NZ	18:A:1152:C:OP1	2.09	0.86
18:A:514:A:N3	18:A:581:C:O2'	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:2647:U:O2	18:A:2673:G:O6	1.95	0.85
18:A:1528:A:N6	18:A:1543:G:O2'	2.10	0.85
18:A:299:A:O2'	18:A:300:A:O4'	1.94	0.84
18:A:308:G:C6	18:A:501:A:C6	2.65	0.84
18:A:159:G:O2'	18:A:167:A:N6	2.11	0.84
16:2:34:ARG:NH2	18:A:466:A:OP1	2.11	0.83
8:P:61:ARG:NH1	8:P:70:GLU:OE2	2.12	0.83
18:A:228:C:N4	18:A:416:U:O2	2.11	0.83
2:D:174:SER:OG	18:A:2730:C:O3'	1.98	0.82
18:A:1007:C:OP2	18:A:1008:A:O2'	1.99	0.81
18:A:1351:C:O2'	18:A:1571:A:O2'	1.91	0.81
18:A:1496:A:N3	18:A:1577:C:O2'	2.12	0.81
18:A:1992:G:N2	18:A:1996:C:O2'	2.14	0.81
18:A:2646:C:OP2	18:A:2732:G:O2'	1.99	0.80
18:A:261:G:HO2'	18:A:610:C:HO2'	1.15	0.80
18:A:1019:U:O2'	18:A:1021:A:N7	2.15	0.80
4:J:65:THR:OG1	18:A:1140:C:OP1	1.99	0.80
8:P:16:VAL:HG13	8:P:83:ILE:HD11	1.64	0.80
18:A:685:A:O2'	18:A:773:U:O4	2.01	0.79
18:A:83:A:O2'	18:A:103:A:N6	2.16	0.79
6:L:29:LYS:O	6:L:30:THR:OG1	2.01	0.79
4:J:120:ARG:NE	18:A:2780:G:OP2	2.15	0.78
18:A:1363:C:O2'	18:A:1809:A:N3	2.17	0.78
18:A:176:A:O2'	18:A:177:G:O4'	2.02	0.78
18:A:745:G:O2'	18:A:750:A:N6	2.16	0.78
7:N:77:ALA:O	7:N:81:ASN:ND2	2.17	0.77
2:D:16:THR:OG1	2:D:18:ASP:OD1	2.01	0.77
18:A:1796:U:O2	18:A:1823:G:O6	2.02	0.77
6:L:21:ARG:NH2	18:A:587:C:OP1	2.19	0.76
8:P:55:HIS:HD1	18:A:2682:A:HO2'	1.31	0.76
12:T:73:ARG:NH2	18:A:65:U:O3'	2.18	0.76
18:A:453:A:N3	18:A:457:A:O2'	2.19	0.76
6:L:135:ILE:HG21	6:L:142:ILE:HD11	1.68	0.76
18:A:1135:C:N4	18:A:1138:G:OP2	2.18	0.75
18:A:1359:A:OP2	18:A:1371:G:N2	2.19	0.75
18:A:1629:U:O4	18:A:1630:A:N6	2.19	0.75
18:A:779:U:O2	18:A:785:G:O6	2.04	0.75
18:A:1753:G:N2	18:A:1756:G:O5'	2.19	0.75
18:A:2645:G:OP2	18:A:2645:G:N2	2.18	0.75
18:A:1322:A:N1	18:A:1333:G:O2'	2.20	0.75
18:A:1521:G:OP2	18:A:1522:A:O2'	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:8:ARG:NE	18:A:1652:A:OP1	2.20	0.74
16:2:34:ARG:NH1	16:2:42:LEU:O	2.21	0.74
18:A:31:C:O2'	18:A:1238:G:OP1	2.04	0.74
18:A:636:G:O2'	18:A:638:G:O2'	1.93	0.74
18:A:1447:C:O2'	18:A:1544:A:N3	2.20	0.74
14:Y:52:ARG:NH2	18:A:76:C:O3'	2.20	0.73
18:A:465:G:N2	18:A:684:G:O2'	2.21	0.73
18:A:1791:A:N6	18:A:1828:G:O2'	2.22	0.73
5:K:48:PRO:O	5:K:53:LYS:NZ	2.22	0.73
18:A:860:U:O2	18:A:917:A:N7	2.21	0.73
3:E:48:THR:OG1	3:E:51:GLU:OE1	2.06	0.73
18:A:541:A:N6	18:A:553:G:O6	2.21	0.73
18:A:2865:U:OP2	18:A:2866:U:O2'	2.04	0.73
18:A:1358:G:N2	18:A:1372:U:OP2	2.22	0.73
18:A:9:G:O2'	18:A:2800:A:N6	2.22	0.72
18:A:247:G:O2'	18:A:250:G:O6	2.08	0.72
18:A:1721:G:O2'	18:A:1739:A:N6	2.23	0.72
18:A:2857:G:N2	18:A:2860:A:OP2	2.22	0.71
13:U:36:GLU:N	13:U:36:GLU:OE1	2.24	0.71
18:A:395:U:O2'	18:A:396:G:N7	2.20	0.71
6:L:112:LEU:HD22	6:L:135:ILE:HG13	1.72	0.71
15:0:39:ARG:NH2	18:A:2885:G:O6	2.23	0.71
18:A:308:G:O6	18:A:501:A:C6	2.44	0.71
8:P:33:GLU:OE2	8:P:36:LYS:NZ	2.23	0.71
18:A:1009:A:O2'	18:A:1010:A:O4'	2.02	0.70
9:Q:97:ILE:HD11	9:Q:104:ALA:HB1	1.73	0.70
18:A:1475:G:O2'	18:A:1514:G:O6	2.09	0.70
17:Z:7:THR:HG22	17:Z:34:THR:HG22	1.74	0.70
1:C:151:GLY:O	1:C:155:ARG:NE	2.25	0.69
1:C:95:TYR:OH	1:C:101:ARG:NH2	2.24	0.69
6:L:128:THR:O	6:L:132:ARG:NH1	2.25	0.69
18:A:1217:U:O2	18:A:1232:G:O6	2.10	0.69
9:Q:48:ASP:OD2	18:A:534:U:O2'	2.06	0.69
4:J:135:GLN:NE2	18:A:6:A:N3	2.41	0.69
14:Y:45:GLN:N	14:Y:45:GLN:OE1	2.26	0.69
18:A:1288:G:OP2	18:A:1288:G:N2	2.26	0.69
9:Q:91:ARG:NH2	18:A:1153:C:OP1	2.26	0.69
18:A:136:G:O2'	18:A:137:U:O5'	2.07	0.69
18:A:1800:C:O2	18:A:1817:G:O6	2.11	0.68
8:P:55:HIS:ND1	18:A:2682:A:O2'	2.22	0.68
8:P:102:ARG:NH2	18:A:1754:A:O2'	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:727:A:OP1	18:A:1431:A:O2'	2.04	0.68
18:A:2043:C:OP1	18:A:2777:G:O2'	2.08	0.68
7:N:37:THR:HG22	7:N:39:PRO:HD2	1.76	0.67
18:A:1326:U:N3	18:A:1648:U:O2'	2.28	0.67
2:D:162:ALA:O	18:A:2620:C:O2'	2.09	0.67
12:T:11:LEU:O	14:Y:29:ARG:NH1	2.26	0.67
7:N:4:ARG:NH2	18:A:2874:C:OP1	2.28	0.66
3:E:156:ASN:OD1	3:E:157:LEU:N	2.28	0.66
13:U:9:GLU:OE2	13:U:21:ARG:NH1	2.29	0.66
18:A:1329:U:OP2	18:A:1330:C:N4	2.29	0.65
5:K:106:GLU:OE1	5:K:106:GLU:N	2.29	0.65
5:K:104:THR:OG1	5:K:106:GLU:OE1	2.09	0.65
18:A:378:C:N4	18:A:379:G:O6	2.29	0.65
18:A:951:C:N4	18:A:952:G:O6	2.30	0.65
7:N:41:ALA:CB	7:N:113:ILE:HD11	2.27	0.65
18:A:948:C:O2	18:A:984:A:O2'	2.11	0.65
3:E:40:ARG:NH2	18:A:444:C:OP1	2.29	0.65
18:A:117:G:OP2	18:A:119:A:O2'	2.11	0.65
18:A:1472:C:N4	18:A:1473:G:O6	2.28	0.65
16:2:26:ASN:ND2	18:A:682:G:O3'	2.30	0.64
18:A:1286:A:N6	18:A:1329:U:O2	2.31	0.64
18:A:2047:C:O2'	18:A:2823:A:N1	2.28	0.64
8:P:52:ARG:NH2	18:A:2720:U:OP1	2.30	0.64
11:S:80:PRO:O	11:S:100:THR:OG1	2.15	0.64
18:A:1550:C:OP1	18:A:1720:U:O2'	2.05	0.64
18:A:698:C:O2'	18:A:734:A:N6	2.31	0.64
18:A:191:A:O2'	18:A:678:C:O2	2.15	0.63
18:A:2718:G:O2'	18:A:2847:U:OP1	2.17	0.63
18:A:1264:A:N6	18:A:2014:A:OP2	2.32	0.63
8:P:8:GLU:OE2	8:P:54:LEU:N	2.32	0.63
5:K:93:GLN:N	5:K:93:GLN:OE1	2.32	0.63
6:L:93:ASN:O	6:L:94:THR:OG1	2.17	0.63
1:C:34:GLU:N	1:C:34:GLU:OE1	2.32	0.63
18:A:482:A:O2'	18:A:497:A:N1	2.32	0.62
18:A:1681:G:OP2	18:A:1757:A:N6	2.32	0.62
3:E:152:GLU:N	3:E:152:GLU:OE1	2.32	0.62
6:L:112:LEU:HD21	6:L:134:ALA:HB3	1.81	0.62
18:A:629:G:O2'	18:A:649:G:N2	2.32	0.62
11:S:2:GLU:OE1	11:S:2:GLU:N	2.33	0.62
5:K:41:ILE:HD13	5:K:60:ALA:HB3	1.79	0.62
18:A:1636:U:O2'	18:A:1760:C:O2	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:746:U:O4'	18:A:748:G:N2	2.33	0.62
18:A:261:G:O2'	18:A:610:C:O2'	1.99	0.61
18:A:308:G:C6	18:A:501:A:C5	2.86	0.61
18:A:571:U:N3	18:A:575:A:N7	2.48	0.61
4:J:102:GLU:OE1	18:A:2780:G:N1	2.32	0.61
2:D:74:GLU:OE1	2:D:74:GLU:N	2.33	0.61
3:E:51:GLU:OE1	3:E:51:GLU:N	2.34	0.61
3:E:175:ILE:HD11	3:E:180:LEU:HD21	1.82	0.61
18:A:216:A:N7	18:A:431:U:N3	2.48	0.61
18:A:345:A:N3	18:A:347:A:N6	2.49	0.61
18:A:728:G:HO2'	18:A:730:A:H8	1.49	0.61
5:K:30:ARG:NH2	5:K:37:ASP:OD2	2.34	0.60
18:A:1649:G:O6	18:A:2009:A:N6	2.34	0.60
17:Z:7:THR:CG2	17:Z:34:THR:HG22	2.32	0.60
18:A:1223:G:N2	18:A:1226:A:OP2	2.33	0.60
4:J:129:GLU:N	4:J:129:GLU:OE1	2.34	0.60
1:C:169:ALA:O	1:C:185:ALA:N	2.34	0.60
12:T:4:GLU:O	12:T:5:GLU:C	2.40	0.60
14:Y:59:GLU:N	14:Y:59:GLU:OE1	2.32	0.60
2:D:81:GLU:OE2	18:A:2635:A:O2'	2.14	0.60
18:A:36:G:O2'	18:A:451:U:O4'	2.19	0.60
9:Q:58:GLN:NE2	18:A:1009:A:O4'	2.34	0.60
18:A:865:C:O2	18:A:867:C:N4	2.34	0.60
18:A:969:G:N2	18:A:984:A:O2'	2.34	0.60
11:S:45:VAL:HG23	11:S:46:LEU:HD12	1.84	0.60
12:T:73:ARG:NH1	18:A:456:C:O2	2.34	0.59
18:A:373:U:O2'	18:A:423:A:N6	2.34	0.59
3:E:47:LYS:NZ	18:A:451:U:O3'	2.36	0.59
15:O:53:VAL:HG22	15:O:54:ILE:H	1.67	0.59
18:A:821:A:N6	18:A:972:A:O2'	2.36	0.59
5:K:12:ASP:OD1	5:K:13:ASN:N	2.36	0.59
18:A:976:G:O2'	18:A:1155:A:O2'	2.21	0.59
4:J:135:GLN:N	4:J:135:GLN:OE1	2.36	0.59
6:L:127:VAL:HG11	6:L:142:ILE:HD12	1.85	0.59
7:N:69:ARG:O	7:N:70:THR:OG1	2.20	0.59
8:P:101:GLU:OE1	8:P:101:GLU:N	2.36	0.58
3:E:155:GLU:OE1	3:E:155:GLU:N	2.35	0.58
12:T:4:GLU:O	12:T:7:LEU:N	2.37	0.58
18:A:375:G:O2'	18:A:376:G:O4'	2.16	0.58
18:A:1216:G:N1	18:A:1234:U:O4	2.36	0.58
12:T:59:ASN:OD1	12:T:60:THR:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:175:G:HO2'	18:A:176:A:C5'	2.10	0.58
8:P:1:SER:OG	18:A:2876:G:OP1	2.16	0.58
2:D:17:GLU:N	2:D:17:GLU:OE1	2.36	0.58
5:K:34:GLY:N	5:K:37:ASP:OD2	2.37	0.57
14:Y:58:ASN:OD1	14:Y:59:GLU:N	2.37	0.57
18:A:987:C:O2'	18:A:1000:A:N3	2.32	0.57
18:A:1140:C:O2	18:A:1143:A:O2'	2.23	0.57
18:A:1582:C:O2'	18:A:1585:C:N3	2.34	0.57
18:A:1384:A:O2'	18:A:1404:C:O2	2.18	0.57
1:C:152:GLN:O	18:A:1818:U:O2'	2.21	0.57
18:A:750:A:OP1	18:A:1615:C:N4	2.38	0.57
18:A:1814:G:OP2	18:A:1815:A:O2'	2.15	0.57
2:D:169:ARG:NH2	18:A:2774:C:OP2	2.37	0.57
18:A:714:U:N3	18:A:717:C:OP2	2.38	0.56
4:J:13:ARG:NH2	4:J:49:ASP:O	2.38	0.56
16:2:35:ARG:NH1	18:A:54:G:O2'	2.39	0.56
18:A:2006:C:O2'	18:A:2823:A:N3	2.37	0.56
15:0:3:GLN:NE2	15:0:5:ASN:O	2.38	0.56
18:A:1673:G:N2	18:A:1675:C:O4'	2.39	0.56
1:C:96:LYS:O	18:A:1501:G:O2'	2.17	0.56
2:D:103:ASP:OD1	2:D:105:LYS:NZ	2.39	0.56
18:A:65:U:O2'	18:A:456:C:N3	2.36	0.55
18:A:308:G:O6	18:A:501:A:N1	2.40	0.55
1:C:114:GLN:N	1:C:114:GLN:OE1	2.40	0.55
5:K:59:LYS:NZ	5:K:88:ASN:O	2.39	0.55
11:S:77:ASP:OD1	11:S:77:ASP:N	2.38	0.55
18:A:239:C:HO2'	18:A:622:G:HO2'	1.54	0.55
4:J:21:THR:OG1	4:J:58:ASN:ND2	2.40	0.55
3:E:171:ASP:OD1	3:E:172:ALA:N	2.39	0.55
18:A:1173:U:O2'	18:A:1176:U:O2	2.13	0.55
1:C:132:ARG:O	1:C:166:ARG:NE	2.39	0.55
18:A:532:A:OP1	18:A:561:G:N2	2.39	0.55
18:A:774:G:O2'	18:A:775:G:OP2	2.16	0.55
3:E:46:GLN:N	3:E:46:GLN:OE1	2.40	0.55
18:A:1754:A:N6	18:A:2717:C:O4'	2.40	0.55
17:Z:57:GLU:N	17:Z:57:GLU:OE1	2.39	0.54
18:A:409:G:N1	18:A:419:U:O4	2.41	0.54
18:A:1024:G:OP2	18:A:1025:G:O2'	2.20	0.54
18:A:2637:U:O4	18:A:2776:A:N7	2.40	0.54
6:L:21:ARG:NH1	18:A:1250:G:OP2	2.41	0.54
7:N:103:ARG:O	7:N:107:ASN:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:106:ASP:OD2	18:A:1287:A:N6	2.41	0.54
18:A:1271:G:O2'	18:A:1618:A:N7	2.39	0.54
18:A:2834:G:O2'	18:A:2835:A:O5'	2.23	0.54
3:E:79:ARG:NH1	18:A:471:A:OP1	2.38	0.54
13:U:50:ALA:C	13:U:51:LEU:HD23	2.28	0.54
18:A:1726:C:N3	18:A:1735:A:N6	2.56	0.54
1:C:122:ALA:O	1:C:127:ASN:ND2	2.38	0.54
10:R:23:GLU:N	10:R:23:GLU:OE1	2.39	0.54
18:A:1712:U:OP2	18:A:1713:A:O2'	2.11	0.54
7:N:12:ARG:NH2	18:A:1650:A:OP1	2.41	0.54
18:A:2731:G:O2'	18:A:2732:G:O4'	2.23	0.54
11:S:52:GLU:OE1	18:A:487:C:O2'	2.18	0.54
16:2:13:ASN:O	16:2:17:GLY:N	2.41	0.54
18:A:728:G:O2'	18:A:730:A:O4'	2.26	0.54
14:Y:50:VAL:HA	14:Y:53:VAL:HG22	1.90	0.53
18:A:1346:G:N1	18:A:1601:G:O6	2.42	0.53
18:A:1726:C:H2'	18:A:1727:C:C1'	2.39	0.53
3:E:108:ILE:O	3:E:112:LEU:HD23	2.09	0.53
12:T:3:ARG:O	12:T:5:GLU:N	2.41	0.53
18:A:789:A:N6	18:A:1613:G:O3'	2.42	0.53
18:A:1668:A:N3	18:A:1670:C:N4	2.56	0.53
18:A:1426:G:O2'	18:A:1572:A:N6	2.41	0.53
4:J:37:ARG:NE	4:J:44:TYR:OH	2.42	0.53
18:A:1428:C:N4	18:A:1570:A:OP2	2.42	0.53
18:A:49:A:N1	18:A:177:G:N2	2.56	0.53
18:A:2059:A:N3	18:A:2609:U:O2'	2.37	0.53
16:2:37:LYS:NZ	18:A:469:G:O6	2.42	0.53
18:A:31:C:H2'	18:A:32:C:C1'	2.39	0.53
18:A:2788:C:O2'	18:A:2809:A:N3	2.36	0.53
18:A:262:A:N3	18:A:430:A:O2'	2.36	0.53
18:A:381:G:O6	18:A:394:C:N4	2.42	0.53
18:A:1234:U:O2'	18:A:1235:G:OP1	2.20	0.53
12:T:4:GLU:O	12:T:6:ARG:N	2.42	0.52
18:A:1026:G:OP1	18:A:1134:A:O2'	2.25	0.52
3:E:146:VAL:HG21	3:E:187:VAL:HG23	1.91	0.52
5:K:90:ASN:O	5:K:91:SER:OG	2.26	0.52
9:Q:88:GLU:N	9:Q:88:GLU:OE1	2.43	0.52
17:Z:10:ARG:NH1	18:A:988:A:OP1	2.42	0.52
18:A:154:U:O4	18:A:155:A:N6	2.41	0.52
18:A:2643:G:C6	18:A:2644:G:O6	2.62	0.52
15:0:8:THR:HG22	15:0:11:LYS:NZ	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:311:A:N6	18:A:329:G:OP1	2.43	0.52
6:L:3:LEU:HD23	6:L:3:LEU:H	1.74	0.52
18:A:59:U:O2'	18:A:74:A:OP2	2.16	0.52
11:S:8:ARG:NH1	18:A:494:G:OP1	2.43	0.52
1:C:92:LEU:HD12	1:C:101:ARG:O	2.10	0.51
18:A:375:G:H2'	18:A:376:G:C8	2.45	0.51
1:C:92:LEU:HD11	1:C:100:ARG:HB3	1.92	0.51
1:C:68:ARG:NH1	1:C:128:THR:OG1	2.44	0.51
18:A:48:G:H22	18:A:177:G:P	2.33	0.51
5:K:66:LYS:N	5:K:82:ASN:OD1	2.43	0.51
12:T:2:ILE:CG2	12:T:7:LEU:HD11	2.34	0.51
18:A:225:C:N3	18:A:226:A:N6	2.59	0.51
18:A:2659:G:N2	18:A:2662:A:OP2	2.32	0.51
4:J:36:LEU:HD21	4:J:54:ILE:HG22	1.93	0.51
7:N:96:ARG:NH1	18:A:2882:A:OP1	2.42	0.51
7:N:100:CYS:HA	15:0:42:ILE:HG22	1.91	0.51
18:A:677:A:N6	18:A:802:A:N1	2.58	0.51
18:A:136:G:HO2'	18:A:137:U:C5'	2.22	0.51
3:E:117:ARG:NH1	6:L:2:ARG:O	2.40	0.50
5:K:60:ALA:HB1	5:K:84:CYS:SG	2.51	0.50
10:R:83:TYR:OH	10:R:85:LYS:NZ	2.43	0.50
4:J:90:GLU:OE1	4:J:90:GLU:N	2.42	0.50
8:P:55:HIS:CG	18:A:2682:A:HO2'	2.24	0.50
3:E:25:GLU:OE2	6:L:7:SER:N	2.40	0.50
18:A:956:G:N1	18:A:960:A:OP2	2.44	0.50
7:N:64:ARG:NH1	18:A:2851:A:O2'	2.44	0.50
18:A:239:C:O2'	18:A:622:G:O2'	2.23	0.50
18:A:1383:A:O2'	18:A:1384:A:O4'	2.20	0.50
18:A:308:G:N2	18:A:477:A:N7	2.59	0.50
18:A:2647:U:O2	18:A:2673:G:C6	2.63	0.50
18:A:728:G:H3'	18:A:729:G:C5'	2.42	0.50
2:D:164:GLN:NE2	18:A:2822:G:OP1	2.45	0.49
12:T:18:GLU:OE1	18:A:1392:A:N6	2.45	0.49
18:A:2853:C:N4	18:A:2854:G:O6	2.45	0.49
11:S:78:GLU:OE2	18:A:24:G:N2	2.43	0.49
11:S:82:MET:SD	11:S:82:MET:N	2.86	0.49
18:A:2776:A:O2'	18:A:2782:G:N7	2.32	0.49
18:A:136:G:O2'	18:A:137:U:P	2.70	0.49
18:A:1332:G:HO2'	18:A:1609:A:H2	1.58	0.49
18:A:1532:A:N6	18:A:1540:G:O6	2.46	0.49
18:A:1572:A:C2	18:A:1573:G:C8	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:2821:A:O2'	18:A:2822:G:O4'	2.28	0.49
2:D:78:GLY:C	2:D:79:LEU:HD12	2.33	0.49
4:J:67:ASN:ND2	4:J:71:ASP:OD2	2.45	0.49
18:A:978:G:HO2'	18:A:1002:G:HO2'	1.57	0.49
7:N:6:SER:OG	18:A:2873:A:O4'	2.23	0.49
11:S:66:ILE:HA	11:S:69:LEU:HD23	1.94	0.49
14:Y:8:GLU:N	14:Y:8:GLU:OE1	2.46	0.49
18:A:404:A:N3	18:A:406:G:N1	2.60	0.49
18:A:2734:A:N6	18:A:2770:G:O2'	2.45	0.49
18:A:2743:U:OP2	18:A:2755:C:N4	2.35	0.49
18:A:2688:G:N1	18:A:2720:U:OP2	2.43	0.48
18:A:1234:U:HO2'	18:A:1235:G:P	2.34	0.48
18:A:1728:C:N4	18:A:1731:G:H22	2.10	0.48
5:K:40:LYS:C	5:K:41:ILE:HD12	2.34	0.48
15:O:8:THR:HG23	15:O:10:SER:H	1.77	0.48
18:A:1328:A:O2'	18:A:1329:U:O5'	2.29	0.48
18:A:860:U:C2	18:A:917:A:N7	2.81	0.48
4:J:25:LEU:HD11	18:A:1139:G:O3'	2.14	0.48
7:N:8:ARG:HG3	7:N:10:LEU:HD23	1.96	0.48
14:Y:17:GLU:OE1	14:Y:18:LEU:N	2.46	0.48
18:A:644:A:O2'	18:A:645:C:O5'	2.29	0.48
3:E:43:THR:OG1	18:A:38:A:N3	2.42	0.48
18:A:243:U:O2	18:A:255:A:N7	2.47	0.48
18:A:2703:C:C2	18:A:2704:C:C5	3.01	0.48
8:P:32:VAL:HG22	8:P:37:LYS:CD	2.44	0.48
18:A:532:A:N7	18:A:2021:C:O2'	2.40	0.48
9:Q:52:ARG:NH2	18:A:995:C:OP2	2.46	0.48
18:A:324:A:OP2	18:A:1205:A:N6	2.46	0.48
18:A:213:A:H2'	18:A:214:G:C8	2.49	0.48
3:E:7:ASP:OD1	3:E:8:ALA:N	2.45	0.47
18:A:687:C:O2'	18:A:1780:A:N6	2.35	0.47
2:D:169:ARG:NE	18:A:2773:C:OP1	2.44	0.47
2:D:58:ASN:OD1	2:D:59:ARG:N	2.46	0.47
3:E:94:GLN:NE2	18:A:659:G:O2'	2.47	0.47
4:J:28:LEU:O	4:J:32:LEU:HD13	2.14	0.47
8:P:27:VAL:HG22	8:P:83:ILE:HG22	1.96	0.47
15:O:11:LYS:NZ	18:A:2021:C:OP1	2.41	0.47
18:A:212:G:H2'	18:A:213:A:C8	2.50	0.47
18:A:451:U:C4	18:A:453:A:C8	3.03	0.47
18:A:1573:G:C5	18:A:1574:C:C5	3.02	0.47
18:A:582:A:N6	18:A:1259:G:O6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1358:G:O2'	18:A:1373:A:N6	2.47	0.47
14:Y:18:LEU:HD23	14:Y:22:LEU:HD23	1.97	0.47
3:E:94:GLN:NE2	18:A:659:G:O3'	2.47	0.47
16:2:9:VAL:HG12	18:A:1309:G:OP1	2.14	0.47
18:A:1574:C:C2	18:A:1575:C:C5	3.03	0.47
11:S:42:LYS:O	11:S:45:VAL:HG22	2.15	0.47
14:Y:9:LYS:N	14:Y:12:GLU:OE2	2.45	0.47
18:A:2687:U:H2'	18:A:2688:G:O4'	2.15	0.47
7:N:49:GLU:N	7:N:50:PRO:CD	2.78	0.46
18:A:705:A:N6	18:A:727:A:N7	2.64	0.46
18:A:1328:A:HO2'	18:A:1329:U:P	2.37	0.46
18:A:1728:C:N4	18:A:1730:C:O2	2.48	0.46
12:T:59:ASN:ND2	18:A:1341:G:O3'	2.45	0.46
18:A:1432:G:H2'	18:A:1433:A:C8	2.51	0.46
1:C:181:ARG:NH1	18:A:1799:G:O2'	2.49	0.46
18:A:176:A:H2'	18:A:177:G:C4	2.51	0.46
18:A:235:U:O4	18:A:263:G:N2	2.49	0.46
6:L:100:ILE:HG23	6:L:101:ILE:HG12	1.98	0.46
17:Z:31:ILE:N	17:Z:31:ILE:HD12	2.30	0.46
5:K:31:ARG:NE	18:A:1996:C:OP2	2.49	0.46
17:Z:50:VAL:HG13	17:Z:53:MET:HE2	1.98	0.46
5:K:79:PHE:HE1	8:P:69:VAL:HG13	1.82	0.46
18:A:307:G:N1	18:A:309:A:O5'	2.49	0.46
18:A:789:A:N6	18:A:1613:G:O2'	2.45	0.46
1:C:166:ARG:HA	1:C:171:VAL:HG11	1.98	0.45
8:P:70:GLU:OE1	8:P:70:GLU:N	2.49	0.45
11:S:17:VAL:HG23	11:S:76:VAL:HG21	1.97	0.45
13:U:98:ASN:C	13:U:98:ASN:OD1	2.54	0.45
1:C:81:GLU:OE1	1:C:81:GLU:N	2.49	0.45
18:A:68:G:N2	18:A:74:A:O4'	2.50	0.45
1:C:121:ALA:HB1	1:C:129:LEU:HD23	1.98	0.45
15:0:9:ARG:NE	18:A:517:C:OP2	2.50	0.45
2:D:77:ARG:NH2	2:D:200:ASP:OD1	2.49	0.45
2:D:117:GLY:N	18:A:2822:G:OP1	2.46	0.45
18:A:1378:A:C4'	18:A:1379:U:OP1	2.65	0.45
18:A:540:C:N4	18:A:541:A:H62	2.13	0.45
3:E:55:SER:OG	18:A:468:G:O3'	2.28	0.45
18:A:680:C:N4	18:A:681:G:O6	2.50	0.45
3:E:190:ALA:O	3:E:194:LYS:NZ	2.47	0.45
8:P:55:HIS:CE1	18:A:2682:A:HO2'	2.28	0.45
18:A:476:G:N2	18:A:479:A:O4'	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:1969:A:H2'	18:A:1972:G:H21	1.80	0.45
12:T:91:GLN:N	12:T:91:GLN:OE1	2.50	0.45
18:A:402:A:N3	18:A:407:G:O2'	2.48	0.45
18:A:554:U:H2'	18:A:555:G:O4'	2.17	0.45
18:A:572:A:N6	18:A:573:U:O2	2.50	0.45
18:A:1800:C:O2	18:A:1817:G:C6	2.69	0.45
18:A:2704:C:C2	18:A:2705:A:C8	3.05	0.45
2:D:34:VAL:HG13	2:D:48:ILE:HD11	1.99	0.44
6:L:4:ASN:OD1	18:A:1202:G:N2	2.50	0.44
10:R:39:LEU:O	10:R:49:ILE:HG21	2.17	0.44
18:A:306:U:H3	18:A:310:A:H62	1.66	0.44
3:E:111:GLU:OE2	3:E:115:GLN:NE2	2.50	0.44
11:S:109:ASP:OD1	11:S:110:ARG:N	2.49	0.44
16:2:14:ARG:NH2	18:A:770:G:O3'	2.51	0.44
18:A:965:C:N4	18:A:966:G:O6	2.51	0.44
18:A:981:A:O2'	18:A:2036:C:O2'	2.33	0.44
18:A:1630:A:H2'	18:A:1631:G:O4'	2.18	0.44
18:A:306:U:O4	18:A:310:A:N7	2.51	0.44
18:A:573:U:N3	18:A:2029:G:O2'	2.45	0.44
1:C:174:ARG:NH1	1:C:175:LEU:O	2.49	0.44
3:E:133:LEU:HD23	3:E:133:LEU:O	2.18	0.44
11:S:15:GLN:N	11:S:15:GLN:OE1	2.51	0.44
18:A:301:G:O2'	18:A:302:C:O5'	2.33	0.43
2:D:113:SER:OG	2:D:168:GLU:OE2	2.35	0.43
6:L:5:THR:HG22	6:L:5:THR:O	2.18	0.43
7:N:82:GLU:HG2	7:N:83:LEU:HD12	2.00	0.43
2:D:116:LYS:NZ	18:A:2723:C:O3'	2.46	0.43
11:S:83:LYS:HD3	11:S:97:LEU:HD11	2.00	0.43
18:A:175:G:C2'	18:A:176:A:O5'	2.65	0.43
18:A:629:G:H21	18:A:640:C:H4'	1.83	0.43
13:U:76:THR:HG23	13:U:78:LYS:H	1.83	0.43
11:S:57:ASN:O	11:S:61:ASN:ND2	2.50	0.43
18:A:390:U:O2	18:A:391:A:N6	2.49	0.43
3:E:149:ILE:HD12	3:E:170:ARG:O	2.19	0.43
18:A:226:A:N6	18:A:230:G:C6	2.87	0.43
18:A:532:A:N1	18:A:2035:G:N2	2.64	0.43
18:A:1021:A:N1	18:A:1022:G:N2	2.66	0.43
18:A:1353:A:N7	18:A:1377:G:N2	2.66	0.43
4:J:10:THR:HG22	4:J:10:THR:O	2.19	0.43
10:R:45:GLU:N	10:R:45:GLU:OE1	2.51	0.43
14:Y:17:GLU:HG3	14:Y:53:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:151:C:N4	18:A:152:A:N6	2.66	0.43
10:R:29:THR:HA	10:R:63:VAL:HG23	2.00	0.43
18:A:499:U:H2'	18:A:500:G:O4'	2.18	0.43
3:E:21:ARG:O	3:E:114:ARG:NH2	2.50	0.43
6:L:108:ALA:O	6:L:125:LEU:HD23	2.18	0.43
18:A:1146:C:C2	18:A:1147:A:C8	3.07	0.43
12:T:31:VAL:HG22	12:T:84:TYR:CD1	2.54	0.42
13:U:48:VAL:HG21	13:U:51:LEU:HD21	2.00	0.42
18:A:1528:A:N6	18:A:1543:G:HO2'	2.15	0.42
14:Y:14:LEU:C	14:Y:14:LEU:HD23	2.40	0.42
5:K:111:LYS:HZ2	5:K:112:PHE:HE1	1.66	0.42
18:A:820:A:N3	18:A:943:A:O2'	2.50	0.42
7:N:65:LEU:HD23	7:N:65:LEU:O	2.19	0.42
13:U:102:ILE:N	13:U:102:ILE:HD12	2.35	0.42
18:A:1738:G:HO2'	18:A:1739:A:C5'	2.32	0.42
4:J:39:LYS:O	9:Q:66:ALA:HB2	2.20	0.42
18:A:106:C:O2	18:A:294:A:O2'	2.36	0.42
18:A:1416:G:O2'	18:A:1417:C:OP2	2.26	0.42
18:A:2637:U:H3	18:A:2776:A:H62	1.68	0.42
5:K:11:ALA:HB2	5:K:83:ALA:HB1	2.01	0.42
18:A:401:A:H3'	18:A:402:A:H5'	2.00	0.42
18:A:1017:G:C6	18:A:1146:C:N4	2.88	0.42
2:D:110:THR:HG22	2:D:171:THR:HG23	2.02	0.42
9:Q:79:ILE:HG22	9:Q:83:LYS:HE3	2.01	0.42
10:R:82:HIS:NE2	18:A:566:U:OP1	2.53	0.42
18:A:727:A:P	18:A:1431:A:HO2'	2.31	0.42
2:D:173:GLN:O	2:D:174:SER:OG	2.38	0.42
18:A:175:G:HO2'	18:A:176:A:P	2.32	0.42
4:J:59:ALA:O	4:J:62:VAL:HG13	2.20	0.42
18:A:1328:A:O2'	18:A:1329:U:P	2.78	0.42
18:A:1721:G:N1	18:A:1738:G:N7	2.67	0.42
18:A:2679:A:N6	18:A:2729:G:O6	2.53	0.42
10:R:18:GLN:NE2	10:R:19:THR:O	2.52	0.41
18:A:2816:G:N3	18:A:2883:A:O2'	2.45	0.41
6:L:77:ILE:HD11	6:L:101:ILE:HD13	2.03	0.41
6:L:128:THR:HG21	18:A:636:G:OP2	2.20	0.41
10:R:91:GLN:NE2	18:A:993:G:N3	2.60	0.41
13:U:44:HIS:N	18:A:481:G:OP2	2.51	0.41
14:Y:17:GLU:CG	14:Y:53:VAL:HG21	2.51	0.41
16:2:39:ARG:NH1	18:A:469:G:O6	2.53	0.41
18:A:42:A:N6	18:A:438:G:O6	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:500:G:H22	18:A:503:A:H5'	1.86	0.41
1:C:121:ALA:CB	1:C:129:LEU:HD23	2.50	0.41
13:U:102:ILE:HD12	13:U:102:ILE:H	1.85	0.41
18:A:526:A:O2'	18:A:2043:C:O2	2.33	0.41
18:A:2050:C:C3'	18:A:2051:A:O4'	2.69	0.41
6:L:91:ASP:OD1	6:L:91:ASP:N	2.51	0.41
7:N:10:LEU:O	7:N:12:ARG:N	2.54	0.41
18:A:176:A:H2'	18:A:177:G:N3	2.35	0.41
13:U:71:ILE:HD12	13:U:95:PHE:CE1	2.56	0.41
18:A:463:G:N2	18:A:466:A:OP2	2.42	0.41
18:A:1437:C:O2'	18:A:1516:G:O2'	2.08	0.41
5:K:16:ALA:HB1	5:K:43:ILE:HD13	2.03	0.41
8:P:23:ASP:OD1	8:P:89:GLY:N	2.48	0.41
13:U:46:LYS:NZ	18:A:483:A:OP1	2.33	0.41
18:A:289:G:O6	18:A:352:A:N6	2.54	0.41
18:A:399:U:H2'	18:A:400:G:O4'	2.21	0.41
18:A:1667:G:O2'	18:A:1991:U:O4	2.35	0.41
18:A:1720:U:H2'	18:A:1721:G:O4'	2.21	0.41
12:T:4:GLU:HG3	12:T:5:GLU:N	2.35	0.41
18:A:2702:G:C2	18:A:2703:C:C6	3.09	0.41
14:Y:43:LEU:N	14:Y:43:LEU:HD12	2.36	0.40
18:A:2725:A:O2'	18:A:2726:A:H2'	2.22	0.40
18:A:312:G:C2	18:A:313:G:N7	2.89	0.40
18:A:1571:A:HO2'	18:A:1572:A:H5'	1.86	0.40
3:E:4:VAL:HG12	3:E:6:LYS:H	1.86	0.40
15:O:25:THR:O	15:O:25:THR:HG22	2.21	0.40
18:A:751:A:HO2'	18:A:752:A:H2	1.70	0.40
18:A:1138:G:H2'	18:A:1139:G:O4'	2.22	0.40
18:A:2666:C:C5	18:A:2667:C:C5	3.09	0.40
9:Q:36:GLN:NE2	18:A:1252:G:O6	2.54	0.40
18:A:953:G:H2'	18:A:954:G:C8	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	152/273 (56%)	143 (94%)	9 (6%)	0	100	100
2	D	176/209 (84%)	172 (98%)	4 (2%)	0	100	100
3	E	186/201 (92%)	184 (99%)	2 (1%)	0	100	100
4	J	136/142 (96%)	132 (97%)	4 (3%)	0	100	100
5	K	117/123 (95%)	114 (97%)	3 (3%)	0	100	100
6	L	104/144 (72%)	96 (92%)	7 (7%)	1 (1%)	15	54
7	N	118/127 (93%)	111 (94%)	7 (6%)	0	100	100
8	P	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
9	Q	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
10	R	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
11	S	97/110 (88%)	93 (96%)	4 (4%)	0	100	100
12	T	90/100 (90%)	84 (93%)	4 (4%)	2 (2%)	6	38
13	U	100/104 (96%)	89 (89%)	11 (11%)	0	100	100
14	Y	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
15	0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
16	2	37/46 (80%)	36 (97%)	1 (3%)	0	100	100
17	Z	56/59 (95%)	56 (100%)	0	0	100	100
All	All	1812/2094 (86%)	1741 (96%)	68 (4%)	3 (0%)	50	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	T	4	GLU
12	T	5	GLU
6	L	111	ILE

### 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	C	124/218 (57%)	124 (100%)	0	100	100
2	D	140/164 (85%)	140 (100%)	0	100	100
3	E	157/165 (95%)	155 (99%)	2 (1%)	69	82
4	J	116/116 (100%)	116 (100%)	0	100	100
5	K	102/104 (98%)	102 (100%)	0	100	100
6	L	75/103 (73%)	74 (99%)	1 (1%)	69	82
7	N	100/103 (97%)	100 (100%)	0	100	100
8	P	99/100 (99%)	99 (100%)	0	100	100
9	Q	89/90 (99%)	89 (100%)	0	100	100
10	R	84/84 (100%)	84 (100%)	0	100	100
11	S	87/93 (94%)	87 (100%)	0	100	100
12	T	79/84 (94%)	77 (98%)	2 (2%)	47	68
13	U	83/85 (98%)	83 (100%)	0	100	100
14	Y	55/55 (100%)	55 (100%)	0	100	100
15	0	47/48 (98%)	47 (100%)	0	100	100
16	2	31/38 (82%)	31 (100%)	0	100	100
17	Z	48/49 (98%)	48 (100%)	0	100	100
All	All	1516/1699 (89%)	1511 (100%)	5 (0%)	92	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	57	LYS
3	E	136	GLN
6	L	126	ARG
12	T	2	ILE
12	T	64	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	94	GLN
4	J	58	ASN
6	L	99	ASN
17	Z	19	HIS

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	A	2071/2904 (71%)	295 (14%)	11 (0%)

All (295) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	A	10	A
18	A	12	U
18	A	26	G
18	A	27	G
18	A	34	U
18	A	45	G
18	A	46	G
18	A	63	A
18	A	74	A
18	A	75	G
18	A	101	A
18	A	103	A
18	A	118	A
18	A	120	U
18	A	131	A
18	A	137	U
18	A	139	U
18	A	140	C
18	A	144	A
18	A	160	A
18	A	176	A
18	A	196	A
18	A	215	G
18	A	216	A
18	A	221	A
18	A	222	A
18	A	224	U
18	A	228	C
18	A	230	G
18	A	233	A
18	A	248	G
18	A	254	G
18	A	255	A
18	A	264	C
18	A	265	A
18	A	266	G

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	A	271	G
18	A	272	A
18	A	276	U
18	A	278	A
18	A	299	A
18	A	302	C
18	A	311	A
18	A	323	C
18	A	329	G
18	A	330	A
18	A	331	C
18	A	335	C
18	A	362	A
18	A	370	G
18	A	371	A
18	A	372	G
18	A	386	G
18	A	387	U
18	A	396	G
18	A	399	U
18	A	402	A
18	A	405	U
18	A	406	G
18	A	411	G
18	A	412	A
18	A	420	C
18	A	422	A
18	A	424	G
18	A	430	A
18	A	435	C
18	A	451	U
18	A	456	C
18	A	473	G
18	A	475	C
18	A	479	A
18	A	480	A
18	A	481	G
18	A	490	C
18	A	491	G
18	A	502	A
18	A	505	A
18	A	509	C

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	A	531	C
18	A	532	A
18	A	541	A
18	A	546	U
18	A	547	A
18	A	548	G
18	A	550	C
18	A	563	A
18	A	573	U
18	A	574	A
18	A	586	A
18	A	603	A
18	A	614	A
18	A	621	A
18	A	627	A
18	A	637	A
18	A	645	C
18	A	646	U
18	A	647	G
18	A	654	A
18	A	669	G
18	A	683	U
18	A	684	G
18	A	686	U
18	A	705	A
18	A	726	G
18	A	730	A
18	A	739	A
18	A	747	U
18	A	762	U
18	A	775	G
18	A	776	G
18	A	777	G
18	A	782	A
18	A	784	G
18	A	785	G
18	A	804	A
18	A	812	C
18	A	819	A
18	A	827	U
18	A	828	U
18	A	830	G

*Continued on next page...*



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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	A	845	A
18	A	846	U
18	A	847	U
18	A	910	A
18	A	914	G
18	A	915	C
18	A	931	U
18	A	932	U
18	A	956	G
18	A	958	U
18	A	973	A
18	A	974	G
18	A	981	A
18	A	983	A
18	A	985	C
18	A	995	C
18	A	1009	A
18	A	1012	U
18	A	1013	C
18	A	1020	A
18	A	1022	G
18	A	1026	G
18	A	1132	U
18	A	1133	A
18	A	1135	C
18	A	1138	G
18	A	1142	A
18	A	1157	G
18	A	1171	G
18	A	1174	U
18	A	1175	A
18	A	1176	U
18	A	1180	U
18	A	1186	G
18	A	1212	G
18	A	1235	G
18	A	1236	G
18	A	1238	G
18	A	1253	A
18	A	1256	G
18	A	1264	A
18	A	1266	G

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	A	1271	G
18	A	1272	A
18	A	1277	G
18	A	1300	G
18	A	1301	A
18	A	1314	C
18	A	1329	U
18	A	1341	G
18	A	1345	C
18	A	1365	A
18	A	1378	A
18	A	1379	U
18	A	1383	A
18	A	1395	A
18	A	1416	G
18	A	1417	C
18	A	1428	C
18	A	1452	G
18	A	1453	A
18	A	1458	U
18	A	1467	U
18	A	1482	G
18	A	1490	A
18	A	1493	C
18	A	1495	A
18	A	1496	A
18	A	1497	U
18	A	1508	A
18	A	1515	A
18	A	1523	U
18	A	1524	G
18	A	1528	A
18	A	1532	A
18	A	1535	A
18	A	1548	A
18	A	1554	U
18	A	1555	G
18	A	1556	C
18	A	1566	A
18	A	1569	A
18	A	1578	U
18	A	1583	A

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	A	1585	C
18	A	1587	G
18	A	1598	A
18	A	1608	A
18	A	1616	A
18	A	1617	C
18	A	1634	A
18	A	1646	C
18	A	1647	U
18	A	1648	U
18	A	1654	A
18	A	1660	G
18	A	1665	A
18	A	1674	G
18	A	1710	G
18	A	1729	U
18	A	1730	C
18	A	1732	C
18	A	1737	G
18	A	1738	G
18	A	1757	A
18	A	1758	U
18	A	1764	C
18	A	1769	U
18	A	1773	A
18	A	1781	U
18	A	1800	C
18	A	1801	A
18	A	1808	A
18	A	1809	A
18	A	1816	C
18	A	1819	A
18	A	1829	A
18	A	1833	C
18	A	1972	G
18	A	1991	U
18	A	1992	G
18	A	1993	U
18	A	1997	C
18	A	2021	C
18	A	2022	U
18	A	2023	C

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	A	2025	C
18	A	2030	A
18	A	2031	A
18	A	2043	C
18	A	2051	A
18	A	2052	A
18	A	2054	A
18	A	2055	C
18	A	2056	G
18	A	2060	A
18	A	2610	C
18	A	2611	C
18	A	2614	A
18	A	2615	U
18	A	2623	G
18	A	2629	U
18	A	2636	C
18	A	2639	A
18	A	2646	C
18	A	2682	A
18	A	2684	U
18	A	2689	U
18	A	2690	U
18	A	2707	U
18	A	2714	G
18	A	2725	A
18	A	2726	A
18	A	2733	A
18	A	2739	U
18	A	2748	A
18	A	2755	C
18	A	2757	A
18	A	2758	A
18	A	2765	A
18	A	2766	A
18	A	2771	C
18	A	2778	A
18	A	2791	G
18	A	2818	U
18	A	2820	A
18	A	2835	A
18	A	2849	U

*Continued on next page...*

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Mol	Chain	Res	Type
18	A	2858	C
18	A	2867	G
18	A	2874	C
18	A	2879	A
18	A	2880	C
18	A	2884	U
18	A	2901	C

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	A	25	U
18	A	136	G
18	A	175	G
18	A	271	G
18	A	644	A
18	A	725	G
18	A	1234	U
18	A	1235	G
18	A	1328	A
18	A	1378	A
18	A	2834	G

#### 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](#)

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

There are no chain breaks in this entry.

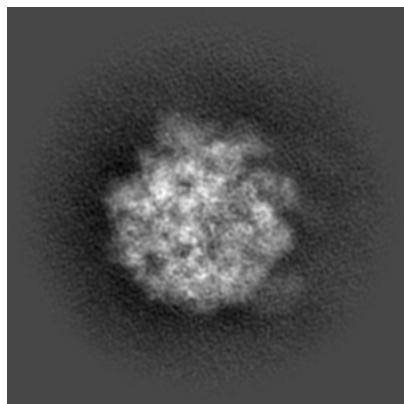
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16498. These allow visual inspection of the internal detail of the map and identification of artifacts.

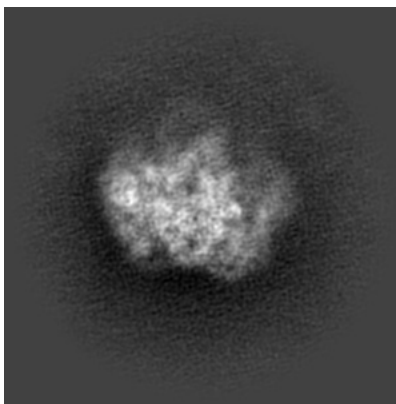
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

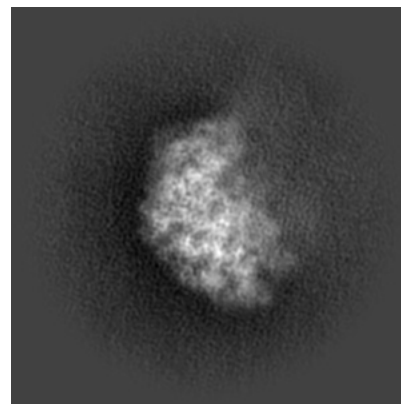
#### 6.1.1 Primary map



X

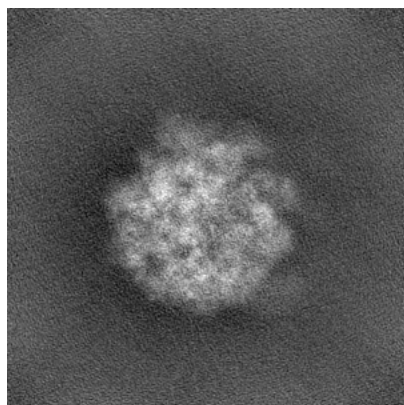


Y

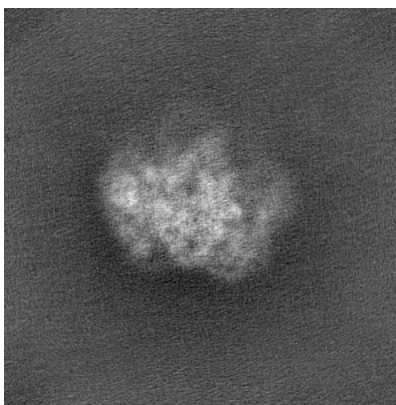


Z

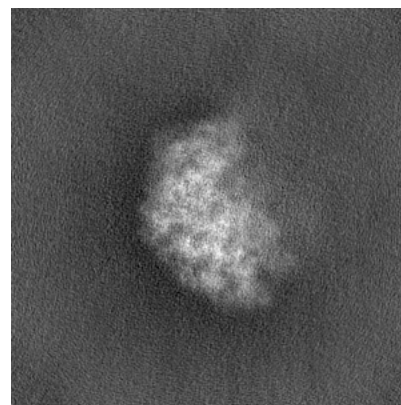
#### 6.1.2 Raw map



X



Y

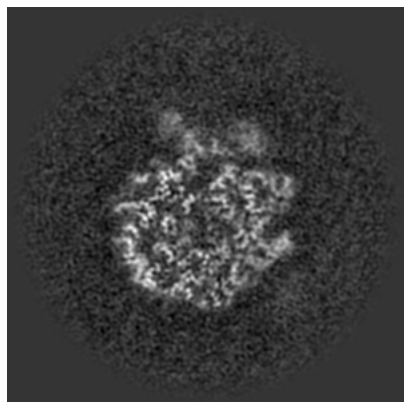


Z

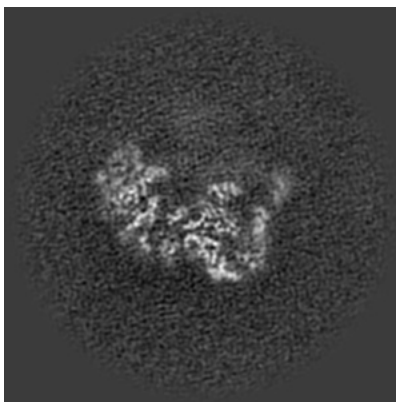
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

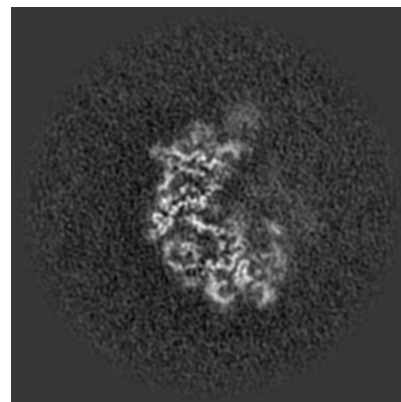
### 6.2.1 Primary map



X Index: 150

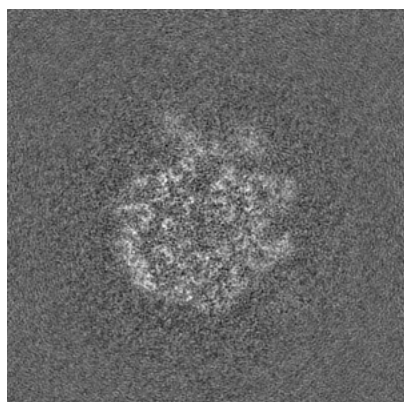


Y Index: 150

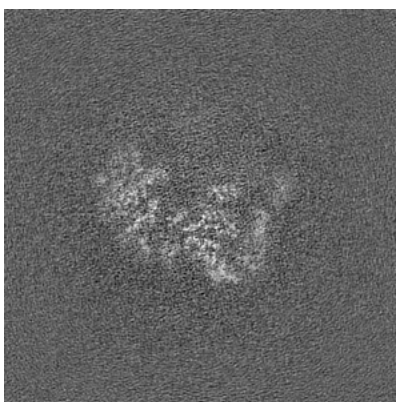


Z Index: 150

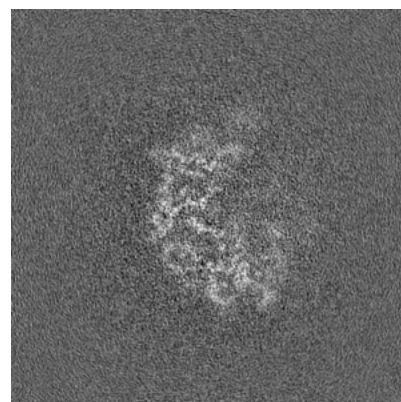
### 6.2.2 Raw map



X Index: 150



Y Index: 150



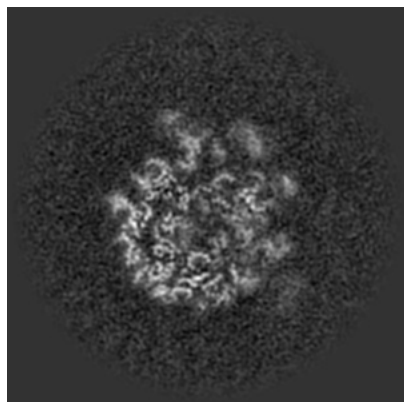
Z Index: 150

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

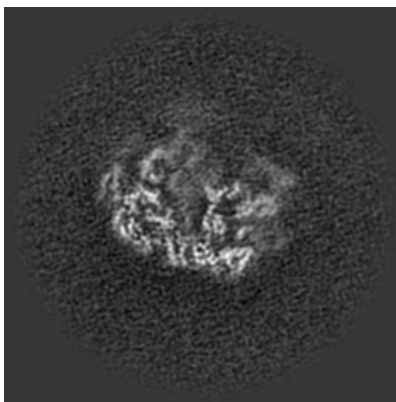


## 6.3 Largest variance slices [i](#)

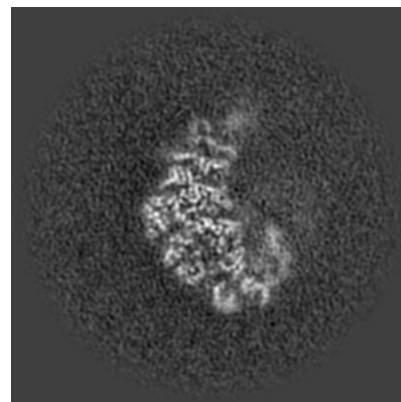
### 6.3.1 Primary map



X Index: 153

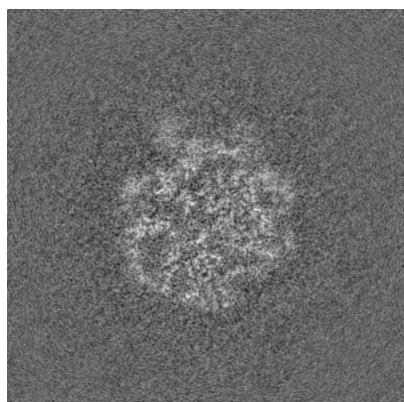


Y Index: 139

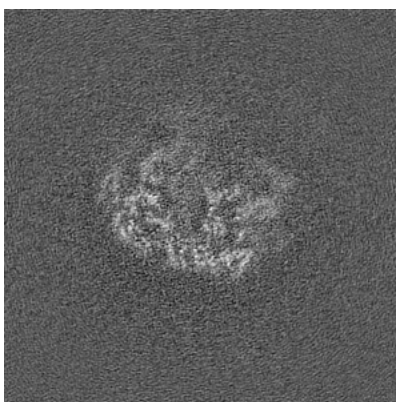


Z Index: 154

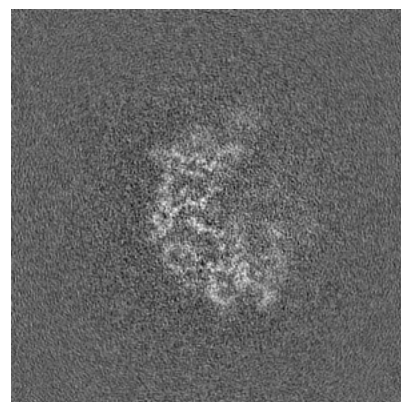
### 6.3.2 Raw map



X Index: 145



Y Index: 139

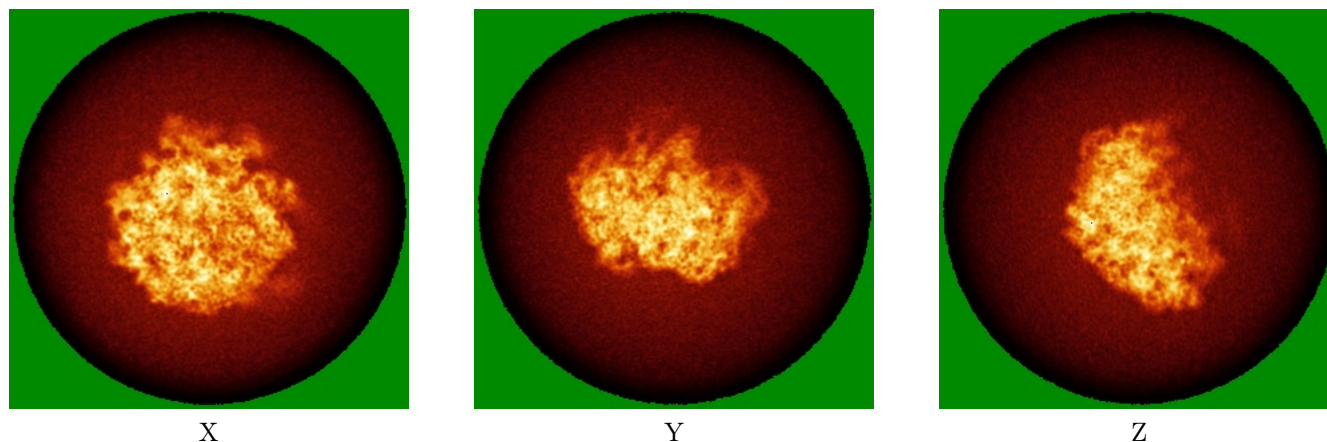


Z Index: 150

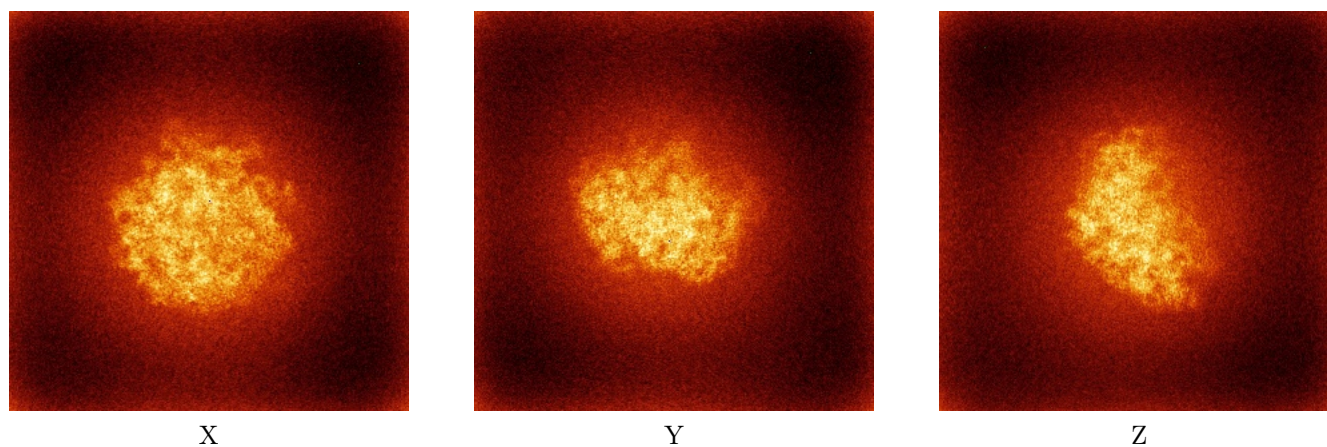
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



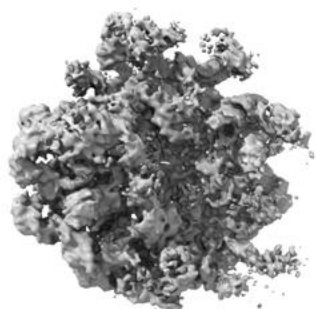
### 6.4.2 Raw map



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



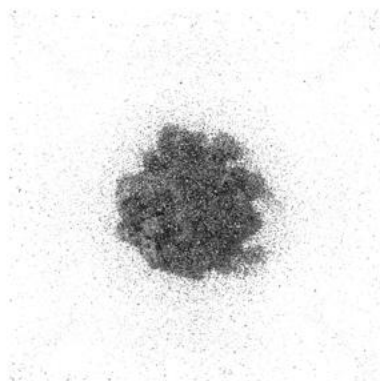
Y



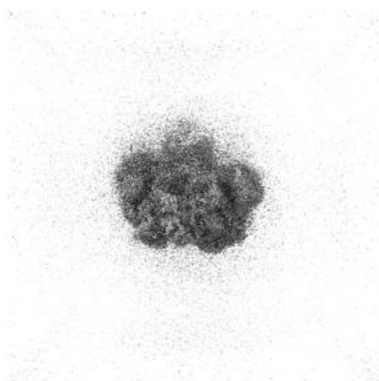
Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

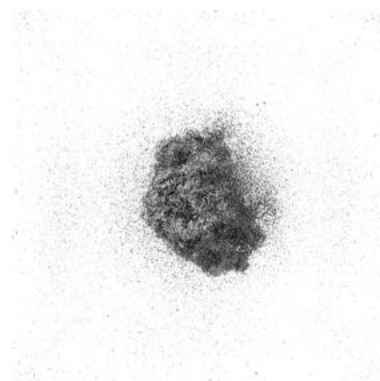
### 6.5.2 Raw map



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.

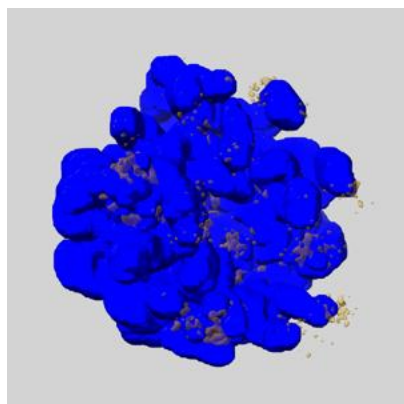
## 6.6 Mask visualisation [i](#)

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

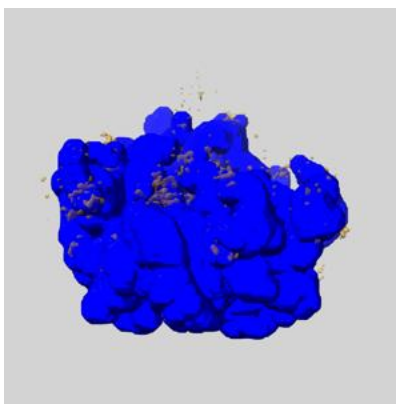
A mask typically either:

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

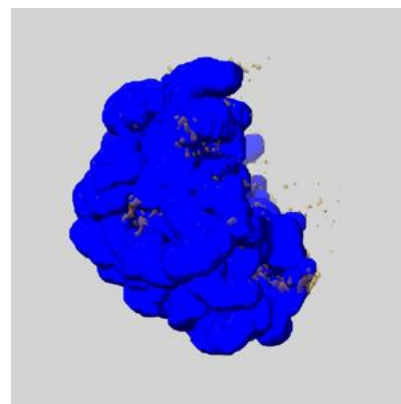
### 6.6.1 emd\_16498\_msk\_1.map [i](#)



X



Y

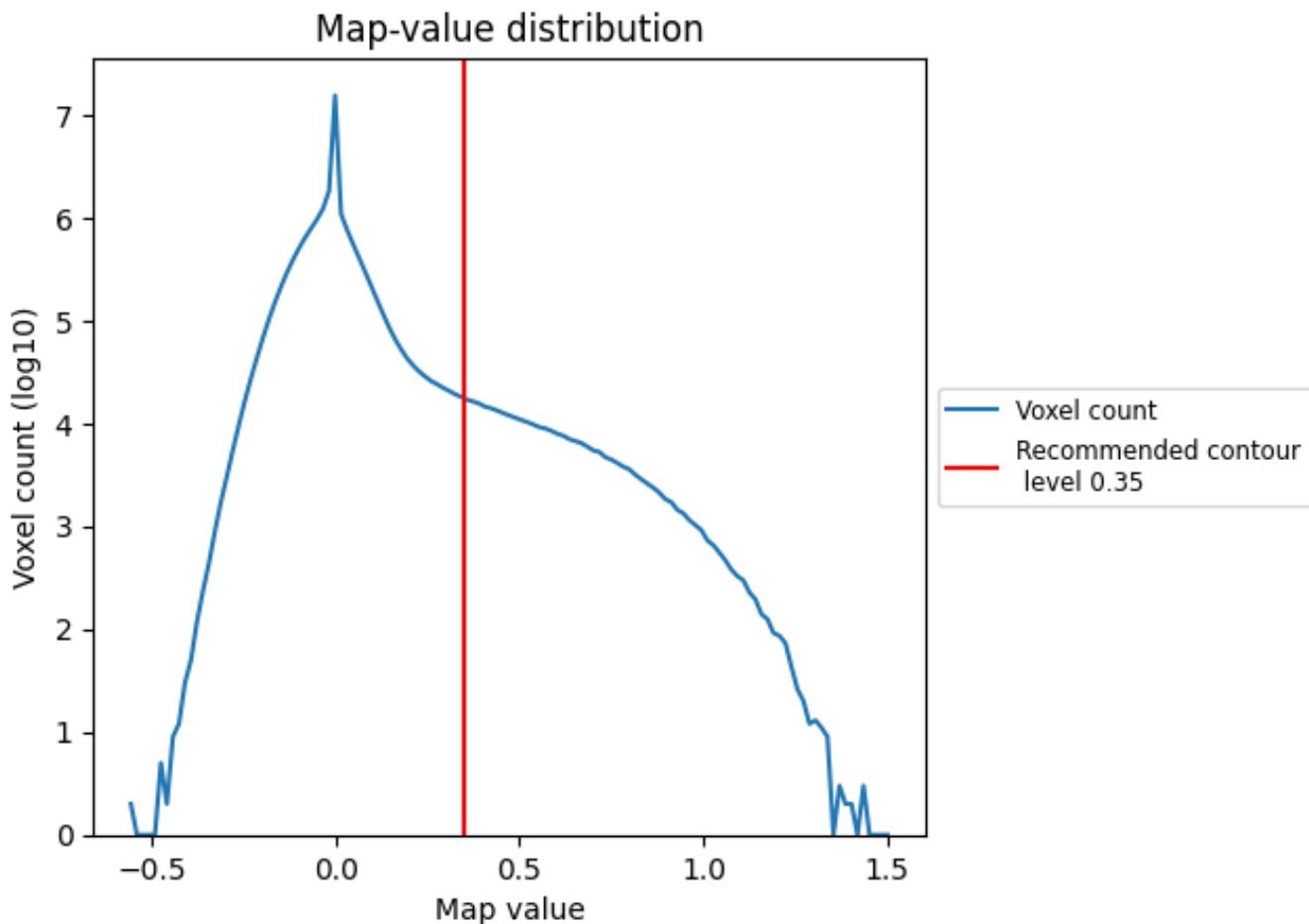


Z

## 7 Map analysis [i](#)

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

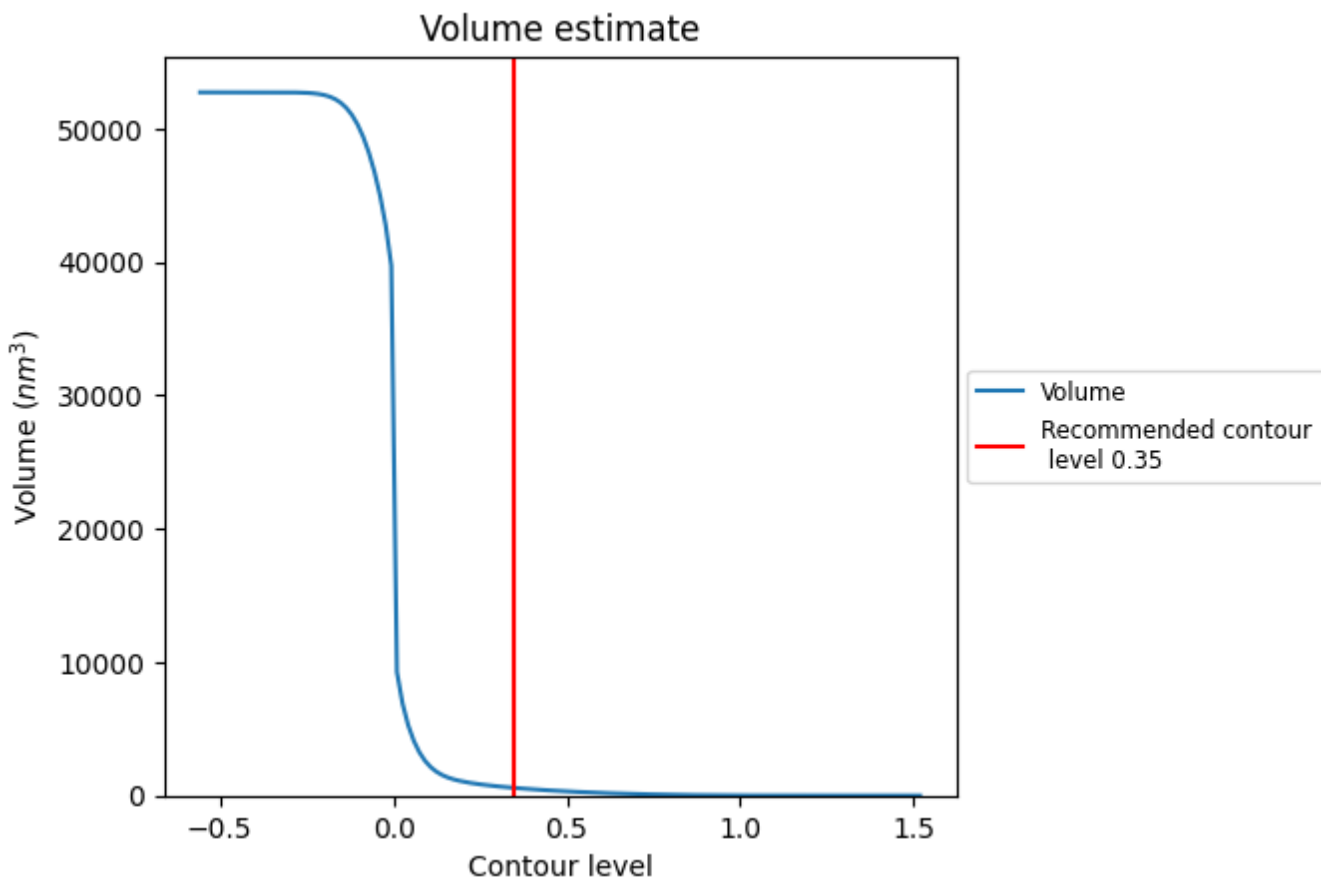
### 7.1 Map-value distribution [i](#)



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.



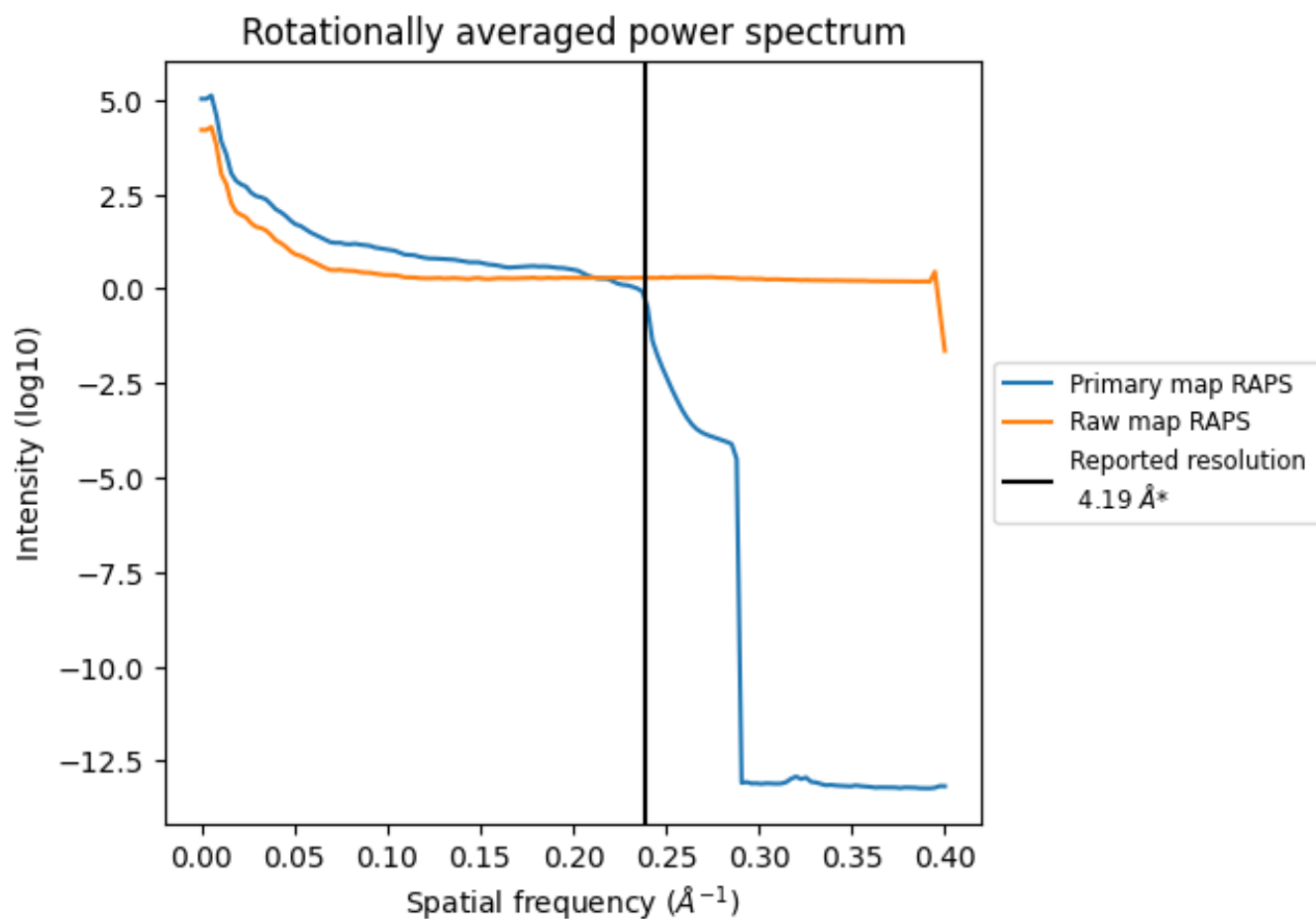
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 571 nm<sup>3</sup>; this corresponds to an approximate mass of 516 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](#)

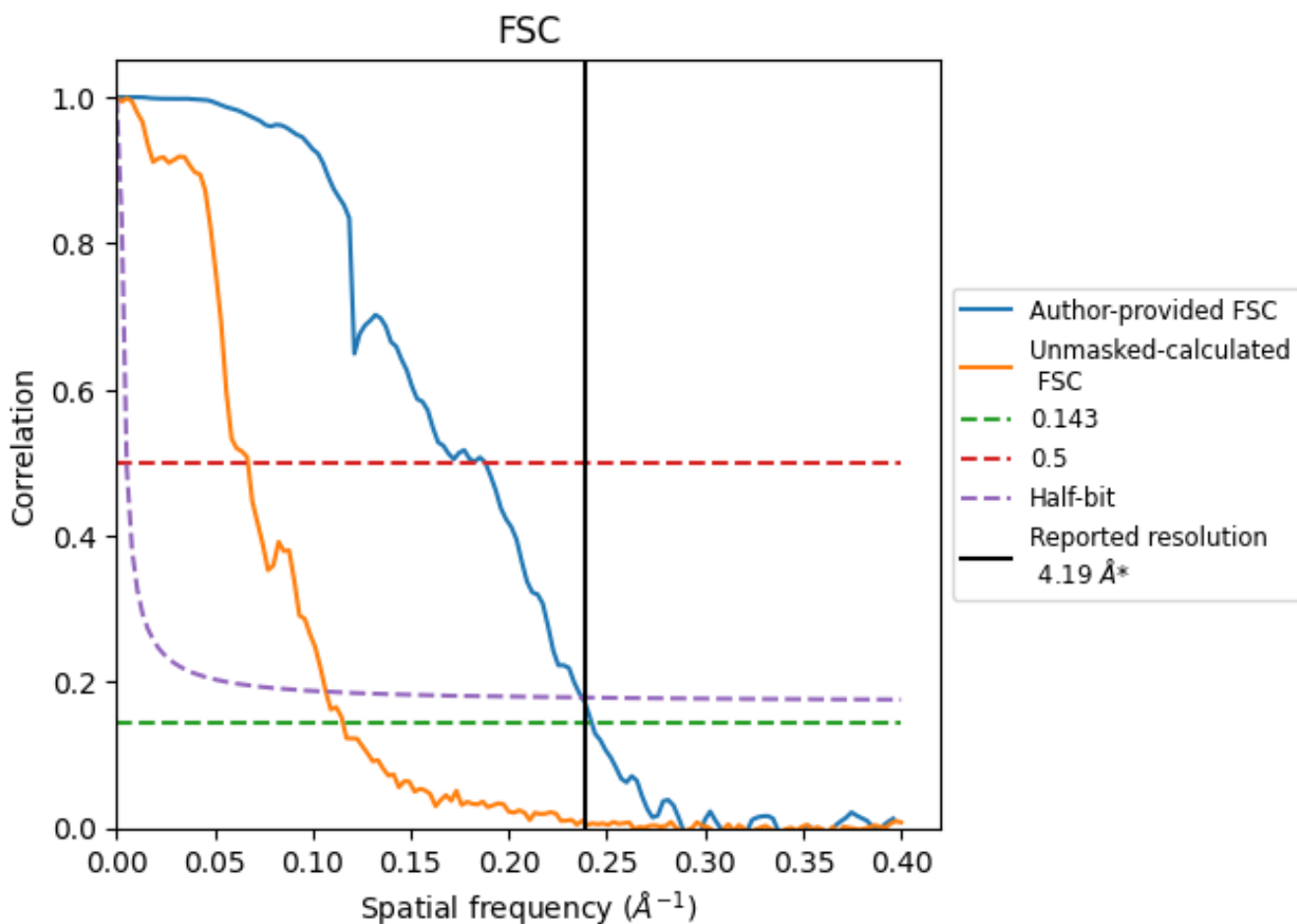


\*Reported resolution corresponds to spatial frequency of 0.239 Å<sup>-1</sup>

## 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 0.239 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

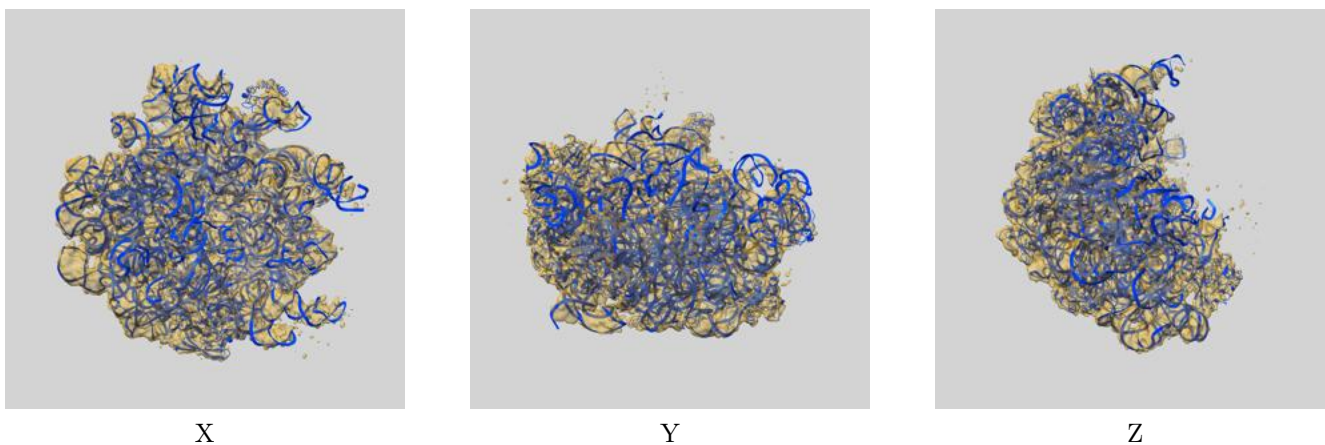
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.19	-	-
Author-provided FSC curve	4.13	5.32	4.21
Unmasked-calculated*	8.66	14.93	9.37

\*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 8.66 differs from the reported value 4.19 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16498 and PDB model 8C91. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



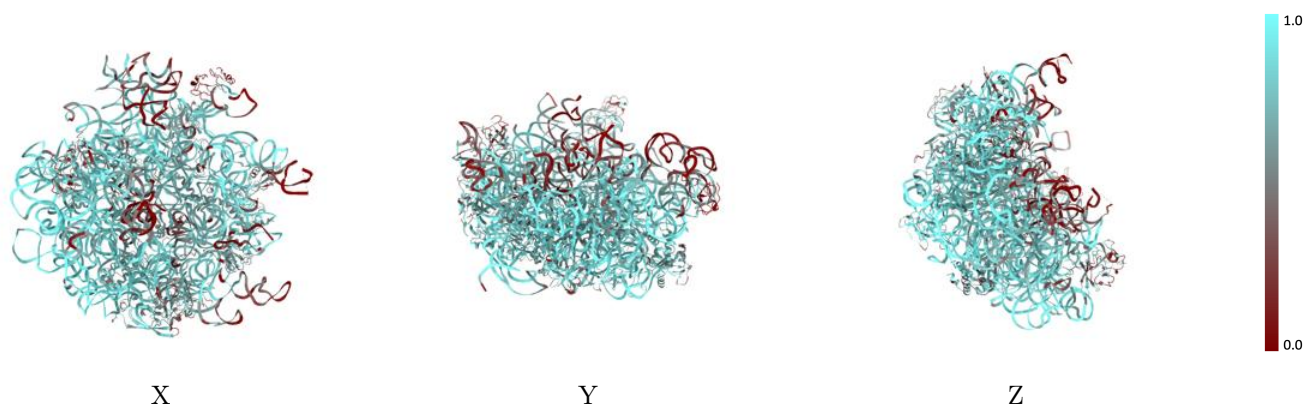
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



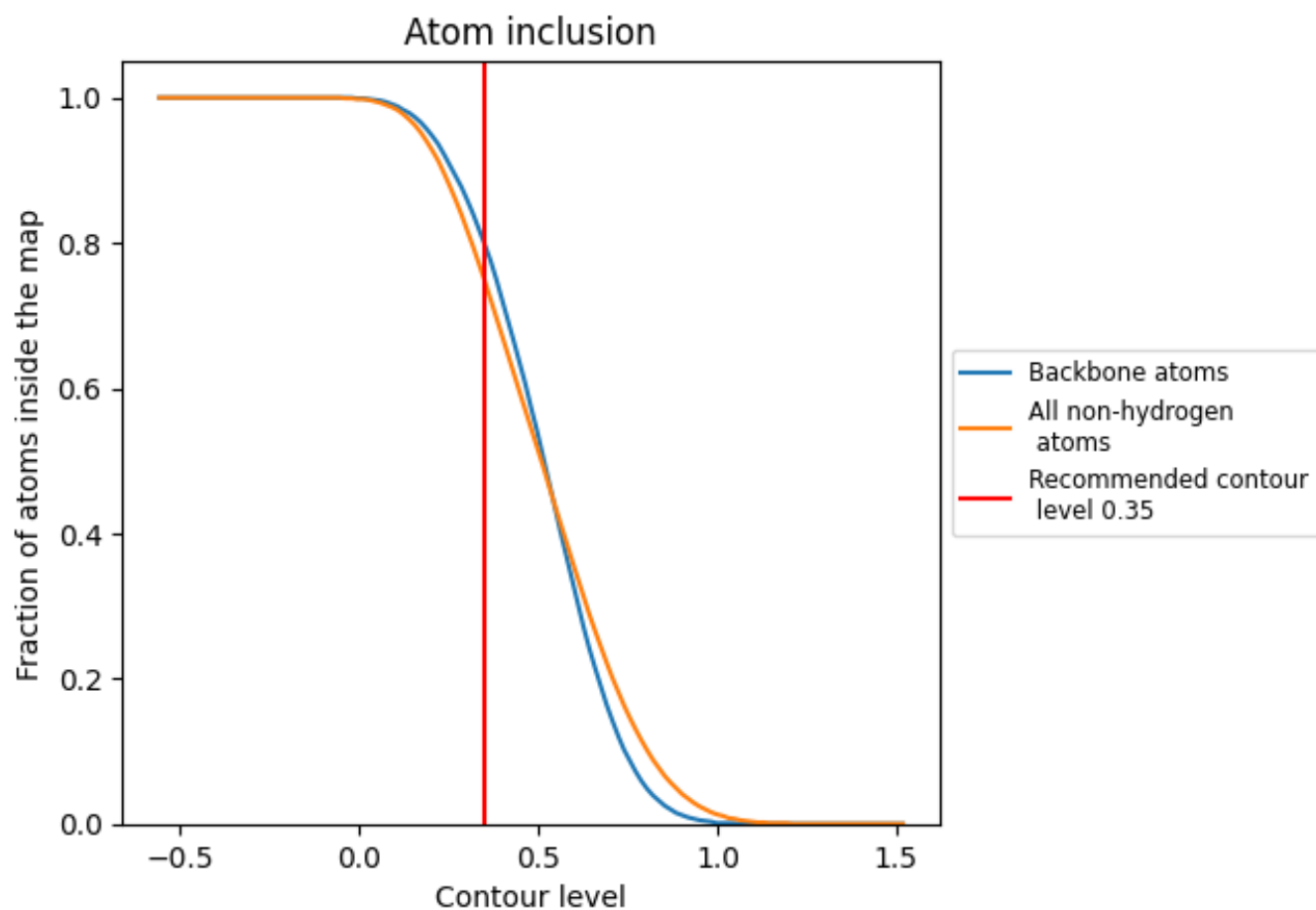
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7490	 0.2760
0	 0.5750	 0.3060
2	 0.6640	 0.3390
A	 0.7870	 0.2700
C	 0.4900	 0.2290
D	 0.6560	 0.3330
E	 0.6870	 0.3090
J	 0.6720	 0.2980
K	 0.4670	 0.2460
L	 0.2760	 0.1400
N	 0.7530	 0.3350
P	 0.6820	 0.3010
Q	 0.7400	 0.3100
R	 0.6550	 0.3110
S	 0.6670	 0.3370
T	 0.6960	 0.3470
U	 0.7760	 0.3180
Y	 0.6720	 0.2530
Z	 0.5060	 0.2620

