Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 04:17 pm GMT

PDB ID	:	7AQC
EMDB ID	:	EMD-11862
Title	:	Structure of the bacterial RQC complex (Decoding State)
Authors	:	Filbeck, S.; Pfeffer, S.
Deposited on	:	2020-10-21
Resolution	:	2.99 Å(reported)
Based on initial models	:	1DM9, 5H3X, 5H3W, 3J9W

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

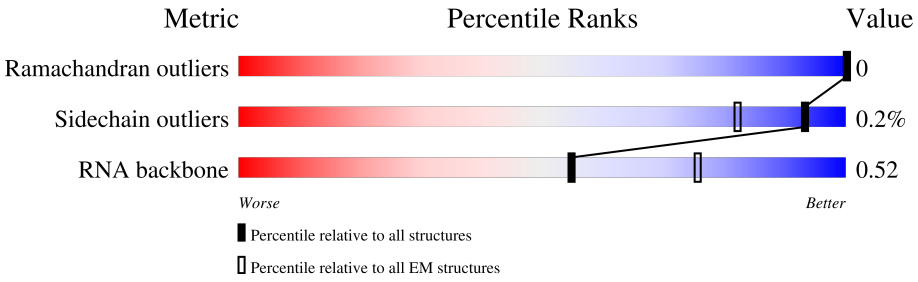
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.99 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2820	75% 23%
2	B	112	67% 31%
3	C	277	99%
4	D	209	99%
5	E	207	99%
6	F	179	61% 98%
7	G	179	15% 97%
8	I	141	52% 94% 6%

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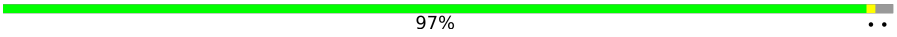
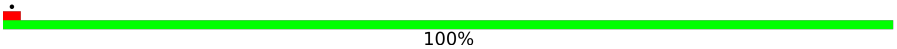
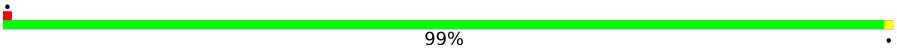
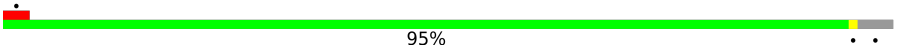
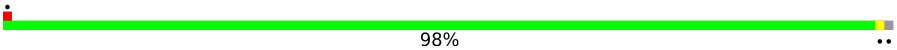
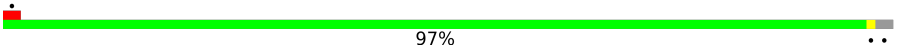
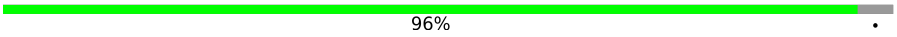
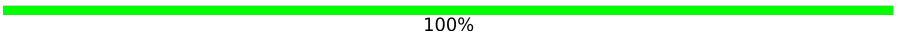
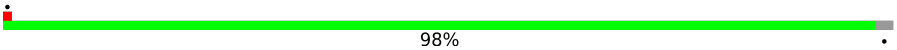
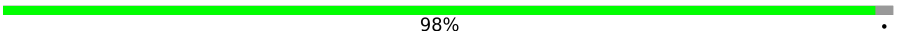
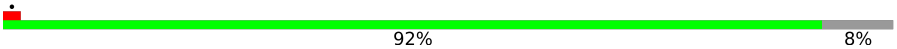
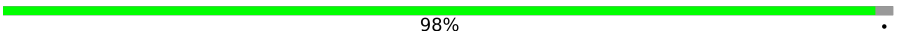
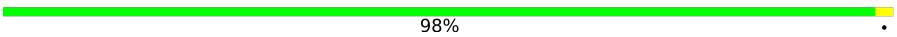
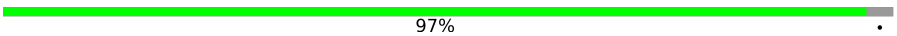
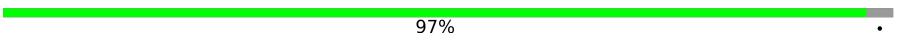
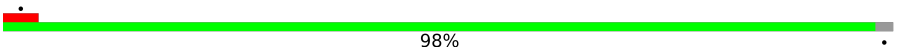
Mol	Chain	Length	Quality of chain
9	J	145	
10	K	122	
11	L	146	
12	M	144	
13	N	120	
14	O	120	
15	P	76	
15	T	76	
16	Q	119	
17	R	570	
18	S	113	
19	U	103	
20	V	94	
21	W	7	
22	X	62	
23	Y	86	
24	Z	59	
25	a	115	
26	b	59	
27	c	49	
28	d	44	
29	e	66	
30	f	37	
31	g	102	
32	h	95	

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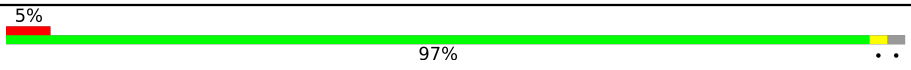
Mol	Chain	Length	Quality of chain
33	i	66	

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 95378 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2820	60561	27019	11193	19529	2820	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	112	2395	1068	435	780	112	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	275	2111	1312	416	377	6	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	207	1575	988	290	292	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	205	1561	980	289	290	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	178	1404	893	245	259	7	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	133	Total	C	N	O	S	0	0
			981	617	173	185	6		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	146	Total	C	N	O	S	0	0
			1081	671	207	201	2		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	138	Total	C	N	O	S	0	0
			1097	703	208	181	5		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	120	Total	C	N	O	S	0	0
			912	564	176	171	1		

- Molecule 15 is a RNA chain called Ala-tRNA (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	69	Total	C	N	O	P	0	0
			1477	657	268	483	69		
15	T	76	Total	C	N	O	P	0	0
			1622	722	290	534	76		

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 17 is a protein called Rqc2 homolog RqcH.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	558	Total	C	N	O	S	0	0
			4498	2855	782	850	11		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	100	Total	C	N	O	S	0	0
			754	473	141	137	3		

- Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	V	82	Total	C	N	O	0	0
			630	390	123	117		

- Molecule 21 is a protein called nascent polyalanine.

Mol	Chain	Residues	Atoms	AltConf	Trace
21	W	7	Total C N O 35 21 7 7	0	0

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms	AltConf	Trace
22	X	58	Total C N O S 444 275 92 75 2	0	0

- Molecule 23 is a protein called Uncharacterized protein YabO.

Mol	Chain	Residues	Atoms	AltConf	Trace
23	Y	84	Total C N O S 667 416 122 127 2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms	AltConf	Trace
24	Z	58	Total C N O S 455 281 89 84 1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms	AltConf	Trace
25	a	114	Total C N O 936 595 184 157	0	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms	AltConf	Trace
26	b	54	Total C N O S 426 262 86 71 7	0	0

- Molecule 27 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms	AltConf	Trace
27	c	48	Total C N O S 401 244 80 73 4	0	0

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	36	Total	C	N	O	S	0	0
			288	181	59	44	4		

- Molecule 31 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	g	101	Total	C	N	O	0	0
			786	501	139	146		

- Molecule 32 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	93	Total	C	N	O	S	0	0
			752	472	137	139	4		

- Molecule 33 is a protein called 50S ribosomal protein L29.

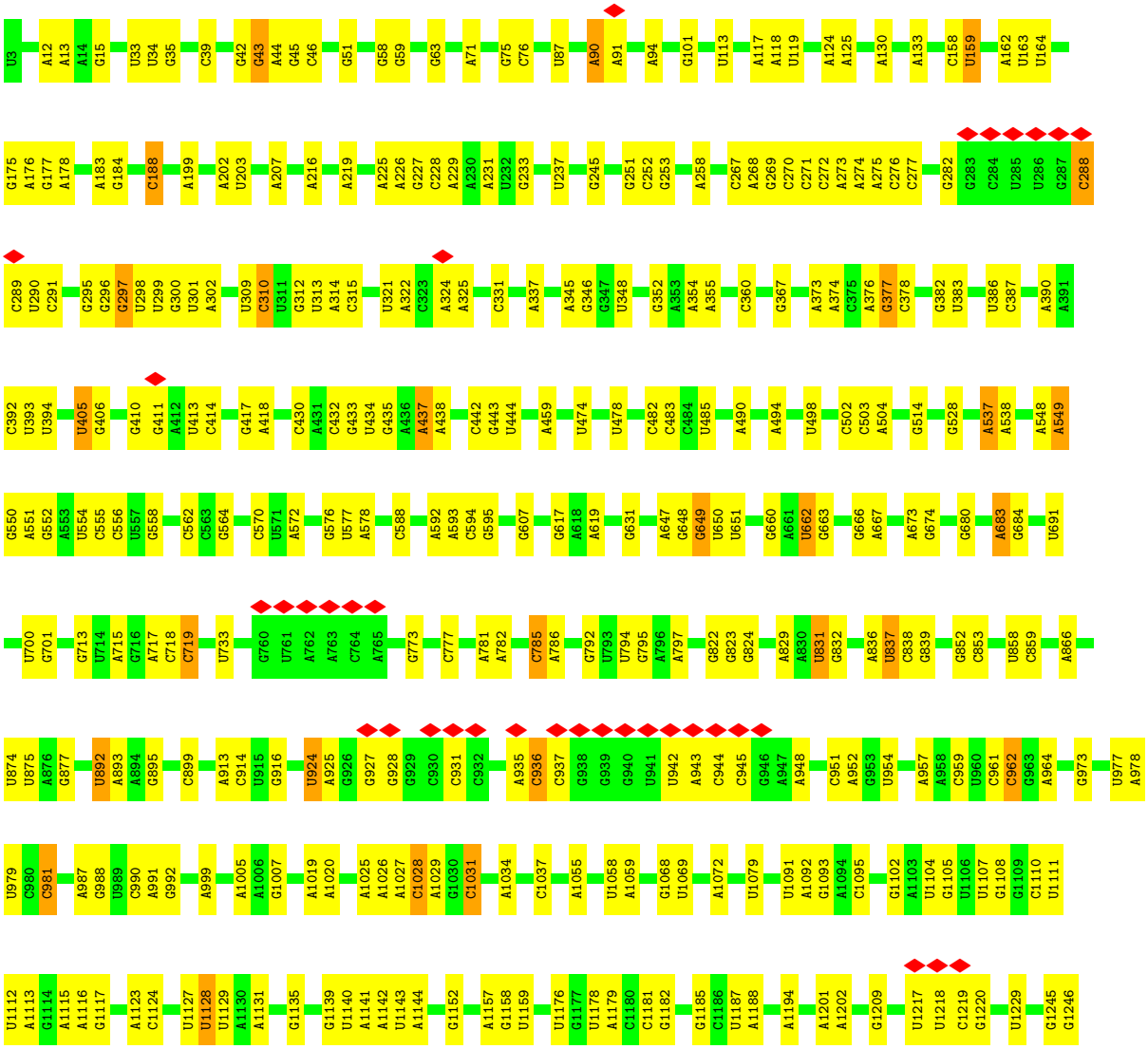
Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

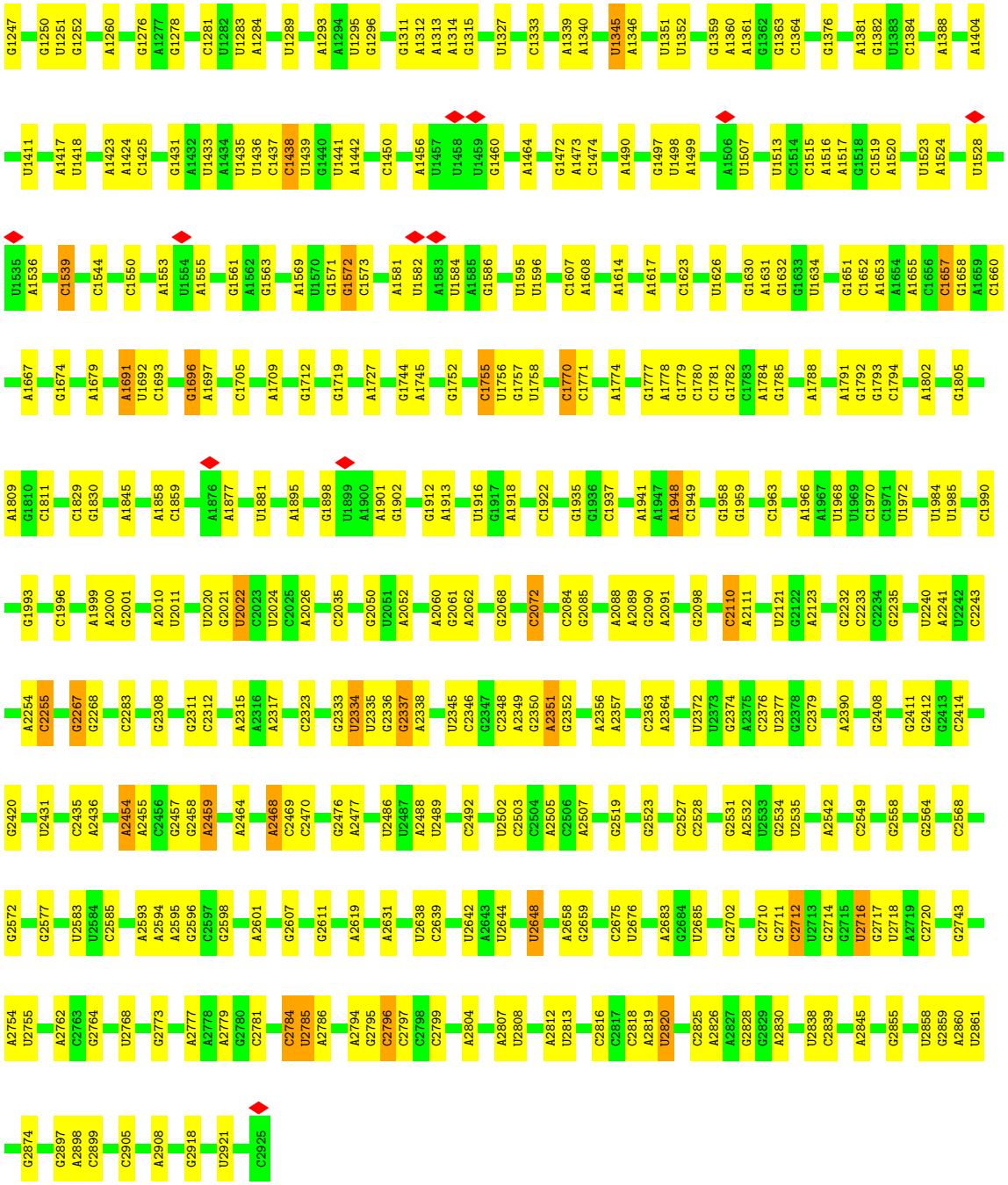
3 Residue-property plots (i)

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 ribosomal RNA

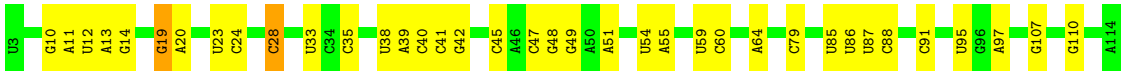
Chain A:





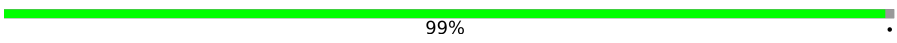
• Molecule 2: 5S ribosomal RNA

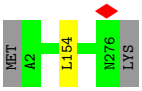
Chain B:



• Molecule 3: 50S ribosomal protein L2

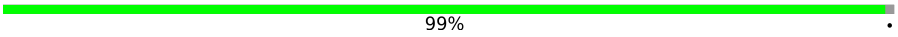
Chain C:

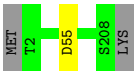




• Molecule 4: 50S ribosomal protein L3

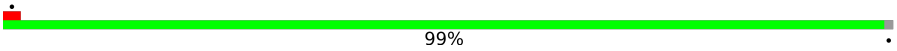
Chain D:

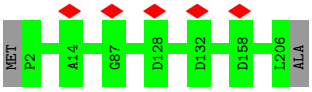




• Molecule 5: 50S ribosomal protein L4

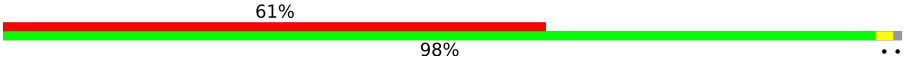
Chain E:





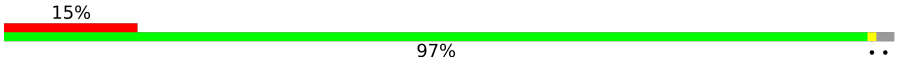
• Molecule 6: 50S ribosomal protein L5

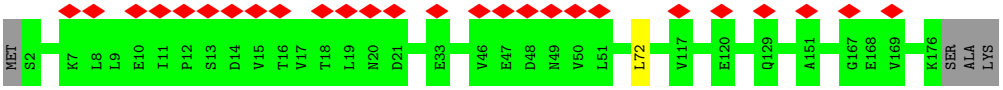
Chain F:



• Molecule 7: 50S ribosomal protein L6

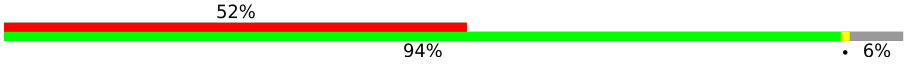
Chain G:

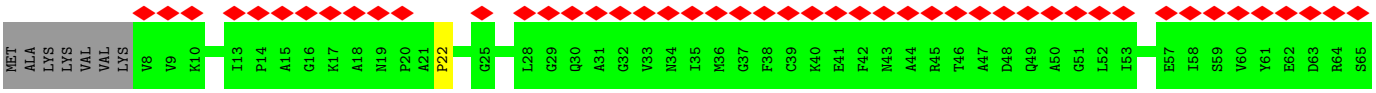


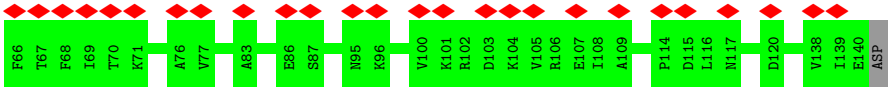


• Molecule 8: 50S ribosomal protein L11

Chain I:

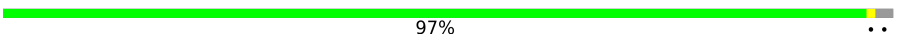


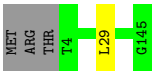




• Molecule 9: 50S ribosomal protein L13

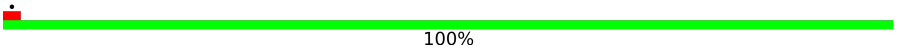
Chain J:

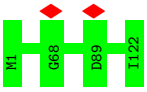




• Molecule 10: 50S ribosomal protein L14

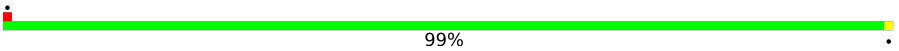
Chain K:

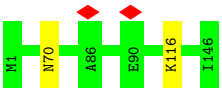




• Molecule 11: 50S ribosomal protein L15

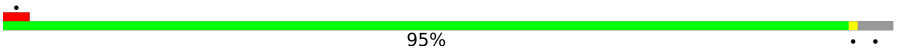
Chain L:

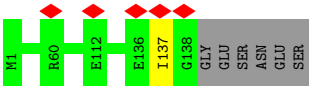




• Molecule 12: 50S ribosomal protein L16

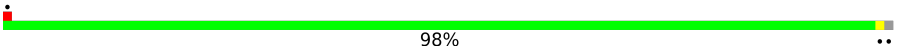
Chain M:

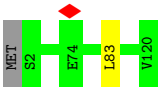




• Molecule 13: 50S ribosomal protein L17

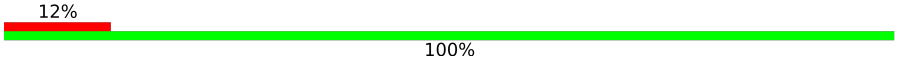
Chain N:

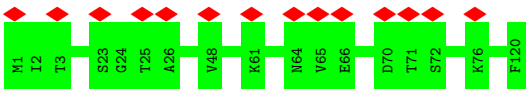




• Molecule 14: 50S ribosomal protein L18

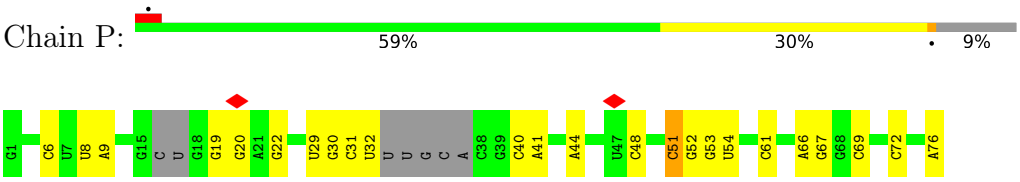
Chain O:





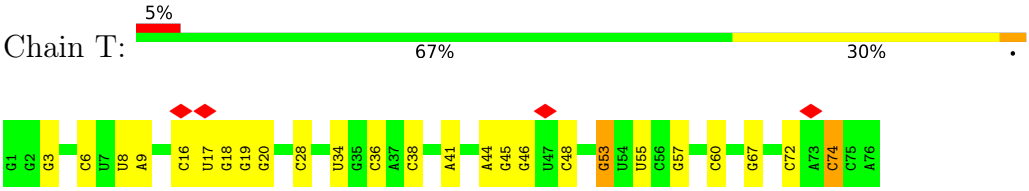
• Molecule 15: Ala-tRNA (P-site)

Chain P:



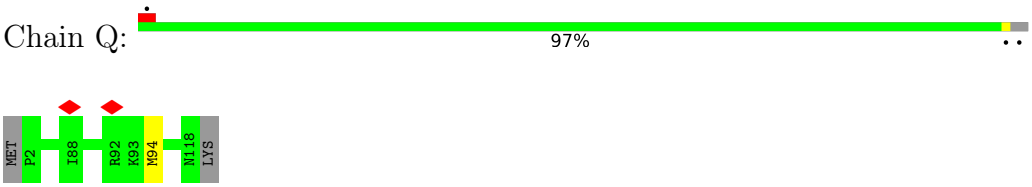
• Molecule 15: Ala-tRNA (P-site)

Chain T:



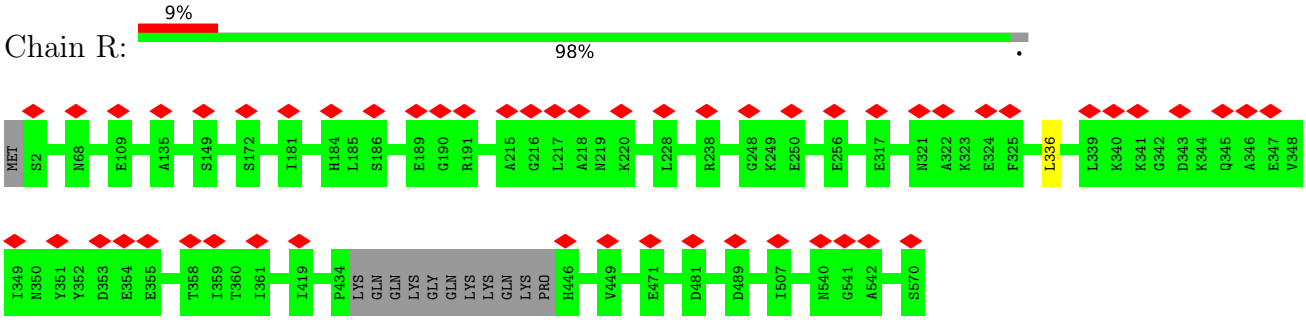
• Molecule 16: 50S ribosomal protein L20

Chain Q:



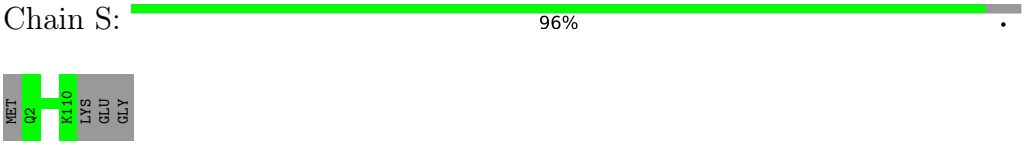
• Molecule 17: Rqc2 homolog RqcH

Chain R:



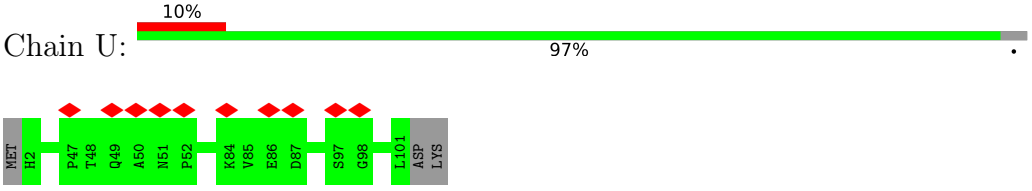
• Molecule 18: 50S ribosomal protein L22

Chain S:



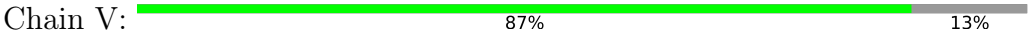
• Molecule 19: 50S ribosomal protein L24

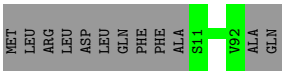
Chain U:



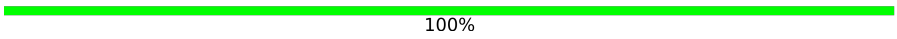
• Molecule 20: 50S ribosomal protein L27

Chain V:



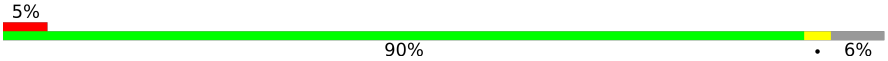


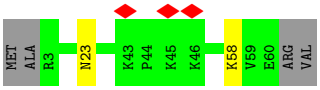
• Molecule 21: nascent polyalanine

Chain W: 

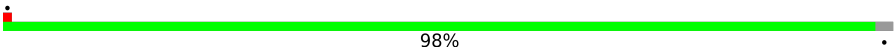
There are no outlier residues recorded for this chain.

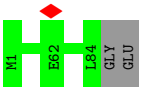
• Molecule 22: 50S ribosomal protein L28

Chain X: 

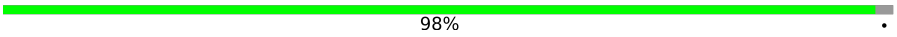


• Molecule 23: Uncharacterized protein YabO

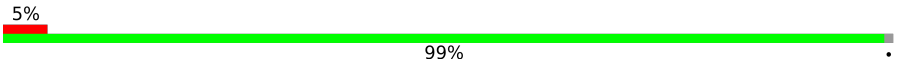
Chain Y: 

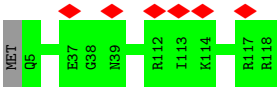


• Molecule 24: 50S ribosomal protein L30

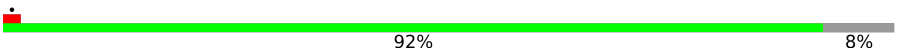
Chain Z: 

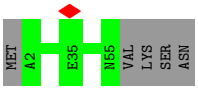
• Molecule 25: 50S ribosomal protein L19

Chain a: 

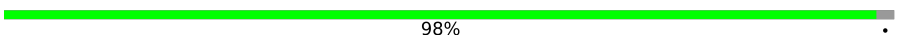


• Molecule 26: 50S ribosomal protein L32

Chain b: 

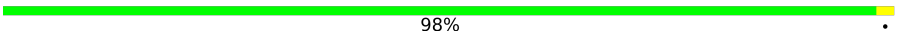


• Molecule 27: 50S ribosomal protein L33 1

Chain c: 

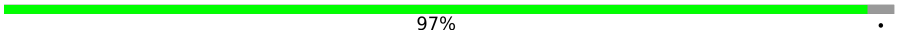
• Molecule 28: 50S ribosomal protein L34

Chain d:



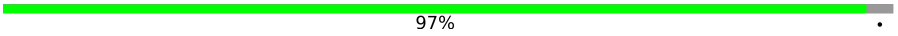
• Molecule 29: 50S ribosomal protein L35

Chain e:



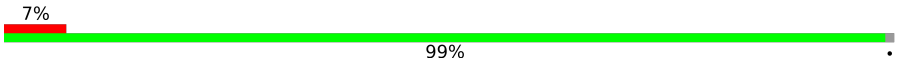
• Molecule 30: 50S ribosomal protein L36

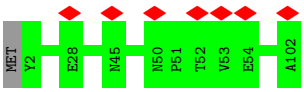
Chain f:



• Molecule 31: 50S ribosomal protein L21

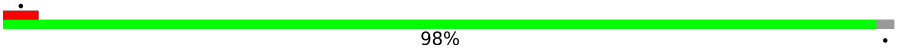
Chain g:

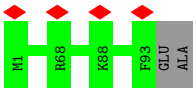




• Molecule 32: 50S ribosomal protein L23

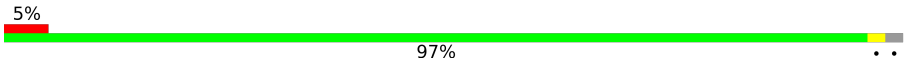
Chain h:

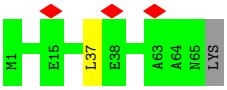




• Molecule 33: 50S ribosomal protein L29

Chain i:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	138382	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.300	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	410.88, 410.88, 410.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.30	1/67837 (0.0%)	1.00	159/105829 (0.2%)
2	B	0.31	0/2678	1.10	17/4174 (0.4%)
3	C	0.26	0/2148	0.54	0/2881
4	D	0.28	0/1597	0.55	1/2140 (0.0%)
5	E	0.28	0/1580	0.56	0/2132
6	F	0.29	0/1423	0.65	1/1910 (0.1%)
7	G	0.28	0/1360	0.56	1/1832 (0.1%)
8	I	0.29	0/995	0.59	0/1346
9	J	0.30	0/1146	0.60	1/1542 (0.1%)
10	K	0.28	0/927	0.58	0/1245
11	L	0.28	0/1093	0.52	0/1457
12	M	0.29	0/1120	0.54	1/1496 (0.1%)
13	N	0.26	0/960	0.51	1/1284 (0.1%)
14	O	0.27	0/921	0.58	0/1236
15	P	0.32	0/1648	1.06	5/2564 (0.2%)
15	T	0.31	0/1811	1.12	12/2822 (0.4%)
16	Q	0.28	0/952	0.54	1/1266 (0.1%)
17	R	0.44	0/4590	0.58	1/6195 (0.0%)
18	S	0.26	0/851	0.57	0/1146
19	U	0.27	0/764	0.53	0/1022
20	V	0.30	0/638	0.58	0/847
21	W	0.25	0/34	0.53	0/46
22	X	0.27	0/448	0.68	1/596 (0.2%)
23	Y	0.24	0/670	0.47	0/893
24	Z	0.28	0/457	0.54	0/613
25	a	0.25	0/949	0.51	0/1269
26	b	0.29	0/433	0.61	0/574
27	c	0.27	0/406	0.52	0/540
28	d	0.24	0/370	0.45	0/483
29	e	0.28	0/519	0.55	0/680
30	f	0.24	0/291	0.44	0/383
31	g	0.30	0/797	0.66	0/1070
32	h	0.26	0/759	0.50	0/1011
33	i	0.28	0/531	0.65	1/707 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.31	1/103703 (0.0%)	0.92	203/155231 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
8	I	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2010	A	N9-C4	5.24	1.41	1.37

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1657	C	C5-C6-N1	9.09	125.55	121.00
15	T	74	C	N1-C2-O2	8.91	124.25	118.90
1	A	2712	C	N1-C2-O2	8.78	124.17	118.90
15	T	74	C	C2-N1-C1'	8.53	128.19	118.80
1	A	2489	U	N3-C2-O2	-8.38	116.33	122.20
2	B	28	C	N1-C2-O2	7.78	123.56	118.90
1	A	2712	C	C2-N1-C1'	7.59	127.15	118.80
6	F	83	MET	CA-CB-CG	7.55	126.13	113.30
1	A	1345	U	O4'-C1'-N1	7.35	114.08	108.20
1	A	2489	U	N1-C2-O2	7.30	127.91	122.80
1	A	1544	C	N1-C2-O2	7.24	123.25	118.90
1	A	2376	C	O4'-C1'-N1	7.21	113.97	108.20
1	A	2785	U	P-O3'-C3'	7.13	128.25	119.70
17	R	336	LEU	CA-CB-CG	7.12	131.67	115.30
1	A	1963	C	C2-N1-C1'	7.07	126.57	118.80
1	A	237	U	N1-C2-O2	7.03	127.72	122.80
1	A	1696	G	O4'-C1'-N9	7.03	113.82	108.20
1	A	2010	A	C2-N3-C4	7.02	114.11	110.60
1	A	1550	C	N1-C2-O2	7.00	123.10	118.90
1	A	2489	U	C2-N1-C1'	6.97	126.07	117.70
15	T	74	C	N3-C2-O2	-6.96	117.03	121.90
1	A	2255	C	N1-C2-O2	6.90	123.04	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	43	G	C2'-C3'-O3'	6.84	124.64	113.70
1	A	377	G	P-O3'-C3'	6.78	127.84	119.70
1	A	2459	A	C2-N3-C4	6.76	113.98	110.60
1	A	936	C	P-O3'-C3'	6.76	127.81	119.70
1	A	2712	C	N3-C2-O2	-6.74	117.18	121.90
1	A	2568	C	C2-N1-C1'	6.72	126.19	118.80
1	A	1229	U	N1-C2-O2	6.70	127.49	122.80
1	A	1657	C	C6-N1-C2	-6.70	117.62	120.30
15	T	6	C	C2-N1-C1'	6.70	126.17	118.80
1	A	683	A	P-O3'-C3'	6.67	127.71	119.70
1	A	1028	C	N1-C2-O2	6.67	122.91	118.90
1	A	188	C	C5-C6-N1	6.66	124.33	121.00
1	A	1985	U	N1-C2-O2	6.65	127.45	122.80
1	A	1970	C	N1-C2-O2	6.57	122.84	118.90
1	A	237	U	N3-C2-O2	-6.55	117.61	122.20
1	A	113	U	C2-N1-C1'	6.55	125.56	117.70
2	B	28	C	C2-N1-C1'	6.45	125.90	118.80
1	A	2503	C	C2-N1-C1'	6.44	125.89	118.80
1	A	1771	C	C2-N1-C1'	6.44	125.88	118.80
15	P	72	C	N1-C2-O2	6.40	122.74	118.90
13	N	83	LEU	CA-CB-CG	6.38	129.98	115.30
1	A	1922	C	N1-C2-O2	6.36	122.71	118.90
1	A	1922	C	N3-C2-O2	-6.31	117.48	121.90
1	A	1985	U	N3-C2-O2	-6.27	117.81	122.20
2	B	28	C	N3-C2-O2	-6.26	117.52	121.90
15	P	69	C	C2-N1-C1'	6.25	125.68	118.80
1	A	1411	U	N3-C2-O2	-6.24	117.83	122.20
1	A	1069	U	N1-C2-O2	6.24	127.17	122.80
1	A	2712	C	C6-N1-C2	-6.19	117.83	120.30
1	A	719	C	C2-N1-C1'	6.18	125.60	118.80
1	A	1970	C	C2-N1-C1'	6.17	125.59	118.80
2	B	79	C	N1-C2-O2	6.17	122.60	118.90
1	A	2468	A	P-O3'-C3'	6.14	127.06	119.70
1	A	1572	G	O4'-C1'-N9	6.11	113.09	108.20
1	A	649	G	C2'-C3'-O3'	6.10	123.46	113.70
15	P	51	C	P-O3'-C3'	6.10	127.02	119.70
2	B	35	C	N1-C2-O2	6.07	122.54	118.90
1	A	2072	C	C2-N1-C1'	6.06	125.47	118.80
1	A	981	C	C2-N1-C1'	6.04	125.44	118.80
1	A	2838	U	N3-C2-O2	-6.02	117.98	122.20
1	A	437	A	P-O3'-C3'	6.02	126.92	119.70
1	A	2585	C	N1-C2-O2	6.00	122.50	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	24	C	N1-C2-O2	5.99	122.50	118.90
1	A	188	C	C6-N1-C2	-5.98	117.91	120.30
1	A	588	C	C2-N1-C1'	5.97	125.37	118.80
1	A	1859	C	C5-C6-N1	5.95	123.97	121.00
1	A	90	A	P-O3'-C3'	5.95	126.83	119.70
15	T	74	C	C6-N1-C1'	-5.93	113.68	120.80
1	A	2648	U	N3-C2-O2	-5.92	118.06	122.20
1	A	1963	C	C6-N1-C2	-5.91	117.94	120.30
1	A	2839	C	N1-C2-O2	5.90	122.44	118.90
2	B	91	C	C2-N1-C1'	5.89	125.28	118.80
2	B	28	C	C6-N1-C2	-5.88	117.95	120.30
1	A	1028	C	C2-N1-C1'	5.88	125.27	118.80
1	A	1859	C	C6-N1-C2	-5.87	117.95	120.30
1	A	1544	C	N3-C2-O2	-5.86	117.80	121.90
1	A	537	A	P-O3'-C3'	5.85	126.72	119.70
1	A	2454	A	P-O3'-C3'	5.85	126.72	119.70
1	A	288	C	N3-C2-O2	-5.83	117.82	121.90
33	i	37	LEU	CA-CB-CG	5.83	128.71	115.30
2	B	45	C	N1-C2-O2	5.83	122.40	118.90
1	A	2796	C	P-O3'-C3'	5.83	126.69	119.70
1	A	962	C	C2-N1-C1'	5.82	125.20	118.80
1	A	2022	U	N3-C2-O2	-5.81	118.13	122.20
1	A	1755	C	P-O3'-C3'	5.77	126.62	119.70
1	A	310	C	C2-N1-C1'	5.76	125.14	118.80
1	A	945	C	N1-C2-O2	5.76	122.36	118.90
1	A	2568	C	C6-N1-C2	-5.74	118.00	120.30
1	A	1794	C	C2-N1-C1'	5.73	125.11	118.80
1	A	1550	C	C2-N1-C1'	5.73	125.10	118.80
1	A	979	U	N1-C2-O2	5.72	126.81	122.80
1	A	413	U	N3-C2-O2	-5.70	118.21	122.20
1	A	1916	U	N1-C2-O2	5.70	126.79	122.80
1	A	1069	U	N3-C2-O2	-5.69	118.22	122.20
1	A	924	U	N1-C2-O2	5.68	126.78	122.80
15	P	6	C	C2-N1-C1'	5.67	125.03	118.80
1	A	549	A	P-O3'-C3'	5.67	126.50	119.70
1	A	1437	C	C2-N1-C1'	5.67	125.03	118.80
1	A	413	U	N1-C2-O2	5.65	126.76	122.80
1	A	2072	C	C6-N1-C2	-5.65	118.04	120.30
2	B	19	G	C4-N9-C1'	5.64	133.84	126.50
1	A	1069	U	C2-N1-C1'	5.64	124.47	117.70
1	A	2351	A	P-O3'-C3'	5.64	126.47	119.70
1	A	2503	C	N1-C2-O2	5.64	122.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1691	A	C2-N3-C4	5.63	113.42	110.60
1	A	2781	C	N1-C2-O2	5.63	122.28	118.90
1	A	1229	U	N3-C2-O2	-5.61	118.27	122.20
1	A	2255	C	N3-C2-O2	-5.61	117.97	121.90
15	T	74	C	C6-N1-C2	-5.61	118.06	120.30
1	A	899	C	N3-C2-O2	-5.58	117.99	121.90
1	A	1031	C	C2-N1-C1'	5.58	124.94	118.80
1	A	892	U	C2-N1-C1'	5.57	124.39	117.70
15	T	53	G	C4-N9-C1'	5.57	133.74	126.50
1	A	2685	U	N1-C2-O2	5.57	126.69	122.80
1	A	2712	C	C5-C6-N1	5.56	123.78	121.00
1	A	1438	C	P-O3'-C3'	5.55	126.36	119.70
16	Q	94	MET	CA-CB-CG	5.54	122.73	113.30
1	A	309	U	C2-N1-C1'	5.53	124.33	117.70
1	A	2784	C	P-O3'-C3'	5.51	126.32	119.70
1	A	899	C	N1-C2-O2	5.51	122.21	118.90
15	T	28	C	C2-N1-C1'	5.50	124.85	118.80
1	A	1411	U	C2-N1-C1'	5.49	124.29	117.70
1	A	288	C	N1-C2-O2	5.49	122.19	118.90
1	A	2283	C	N1-C2-O2	5.45	122.17	118.90
1	A	297	G	C4'-C3'-O3'	5.45	123.90	113.00
1	A	1411	U	N1-C2-O2	5.45	126.61	122.80
1	A	2010	A	N3-C4-C5	-5.45	122.99	126.80
1	A	1916	U	N3-C2-O2	-5.44	118.39	122.20
1	A	1963	C	N1-C2-O2	5.43	122.16	118.90
1	A	1859	C	C2-N1-C1'	5.43	124.77	118.80
1	A	2838	U	N1-C2-O2	5.43	126.60	122.80
1	A	2334	U	P-O3'-C3'	5.41	126.19	119.70
1	A	2816	C	C2-N1-C1'	5.41	124.75	118.80
7	G	72	LEU	CA-CB-CG	5.39	127.71	115.30
1	A	924	U	C2-N1-C1'	5.38	124.16	117.70
1	A	662	U	P-O3'-C3'	5.38	126.16	119.70
15	T	53	G	O4'-C1'-N9	5.34	112.47	108.20
15	T	60	C	C2-N1-C1'	5.34	124.67	118.80
12	M	137	ILE	C-N-CA	5.32	133.47	122.30
1	A	2323	C	C2-N1-C1'	5.29	124.62	118.80
1	A	1657	C	C2-N1-C1'	5.28	124.61	118.80
1	A	924	U	N3-C2-O2	-5.28	118.50	122.20
2	B	95	U	N1-C2-O2	5.28	126.49	122.80
1	A	310	C	N1-C2-O2	5.28	122.06	118.90
1	A	1916	U	C2-N1-C1'	5.27	124.03	117.70
1	A	413	U	C2-N1-C1'	5.26	124.01	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	19	G	OP1-P-O3'	5.25	116.74	105.20
2	B	35	C	N3-C2-O2	-5.24	118.23	121.90
1	A	936	C	OP1-P-O3'	5.23	116.70	105.20
1	A	2492	C	C2-N1-C1'	5.23	124.55	118.80
1	A	158	C	C2-N1-C1'	5.23	124.55	118.80
1	A	1963	C	C5-C6-N1	5.22	123.61	121.00
1	A	2010	A	N3-C4-N9	5.20	131.56	127.40
1	A	837	U	P-O3'-C3'	5.20	125.94	119.70
1	A	1544	C	C2-N1-C1'	5.19	124.51	118.80
1	A	2839	C	N3-C2-O2	-5.19	118.27	121.90
1	A	2337	G	N3-C4-C5	-5.19	126.01	128.60
15	P	72	C	N3-C2-O2	-5.18	118.28	121.90
1	A	2035	C	C2-N1-C1'	5.17	124.49	118.80
1	A	1028	C	N3-C2-O2	-5.17	118.28	121.90
1	A	1437	C	C6-N1-C2	-5.16	118.24	120.30
1	A	1539	C	N1-C2-O2	5.16	121.99	118.90
1	A	1937	C	C2-N1-C1'	5.14	124.46	118.80
1	A	831	U	N3-C2-O2	-5.14	118.60	122.20
9	J	29	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	979	U	N3-C2-O2	-5.13	118.61	122.20
15	T	6	C	C6-N1-C2	-5.13	118.25	120.30
1	A	1095	C	N1-C2-O2	5.12	121.97	118.90
1	A	159	U	N1-C2-O2	5.12	126.38	122.80
4	D	55	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	785	C	P-O3'-C3'	5.11	125.83	119.70
1	A	2685	U	N3-C2-O2	-5.11	118.62	122.20
1	A	1691	A	C4-N9-C1'	5.10	135.48	126.30
1	A	2267	G	P-O3'-C3'	5.10	125.82	119.70
1	A	1550	C	N3-C2-O2	-5.09	118.34	121.90
1	A	1970	C	N3-C2-O2	-5.09	118.34	121.90
1	A	2489	U	C6-N1-C2	-5.09	117.94	121.00
1	A	2820	U	C2-N1-C1'	5.09	123.81	117.70
1	A	2255	C	C6-N1-C2	-5.09	118.27	120.30
1	A	1937	C	N1-C2-O2	5.08	121.95	118.90
1	A	1333	C	C2-N1-C1'	5.07	124.38	118.80
1	A	383	U	N3-C2-O2	-5.07	118.65	122.20
1	A	1128	U	C5-C6-N1	5.07	125.24	122.70
2	B	35	C	C6-N1-C2	-5.07	118.27	120.30
1	A	570	C	C2-N1-C1'	5.07	124.37	118.80
1	A	1544	C	C6-N1-C2	-5.06	118.28	120.30
1	A	1770	C	C2-N1-C1'	5.05	124.36	118.80
1	A	2110	C	C2-N1-C1'	5.05	124.35	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	X	23	ASN	C-N-CA	5.05	134.32	121.70
2	B	19	G	P-O3'-C3'	5.04	125.75	119.70
1	A	1948	A	P-O3'-C3'	5.03	125.74	119.70
1	A	2372	U	N1-C2-O2	5.03	126.32	122.80
1	A	2716	U	P-O3'-C3'	5.03	125.73	119.70
1	A	1794	C	C6-N1-C2	-5.03	118.29	120.30
2	B	79	C	N3-C2-O2	-5.03	118.38	121.90
1	A	1229	U	C5-C6-N1	5.02	125.21	122.70
2	B	95	U	C2-N1-C1'	5.02	123.73	117.70
1	A	405	U	P-O3'-C3'	5.02	125.73	119.70
15	T	74	C	O4'-C1'-N1	5.02	112.22	108.20
1	A	237	U	C2-N1-C1'	5.02	123.72	117.70
1	A	2323	C	N1-C2-O2	5.01	121.91	118.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	154	LEU	Peptide
8	I	22	PRO	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
3	C	273/277 (99%)	261 (96%)	12 (4%)	0	100	100
4	D	205/209 (98%)	197 (96%)	8 (4%)	0	100	100
5	E	203/207 (98%)	189 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	176/179 (98%)	163 (93%)	13 (7%)	0	100	100
7	G	173/179 (97%)	165 (95%)	8 (5%)	0	100	100
8	I	131/141 (93%)	126 (96%)	5 (4%)	0	100	100
9	J	140/145 (97%)	133 (95%)	7 (5%)	0	100	100
10	K	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	L	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
12	M	136/144 (94%)	133 (98%)	3 (2%)	0	100	100
13	N	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
14	O	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
16	Q	115/119 (97%)	110 (96%)	5 (4%)	0	100	100
17	R	554/570 (97%)	520 (94%)	34 (6%)	0	100	100
18	S	107/113 (95%)	94 (88%)	13 (12%)	0	100	100
19	U	98/103 (95%)	87 (89%)	11 (11%)	0	100	100
20	V	80/94 (85%)	80 (100%)	0	0	100	100
21	W	5/7 (71%)	5 (100%)	0	0	100	100
22	X	56/62 (90%)	51 (91%)	5 (9%)	0	100	100
23	Y	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
24	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
25	a	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
26	b	52/59 (88%)	48 (92%)	4 (8%)	0	100	100
27	c	46/49 (94%)	46 (100%)	0	0	100	100
28	d	42/44 (96%)	42 (100%)	0	0	100	100
29	e	62/66 (94%)	59 (95%)	3 (5%)	0	100	100
30	f	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
31	g	99/102 (97%)	86 (87%)	13 (13%)	0	100	100
32	h	91/95 (96%)	87 (96%)	4 (4%)	0	100	100
33	i	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
All	All	3690/3835 (96%)	3492 (95%)	198 (5%)	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
3	C	223/225 (99%)	223 (100%)	0	100 100
4	D	168/170 (99%)	168 (100%)	0	100 100
5	E	169/170 (99%)	169 (100%)	0	100 100
6	F	153/154 (99%)	151 (99%)	2 (1%)	69 89
7	G	148/151 (98%)	148 (100%)	0	100 100
8	I	103/110 (94%)	103 (100%)	0	100 100
9	J	120/123 (98%)	120 (100%)	0	100 100
10	K	101/101 (100%)	101 (100%)	0	100 100
11	L	110/110 (100%)	108 (98%)	2 (2%)	59 85
12	M	111/116 (96%)	111 (100%)	0	100 100
13	N	99/100 (99%)	99 (100%)	0	100 100
14	O	93/93 (100%)	93 (100%)	0	100 100
16	Q	96/98 (98%)	96 (100%)	0	100 100
17	R	494/505 (98%)	494 (100%)	0	100 100
18	S	90/93 (97%)	90 (100%)	0	100 100
19	U	84/87 (97%)	84 (100%)	0	100 100
20	V	64/74 (86%)	64 (100%)	0	100 100
22	X	47/50 (94%)	46 (98%)	1 (2%)	53 82
23	Y	74/75 (99%)	74 (100%)	0	100 100
24	Z	52/53 (98%)	52 (100%)	0	100 100
25	a	99/100 (99%)	99 (100%)	0	100 100
26	b	48/53 (91%)	48 (100%)	0	100 100
27	c	46/47 (98%)	46 (100%)	0	100 100
28	d	39/39 (100%)	38 (97%)	1 (3%)	46 78
29	e	54/56 (96%)	54 (100%)	0	100 100
30	f	34/35 (97%)	34 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	g	83/84 (99%)	83 (100%)	0	100 100
32	h	84/85 (99%)	84 (100%)	0	100 100
33	i	56/57 (98%)	56 (100%)	0	100 100
All	All	3142/3214 (98%)	3136 (100%)	6 (0%)	93 98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	110	ARG
6	F	115	ARG
11	L	70	ASN
11	L	116	LYS
22	X	58	LYS
28	d	25	LYS

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

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2817/2820 (99%)	644 (22%)	56 (1%)
15	P	66/76 (86%)	20 (30%)	1 (1%)
15	T	75/76 (98%)	22 (29%)	0
2	B	111/112 (99%)	30 (27%)	2 (1%)
All	All	3069/3084 (99%)	716 (23%)	59 (1%)

All (716) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	15	G
1	A	33	U
1	A	34	U
1	A	35	G
1	A	39	C
1	A	42	G
1	A	43	G
1	A	44	A

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Mol	Chain	Res	Type
1	A	45	G
1	A	46	C
1	A	51	G
1	A	59	G
1	A	63	G
1	A	71	A
1	A	75	G
1	A	76	C
1	A	87	U
1	A	91	A
1	A	94	A
1	A	101	G
1	A	117	A
1	A	118	A
1	A	119	U
1	A	124	A
1	A	125	A
1	A	130	A
1	A	133	A
1	A	159	U
1	A	162	A
1	A	163	U
1	A	164	U
1	A	175	G
1	A	176	A
1	A	177	G
1	A	178	A
1	A	183	A
1	A	184	G
1	A	188	C
1	A	199	A
1	A	202	A
1	A	203	U
1	A	207	A
1	A	216	A
1	A	219	A
1	A	225	A
1	A	226	A
1	A	227	G
1	A	228	C
1	A	229	A
1	A	231	A

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Mol	Chain	Res	Type
1	A	233	G
1	A	245	G
1	A	251	G
1	A	252	C
1	A	253	G
1	A	258	A
1	A	267	C
1	A	268	A
1	A	269	G
1	A	270	C
1	A	271	C
1	A	272	C
1	A	273	A
1	A	274	A
1	A	275	A
1	A	276	C
1	A	277	C
1	A	282	G
1	A	289	C
1	A	290	U
1	A	291	C
1	A	295	G
1	A	296	G
1	A	297	G
1	A	298	U
1	A	299	U
1	A	300	G
1	A	301	U
1	A	302	A
1	A	310	C
1	A	312	G
1	A	313	U
1	A	314	A
1	A	315	C
1	A	321	U
1	A	322	A
1	A	324	A
1	A	325	A
1	A	331	C
1	A	337	A
1	A	345	A
1	A	346	G

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Mol	Chain	Res	Type
1	A	348	U
1	A	352	G
1	A	354	A
1	A	355	A
1	A	360	C
1	A	367	G
1	A	373	A
1	A	374	A
1	A	376	A
1	A	378	C
1	A	382	G
1	A	386	U
1	A	387	C
1	A	390	A
1	A	392	C
1	A	393	U
1	A	394	U
1	A	405	U
1	A	406	G
1	A	410	G
1	A	411	G
1	A	414	C
1	A	417	G
1	A	418	A
1	A	430	C
1	A	432	C
1	A	433	G
1	A	434	U
1	A	435	G
1	A	438	A
1	A	442	C
1	A	443	G
1	A	444	U
1	A	459	A
1	A	474	U
1	A	478	U
1	A	482	C
1	A	483	C
1	A	485	U
1	A	490	A
1	A	494	A
1	A	498	U

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Mol	Chain	Res	Type
1	A	502	C
1	A	503	C
1	A	504	A
1	A	514	G
1	A	528	G
1	A	538	A
1	A	548	A
1	A	550	G
1	A	551	A
1	A	552	G
1	A	554	U
1	A	555	C
1	A	556	C
1	A	558	G
1	A	562	C
1	A	564	G
1	A	572	A
1	A	576	G
1	A	577	U
1	A	578	A
1	A	592	A
1	A	593	A
1	A	594	C
1	A	595	G
1	A	607	G
1	A	617	G
1	A	619	A
1	A	631	G
1	A	647	A
1	A	648	G
1	A	649	G
1	A	650	U
1	A	651	U
1	A	660	G
1	A	663	G
1	A	666	G
1	A	667	A
1	A	673	A
1	A	674	G
1	A	680	G
1	A	683	A
1	A	684	G

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Mol	Chain	Res	Type
1	A	691	U
1	A	700	U
1	A	701	G
1	A	713	G
1	A	715	A
1	A	717	A
1	A	718	C
1	A	719	C
1	A	733	U
1	A	773	G
1	A	777	C
1	A	781	A
1	A	782	A
1	A	786	A
1	A	792	G
1	A	794	U
1	A	795	G
1	A	797	A
1	A	822	G
1	A	823	G
1	A	824	G
1	A	829	A
1	A	831	U
1	A	832	G
1	A	836	A
1	A	837	U
1	A	838	C
1	A	839	G
1	A	852	G
1	A	853	C
1	A	858	U
1	A	859	C
1	A	866	A
1	A	874	U
1	A	875	U
1	A	877	G
1	A	892	U
1	A	893	A
1	A	895	G
1	A	913	A
1	A	914	C
1	A	916	G

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Mol	Chain	Res	Type
1	A	924	U
1	A	925	A
1	A	927	G
1	A	928	G
1	A	931	C
1	A	935	A
1	A	937	C
1	A	942	U
1	A	943	A
1	A	944	C
1	A	948	A
1	A	951	C
1	A	952	A
1	A	954	U
1	A	957	A
1	A	959	C
1	A	961	C
1	A	962	C
1	A	964	A
1	A	973	G
1	A	977	U
1	A	978	A
1	A	981	C
1	A	987	A
1	A	988	G
1	A	990	C
1	A	991	A
1	A	992	G
1	A	999	A
1	A	1005	A
1	A	1007	G
1	A	1019	A
1	A	1020	A
1	A	1025	A
1	A	1026	A
1	A	1027	A
1	A	1028	C
1	A	1029	A
1	A	1031	C
1	A	1034	A
1	A	1037	C
1	A	1055	A

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Mol	Chain	Res	Type
1	A	1058	U
1	A	1059	A
1	A	1068	G
1	A	1072	A
1	A	1079	U
1	A	1091	U
1	A	1092	A
1	A	1093	G
1	A	1102	G
1	A	1104	U
1	A	1105	G
1	A	1107	U
1	A	1108	G
1	A	1110	C
1	A	1112	U
1	A	1113	A
1	A	1115	A
1	A	1116	A
1	A	1117	G
1	A	1123	A
1	A	1124	C
1	A	1127	U
1	A	1128	U
1	A	1129	U
1	A	1131	A
1	A	1135	G
1	A	1139	G
1	A	1140	U
1	A	1141	A
1	A	1142	A
1	A	1143	U
1	A	1144	A
1	A	1152	G
1	A	1157	A
1	A	1158	G
1	A	1159	U
1	A	1176	U
1	A	1178	U
1	A	1179	A
1	A	1181	C
1	A	1182	G
1	A	1185	G

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Mol	Chain	Res	Type
1	A	1187	U
1	A	1188	A
1	A	1194	A
1	A	1201	A
1	A	1202	A
1	A	1209	G
1	A	1217	U
1	A	1218	U
1	A	1219	C
1	A	1220	G
1	A	1246	G
1	A	1247	G
1	A	1251	U
1	A	1252	G
1	A	1260	A
1	A	1276	G
1	A	1278	G
1	A	1281	C
1	A	1283	U
1	A	1284	A
1	A	1289	U
1	A	1293	A
1	A	1295	U
1	A	1296	G
1	A	1311	G
1	A	1312	A
1	A	1313	A
1	A	1314	A
1	A	1315	G
1	A	1327	U
1	A	1339	A
1	A	1340	A
1	A	1345	U
1	A	1346	A
1	A	1351	U
1	A	1352	U
1	A	1359	G
1	A	1360	A
1	A	1361	A
1	A	1363	G
1	A	1364	C
1	A	1376	G

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Mol	Chain	Res	Type
1	A	1381	A
1	A	1382	G
1	A	1384	C
1	A	1388	A
1	A	1404	A
1	A	1417	A
1	A	1418	U
1	A	1423	A
1	A	1424	A
1	A	1425	C
1	A	1431	G
1	A	1433	U
1	A	1435	U
1	A	1436	U
1	A	1439	U
1	A	1441	U
1	A	1442	A
1	A	1450	C
1	A	1456	A
1	A	1460	G
1	A	1464	A
1	A	1472	G
1	A	1473	A
1	A	1474	C
1	A	1490	A
1	A	1497	G
1	A	1498	U
1	A	1499	A
1	A	1507	U
1	A	1513	U
1	A	1515	C
1	A	1516	A
1	A	1517	A
1	A	1519	C
1	A	1520	A
1	A	1523	U
1	A	1524	A
1	A	1528	U
1	A	1536	A
1	A	1539	C
1	A	1553	A
1	A	1555	A

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Mol	Chain	Res	Type
1	A	1561	G
1	A	1563	G
1	A	1569	A
1	A	1571	G
1	A	1572	G
1	A	1573	C
1	A	1581	A
1	A	1582	U
1	A	1584	U
1	A	1586	G
1	A	1596	U
1	A	1607	C
1	A	1608	A
1	A	1614	A
1	A	1617	A
1	A	1623	C
1	A	1626	U
1	A	1631	A
1	A	1632	G
1	A	1634	U
1	A	1651	G
1	A	1652	C
1	A	1653	A
1	A	1655	A
1	A	1657	C
1	A	1658	G
1	A	1660	C
1	A	1667	A
1	A	1674	G
1	A	1679	A
1	A	1691	A
1	A	1692	U
1	A	1693	C
1	A	1696	G
1	A	1697	A
1	A	1705	C
1	A	1709	A
1	A	1712	G
1	A	1719	G
1	A	1727	A
1	A	1744	G
1	A	1745	A

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Mol	Chain	Res	Type
1	A	1752	G
1	A	1756	U
1	A	1757	G
1	A	1758	U
1	A	1770	C
1	A	1774	A
1	A	1777	G
1	A	1778	A
1	A	1779	G
1	A	1780	C
1	A	1781	C
1	A	1782	G
1	A	1785	G
1	A	1788	A
1	A	1791	A
1	A	1792	G
1	A	1793	G
1	A	1802	A
1	A	1805	G
1	A	1809	A
1	A	1811	C
1	A	1829	C
1	A	1830	G
1	A	1845	A
1	A	1858	A
1	A	1877	A
1	A	1881	U
1	A	1895	A
1	A	1898	G
1	A	1901	A
1	A	1902	G
1	A	1912	G
1	A	1913	A
1	A	1918	A
1	A	1935	G
1	A	1941	A
1	A	1949	C
1	A	1958	G
1	A	1959	G
1	A	1966	A
1	A	1968	U
1	A	1972	U

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Mol	Chain	Res	Type
1	A	1984	U
1	A	1990	C
1	A	1993	G
1	A	1996	C
1	A	1999	A
1	A	2000	A
1	A	2001	G
1	A	2011	U
1	A	2020	U
1	A	2021	G
1	A	2022	U
1	A	2024	U
1	A	2026	A
1	A	2050	G
1	A	2052	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2068	G
1	A	2072	C
1	A	2084	C
1	A	2085	G
1	A	2088	A
1	A	2089	A
1	A	2090	G
1	A	2091	A
1	A	2098	G
1	A	2110	C
1	A	2111	A
1	A	2121	U
1	A	2123	A
1	A	2232	G
1	A	2233	C
1	A	2235	G
1	A	2240	U
1	A	2241	A
1	A	2243	C
1	A	2254	A
1	A	2255	C
1	A	2267	G
1	A	2268	G
1	A	2308	G

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Mol	Chain	Res	Type
1	A	2311	G
1	A	2312	C
1	A	2315	A
1	A	2317	A
1	A	2333	G
1	A	2334	U
1	A	2335	U
1	A	2336	G
1	A	2337	G
1	A	2338	A
1	A	2345	U
1	A	2346	C
1	A	2348	C
1	A	2349	A
1	A	2350	G
1	A	2351	A
1	A	2352	G
1	A	2356	A
1	A	2357	A
1	A	2363	C
1	A	2364	A
1	A	2374	G
1	A	2377	U
1	A	2379	C
1	A	2390	A
1	A	2408	G
1	A	2411	G
1	A	2412	G
1	A	2414	C
1	A	2420	G
1	A	2431	U
1	A	2435	C
1	A	2436	A
1	A	2454	A
1	A	2455	A
1	A	2457	G
1	A	2458	G
1	A	2459	A
1	A	2464	A
1	A	2468	A
1	A	2469	C
1	A	2470	C

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Mol	Chain	Res	Type
1	A	2476	G
1	A	2477	A
1	A	2486	U
1	A	2488	A
1	A	2502	U
1	A	2505	A
1	A	2507	A
1	A	2519	G
1	A	2523	G
1	A	2527	C
1	A	2528	C
1	A	2531	G
1	A	2532	A
1	A	2534	G
1	A	2535	U
1	A	2542	A
1	A	2549	C
1	A	2558	G
1	A	2564	G
1	A	2572	G
1	A	2577	G
1	A	2583	U
1	A	2593	A
1	A	2594	A
1	A	2595	A
1	A	2596	G
1	A	2598	G
1	A	2601	A
1	A	2607	G
1	A	2611	G
1	A	2619	A
1	A	2631	A
1	A	2638	U
1	A	2639	C
1	A	2642	U
1	A	2644	U
1	A	2648	U
1	A	2658	A
1	A	2659	G
1	A	2675	C
1	A	2676	U
1	A	2683	A

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Mol	Chain	Res	Type
1	A	2702	G
1	A	2711	G
1	A	2712	C
1	A	2714	G
1	A	2717	G
1	A	2718	U
1	A	2720	C
1	A	2743	G
1	A	2754	A
1	A	2755	U
1	A	2762	A
1	A	2764	G
1	A	2768	U
1	A	2773	G
1	A	2777	A
1	A	2779	A
1	A	2785	U
1	A	2786	A
1	A	2794	A
1	A	2795	G
1	A	2797	C
1	A	2799	C
1	A	2804	A
1	A	2807	A
1	A	2808	U
1	A	2813	U
1	A	2818	C
1	A	2819	A
1	A	2820	U
1	A	2825	C
1	A	2826	A
1	A	2828	G
1	A	2830	A
1	A	2845	A
1	A	2855	G
1	A	2858	U
1	A	2859	G
1	A	2860	A
1	A	2861	U
1	A	2874	G
1	A	2897	G
1	A	2898	A

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Mol	Chain	Res	Type
1	A	2899	C
1	A	2905	C
1	A	2908	A
1	A	2918	G
1	A	2921	U
2	B	10	G
2	B	11	A
2	B	12	U
2	B	13	A
2	B	14	G
2	B	19	G
2	B	20	A
2	B	23	U
2	B	28	C
2	B	33	U
2	B	38	U
2	B	39	A
2	B	40	C
2	B	41	C
2	B	42	G
2	B	48	G
2	B	49	G
2	B	51	A
2	B	54	U
2	B	55	A
2	B	59	U
2	B	60	C
2	B	64	A
2	B	85	U
2	B	86	U
2	B	87	U
2	B	88	C
2	B	97	A
2	B	107	G
2	B	110	G
15	P	8	U
15	P	9	A
15	P	19	G
15	P	20	G
15	P	22	G
15	P	29	U
15	P	30	G

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Mol	Chain	Res	Type
15	P	31	C
15	P	32	U
15	P	40	C
15	P	41	A
15	P	44	A
15	P	48	C
15	P	52	G
15	P	53	G
15	P	54	U
15	P	61	C
15	P	66	A
15	P	67	G
15	P	76	A
15	T	3	G
15	T	8	U
15	T	9	A
15	T	16	C
15	T	17	U
15	T	18	G
15	T	19	G
15	T	20	G
15	T	34	U
15	T	36	C
15	T	38	C
15	T	41	A
15	T	44	A
15	T	45	G
15	T	46	G
15	T	48	C
15	T	53	G
15	T	55	U
15	T	57	G
15	T	67	G
15	T	72	C
15	T	74	C

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	12	A
1	A	43	G
1	A	45	G

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Mol	Chain	Res	Type
1	A	58	G
1	A	90	A
1	A	175	G
1	A	177	G
1	A	183	A
1	A	229	A
1	A	252	C
1	A	272	C
1	A	274	A
1	A	275	A
1	A	276	C
1	A	288	C
1	A	295	G
1	A	296	G
1	A	377	G
1	A	405	U
1	A	437	A
1	A	442	C
1	A	537	A
1	A	549	A
1	A	649	G
1	A	662	U
1	A	683	A
1	A	717	A
1	A	785	C
1	A	837	U
1	A	936	C
1	A	1111	U
1	A	1245	G
1	A	1250	G
1	A	1351	U
1	A	1359	G
1	A	1438	C
1	A	1516	A
1	A	1595	U
1	A	1630	G
1	A	1652	C
1	A	1755	C
1	A	1779	G
1	A	1784	A
1	A	1948	A
1	A	2267	G

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Mol	Chain	Res	Type
1	A	2334	U
1	A	2351	A
1	A	2454	A
1	A	2468	A
1	A	2710	C
1	A	2711	G
1	A	2716	U
1	A	2784	C
1	A	2785	U
1	A	2796	C
1	A	2812	A
2	B	47	C
2	B	59	U
15	P	51	C

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 (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2124:A	O3’	2223:U	P	17.51
1	A	1941:A	O3’	1947:A	P	13.89

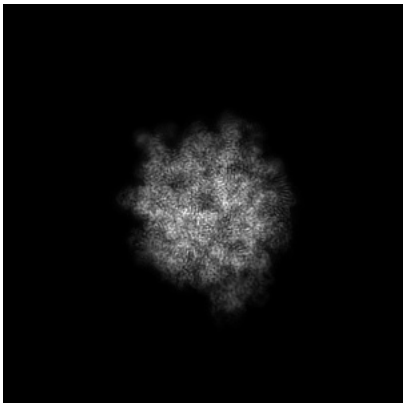
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11862. These allow visual inspection of the internal detail of the map and identification of artifacts.

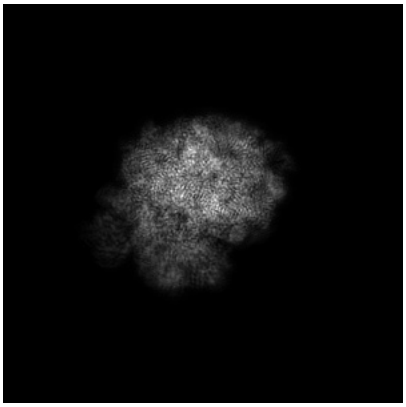
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

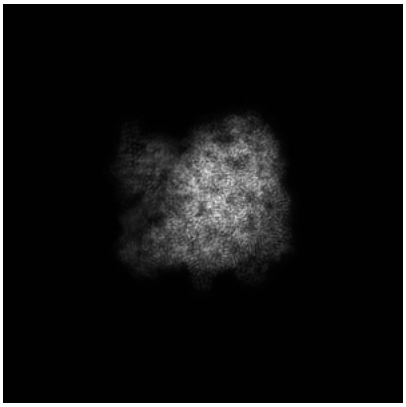
6.1.1 Primary map



X



Y



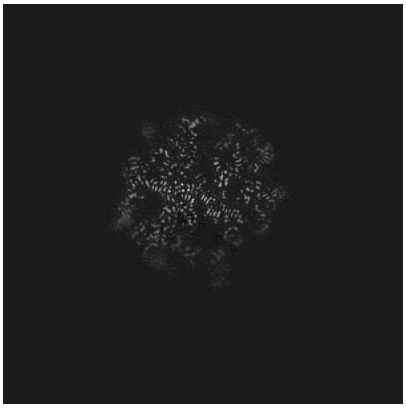
Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 192



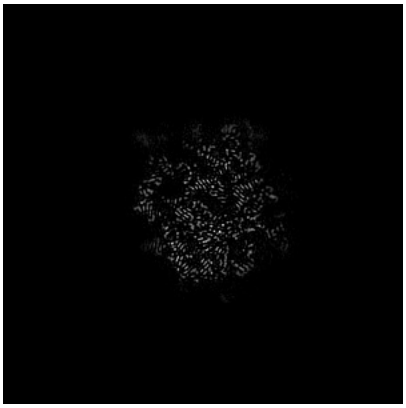
Y Index: 192

Z Index: 192

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: 211

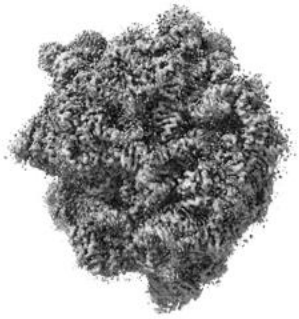
Y Index: 213

Z Index: 182

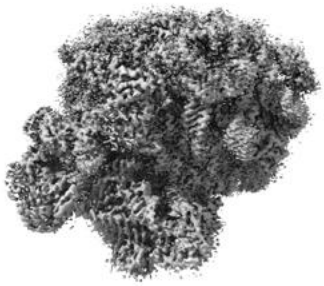
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

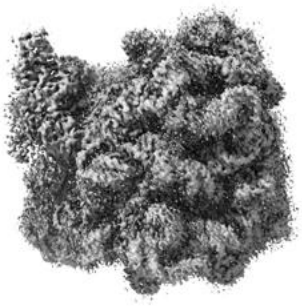
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

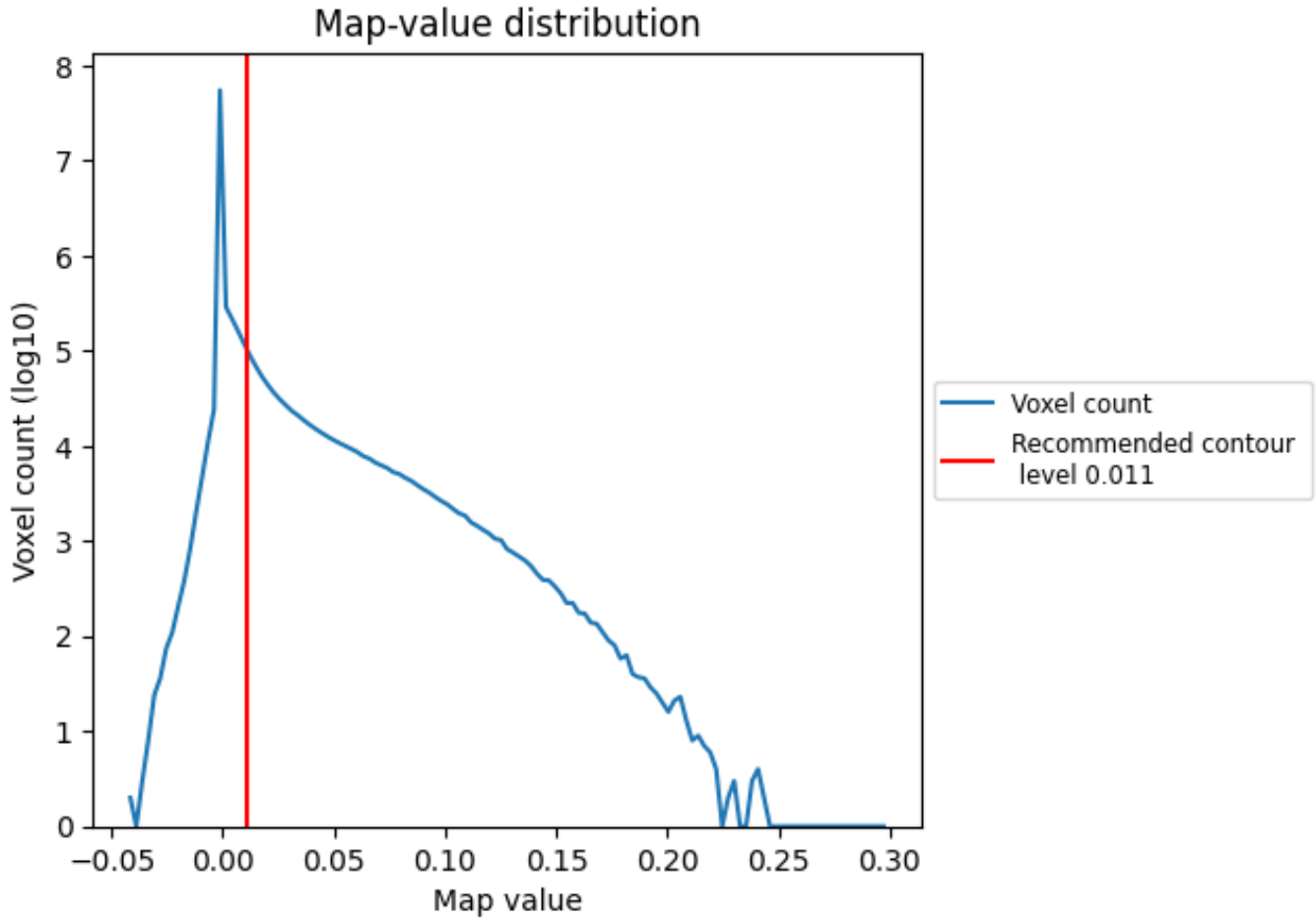
6.5 Mask visualisation (i)

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

7 Map analysis

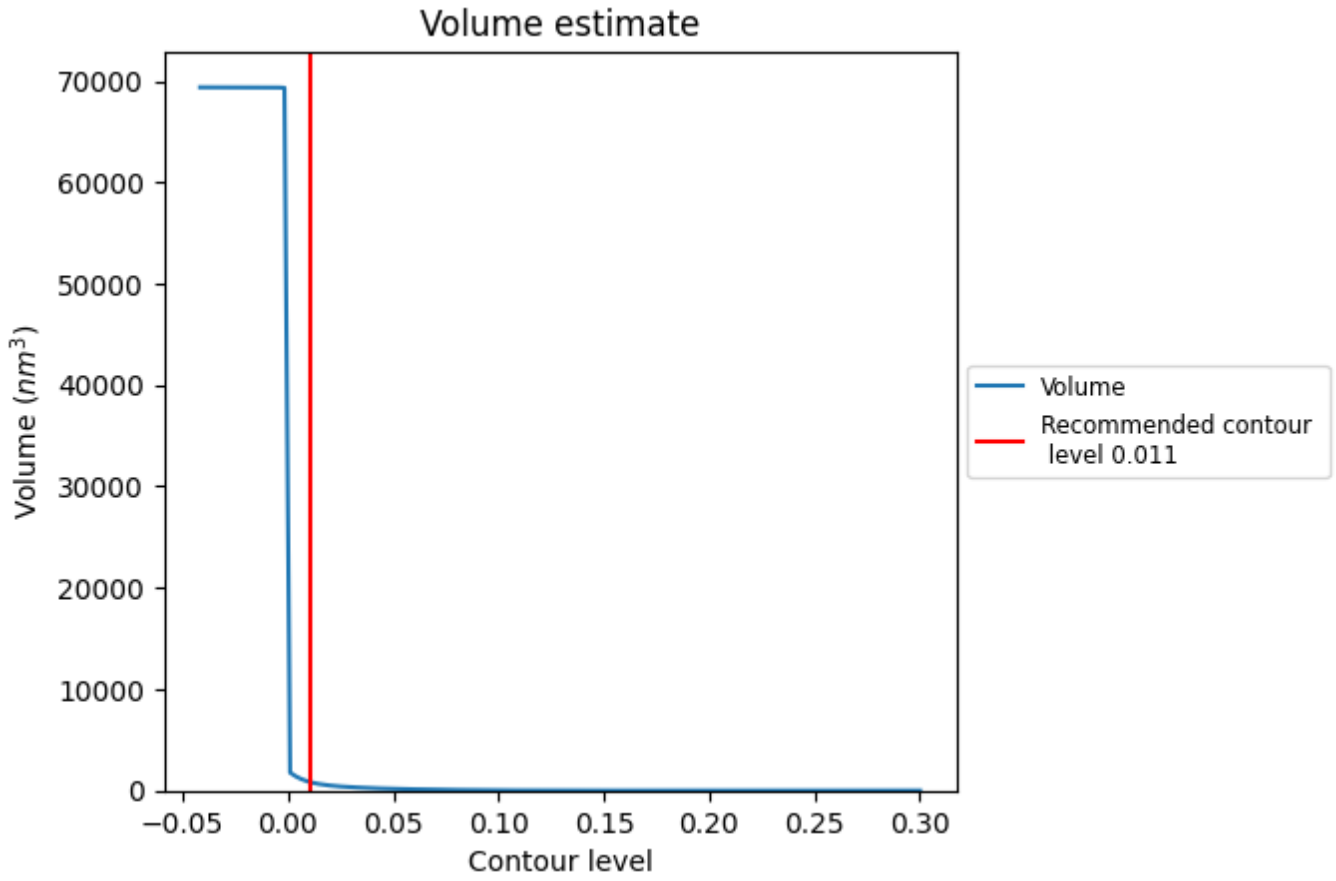
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

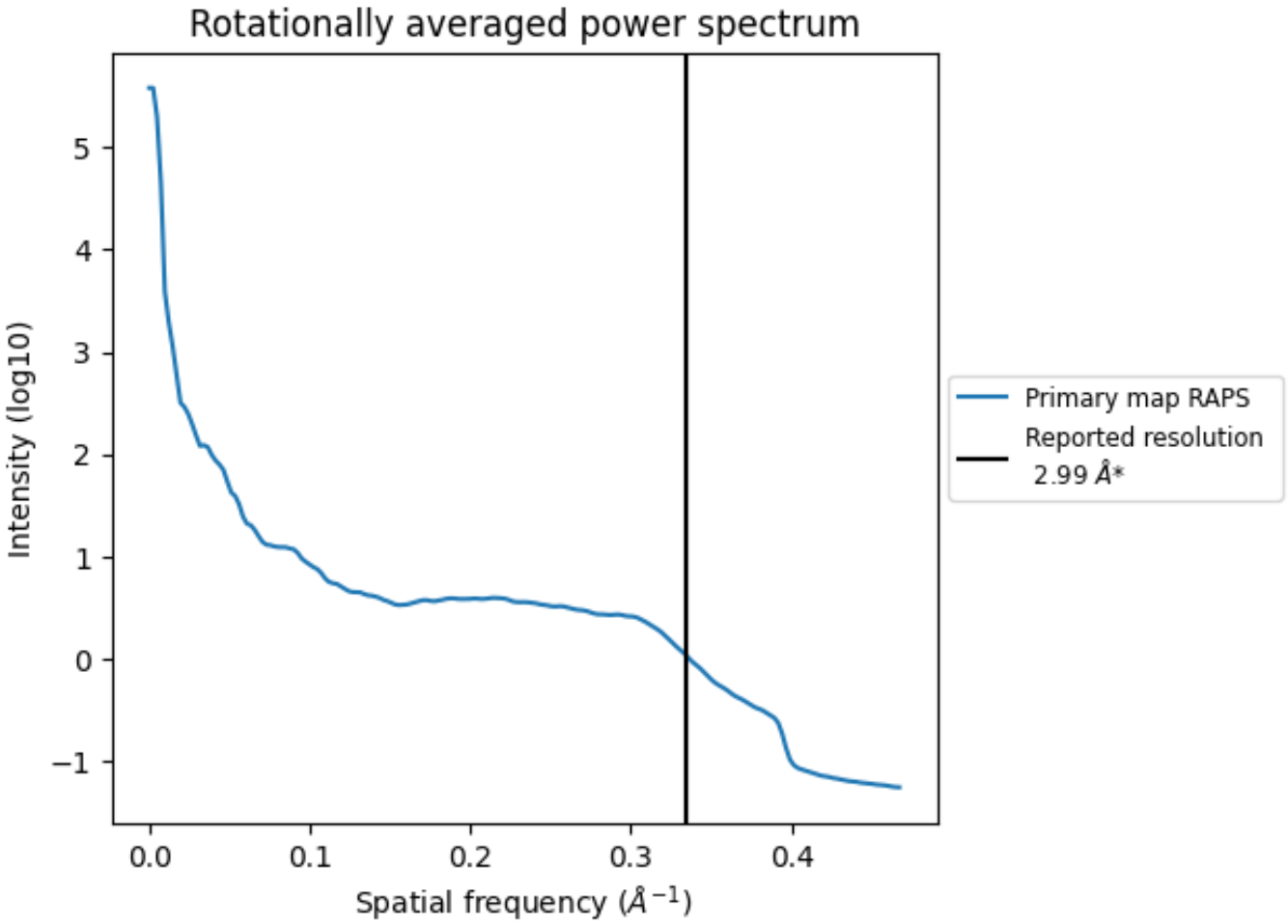
7.2 Volume estimate



The volume at the recommended contour level is 818 nm^3; this corresponds to an approximate mass of 739 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 0.334 $Å^{-1}$

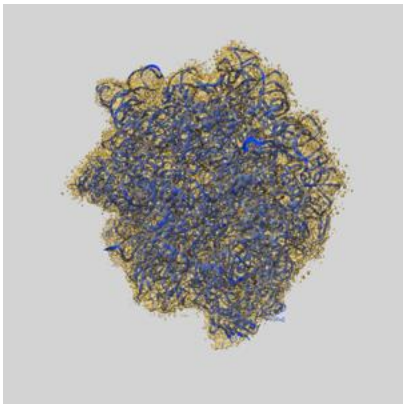
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

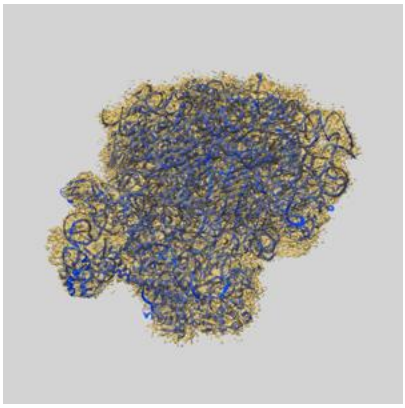
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11862 and PDB model 7AQC. Per-residue inclusion information can be found in section 3 on page 10.

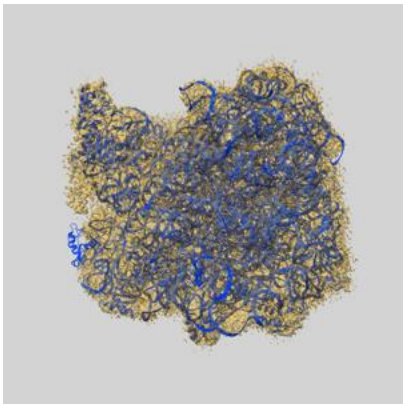
9.1 Map-model overlay



X



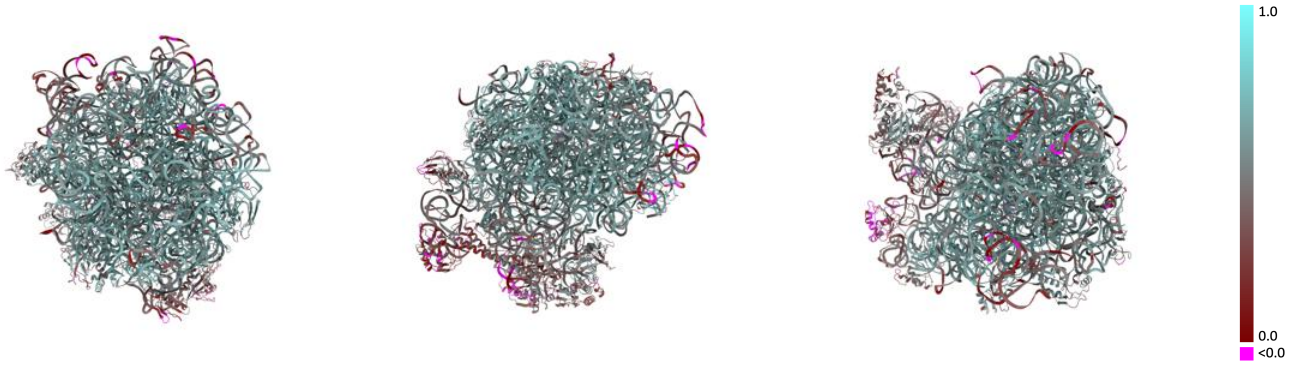
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011 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.

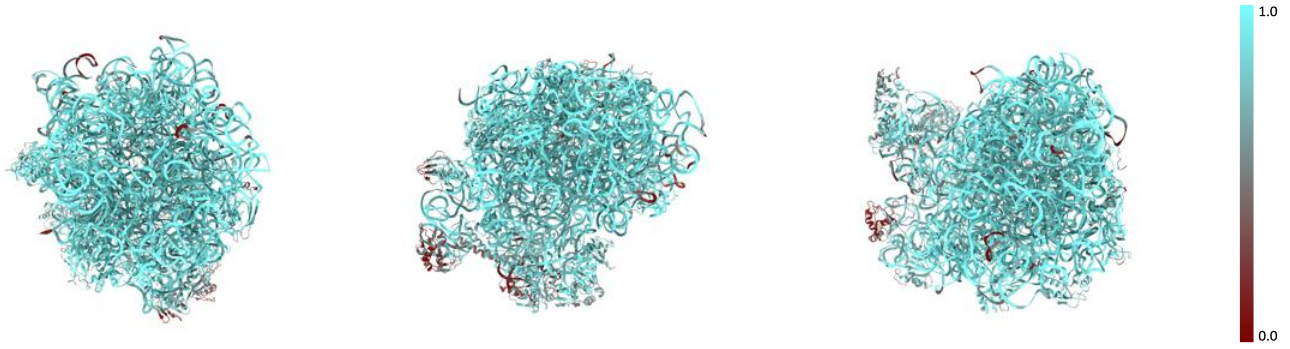
9.2 Q-score mapped to coordinate model (i)



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.

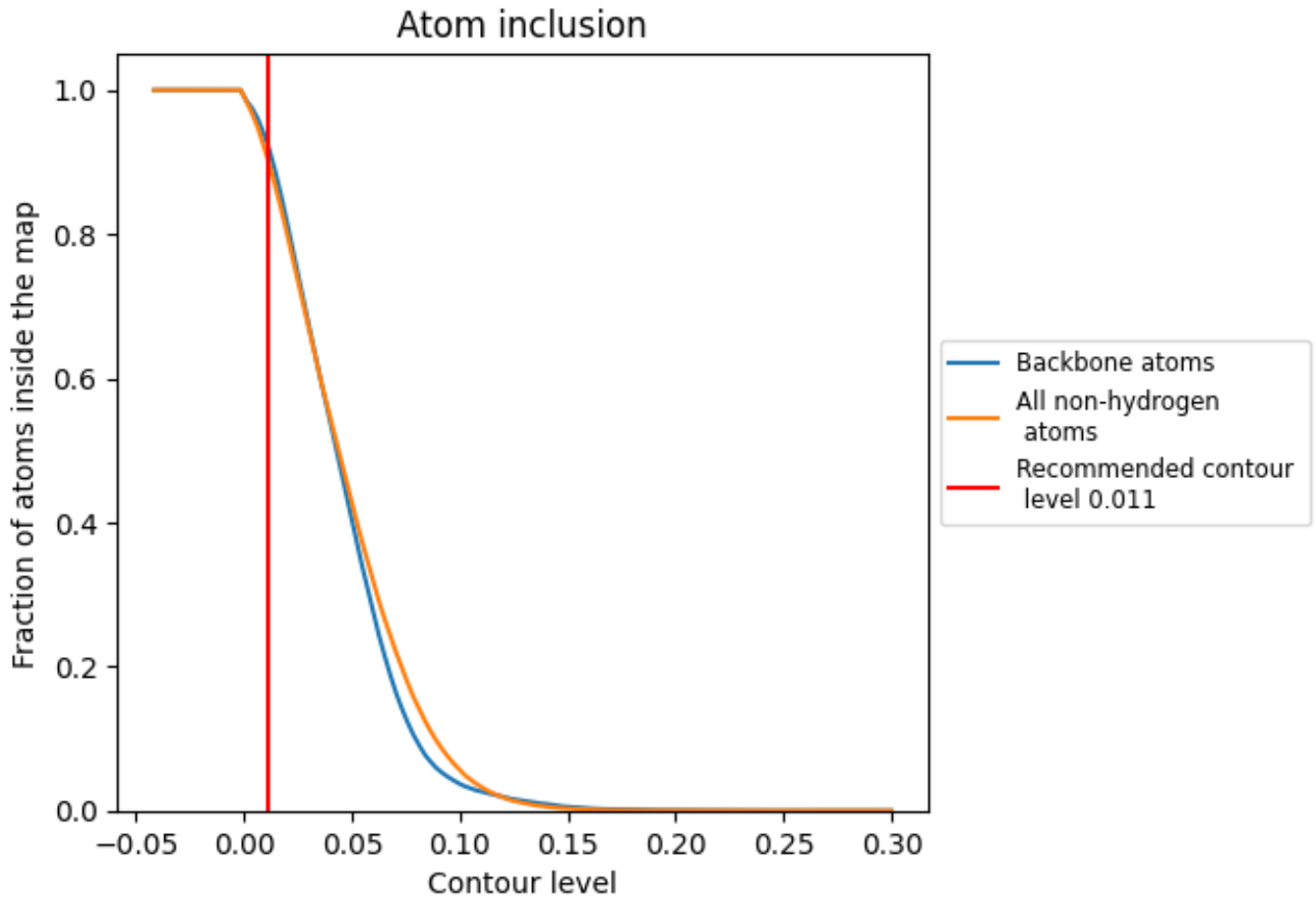
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.011).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9053	0.5390
A	0.9504	0.5720
B	0.9173	0.4680
C	0.9533	0.6210
D	0.9386	0.6100
E	0.8946	0.5480
F	0.2778	0.0930
G	0.6532	0.3320
I	0.3602	0.2060
J	0.9454	0.6000
K	0.9231	0.5770
L	0.9058	0.5560
M	0.9040	0.5680
N	0.9455	0.6240
O	0.7430	0.4020
P	0.8822	0.4160
Q	0.9351	0.5900
R	0.7255	0.3900
S	0.9499	0.6020
T	0.8218	0.3780
U	0.8059	0.4840
V	0.9458	0.6040
W	0.8000	0.4750
X	0.8449	0.4720
Y	0.7905	0.4430
Z	0.9169	0.5850
a	0.8586	0.5370
b	0.9104	0.5730
c	0.9302	0.5900
d	0.9942	0.6850
e	0.9679	0.6270
f	0.9397	0.5950
g	0.8531	0.4880
h	0.8755	0.5400
i	0.7938	0.4210