Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 07:31 AM JST

PDB ID	:	8HKU
EMDB ID	:	EMD-34860
Title	:	Cryo-EM Structures and Translocation Mechanism of Crenarchaeota Ribosome
Authors	:	Wang, Y.H.; Zhou, J.
Deposited on	:	2022-11-28
Resolution	:	2.72 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*
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:

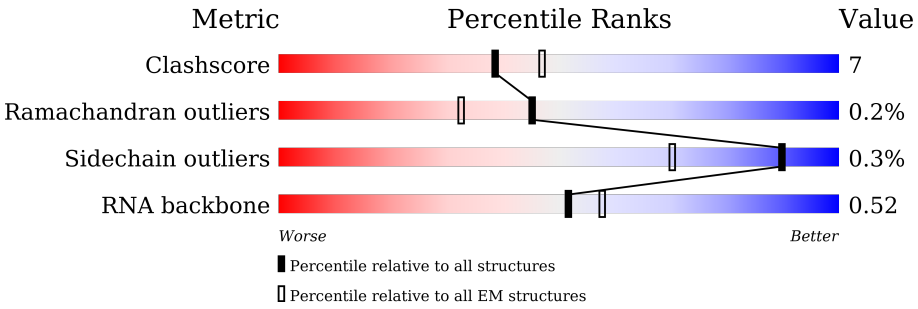
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.72 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A23S	3022	5% 78% 19%
2	A5S	122	75% 19% 7%
3	AL1P	216	100% 100%
4	AL2P	234	100%
5	AL3P	339	99%
6	AL4P	251	100%
7	AL5P	168	6% 100%

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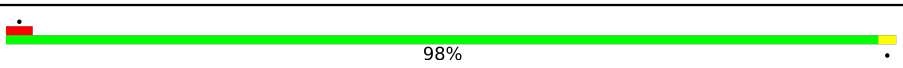
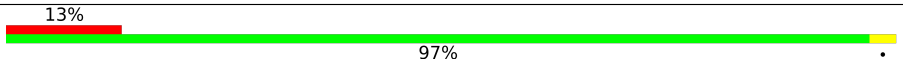
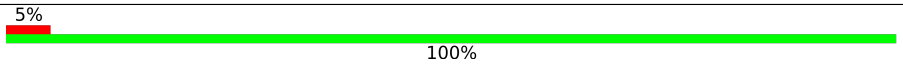
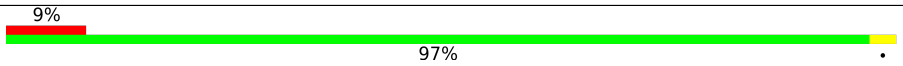
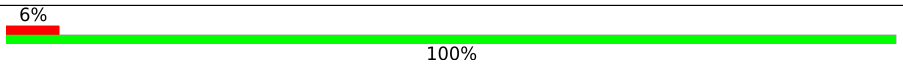
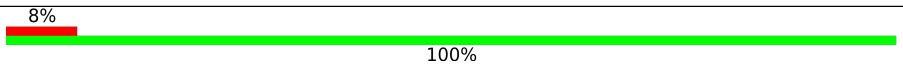
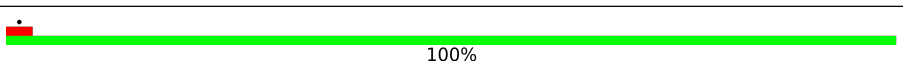
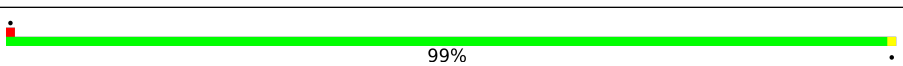
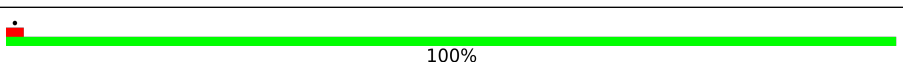
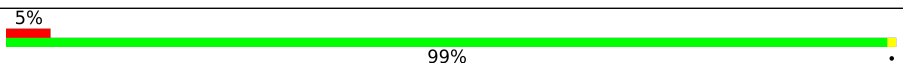
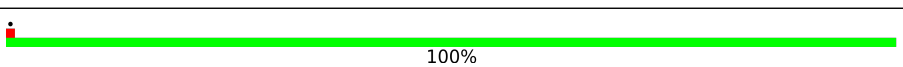
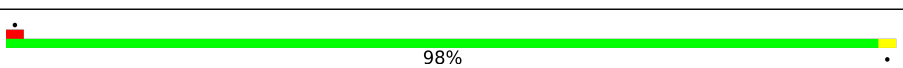
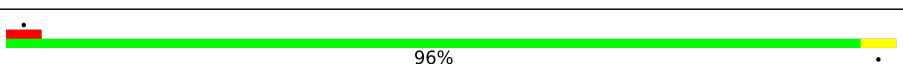
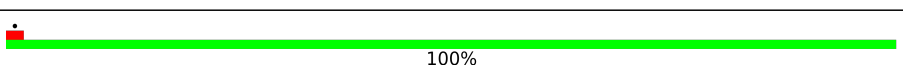
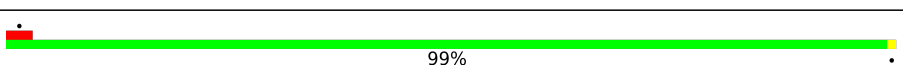
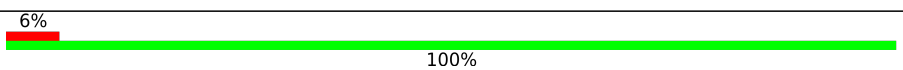
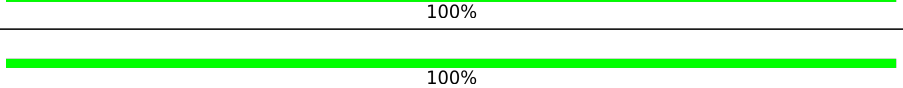
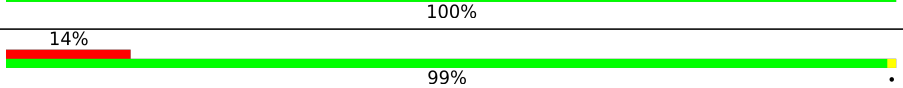
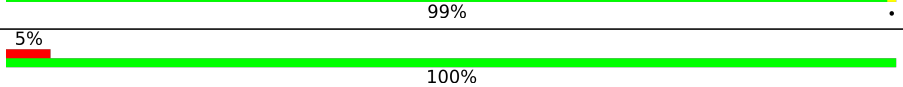
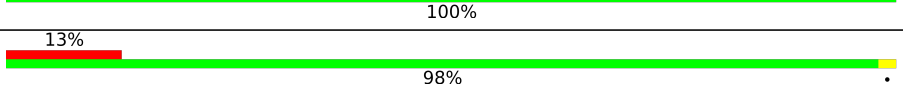
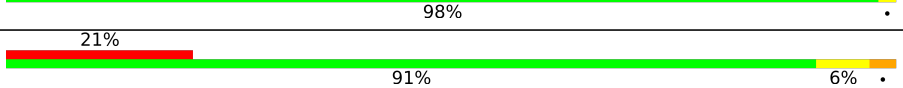
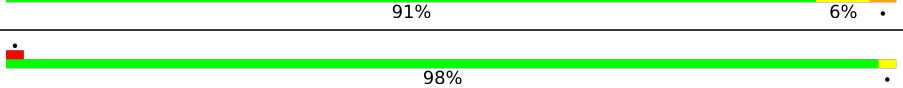
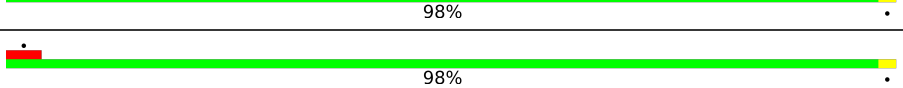
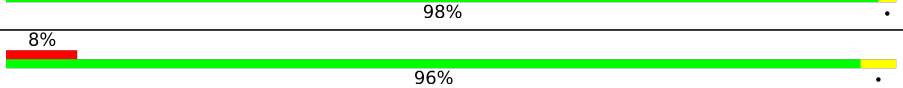
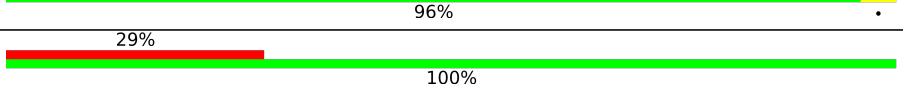
Mol	Chain	Length	Quality of chain
8	AL6P	181	
9	ALX0	76	
10	L10E	164	
11	L13P	140	
12	L141	86	
12	L142	86	
13	L14P	134	
14	L15E	169	
15	L18E	112	
16	L18P	193	
17	L19E	144	
18	L22P	150	
19	L23P	81	
20	L24E	54	
21	L24P	122	
22	L29P	63	
23	L30E	94	
24	L30P	155	
25	L31E	75	
26	L32E	123	
27	L34E	77	
28	L37A	65	
29	L37E	54	
30	L39E	49	
31	L40E	55	

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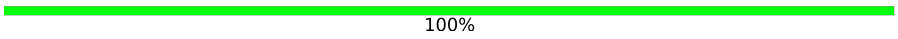
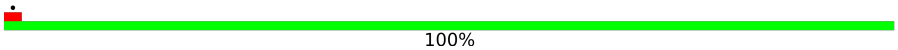
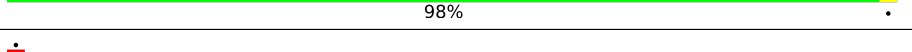
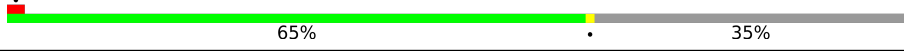
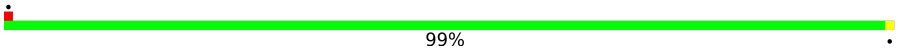
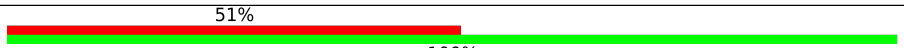
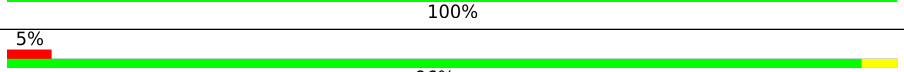
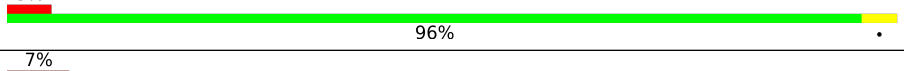
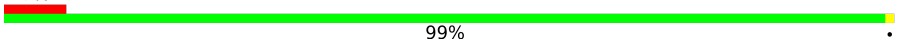
Mol	Chain	Length	Quality of chain
32	L44E	92	
33	L7A1	123	
33	L7A2	123	
34	L15P	144	
35	L21E	97	
36	ARF1	232	
37	L45A	101	
38	L46A	70	
39	L47A	80	
40	AETN	19	

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 106630 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 rRNA (2996-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A23S	2995	64335	28663	11905	20772	2995	0	0

- Molecule 2 is a RNA chain called 5s rRNA (122-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	A5S	122	2609	1163	476	849	121	0	0

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AL1P	216	1715	1096	303	312	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AL2P	234	1754	1101	344	307	2	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AL3P	339	2695	1730	484	477	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AL4P	251	1926	1223	356	345	2	0	0

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AL5P	168	Total	C	N	O	S	0	0
			1343	854	253	232	4		

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AL6P	181	Total	C	N	O	S	0	0
			1431	920	246	264	1		

- Molecule 9 is a protein called 50S ribosomal protein L18Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	ALX0	76	Total	C	N	O	S	0	0
			629	403	110	115	1		

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L10E	164	Total	C	N	O	S	0	0
			1310	837	239	227	7		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L13P	140	Total	C	N	O	S	0	0
			1109	707	208	190	4		

- Molecule 12 is a protein called 50S ribosomal protein L14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L141	86	Total	C	N	O	S	0	0
			669	417	123	127	2		
12	L142	86	Total	C	N	O	S	0	0
			669	417	123	127	2		

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L14P	134	Total	C	N	O	S	0	0
			1034	655	194	181	4		

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L15E	169	Total	C	N	O	S	0	0
			1423	899	283	236	5		

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L18E	112	Total	C	N	O	S	0	0
			895	576	163	153	3		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L18P	193	Total	C	N	O	S	0	0
			1539	990	274	274	1		

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	L19E	144	Total	C	N	O	0	0
			1206	753	247	206		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L22P	150	Total	C	N	O	S	0	0
			1223	782	225	213	3		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L23P	81	Total	C	N	O	S	0	0
			650	419	109	121	1		

- Molecule 20 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L24E	54	Total	C	N	O	S	0	0
			441	282	80	73	6		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L24P	122	Total	C	N	O	S	0	0
			989	620	189	176	4		

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L29P	63	Total	C	N	O	S	0	0
			513	319	95	96	3		

- Molecule 23 is a protein called 50S ribosomal protein L30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L30E	94	Total	C	N	O	S	0	0
			729	474	116	136	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L30P	155	Total	C	N	O	S	0	0
			1254	804	222	223	5		

- Molecule 25 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L31E	75	Total	C	N	O	S	0	0
			625	398	126	97	4		

- Molecule 26 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L32E	123	Total	C	N	O	S	0	0
			1010	650	193	166	1		

- Molecule 27 is a protein called 50S ribosomal protein L34e.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	L34E	77	Total	C	N	O	S	0	0
			629	395	119	110	5		

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	L37A	65	Total	C	N	O	S	0	0
			527	335	99	87	6		

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L37E	54	Total	C	N	O	S	0	0
			436	267	94	69	6		

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	L39E	49	Total	C	N	O	0	0
			414	265	88	61		

- Molecule 31 is a protein called 50S ribosomal protein L40E.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L40E	55	Total	C	N	O	S	0	0
			439	273	89	72	5		

- Molecule 32 is a protein called 50S ribosomal protein L44e.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L44E	92	Total	C	N	O	S	0	0
			753	474	144	129	6		

- Molecule 33 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L7A1	123	Total	C	N	O	S	0	0
			935	593	155	184	3		
33	L7A2	123	Total	C	N	O	S	0	0
			935	593	155	184	3		

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L15P	94	Total	C	N	O	S	0	0
			752	487	131	133	1		

- Molecule 35 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L21E	97	Total	C	N	O	S	0	0
			785	502	152	129	2		

- Molecule 36 is a protein called Peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	ARF1	232	Total	C	N	O	S	0	0
			1869	1213	299	349	8		

- Molecule 37 is a protein called DUF2280 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L45A	101	Total	C	N	O	S	0	0
			816	515	141	156	4		

- Molecule 38 is a protein called Conserved protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L46A	70	Total	C	N	O	S	0	0
			586	382	101	102	1		

- Molecule 39 is a protein called 50S ribosomal protein L47A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L47A	80	Total	C	N	O	S	0	0
			648	405	113	128	2		

- Molecule 40 is a RNA chain called E-site tRNA.

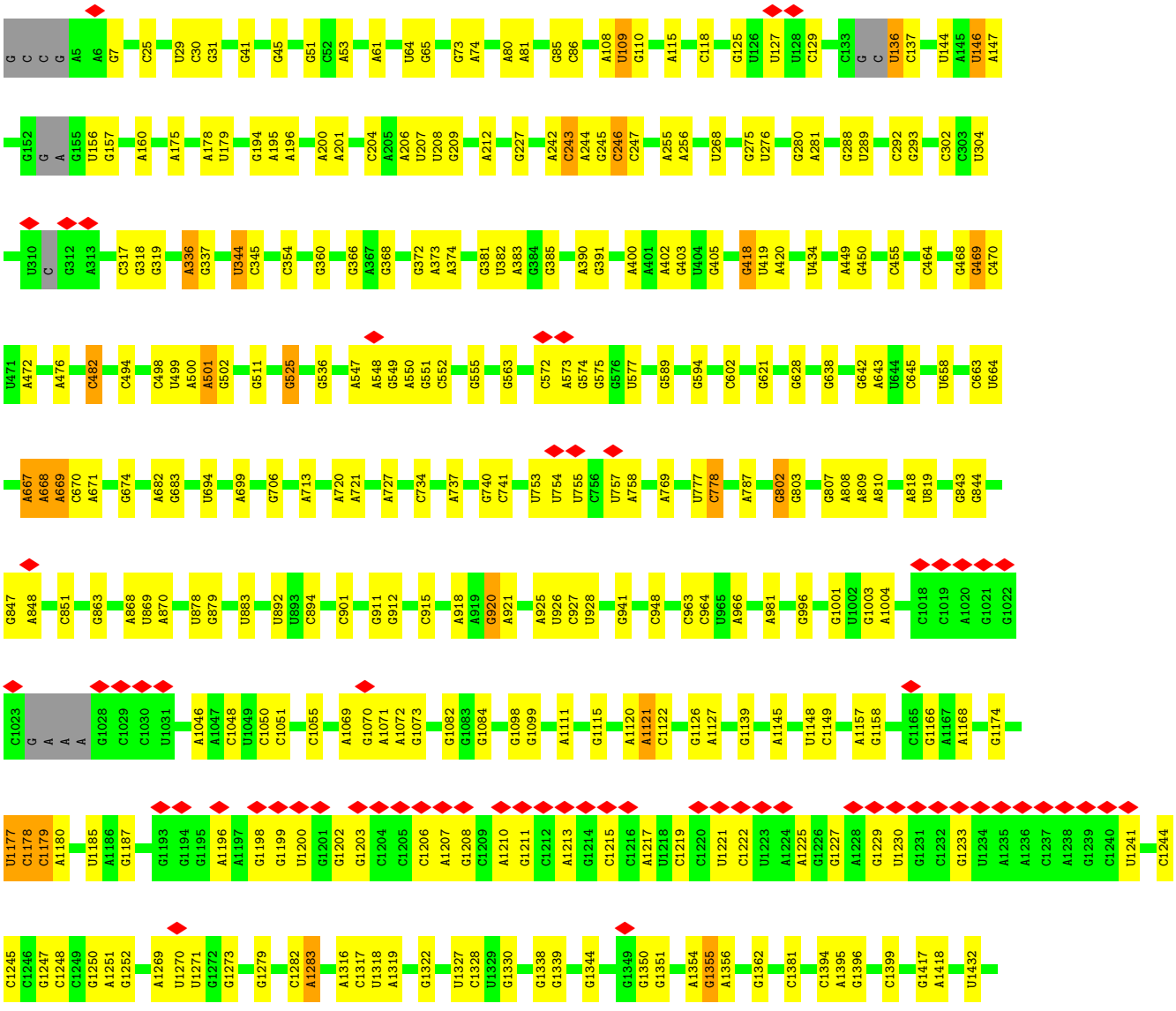
Mol	Chain	Residues	Atoms					AltConf	Trace
40	AETN	18	Total	C	N	O	P	0	0
			381	171	71	122	17		

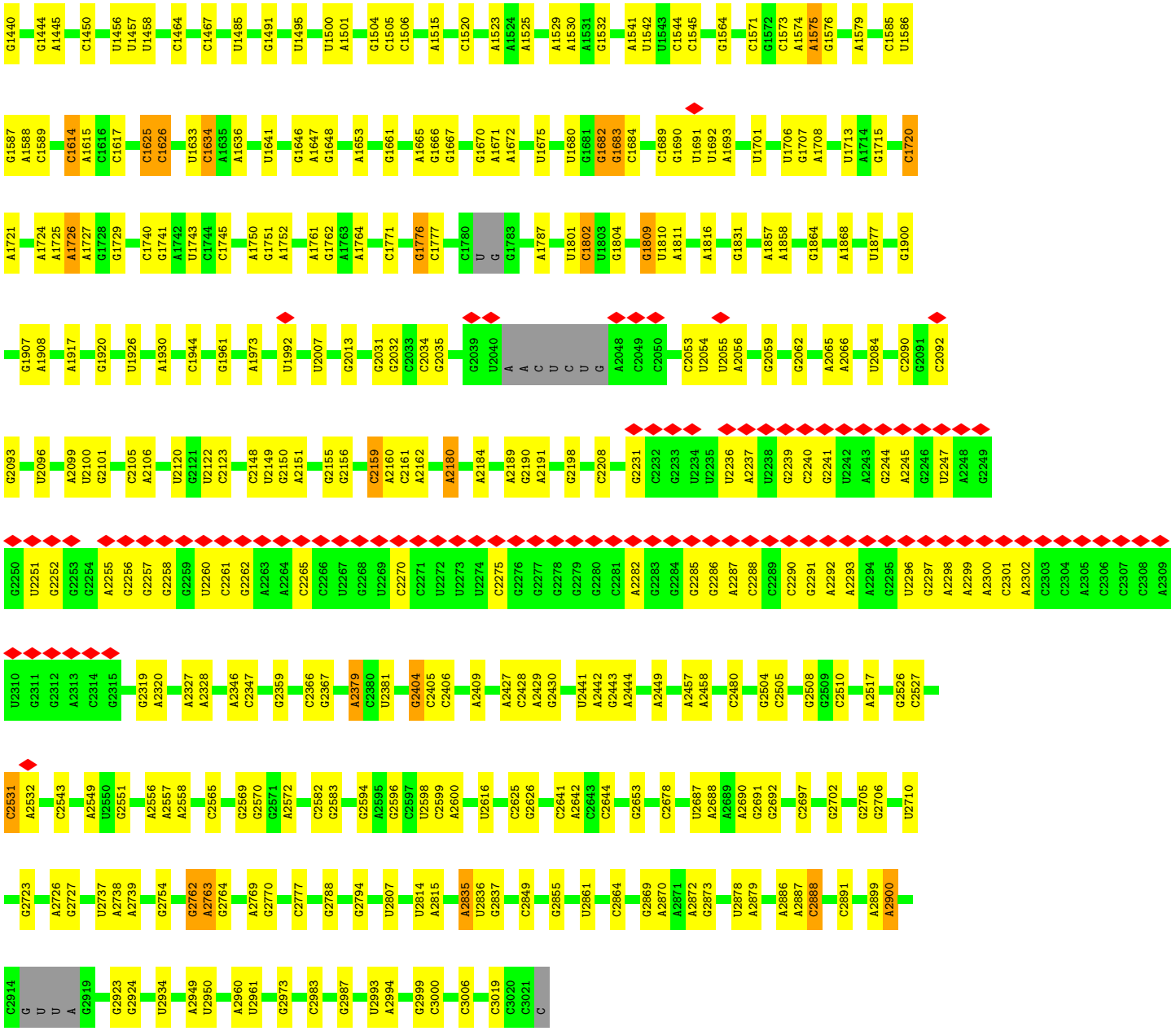
3 Residue-property plots (i)

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

- Molecule 1: 23s rRNA (2996-MER)

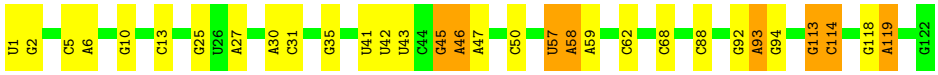
Chain A23S:





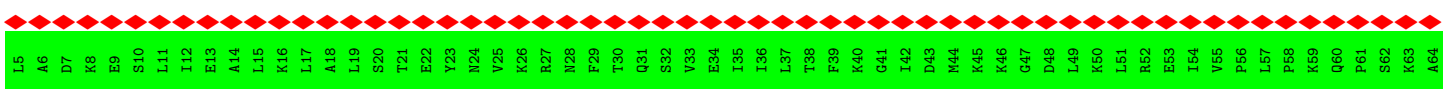
• Molecule 2: 5s rRNA (122-MER)

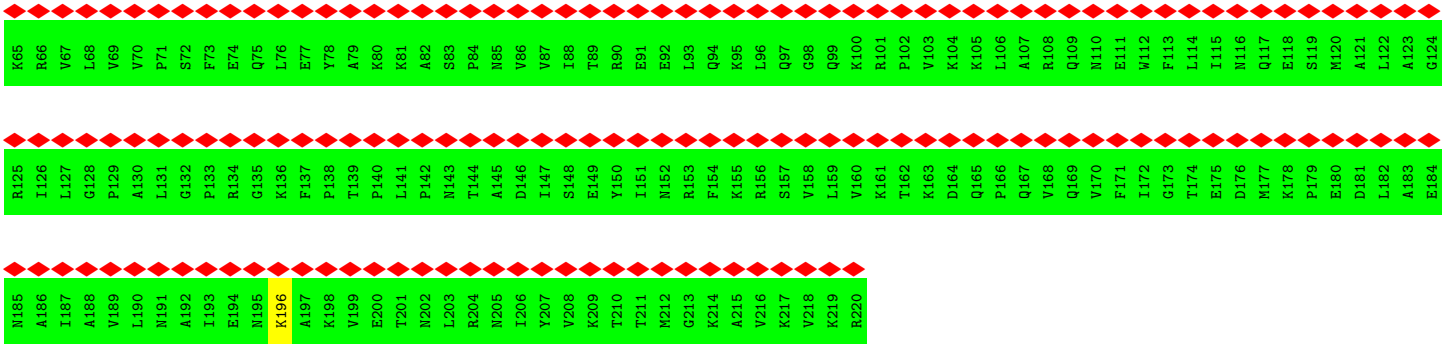
Chain A5S:



• Molecule 3: 50S ribosomal protein L1

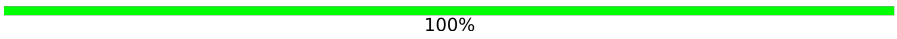
Chain AL1P:





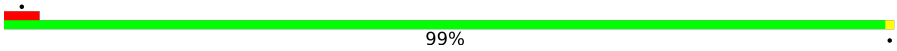
• Molecule 4: 50S ribosomal protein L2

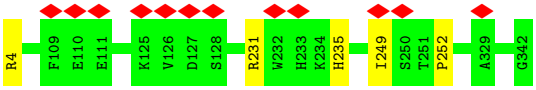
Chain AL2P:



• Molecule 5: 50S ribosomal protein L3

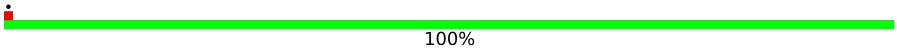
Chain AL3P:

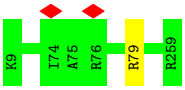




• Molecule 6: 50S ribosomal protein L4

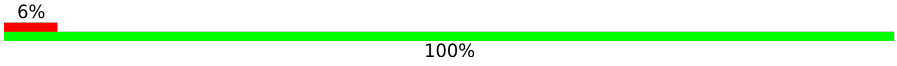
Chain AL4P:

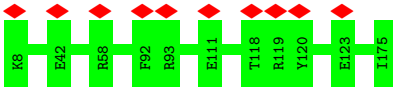




• Molecule 7: 50S ribosomal protein L5

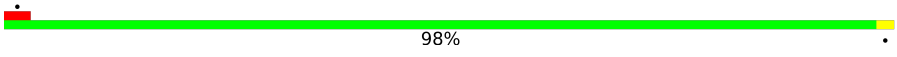
Chain AL5P:

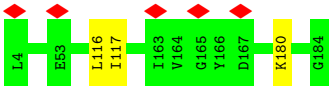




• Molecule 8: 50S ribosomal protein L6

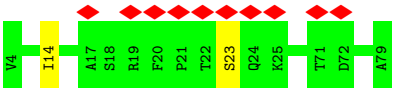
Chain AL6P:





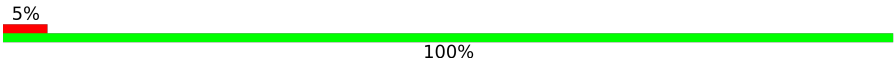
• Molecule 9: 50S ribosomal protein L18Ae

Chain ALX0:



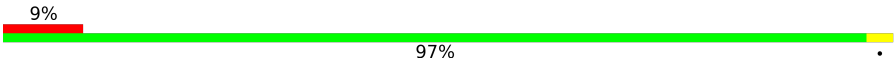
• Molecule 10: 50S ribosomal protein L10e

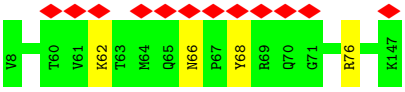
Chain L10E:



• Molecule 11: 50S ribosomal protein L13

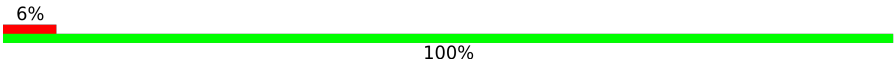
Chain L13P:

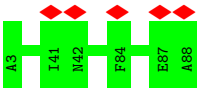




• Molecule 12: 50S ribosomal protein L14e

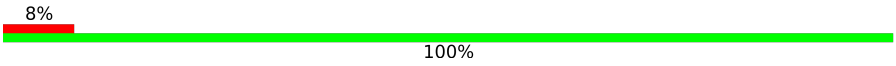
Chain L141:

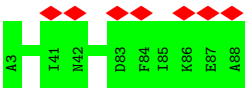




• Molecule 12: 50S ribosomal protein L14e

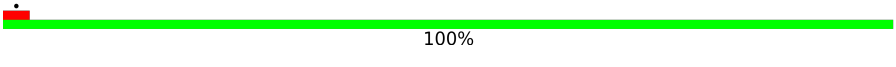
Chain L142:

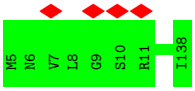




• Molecule 13: 50S ribosomal protein L14

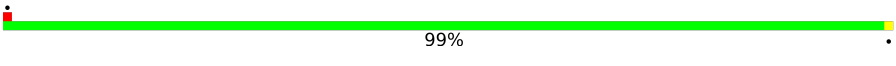
Chain L14P:

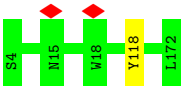




• Molecule 14: 50S ribosomal protein L15e

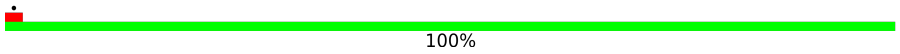
Chain L15E:





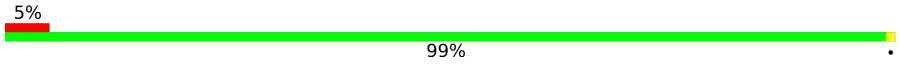
• Molecule 15: 50S ribosomal protein L18e

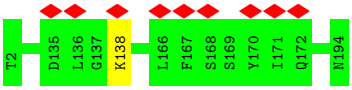
Chain L18E:



• Molecule 16: 50S ribosomal protein L18

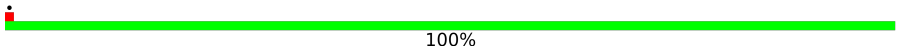
Chain L18P:





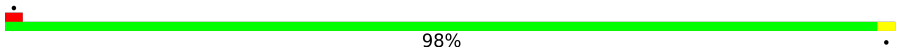
• Molecule 17: 50S ribosomal protein L19e

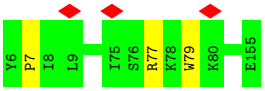
Chain L19E:



• Molecule 18: 50S ribosomal protein L22

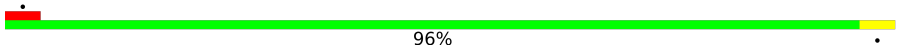
Chain L22P:

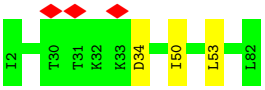




• Molecule 19: 50S ribosomal protein L23

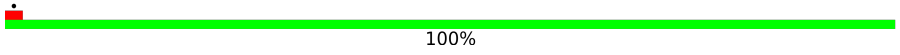
Chain L23P:





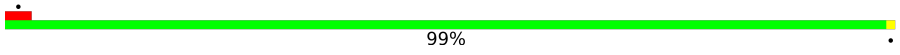
• Molecule 20: 50S ribosomal protein L24e

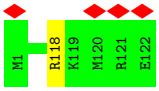
Chain L24E:



• Molecule 21: 50S ribosomal protein L24

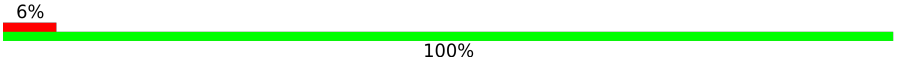
Chain L24P:

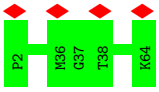




• Molecule 22: 50S ribosomal protein L29

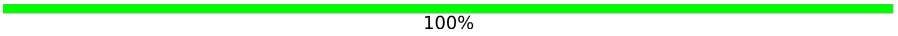
Chain L29P:





• Molecule 23: 50S ribosomal protein L30e

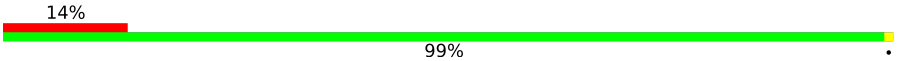
Chain L30E:

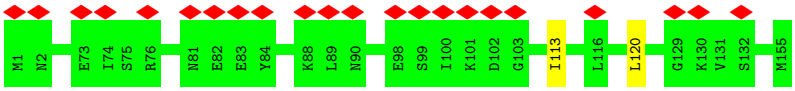


There are no outlier residues recorded for this chain.

• Molecule 24: 50S ribosomal protein L30

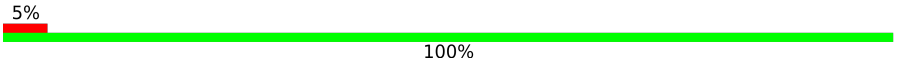
Chain L30P:

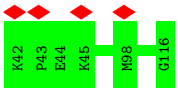




• Molecule 25: 50S ribosomal protein L31e

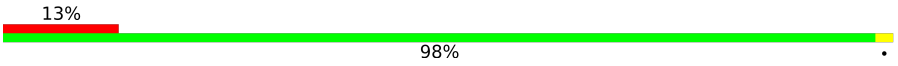
Chain L31E:

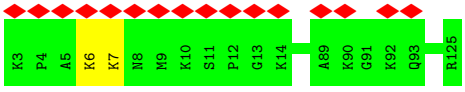




• Molecule 26: 50S ribosomal protein L32e

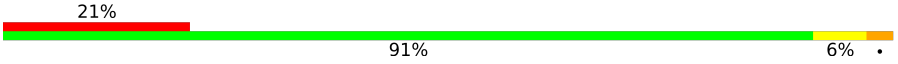
Chain L32E:

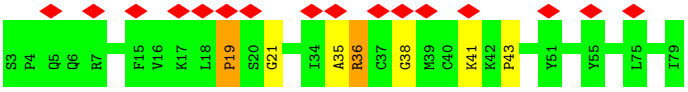




• Molecule 27: 50S ribosomal protein L34e

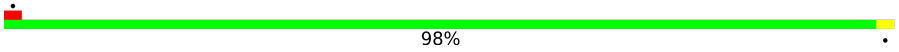
Chain L34E:

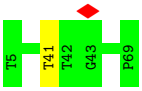




• Molecule 28: 50S ribosomal protein L37Ae

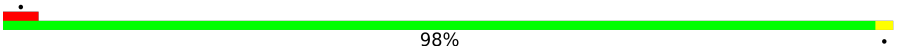
Chain L37A:

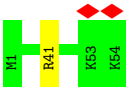




• Molecule 29: 50S ribosomal protein L37e

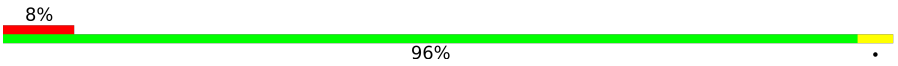
Chain L37E:

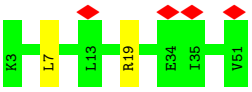




• Molecule 30: 50S ribosomal protein L39e

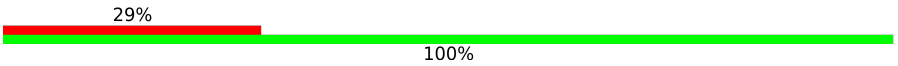
Chain L39E:

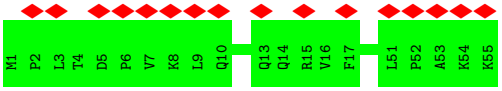




• Molecule 31: 50S ribosomal protein L40E

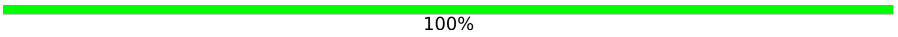
Chain L40E:





• Molecule 32: 50S ribosomal protein L44e

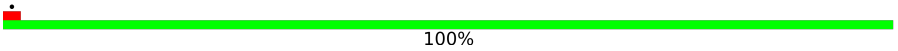
Chain L44E:

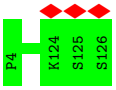


There are no outlier residues recorded for this chain.

• Molecule 33: 50S ribosomal protein L7Ae

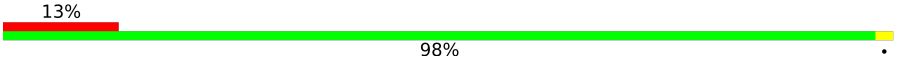
Chain L7A1:

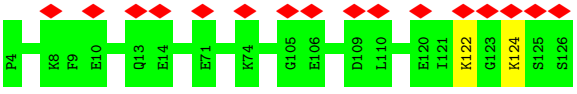




• Molecule 33: 50S ribosomal protein L7Ae

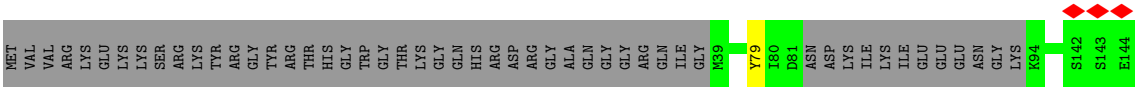
Chain L7A2:





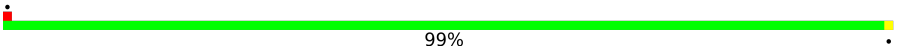
• Molecule 34: 50S ribosomal protein L15

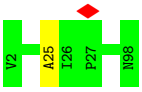
Chain L15P:



• Molecule 35: 50S ribosomal protein L21e

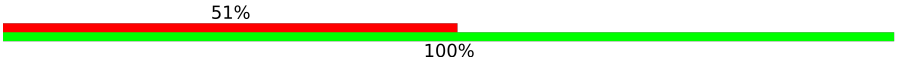
Chain L21E:

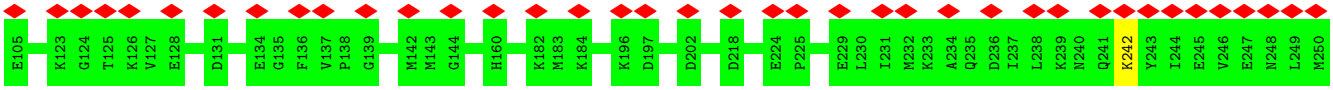


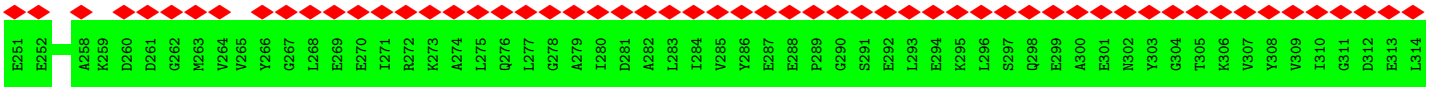


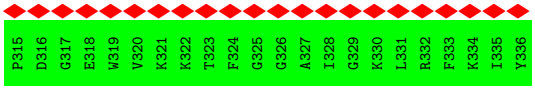
• Molecule 36: Peptide chain release factor subunit 1

Chain ARF1:



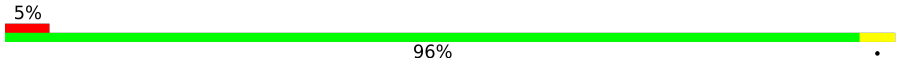


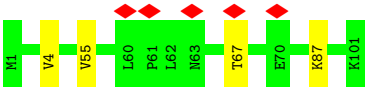




• Molecule 37: DUF2280 domain-containing protein

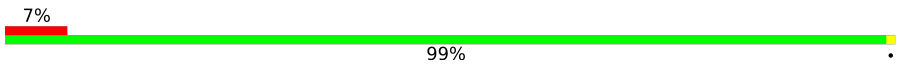
Chain L45A:

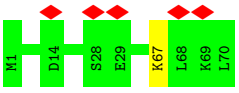




• Molecule 38: Conserved protein

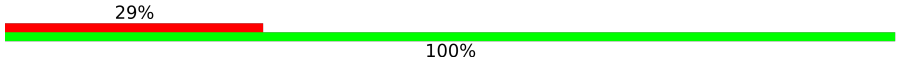
Chain L46A:

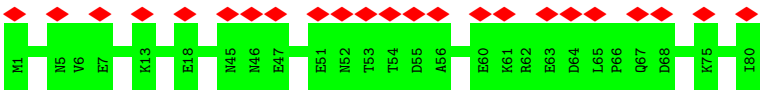




• Molecule 39: 50S ribosomal protein L47A

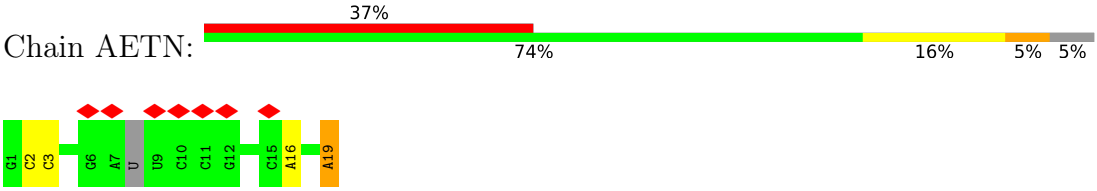
Chain L47A:





• Molecule 40: E-site tRNA

Chain AETN:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	772574	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 ($e^-/Å^2$)	26.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	8.986	Depositor
Minimum map value	-4.723	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.259	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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	A23S	0.89	12/72025 (0.0%)	1.00	230/112376 (0.2%)
2	A5S	0.68	0/2917	0.77	0/4549
3	AL1P	0.24	0/1739	0.49	0/2338
4	AL2P	0.43	0/1787	0.62	1/2409 (0.0%)
5	AL3P	0.46	0/2758	0.62	0/3727
6	AL4P	0.41	0/1956	0.60	1/2635 (0.0%)
7	AL5P	0.31	0/1364	0.57	0/1827
8	AL6P	0.37	0/1450	0.54	0/1949
9	ALX0	0.44	0/638	0.66	0/851
10	L10E	0.41	0/1334	0.60	0/1787
11	L13P	0.45	1/1123 (0.1%)	0.68	1/1502 (0.1%)
12	L141	0.33	0/673	0.54	0/900
12	L142	0.30	0/673	0.52	0/900
13	L14P	0.41	0/1054	0.62	0/1425
14	L15E	0.56	3/1458 (0.2%)	0.67	0/1956
15	L18E	0.38	0/907	0.54	0/1214
16	L18P	0.37	0/1570	0.51	0/2115
17	L19E	0.40	0/1223	0.59	0/1622
18	L22P	0.45	0/1246	0.58	0/1671
19	L23P	0.41	0/655	0.57	1/874 (0.1%)
20	L24E	0.40	0/451	0.53	0/599
21	L24P	0.39	0/1000	0.59	0/1329
22	L29P	0.29	0/513	0.52	0/678
23	L30E	0.38	0/738	0.50	0/985
24	L30P	0.44	0/1278	0.66	1/1713 (0.1%)
25	L31E	0.41	0/632	0.66	0/837
26	L32E	0.48	0/1027	0.61	0/1366
27	L34E	0.51	0/642	0.95	3/854 (0.4%)
28	L37A	0.49	0/542	0.68	0/726
29	L37E	0.49	0/445	0.67	0/585
30	L39E	0.43	0/422	0.76	1/562 (0.2%)
31	L40E	0.32	0/443	0.68	0/587
32	L44E	0.44	0/763	0.61	0/1008
33	L7A1	0.32	0/946	0.44	0/1272

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	L7A2	0.26	0/946	0.44	0/1272
34	L15P	0.38	0/766	0.56	0/1023
35	L21E	0.48	0/800	0.56	0/1067
36	ARF1	0.27	0/1903	0.44	0/2553
37	L45A	0.34	0/824	0.56	0/1094
38	L46A	0.36	0/595	0.51	0/793
39	L47A	0.26	0/652	0.53	0/870
40	AETN	0.50	0/424	0.90	1/657 (0.2%)
All	All	0.75	16/115302 (0.0%)	0.88	240/171057 (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
5	AL3P	0	2
8	AL6P	0	1
9	ALX0	0	2
11	L13P	0	2
18	L22P	0	1
19	L23P	0	1
21	L24P	0	1
24	L30P	0	1
27	L34E	0	4
34	L15P	0	1
35	L21E	0	1
All	All	0	17

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A23S	1179	C	N1-C6	-8.64	1.31	1.37
1	A23S	1179	C	C4-C5	-7.43	1.37	1.43
1	A23S	469	G	C6-N1	-6.18	1.35	1.39
1	A23S	469	G	C8-N7	-6.12	1.27	1.30
1	A23S	1082	G	N9-C4	-5.94	1.33	1.38
14	L15E	118	TYR	CE2-CZ	-5.93	1.30	1.38
1	A23S	2900	A	N9-C4	-5.89	1.34	1.37
1	A23S	1283	A	N9-C4	-5.86	1.34	1.37
1	A23S	2065	A	N9-C4	-5.66	1.34	1.37
1	A23S	2900	A	C5-C6	-5.64	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L13P	76	ARG	C-N	-5.62	1.21	1.34
14	L15E	118	TYR	CD1-CE1	-5.52	1.31	1.39
1	A23S	469	G	C5-C6	-5.34	1.37	1.42
1	A23S	663	C	N3-C4	-5.18	1.30	1.33
1	A23S	469	G	C6-O6	-5.15	1.19	1.24
14	L15E	118	TYR	CD2-CE2	-5.05	1.31	1.39

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A23S	246	C	C2-N1-C1'	18.80	139.48	118.80
1	A23S	246	C	C6-N1-C1'	-18.39	98.74	120.80
1	A23S	469	G	N3-C4-N9	18.33	137.00	126.00
1	A23S	1179	C	C6-N1-C2	-17.79	113.19	120.30
1	A23S	469	G	C8-N9-C1'	-16.41	105.66	127.00
1	A23S	469	G	C6-C5-N7	-15.73	120.96	130.40
1	A23S	469	G	C4-N9-C1'	15.56	146.72	126.50
1	A23S	469	G	N9-C4-C5	-14.84	99.46	105.40
1	A23S	1179	C	C5-C6-N1	14.58	128.29	121.00
1	A23S	469	G	C4-C5-N7	14.15	116.46	110.80
1	A23S	1586	U	C5-C6-N1	14.01	129.70	122.70
1	A23S	1178	C	C6-N1-C2	-13.27	114.99	120.30
1	A23S	1585	C	C6-N1-C2	-13.02	115.09	120.30
1	A23S	1178	C	C2-N1-C1'	12.90	132.99	118.80
1	A23S	1626	C	C6-N1-C2	-12.82	115.17	120.30
1	A23S	2034	C	OP2-P-O3'	-11.78	79.28	105.20
1	A23S	255	A	OP2-P-O3'	-11.13	80.71	105.20
1	A23S	1179	C	N3-C4-N4	10.97	125.68	118.00
1	A23S	1082	G	N3-C4-N9	-10.47	119.72	126.00
1	A23S	469	G	N3-C4-C5	-10.17	123.52	128.60
1	A23S	1179	C	N3-C4-C5	-10.12	117.85	121.90
1	A23S	668	A	O4'-C1'-N9	10.05	116.24	108.20
1	A23S	469	G	C5-C6-O6	-9.95	122.63	128.60
1	A23S	2762	G	N3-C4-C5	-9.87	123.67	128.60
1	A23S	1082	G	N3-C4-C5	9.83	133.52	128.60
1	A23S	246	C	N1-C2-N3	-9.73	112.39	119.20
1	A23S	1625	C	N3-C2-O2	-9.71	115.11	121.90
1	A23S	246	C	C5-C6-N1	9.51	125.75	121.00
1	A23S	2641	C	N3-C2-O2	-9.34	115.36	121.90
1	A23S	246	C	C5-C4-N4	-9.24	113.73	120.20
1	A23S	1625	C	O4'-C1'-N1	9.17	115.54	108.20
1	A23S	246	C	C4-C5-C6	-9.12	112.84	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A23S	246	C	O4'-C1'-N1	9.07	115.45	108.20
1	A23S	255	A	OP1-P-O3'	-8.87	85.69	105.20
1	A23S	2762	G	C8-N9-C4	-8.83	102.87	106.40
1	A23S	2777	C	C2-N1-C1'	-8.82	109.09	118.80
1	A23S	2159	C	C6-N1-C2	8.78	123.81	120.30
1	A23S	2641	C	C6-N1-C2	-8.66	116.84	120.30
1	A23S	2034	C	OP1-P-O3'	-8.60	86.28	105.20
1	A23S	2777	C	C6-N1-C1'	8.58	131.09	120.80
1	A23S	2531	C	O4'-C1'-N1	8.56	115.05	108.20
1	A23S	669	A	O5'-P-OP2	-8.53	98.03	105.70
1	A23S	1585	C	N3-C2-O2	-8.46	115.98	121.90
1	A23S	2035	G	OP1-P-OP2	8.29	132.04	119.60
1	A23S	1179	C	C2-N1-C1'	8.26	127.89	118.80
1	A23S	2159	C	N1-C2-O2	8.20	123.82	118.90
1	A23S	1626	C	N3-C4-C5	-8.19	118.62	121.90
1	A23S	1178	C	N3-C2-O2	-8.17	116.18	121.90
1	A23S	1178	C	N1-C2-O2	8.10	123.76	118.90
1	A23S	1178	C	C5-C6-N1	7.88	124.94	121.00
1	A23S	246	C	N3-C4-C5	7.86	125.05	121.90
1	A23S	2777	C	N3-C4-N4	-7.74	112.58	118.00
1	A23S	668	A	P-O3'-C3'	7.69	128.93	119.70
1	A23S	2159	C	N3-C4-C5	7.69	124.97	121.90
24	L30P	120	LEU	C-N-CA	7.58	140.65	121.70
1	A23S	926	U	C2-N1-C1'	7.56	126.77	117.70
1	A23S	664	U	N1-C2-O2	-7.55	117.52	122.80
1	A23S	336	A	O4'-C1'-N9	7.54	114.23	108.20
1	A23S	668	A	N1-C2-N3	7.49	133.05	129.30
1	A23S	1178	C	C6-N1-C1'	-7.43	111.88	120.80
1	A23S	2762	G	O4'-C1'-N9	7.42	114.14	108.20
1	A23S	1457	U	C2-N1-C1'	7.41	126.59	117.70
1	A23S	2738	A	N1-C6-N6	7.37	123.02	118.60
1	A23S	2159	C	C4-C5-C6	-7.37	113.71	117.40
1	A23S	1082	G	C2-N3-C4	-7.33	108.24	111.90
1	A23S	663	C	C2-N3-C4	7.32	123.56	119.90
1	A23S	2738	A	C5-C6-N6	-7.30	117.86	123.70
1	A23S	247	C	C2-N1-C1'	7.28	126.81	118.80
1	A23S	2900	A	N1-C6-N6	7.22	122.93	118.60
1	A23S	2900	A	N9-C4-C5	-7.19	102.92	105.80
1	A23S	2777	C	C5-C4-N4	7.18	125.23	120.20
1	A23S	2705	G	O4'-C1'-N9	7.10	113.88	108.20
1	A23S	668	A	N9-C1'-C2'	7.09	123.22	114.00
1	A23S	525	G	O4'-C1'-N9	7.02	113.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A23S	2900	A	C4-C5-N7	6.98	114.19	110.70
1	A23S	1157	A	C2-N3-C4	-6.89	107.16	110.60
1	A23S	1179	C	O5'-P-OP2	6.86	118.93	110.70
1	A23S	129	C	N3-C2-O2	-6.85	117.10	121.90
27	L34E	36	ARG	CB-CA-C	-6.79	96.81	110.40
1	A23S	1355	G	C4-N9-C1'	6.78	135.31	126.50
1	A23S	2762	G	C2-N3-C4	6.76	115.28	111.90
1	A23S	1248	C	N3-C2-O2	-6.76	117.17	121.90
1	A23S	1626	C	C5-C6-N1	6.76	124.38	121.00
1	A23S	1586	U	C6-N1-C2	-6.73	116.96	121.00
1	A23S	2180	A	C8-N9-C4	-6.72	103.11	105.80
1	A23S	2159	C	N1-C2-N3	-6.72	114.50	119.20
1	A23S	256	A	OP1-P-OP2	6.71	129.66	119.60
1	A23S	2900	A	C5-C6-N6	-6.66	118.38	123.70
1	A23S	1179	C	N1-C2-O2	6.65	122.89	118.90
1	A23S	1726	A	C2-N3-C4	6.64	113.92	110.60
1	A23S	1614	C	N3-C2-O2	-6.64	117.25	121.90
1	A23S	501	A	O4'-C1'-N9	6.60	113.48	108.20
1	A23S	1355	G	N3-C4-C5	-6.58	125.31	128.60
1	A23S	1283	A	C2-N3-C4	-6.55	107.32	110.60
1	A23S	1585	C	C2-N1-C1'	6.50	125.95	118.80
1	A23S	1179	C	C2-N3-C4	6.50	123.15	119.90
1	A23S	2762	G	N3-C4-N9	6.50	129.90	126.00
1	A23S	1777	C	C5-C6-N1	6.50	124.25	121.00
1	A23S	555	G	O4'-C1'-N9	6.47	113.38	108.20
1	A23S	2404	G	O4'-C1'-N9	6.45	113.36	108.20
1	A23S	1625	C	N1-C2-O2	6.43	122.76	118.90
1	A23S	664	U	N1-C2-N3	6.40	118.74	114.90
1	A23S	1802	C	C2-N1-C1'	6.39	125.83	118.80
1	A23S	1614	C	C6-N1-C2	-6.38	117.75	120.30
1	A23S	2762	G	C4-N9-C1'	6.37	134.78	126.50
30	L39E	7	LEU	CA-CB-CG	6.35	129.90	115.30
1	A23S	469	G	O4'-C1'-N9	6.32	113.25	108.20
1	A23S	469	G	C4-C5-C6	6.29	122.57	118.80
1	A23S	668	A	C3'-C2'-C1'	-6.28	96.47	101.50
1	A23S	1682	G	N1-C6-O6	-6.28	116.13	119.90
1	A23S	1394	C	C6-N1-C2	-6.26	117.80	120.30
1	A23S	1626	C	N3-C2-O2	-6.21	117.55	121.90
1	A23S	1545	C	N3-C2-O2	-6.21	117.56	121.90
1	A23S	1575	A	O4'-C1'-N9	6.19	113.15	108.20
1	A23S	2053	C	N3-C2-O2	-6.18	117.57	121.90
1	A23S	1726	A	N7-C8-N9	6.17	116.89	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A23S	1248	C	N1-C2-O2	6.15	122.59	118.90
1	A23S	1544	C	N3-C2-O2	-6.14	117.60	121.90
1	A23S	1777	C	C6-N1-C2	-6.14	117.84	120.30
1	A23S	2762	G	N7-C8-N9	6.12	116.16	113.10
1	A23S	1355	G	N3-C4-N9	6.08	129.65	126.00
1	A23S	246	C	N3-C2-O2	6.08	126.16	121.90
1	A23S	851	C	N3-C2-O2	-6.07	117.65	121.90
1	A23S	1179	C	O4'-C1'-N1	6.05	113.04	108.20
1	A23S	450	G	O4'-C1'-N9	6.04	113.03	108.20
1	A23S	2900	A	C8-N9-C4	6.00	108.20	105.80
1	A23S	1355	G	C8-N9-C1'	-6.00	119.20	127.00
1	A23S	1178	C	N3-C4-N4	5.96	122.17	118.00
1	A23S	1121	A	P-O3'-C3'	5.92	126.81	119.70
1	A23S	1573	C	O4'-C1'-N1	5.92	112.94	108.20
1	A23S	2738	A	C6-C5-N7	-5.90	128.17	132.30
1	A23S	1450	C	N3-C4-C5	5.90	124.26	121.90
1	A23S	668	A	C2-N3-C4	-5.89	107.65	110.60
1	A23S	668	A	OP1-P-O3'	5.85	118.08	105.20
1	A23S	1682	G	N1-C2-N2	-5.85	110.94	116.20
1	A23S	1614	C	N1-C2-O2	5.84	122.40	118.90
1	A23S	1179	C	C5'-C4'-O4'	5.82	116.08	109.10
1	A23S	1672	A	O4'-C1'-N9	5.81	112.85	108.20
1	A23S	366	G	N3-C4-C5	5.80	131.50	128.60
1	A23S	1071	A	N3-C4-C5	-5.79	122.75	126.80
1	A23S	247	C	C6-N1-C1'	-5.77	113.88	120.80
1	A23S	668	A	C6-C5-N7	-5.75	128.28	132.30
1	A23S	366	G	N3-C4-N9	-5.72	122.57	126.00
1	A23S	778	C	N3-C2-O2	-5.71	117.91	121.90
1	A23S	1082	G	C8-N9-C1'	5.71	134.42	127.00
1	A23S	1585	C	O4'-C1'-N1	5.70	112.76	108.20
1	A23S	1587	G	N1-C2-N2	-5.70	111.07	116.20
1	A23S	1587	G	N3-C4-C5	-5.69	125.75	128.60
1	A23S	1634	C	O4'-C1'-N1	5.69	112.75	108.20
1	A23S	1179	C	N3-C2-O2	-5.68	117.93	121.90
1	A23S	2570	G	N1-C6-O6	-5.66	116.51	119.90
1	A23S	136	U	C5-C6-N1	5.65	125.53	122.70
1	A23S	469	G	C5-C6-N1	5.64	114.32	111.50
1	A23S	920	G	P-O3'-C3'	5.64	126.47	119.70
1	A23S	450	G	N7-C8-N9	5.64	115.92	113.10
1	A23S	1071	A	C8-N9-C4	-5.63	103.55	105.80
1	A23S	482	C	N3-C2-O2	-5.62	117.97	121.90
1	A23S	1395	A	O4'-C1'-N9	-5.61	103.71	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A23S	243	C	N1-C2-O2	5.60	122.26	118.90
1	A23S	1177	U	P-O3'-C3'	5.59	126.41	119.70
1	A23S	1625	C	C4'-C3'-C2'	-5.59	97.01	102.60
1	A23S	1586	U	C4-C5-C6	-5.58	116.35	119.70
1	A23S	778	C	N1-C2-O2	5.58	122.25	118.90
1	A23S	1729	G	N3-C4-N9	5.58	129.35	126.00
1	A23S	2794	G	C5-C6-O6	5.58	131.95	128.60
1	A23S	1458	U	C2-N1-C1'	5.57	124.38	117.70
1	A23S	1776	G	N9-C4-C5	-5.57	103.17	105.40
4	AL2P	176	TRP	CA-CB-CG	-5.52	103.22	113.70
1	A23S	2835	A	OP2-P-O3'	5.50	117.30	105.20
1	A23S	602	C	C2-N1-C1'	5.50	124.85	118.80
1	A23S	2090	C	N3-C2-O2	-5.50	118.05	121.90
1	A23S	450	G	C4-N9-C1'	5.48	133.62	126.50
1	A23S	1776	G	O5'-P-OP1	5.48	117.27	110.70
1	A23S	2835	A	P-O3'-C3'	5.48	126.27	119.70
1	A23S	667	A	C4-C5-C6	5.47	119.74	117.00
1	A23S	1625	C	C3'-C2'-C1'	-5.47	97.12	101.50
1	A23S	450	G	C4-C5-N7	5.44	112.98	110.80
1	A23S	1444	G	C4-C5-N7	5.44	112.98	110.80
1	A23S	2625	C	C6-N1-C2	-5.42	118.13	120.30
1	A23S	1683	G	O4'-C1'-N9	5.41	112.53	108.20
1	A23S	469	G	C5-N7-C8	-5.41	101.59	104.30
1	A23S	1625	C	P-O3'-C3'	5.39	126.17	119.70
1	A23S	926	U	C6-N1-C1'	-5.39	113.66	121.20
1	A23S	2180	A	C4-C5-C6	5.38	119.69	117.00
1	A23S	1179	C	C5-C4-N4	-5.36	116.44	120.20
1	A23S	2777	C	N1-C2-N3	5.33	122.93	119.20
1	A23S	482	C	C6-N1-C2	-5.33	118.17	120.30
1	A23S	450	G	C6-C5-N7	-5.33	127.20	130.40
1	A23S	2053	C	N1-C2-O2	5.32	122.09	118.90
1	A23S	1672	A	N7-C8-N9	5.31	116.45	113.80
1	A23S	1545	C	C2-N1-C1'	5.30	124.63	118.80
40	AETN	19	A	N7-C8-N9	5.30	116.45	113.80
1	A23S	920	G	OP1-P-O3'	5.30	116.86	105.20
19	L23P	53	LEU	CA-CB-CG	5.29	127.48	115.30
1	A23S	2763	A	N1-C2-N3	5.29	131.95	129.30
1	A23S	1545	C	C6-N1-C2	-5.29	118.18	120.30
1	A23S	2549	A	O4'-C1'-N9	5.29	112.43	108.20
1	A23S	1444	G	O4'-C1'-N9	5.29	112.43	108.20
1	A23S	156	U	N3-C2-O2	-5.28	118.50	122.20
1	A23S	663	C	C5-C6-N1	5.28	123.64	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A23S	1444	G	C5-N7-C8	-5.27	101.67	104.30
1	A23S	1585	C	C4-C5-C6	5.26	120.03	117.40
1	A23S	344	U	O4'-C1'-N1	5.26	112.41	108.20
1	A23S	450	G	C5-N7-C8	-5.26	101.67	104.30
1	A23S	2543	C	N3-C2-O2	-5.25	118.22	121.90
1	A23S	482	C	C2-N1-C1'	5.24	124.56	118.80
1	A23S	1809	G	N3-C4-N9	5.22	129.13	126.00
1	A23S	1457	U	C6-N1-C1'	-5.22	113.89	121.20
1	A23S	2180	A	N7-C8-N9	5.21	116.41	113.80
1	A23S	1444	G	C4-N9-C1'	5.21	133.27	126.50
1	A23S	1726	A	C5-C6-N1	5.21	120.31	117.70
1	A23S	1444	G	C6-C5-N7	-5.20	127.28	130.40
1	A23S	2053	C	C6-N1-C2	-5.20	118.22	120.30
1	A23S	663	C	C6-N1-C2	-5.20	118.22	120.30
1	A23S	1444	G	N7-C8-N9	5.20	115.70	113.10
1	A23S	1544	C	C6-N1-C2	-5.20	118.22	120.30
1	A23S	1541	A	O4'-C1'-N9	5.19	112.35	108.20
1	A23S	418	G	N3-C4-N9	-5.18	122.89	126.00
1	A23S	802	G	C4-C5-N7	5.18	112.87	110.80
1	A23S	109	U	P-O3'-C3'	5.16	125.89	119.70
1	A23S	1777	C	O5'-P-OP1	-5.15	101.07	105.70
1	A23S	2888	C	C2-N1-C1'	5.14	124.46	118.80
1	A23S	2180	A	C6-C5-N7	-5.14	128.70	132.30
27	L34E	21	GLY	N-CA-C	5.14	125.95	113.10
1	A23S	1625	C	C6-N1-C2	-5.14	118.25	120.30
1	A23S	2379	A	N1-C2-N3	5.12	131.86	129.30
1	A23S	869	U	C2-N1-C1'	5.11	123.83	117.70
6	AL4P	79	ARG	CB-CG-CD	-5.11	98.32	111.60
1	A23S	469	G	N1-C6-O6	5.11	122.96	119.90
27	L34E	19	PRO	N-CA-C	5.09	125.34	112.10
1	A23S	778	C	C2-N1-C1'	5.09	124.40	118.80
1	A23S	2692	G	N9-C4-C5	5.08	107.43	105.40
1	A23S	2582	C	C2-N1-C1'	5.08	124.39	118.80
1	A23S	1178	C	P-O3'-C3'	5.06	125.77	119.70
1	A23S	1082	G	C4-N9-C1'	-5.05	119.93	126.50
1	A23S	1614	C	C2-N1-C1'	5.04	124.34	118.80
1	A23S	449	A	O4'-C1'-N9	5.02	112.22	108.20
1	A23S	146	U	P-O3'-C3'	5.02	125.72	119.70
1	A23S	1720	C	C6-N1-C2	-5.01	118.29	120.30
11	L13P	66	ASN	N-CA-C	5.01	124.52	111.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AL3P	235	HIS	Peptide
5	AL3P	252	PRO	Peptide
8	AL6P	180	LYS	Peptide
9	ALX0	14	ILE	Peptide
9	ALX0	23	SER	Peptide
11	L13P	62	LYS	Peptide
11	L13P	68	TYR	Peptide
34	L15P	79	TYR	Peptide
35	L21E	25	ALA	Peptide
18	L22P	79	TRP	Peptide
19	L23P	34	ASP	Peptide
21	L24P	118	ARG	Peptide
24	L30P	113	ILE	Peptide
27	L34E	36	ARG	Peptide
27	L34E	38	GLY	Peptide
27	L34E	41	LYS	Peptide
27	L34E	43	PRO	Peptide

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	A23S	64335	0	0	0	0
2	A5S	2609	0	1324	15	0
3	AL1P	1715	0	0	0	0
4	AL2P	1754	0	0	0	0
5	AL3P	2695	0	0	0	0
6	AL4P	1926	0	0	0	0
7	AL5P	1343	0	0	0	0
8	AL6P	1431	0	0	0	0
9	ALX0	629	0	0	0	0
10	L10E	1310	0	0	0	0
11	L13P	1109	0	0	0	0
12	L141	669	0	0	0	0
12	L142	669	0	0	0	0
13	L14P	1034	0	0	0	0
14	L15E	1423	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	L18E	895	0	0	0	0
16	L18P	1539	0	0	0	0
17	L19E	1206	0	0	0	0
18	L22P	1223	0	0	0	0
19	L23P	650	0	0	0	0
20	L24E	441	0	0	0	0
21	L24P	989	0	0	0	0
22	L29P	513	0	0	0	0
23	L30E	729	0	0	0	0
24	L30P	1254	0	0	0	0
25	L31E	625	0	0	0	0
26	L32E	1010	0	0	0	0
27	L34E	629	0	0	0	0
28	L37A	527	0	0	0	0
29	L37E	436	0	0	0	0
30	L39E	414	0	0	0	0
31	L40E	439	0	0	0	0
32	L44E	753	0	0	0	0
33	L7A1	935	0	0	0	0
33	L7A2	935	0	0	0	0
34	L15P	752	0	0	0	0
35	L21E	785	0	0	0	0
36	ARF1	1869	0	0	0	0
37	L45A	816	0	0	0	0
38	L46A	586	0	0	0	0
39	L47A	648	0	0	0	0
40	AETN	381	0	0	0	0
All	All	106630	0	1324	15	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 7.

All (15) 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)
2:A5S:6:A:H61	2:A5S:119:A:H61	1.37	0.72
2:A5S:57:U:H4'	2:A5S:58:A:O5'	2.06	0.56
2:A5S:41:U:O2'	2:A5S:46:A:N6	2.39	0.54
2:A5S:6:A:H61	2:A5S:119:A:N6	2.05	0.53
2:A5S:6:A:N6	2:A5S:119:A:H61	2.08	0.50
2:A5S:113:G:HO2'	2:A5S:114:C:P	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A5S:92:G:H2'	2:A5S:93:A:C8	2.52	0.44
2:A5S:1:U:H2'	2:A5S:2:G:O4'	2.18	0.43
2:A5S:30:A:H2'	2:A5S:31:C:C6	2.53	0.43
2:A5S:1:U:H3'	2:A5S:2:G:H8	1.83	0.43
2:A5S:6:A:N1	2:A5S:119:A:N1	2.67	0.42
2:A5S:6:A:H5'	2:A5S:62:C:H4'	2.03	0.41
2:A5S:35:G:N2	2:A5S:50:C:O2	2.54	0.41
2:A5S:35:G:O6	2:A5S:45:G:H1'	2.20	0.41
2:A5S:41:U:HO2'	2:A5S:46:A:N6	2.17	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AL1P	214/216 (99%)	202 (94%)	12 (6%)	0	100	100
4	AL2P	232/234 (99%)	222 (96%)	10 (4%)	0	100	100
5	AL3P	337/339 (99%)	300 (89%)	36 (11%)	1 (0%)	37	60
6	AL4P	249/251 (99%)	235 (94%)	14 (6%)	0	100	100
7	AL5P	166/168 (99%)	152 (92%)	14 (8%)	0	100	100
8	AL6P	179/181 (99%)	167 (93%)	10 (6%)	2 (1%)	12	28
9	ALX0	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
10	L10E	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
11	L13P	138/140 (99%)	125 (91%)	13 (9%)	0	100	100
12	L141	84/86 (98%)	76 (90%)	8 (10%)	0	100	100
12	L142	84/86 (98%)	77 (92%)	7 (8%)	0	100	100
13	L14P	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
14	L15E	167/169 (99%)	160 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	L18E	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
16	L18P	191/193 (99%)	176 (92%)	15 (8%)	0	100	100
17	L19E	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
18	L22P	148/150 (99%)	135 (91%)	12 (8%)	1 (1%)	19	40
19	L23P	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
20	L24E	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
21	L24P	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
22	L29P	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
23	L30E	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
24	L30P	153/155 (99%)	126 (82%)	27 (18%)	0	100	100
25	L31E	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
26	L32E	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
27	L34E	75/77 (97%)	47 (63%)	26 (35%)	2 (3%)	4	10
28	L37A	63/65 (97%)	56 (89%)	6 (10%)	1 (2%)	8	19
29	L37E	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
30	L39E	47/49 (96%)	39 (83%)	7 (15%)	1 (2%)	5	14
31	L40E	53/55 (96%)	35 (66%)	18 (34%)	0	100	100
32	L44E	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
33	L7A1	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
33	L7A2	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
34	L15P	90/144 (62%)	85 (94%)	5 (6%)	0	100	100
35	L21E	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
36	ARF1	230/232 (99%)	224 (97%)	6 (3%)	0	100	100
37	L45A	99/101 (98%)	73 (74%)	23 (23%)	3 (3%)	3	8
38	L46A	68/70 (97%)	61 (90%)	7 (10%)	0	100	100
39	L47A	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
All	All	4842/4972 (97%)	4452 (92%)	379 (8%)	11 (0%)	45	67

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AL3P	231	ARG
37	L45A	4	VAL

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Mol	Chain	Res	Type
37	L45A	55	VAL
37	L45A	67	THR
8	AL6P	117	ILE
8	AL6P	116	LEU
27	L34E	19	PRO
28	L37A	41	THR
27	L34E	35	ALA
30	L39E	19	ARG
18	L22P	7	PRO

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	AL1P	189/190 (100%)	188 (100%)	1 (0%)	86 95
4	AL2P	181/181 (100%)	181 (100%)	0	100 100
5	AL3P	297/297 (100%)	295 (99%)	2 (1%)	81 92
6	AL4P	212/212 (100%)	212 (100%)	0	100 100
7	AL5P	144/144 (100%)	144 (100%)	0	100 100
8	AL6P	157/157 (100%)	157 (100%)	0	100 100
9	ALX0	68/68 (100%)	68 (100%)	0	100 100
10	L10E	137/137 (100%)	137 (100%)	0	100 100
11	L13P	121/121 (100%)	121 (100%)	0	100 100
12	L141	74/74 (100%)	74 (100%)	0	100 100
12	L142	74/74 (100%)	74 (100%)	0	100 100
13	L14P	110/110 (100%)	110 (100%)	0	100 100
14	L15E	146/146 (100%)	146 (100%)	0	100 100
15	L18E	98/98 (100%)	98 (100%)	0	100 100
16	L18P	162/162 (100%)	161 (99%)	1 (1%)	84 93
17	L19E	126/126 (100%)	126 (100%)	0	100 100
18	L22P	131/131 (100%)	130 (99%)	1 (1%)	79 91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	L23P	74/74 (100%)	73 (99%)	1 (1%)	62 83
20	L24E	50/50 (100%)	50 (100%)	0	100 100
21	L24P	108/108 (100%)	108 (100%)	0	100 100
22	L29P	59/59 (100%)	59 (100%)	0	100 100
23	L30E	83/83 (100%)	83 (100%)	0	100 100
24	L30P	136/136 (100%)	136 (100%)	0	100 100
25	L31E	66/66 (100%)	66 (100%)	0	100 100
26	L32E	106/106 (100%)	104 (98%)	2 (2%)	52 77
27	L34E	70/70 (100%)	70 (100%)	0	100 100
28	L37A	53/53 (100%)	53 (100%)	0	100 100
29	L37E	45/45 (100%)	44 (98%)	1 (2%)	47 74
30	L39E	44/44 (100%)	44 (100%)	0	100 100
31	L40E	50/50 (100%)	50 (100%)	0	100 100
32	L44E	84/84 (100%)	84 (100%)	0	100 100
33	L7A1	104/104 (100%)	104 (100%)	0	100 100
33	L7A2	104/104 (100%)	102 (98%)	2 (2%)	52 77
34	L15P	78/118 (66%)	78 (100%)	0	100 100
35	L21E	85/85 (100%)	85 (100%)	0	100 100
36	ARF1	199/199 (100%)	198 (100%)	1 (0%)	86 95
37	L45A	91/91 (100%)	90 (99%)	1 (1%)	70 87
38	L46A	66/66 (100%)	65 (98%)	1 (2%)	60 82
39	L47A	74/74 (100%)	74 (100%)	0	100 100
All	All	4256/4297 (99%)	4242 (100%)	14 (0%)	90 97

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AL1P	196	LYS
5	AL3P	4	ARG
5	AL3P	249	ILE
16	L18P	138	LYS
18	L22P	77	ARG
19	L23P	50	ILE
26	L32E	6	LYS

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Mol	Chain	Res	Type
26	L32E	7	LYS
29	L37E	41	ARG
33	L7A2	122	LYS
33	L7A2	124	LYS
36	ARF1	242	LYS
37	L45A	87	LYS
38	L46A	67	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	A23S	2988/3022 (98%)	561 (18%)	42 (1%)
2	A5S	121/122 (99%)	19 (15%)	2 (1%)
40	AETN	16/19 (84%)	4 (25%)	1 (6%)
All	All	3125/3163 (98%)	584 (18%)	45 (1%)

All (584) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A23S	7	G
1	A23S	25	C
1	A23S	29	U
1	A23S	30	C
1	A23S	31	G
1	A23S	41	G
1	A23S	45	G
1	A23S	51	G
1	A23S	53	A
1	A23S	61	A
1	A23S	64	U
1	A23S	65	G
1	A23S	74	A
1	A23S	80	A
1	A23S	81	A
1	A23S	85	G
1	A23S	86	C
1	A23S	108	A
1	A23S	109	U

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Mol	Chain	Res	Type
1	A23S	110	G
1	A23S	115	A
1	A23S	118	C
1	A23S	125	G
1	A23S	127	U
1	A23S	137	C
1	A23S	144	U
1	A23S	146	U
1	A23S	147	A
1	A23S	157	G
1	A23S	160	A
1	A23S	175	A
1	A23S	178	A
1	A23S	179	U
1	A23S	194	G
1	A23S	195	A
1	A23S	196	A
1	A23S	200	A
1	A23S	201	A
1	A23S	204	C
1	A23S	206	A
1	A23S	207	U
1	A23S	208	U
1	A23S	209	G
1	A23S	212	A
1	A23S	227	G
1	A23S	242	A
1	A23S	244	A
1	A23S	245	G
1	A23S	246	C
1	A23S	268	U
1	A23S	276	U
1	A23S	281	A
1	A23S	288	G
1	A23S	289	U
1	A23S	292	C
1	A23S	293	G
1	A23S	302	C
1	A23S	304	U
1	A23S	317	C
1	A23S	318	G
1	A23S	319	G

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Mol	Chain	Res	Type
1	A23S	337	G
1	A23S	344	U
1	A23S	345	C
1	A23S	354	C
1	A23S	360	G
1	A23S	368	G
1	A23S	372	G
1	A23S	373	A
1	A23S	374	A
1	A23S	381	G
1	A23S	383	A
1	A23S	385	G
1	A23S	390	A
1	A23S	391	G
1	A23S	400	A
1	A23S	403	G
1	A23S	405	G
1	A23S	418	G
1	A23S	419	U
1	A23S	420	A
1	A23S	434	U
1	A23S	455	C
1	A23S	464	C
1	A23S	468	G
1	A23S	469	G
1	A23S	470	C
1	A23S	472	A
1	A23S	476	A
1	A23S	482	C
1	A23S	494	C
1	A23S	498	C
1	A23S	499	U
1	A23S	500	A
1	A23S	501	A
1	A23S	502	G
1	A23S	511	G
1	A23S	525	G
1	A23S	536	G
1	A23S	547	A
1	A23S	548	A
1	A23S	549	G
1	A23S	550	A

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Mol	Chain	Res	Type
1	A23S	551	G
1	A23S	552	C
1	A23S	563	G
1	A23S	572	C
1	A23S	573	A
1	A23S	574	G
1	A23S	575	G
1	A23S	577	U
1	A23S	589	G
1	A23S	594	G
1	A23S	621	G
1	A23S	628	G
1	A23S	638	G
1	A23S	642	G
1	A23S	643	A
1	A23S	645	C
1	A23S	658	U
1	A23S	667	A
1	A23S	668	A
1	A23S	669	A
1	A23S	670	C
1	A23S	671	A
1	A23S	674	G
1	A23S	682	A
1	A23S	683	G
1	A23S	694	U
1	A23S	699	A
1	A23S	706	G
1	A23S	713	A
1	A23S	720	A
1	A23S	721	A
1	A23S	727	A
1	A23S	734	C
1	A23S	737	A
1	A23S	740	G
1	A23S	741	C
1	A23S	753	U
1	A23S	754	U
1	A23S	755	U
1	A23S	757	U
1	A23S	758	A
1	A23S	769	A

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Mol	Chain	Res	Type
1	A23S	777	U
1	A23S	778	C
1	A23S	787	A
1	A23S	802	G
1	A23S	803	G
1	A23S	807	G
1	A23S	808	A
1	A23S	809	A
1	A23S	810	A
1	A23S	818	A
1	A23S	819	U
1	A23S	844	G
1	A23S	847	G
1	A23S	848	A
1	A23S	863	G
1	A23S	868	A
1	A23S	870	A
1	A23S	878	U
1	A23S	879	G
1	A23S	883	U
1	A23S	892	U
1	A23S	894	C
1	A23S	901	C
1	A23S	911	G
1	A23S	912	G
1	A23S	915	C
1	A23S	918	A
1	A23S	920	G
1	A23S	921	A
1	A23S	925	A
1	A23S	927	C
1	A23S	928	U
1	A23S	941	G
1	A23S	948	C
1	A23S	963	C
1	A23S	964	C
1	A23S	966	A
1	A23S	981	A
1	A23S	996	G
1	A23S	1001	G
1	A23S	1004	A
1	A23S	1046	A

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Mol	Chain	Res	Type
1	A23S	1048	C
1	A23S	1050	C
1	A23S	1051	C
1	A23S	1055	C
1	A23S	1069	A
1	A23S	1070	G
1	A23S	1072	A
1	A23S	1073	G
1	A23S	1084	G
1	A23S	1098	G
1	A23S	1099	G
1	A23S	1111	A
1	A23S	1115	G
1	A23S	1120	A
1	A23S	1122	C
1	A23S	1126	G
1	A23S	1127	A
1	A23S	1139	G
1	A23S	1145	A
1	A23S	1148	U
1	A23S	1149	C
1	A23S	1158	G
1	A23S	1166	G
1	A23S	1168	A
1	A23S	1174	G
1	A23S	1177	U
1	A23S	1178	C
1	A23S	1179	C
1	A23S	1180	A
1	A23S	1185	U
1	A23S	1187	G
1	A23S	1196	A
1	A23S	1199	G
1	A23S	1200	U
1	A23S	1202	G
1	A23S	1203	G
1	A23S	1206	C
1	A23S	1207	A
1	A23S	1208	G
1	A23S	1210	A
1	A23S	1211	G
1	A23S	1213	A

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Mol	Chain	Res	Type
1	A23S	1215	C
1	A23S	1217	A
1	A23S	1219	C
1	A23S	1221	U
1	A23S	1222	C
1	A23S	1225	A
1	A23S	1227	G
1	A23S	1229	G
1	A23S	1230	U
1	A23S	1233	G
1	A23S	1241	U
1	A23S	1244	C
1	A23S	1245	C
1	A23S	1247	G
1	A23S	1250	G
1	A23S	1251	A
1	A23S	1252	G
1	A23S	1269	A
1	A23S	1270	U
1	A23S	1271	U
1	A23S	1273	G
1	A23S	1279	G
1	A23S	1282	C
1	A23S	1283	A
1	A23S	1316	A
1	A23S	1317	C
1	A23S	1318	U
1	A23S	1319	A
1	A23S	1322	G
1	A23S	1328	C
1	A23S	1330	G
1	A23S	1338	G
1	A23S	1339	G
1	A23S	1344	G
1	A23S	1350	G
1	A23S	1351	G
1	A23S	1354	A
1	A23S	1355	G
1	A23S	1356	A
1	A23S	1362	G
1	A23S	1381	C
1	A23S	1396	G

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Mol	Chain	Res	Type
1	A23S	1399	C
1	A23S	1417	G
1	A23S	1418	A
1	A23S	1432	U
1	A23S	1440	G
1	A23S	1445	A
1	A23S	1456	U
1	A23S	1464	C
1	A23S	1467	C
1	A23S	1485	U
1	A23S	1491	G
1	A23S	1495	U
1	A23S	1501	A
1	A23S	1504	G
1	A23S	1505	C
1	A23S	1506	C
1	A23S	1515	A
1	A23S	1520	C
1	A23S	1523	A
1	A23S	1525	A
1	A23S	1529	A
1	A23S	1530	A
1	A23S	1532	G
1	A23S	1542	U
1	A23S	1564	G
1	A23S	1571	C
1	A23S	1574	A
1	A23S	1575	A
1	A23S	1576	G
1	A23S	1579	A
1	A23S	1588	A
1	A23S	1589	C
1	A23S	1614	C
1	A23S	1615	A
1	A23S	1617	C
1	A23S	1625	C
1	A23S	1626	C
1	A23S	1633	U
1	A23S	1634	C
1	A23S	1636	A
1	A23S	1641	U
1	A23S	1647	A

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Mol	Chain	Res	Type
1	A23S	1648	G
1	A23S	1653	A
1	A23S	1661	G
1	A23S	1665	A
1	A23S	1666	G
1	A23S	1667	G
1	A23S	1670	G
1	A23S	1671	A
1	A23S	1675	U
1	A23S	1680	U
1	A23S	1682	G
1	A23S	1683	G
1	A23S	1684	C
1	A23S	1690	G
1	A23S	1691	U
1	A23S	1692	U
1	A23S	1693	A
1	A23S	1701	U
1	A23S	1707	G
1	A23S	1708	A
1	A23S	1713	U
1	A23S	1715	G
1	A23S	1720	C
1	A23S	1721	A
1	A23S	1724	A
1	A23S	1725	A
1	A23S	1726	A
1	A23S	1727	A
1	A23S	1740	C
1	A23S	1741	G
1	A23S	1743	U
1	A23S	1745	C
1	A23S	1751	G
1	A23S	1752	A
1	A23S	1761	A
1	A23S	1762	G
1	A23S	1764	A
1	A23S	1771	C
1	A23S	1776	G
1	A23S	1787	A
1	A23S	1801	U
1	A23S	1802	C

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Mol	Chain	Res	Type
1	A23S	1804	G
1	A23S	1809	G
1	A23S	1810	U
1	A23S	1811	A
1	A23S	1816	A
1	A23S	1831	G
1	A23S	1857	A
1	A23S	1858	A
1	A23S	1864	G
1	A23S	1868	A
1	A23S	1877	U
1	A23S	1900	G
1	A23S	1907	G
1	A23S	1908	A
1	A23S	1917	A
1	A23S	1920	G
1	A23S	1926	U
1	A23S	1930	A
1	A23S	1944	C
1	A23S	1961	G
1	A23S	1973	A
1	A23S	1992	U
1	A23S	2007	U
1	A23S	2013	G
1	A23S	2031	G
1	A23S	2032	G
1	A23S	2054	U
1	A23S	2055	U
1	A23S	2056	A
1	A23S	2059	G
1	A23S	2062	G
1	A23S	2066	A
1	A23S	2084	U
1	A23S	2092	C
1	A23S	2093	G
1	A23S	2096	U
1	A23S	2099	A
1	A23S	2100	U
1	A23S	2101	G
1	A23S	2105	C
1	A23S	2106	A
1	A23S	2120	U

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Mol	Chain	Res	Type
1	A23S	2122	U
1	A23S	2123	C
1	A23S	2149	U
1	A23S	2150	G
1	A23S	2151	A
1	A23S	2155	G
1	A23S	2156	G
1	A23S	2159	C
1	A23S	2160	A
1	A23S	2161	C
1	A23S	2162	A
1	A23S	2180	A
1	A23S	2184	A
1	A23S	2189	A
1	A23S	2190	G
1	A23S	2191	A
1	A23S	2198	G
1	A23S	2208	C
1	A23S	2231	G
1	A23S	2236	U
1	A23S	2237	A
1	A23S	2239	G
1	A23S	2240	C
1	A23S	2241	G
1	A23S	2244	G
1	A23S	2245	A
1	A23S	2247	U
1	A23S	2251	U
1	A23S	2252	G
1	A23S	2255	A
1	A23S	2257	G
1	A23S	2258	G
1	A23S	2260	U
1	A23S	2261	C
1	A23S	2262	G
1	A23S	2265	C
1	A23S	2270	C
1	A23S	2275	C
1	A23S	2282	A
1	A23S	2285	G
1	A23S	2286	G
1	A23S	2287	A

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Mol	Chain	Res	Type
1	A23S	2288	C
1	A23S	2290	C
1	A23S	2291	G
1	A23S	2292	A
1	A23S	2293	A
1	A23S	2296	U
1	A23S	2297	G
1	A23S	2298	A
1	A23S	2299	A
1	A23S	2300	A
1	A23S	2301	C
1	A23S	2302	A
1	A23S	2319	G
1	A23S	2320	A
1	A23S	2327	A
1	A23S	2328	A
1	A23S	2346	A
1	A23S	2347	C
1	A23S	2359	G
1	A23S	2366	C
1	A23S	2367	G
1	A23S	2379	A
1	A23S	2381	U
1	A23S	2404	G
1	A23S	2405	C
1	A23S	2406	C
1	A23S	2409	A
1	A23S	2427	A
1	A23S	2428	C
1	A23S	2429	A
1	A23S	2430	G
1	A23S	2441	U
1	A23S	2442	A
1	A23S	2443	G
1	A23S	2444	A
1	A23S	2449	A
1	A23S	2457	A
1	A23S	2458	A
1	A23S	2480	C
1	A23S	2504	G
1	A23S	2505	C
1	A23S	2508	G

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Mol	Chain	Res	Type
1	A23S	2510	C
1	A23S	2517	A
1	A23S	2526	G
1	A23S	2527	C
1	A23S	2531	C
1	A23S	2532	A
1	A23S	2551	G
1	A23S	2556	A
1	A23S	2557	A
1	A23S	2558	A
1	A23S	2565	C
1	A23S	2569	G
1	A23S	2572	A
1	A23S	2583	G
1	A23S	2594	G
1	A23S	2596	G
1	A23S	2599	C
1	A23S	2600	A
1	A23S	2616	U
1	A23S	2626	G
1	A23S	2642	A
1	A23S	2644	C
1	A23S	2653	G
1	A23S	2678	C
1	A23S	2687	U
1	A23S	2688	A
1	A23S	2690	A
1	A23S	2691	G
1	A23S	2697	C
1	A23S	2702	G
1	A23S	2706	G
1	A23S	2710	U
1	A23S	2723	G
1	A23S	2726	A
1	A23S	2727	G
1	A23S	2737	U
1	A23S	2739	A
1	A23S	2754	G
1	A23S	2762	G
1	A23S	2763	A
1	A23S	2764	G
1	A23S	2769	A

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Mol	Chain	Res	Type
1	A23S	2770	G
1	A23S	2788	G
1	A23S	2807	U
1	A23S	2814	U
1	A23S	2815	A
1	A23S	2835	A
1	A23S	2836	U
1	A23S	2837	G
1	A23S	2849	C
1	A23S	2855	G
1	A23S	2861	U
1	A23S	2864	C
1	A23S	2869	G
1	A23S	2870	A
1	A23S	2872	A
1	A23S	2873	G
1	A23S	2879	A
1	A23S	2886	A
1	A23S	2887	A
1	A23S	2888	C
1	A23S	2891	C
1	A23S	2899	A
1	A23S	2900	A
1	A23S	2924	G
1	A23S	2934	U
1	A23S	2949	A
1	A23S	2950	U
1	A23S	2960	A
1	A23S	2961	U
1	A23S	2973	G
1	A23S	2983	C
1	A23S	2987	G
1	A23S	2993	U
1	A23S	2994	A
1	A23S	2999	G
1	A23S	3000	C
1	A23S	3006	C
1	A23S	3019	C
2	A5S	5	C
2	A5S	10	G
2	A5S	13	C
2	A5S	25	G

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Mol	Chain	Res	Type
2	A5S	27	A
2	A5S	42	U
2	A5S	43	U
2	A5S	46	A
2	A5S	47	A
2	A5S	58	A
2	A5S	59	A
2	A5S	68	C
2	A5S	88	C
2	A5S	93	A
2	A5S	94	G
2	A5S	113	G
2	A5S	114	C
2	A5S	118	G
2	A5S	119	A
40	AETN	2	C
40	AETN	3	C
40	AETN	16	A
40	AETN	19	A

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A23S	73	G
1	A23S	109	U
1	A23S	136	U
1	A23S	146	U
1	A23S	243	C
1	A23S	275	G
1	A23S	280	G
1	A23S	336	A
1	A23S	382	U
1	A23S	402	A
1	A23S	574	G
1	A23S	668	A
1	A23S	740	G
1	A23S	802	G
1	A23S	843	G
1	A23S	920	G
1	A23S	1003	G
1	A23S	1072	A
1	A23S	1121	A

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Mol	Chain	Res	Type
1	A23S	1177	U
1	A23S	1179	C
1	A23S	1198	G
1	A23S	1270	U
1	A23S	1327	U
1	A23S	1500	U
1	A23S	1625	C
1	A23S	1646	G
1	A23S	1647	A
1	A23S	1689	C
1	A23S	1706	U
1	A23S	1750	A
1	A23S	1751	G
1	A23S	1776	G
1	A23S	2148	C
1	A23S	2256	G
1	A23S	2429	A
1	A23S	2504	G
1	A23S	2598	U
1	A23S	2726	A
1	A23S	2835	A
1	A23S	2878	U
1	A23S	2923	G
2	A5S	45	G
2	A5S	57	U
40	AETN	2	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

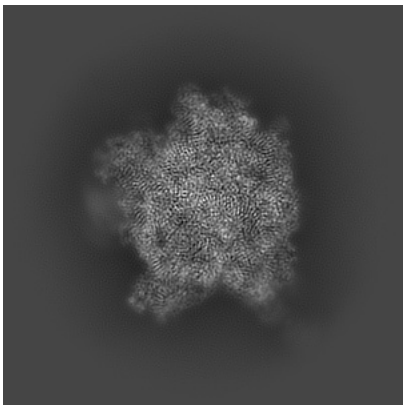
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34860. These allow visual inspection of the internal detail of the map and identification of artifacts.

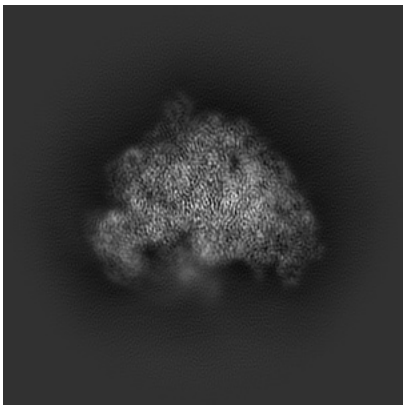
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

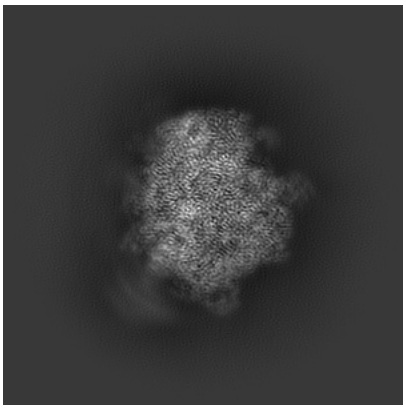
6.1.1 Primary map



X

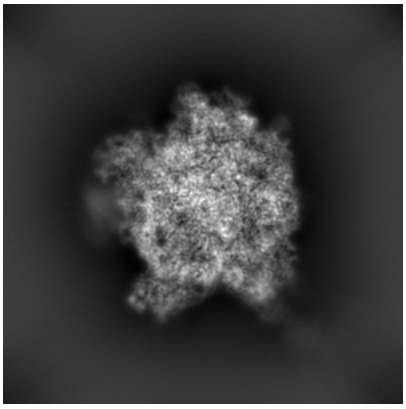


Y

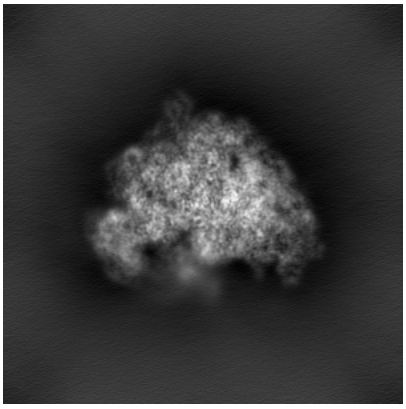


Z

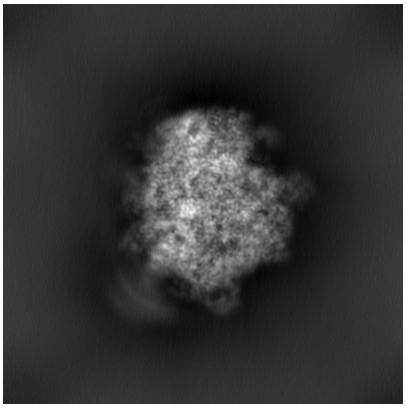
6.1.2 Raw map



X



Y

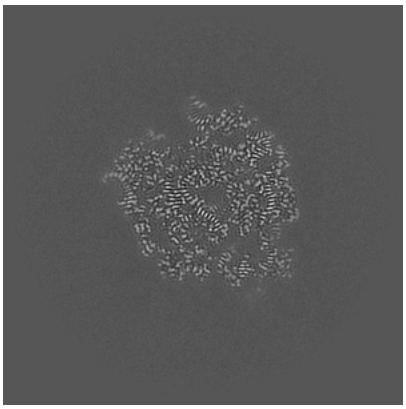


Z

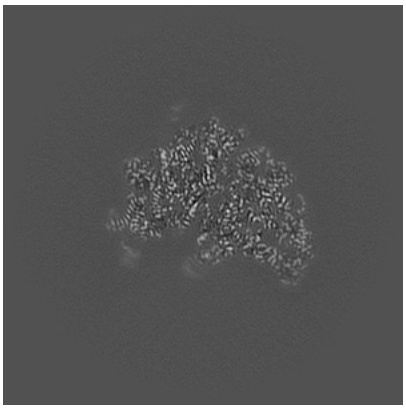
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

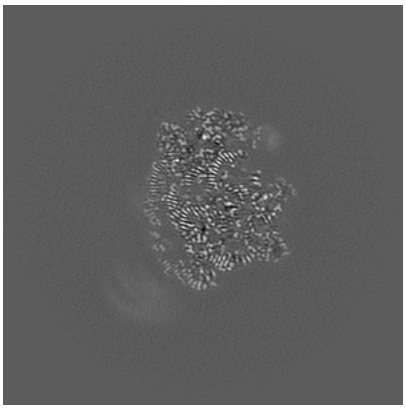
6.2.1 Primary map



X Index: 180

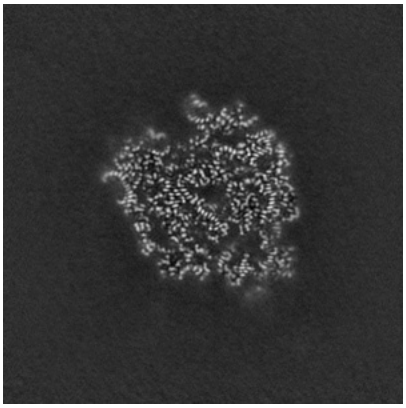


Y Index: 180

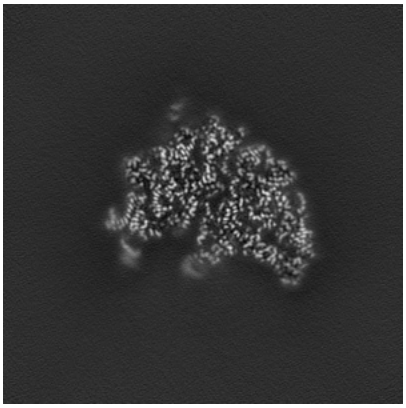


Z Index: 180

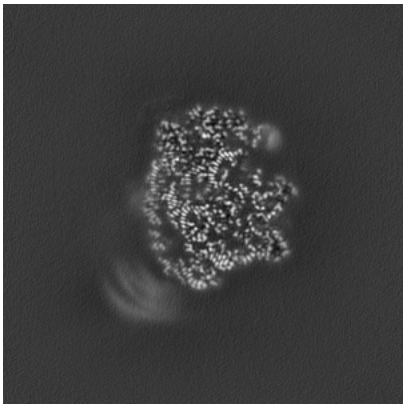
6.2.2 Raw map



X Index: 180



Y Index: 180

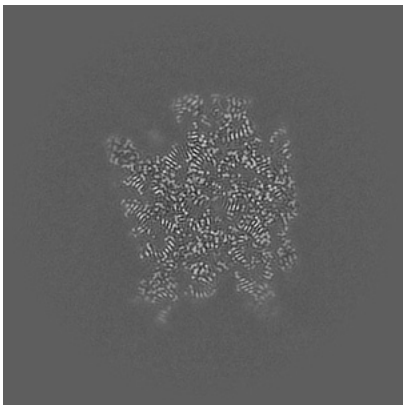


Z Index: 180

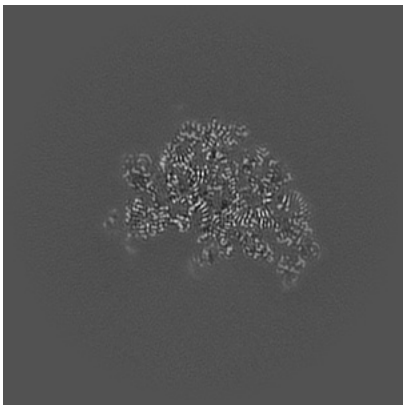
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

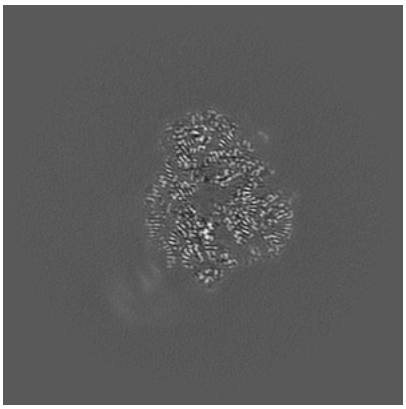
6.3.1 Primary map



X Index: 169

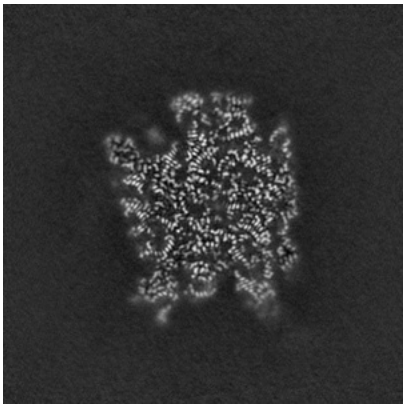


Y Index: 176

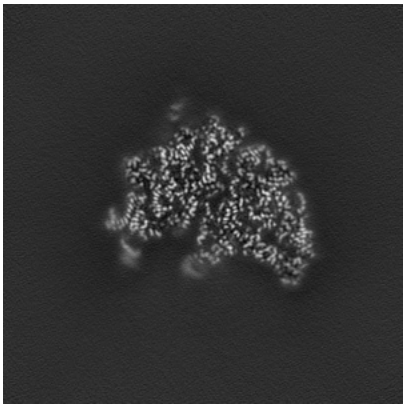


Z Index: 191

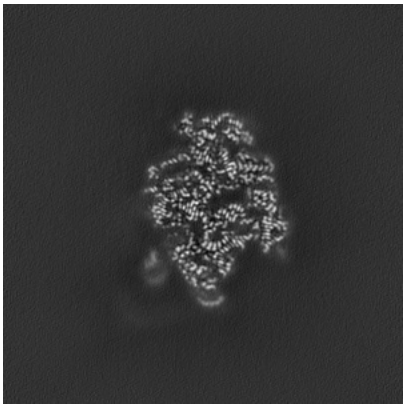
6.3.2 Raw map



X Index: 169



Y Index: 180

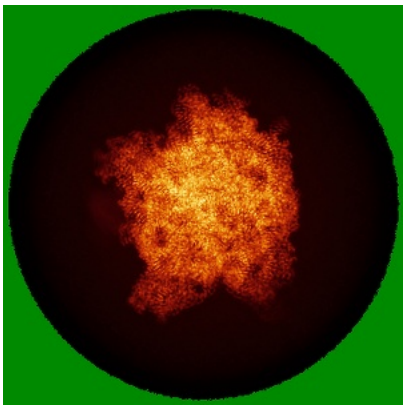


Z Index: 202

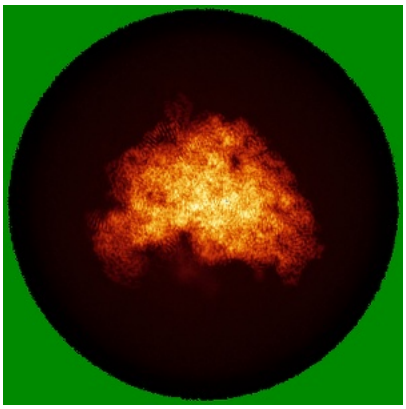
The images above show the largest variance slices of the map in three orthogonal directions.

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

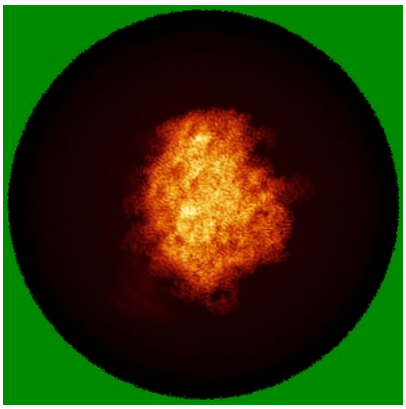
6.4.1 Primary map



X

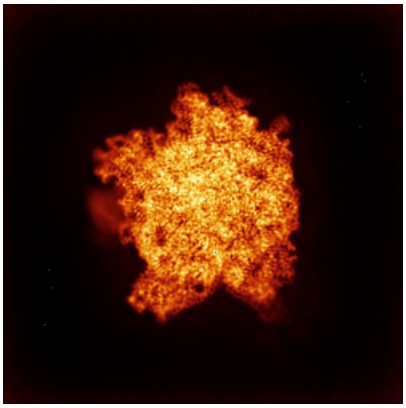


Y

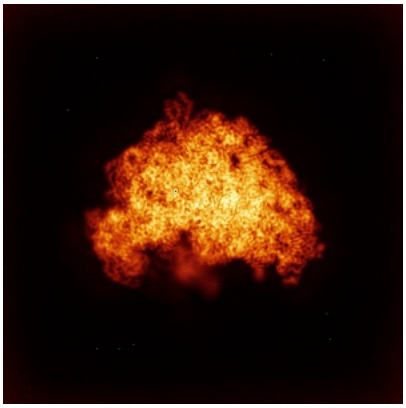


Z

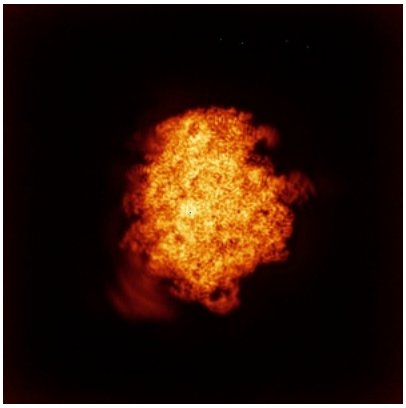
6.4.2 Raw map



X



Y

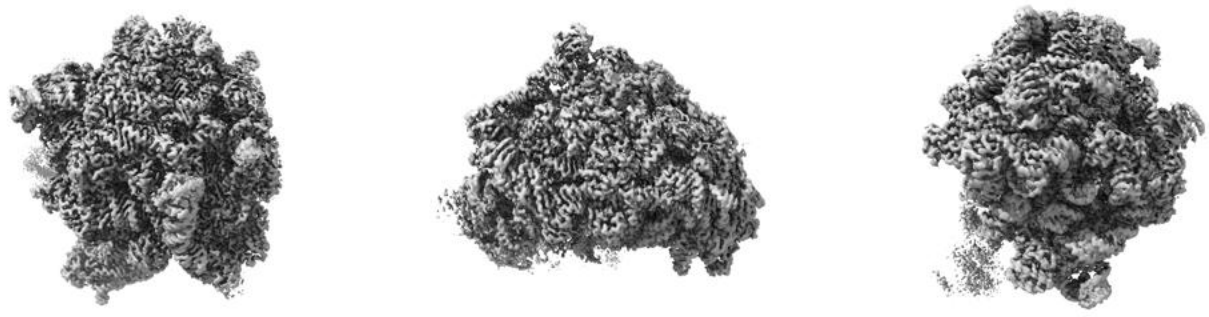


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

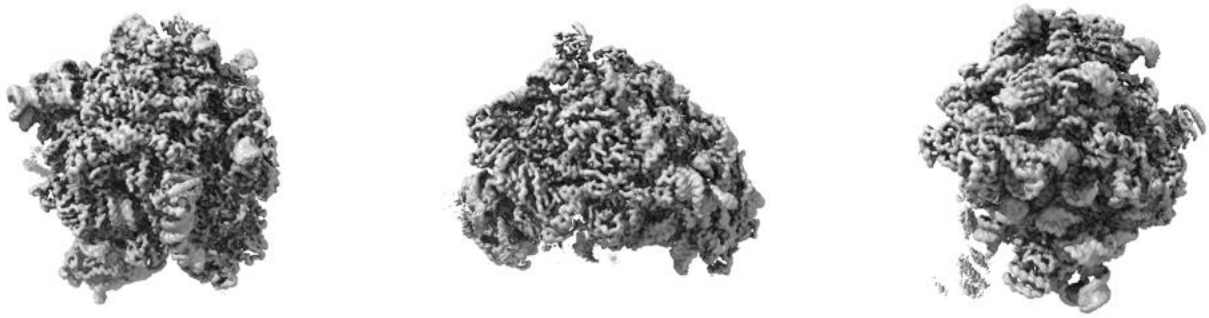
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. 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.

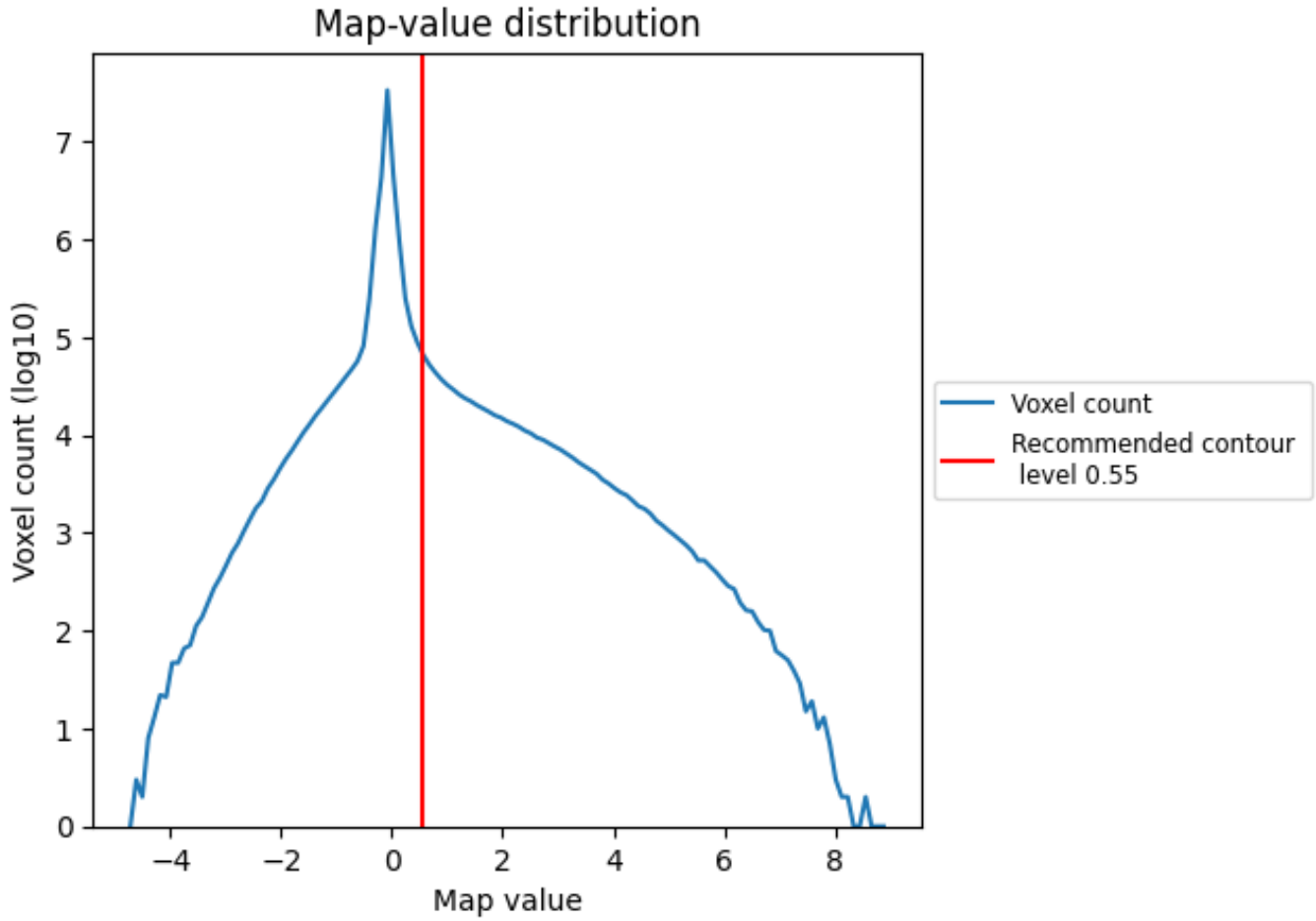
6.6 Mask visualisation (i)

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

7 Map analysis

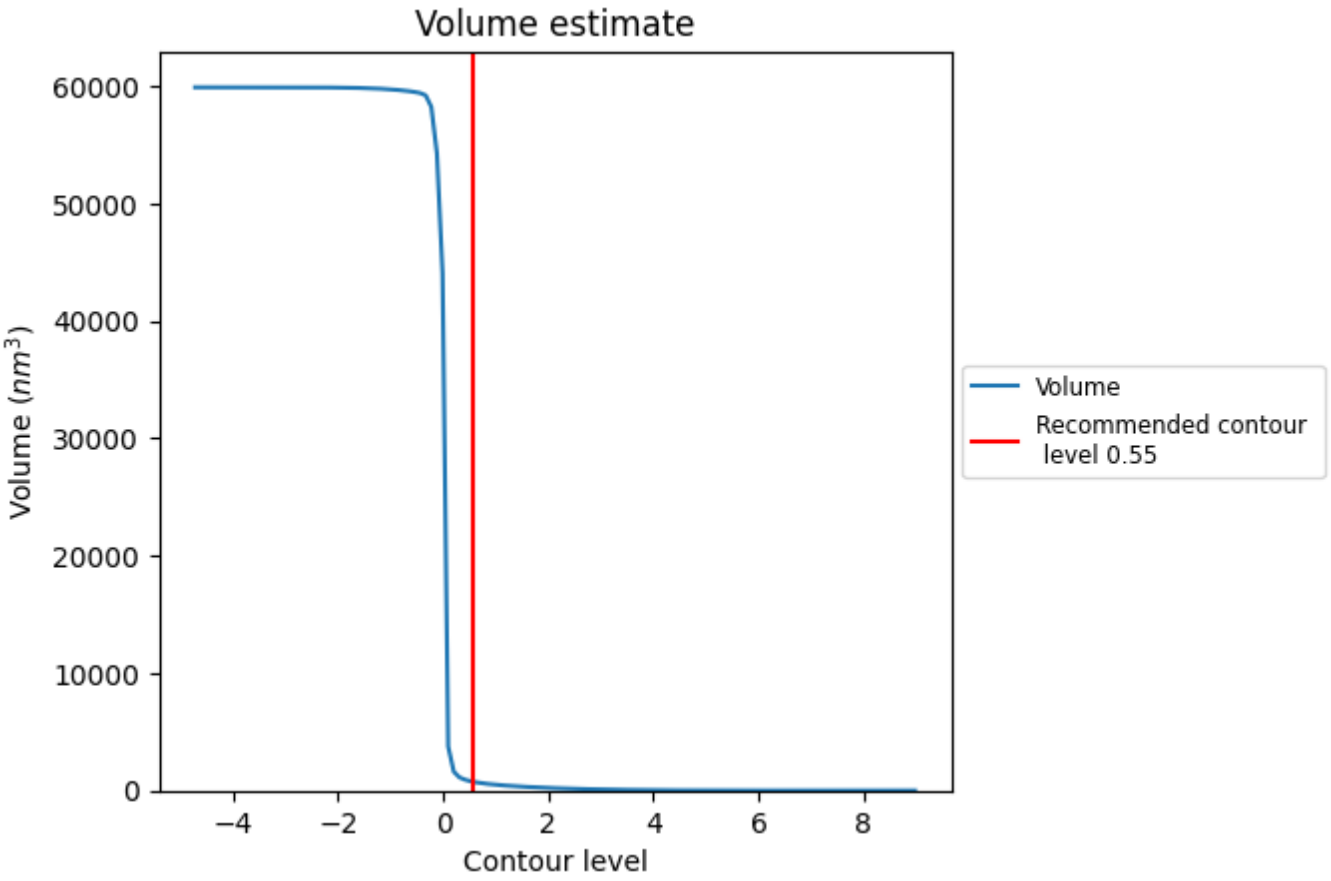
This section contains the results of statistical analysis of the map.

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.

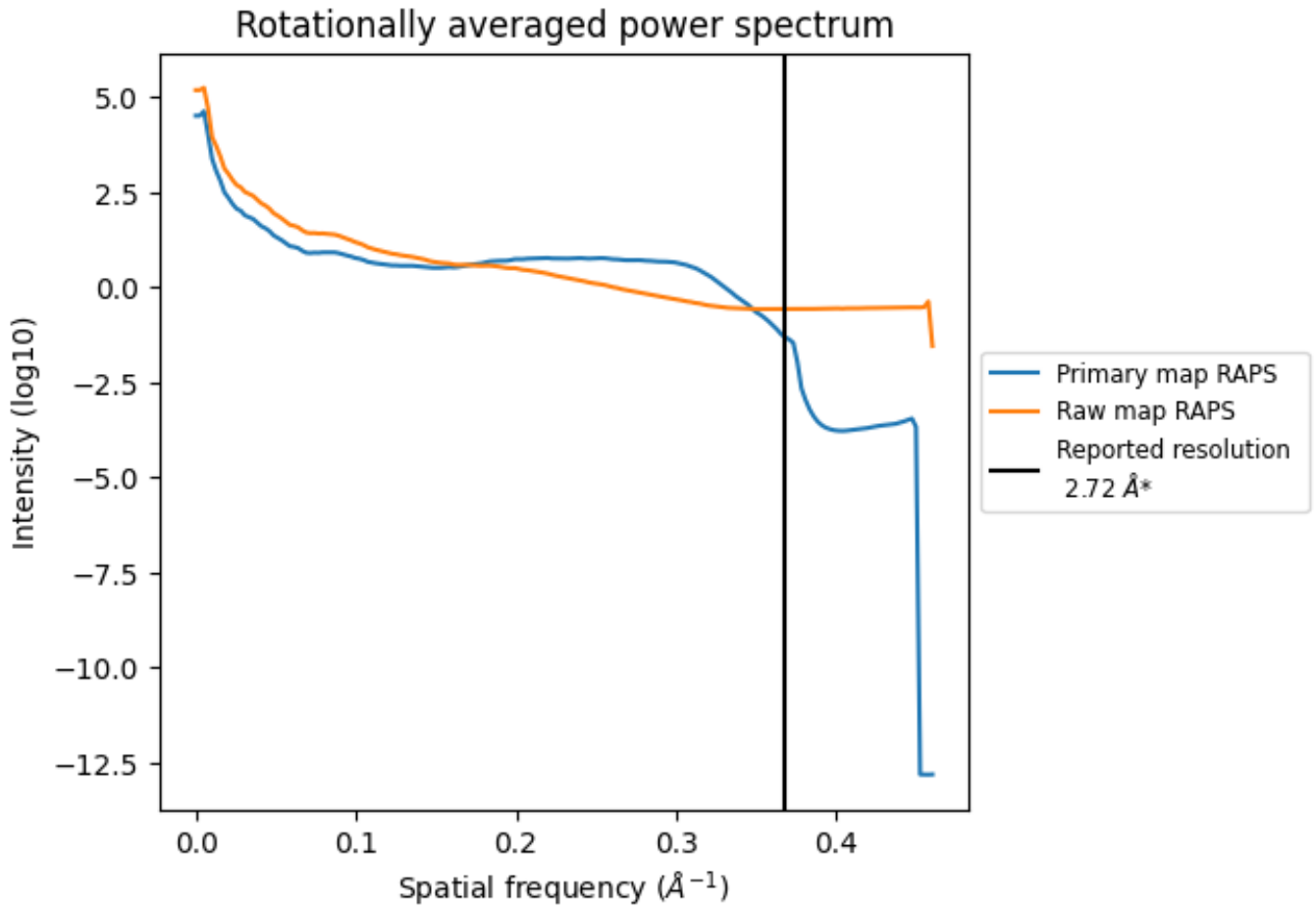
7.2 Volume estimate



The volume at the recommended contour level is 772 nm^3; this corresponds to an approximate mass of 698 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)

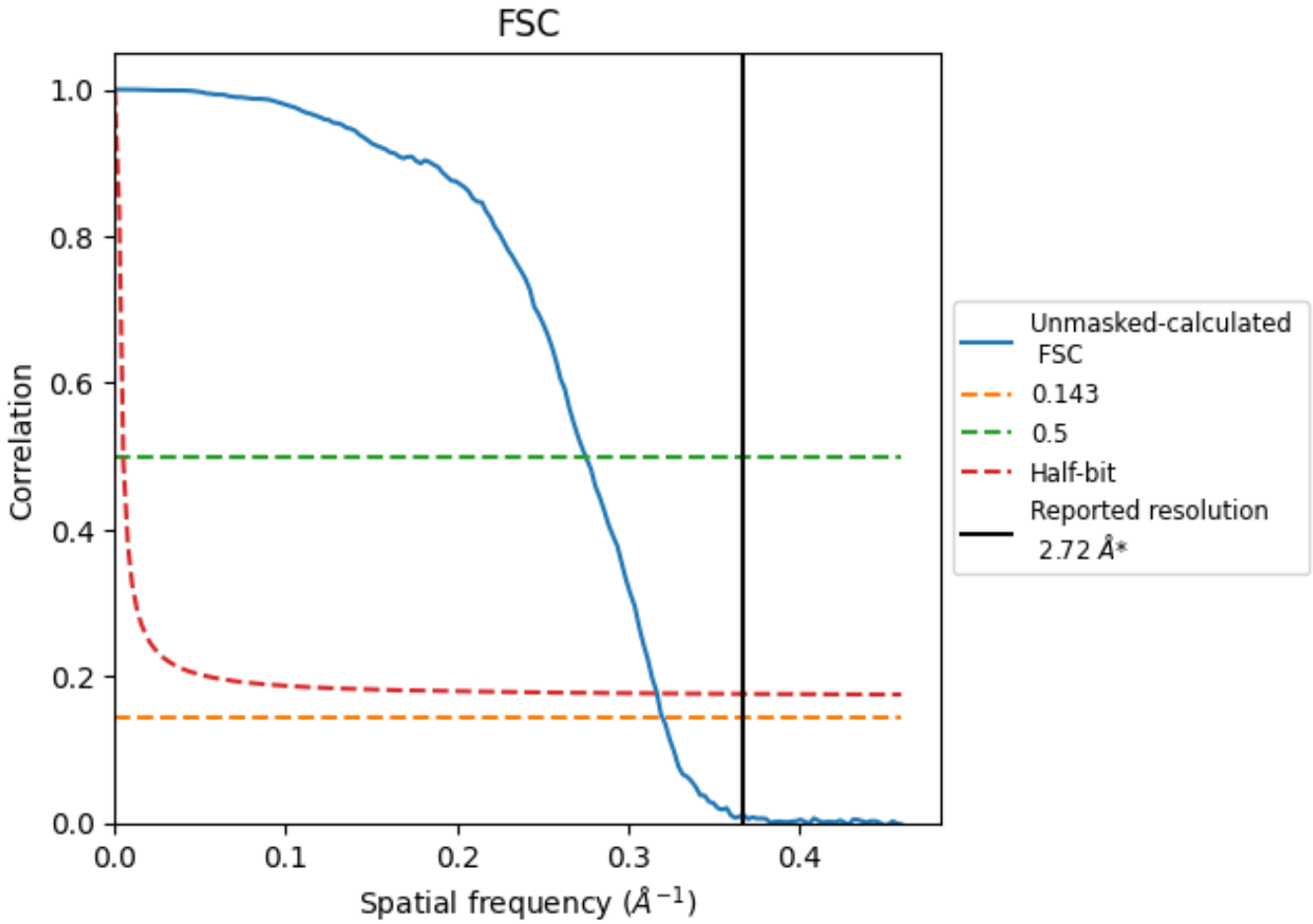


*Reported resolution corresponds to spatial frequency of 0.368 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.368 Å^{-1}

8.2 Resolution estimates (i)

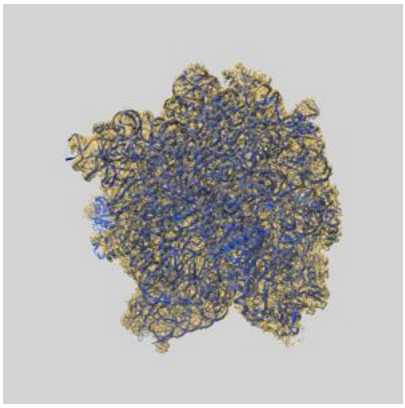
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.12	3.63	3.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.72 by more than 10 %

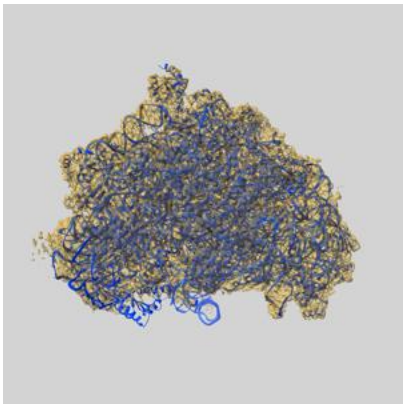
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34860 and PDB model 8HKU. Per-residue inclusion information can be found in section 3 on page 11.

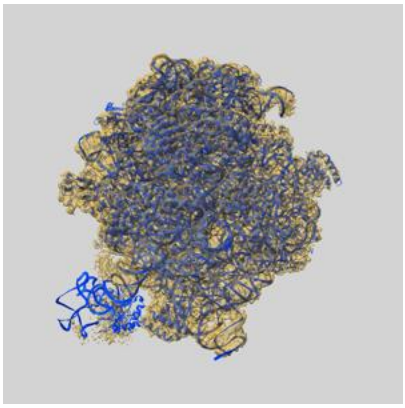
9.1 Map-model overlay



X



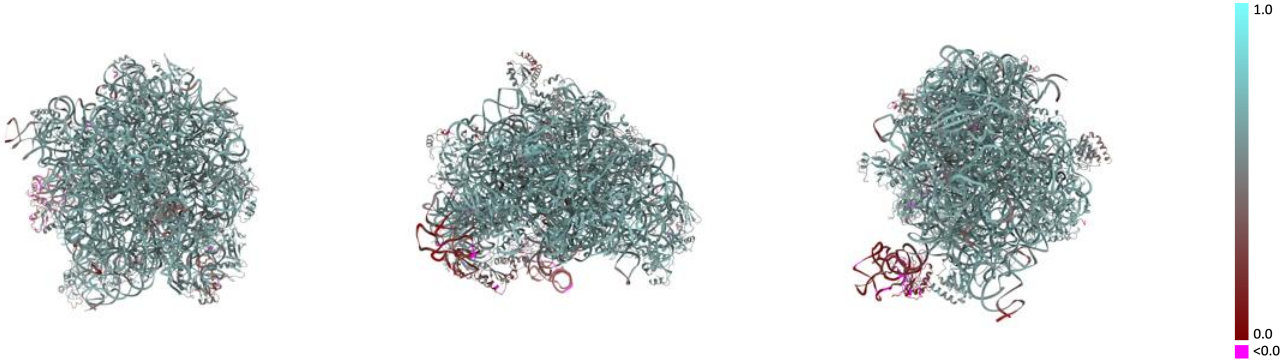
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 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.

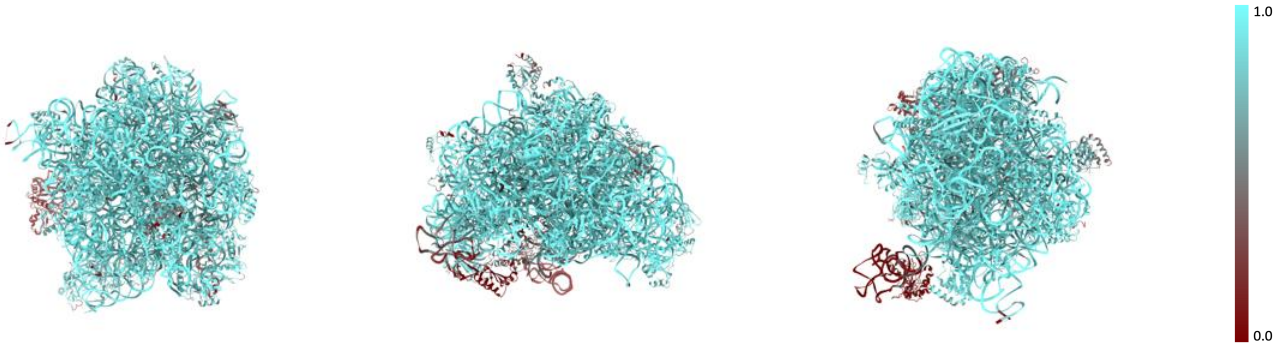
9.2 Q-score mapped to coordinate model (i)



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.

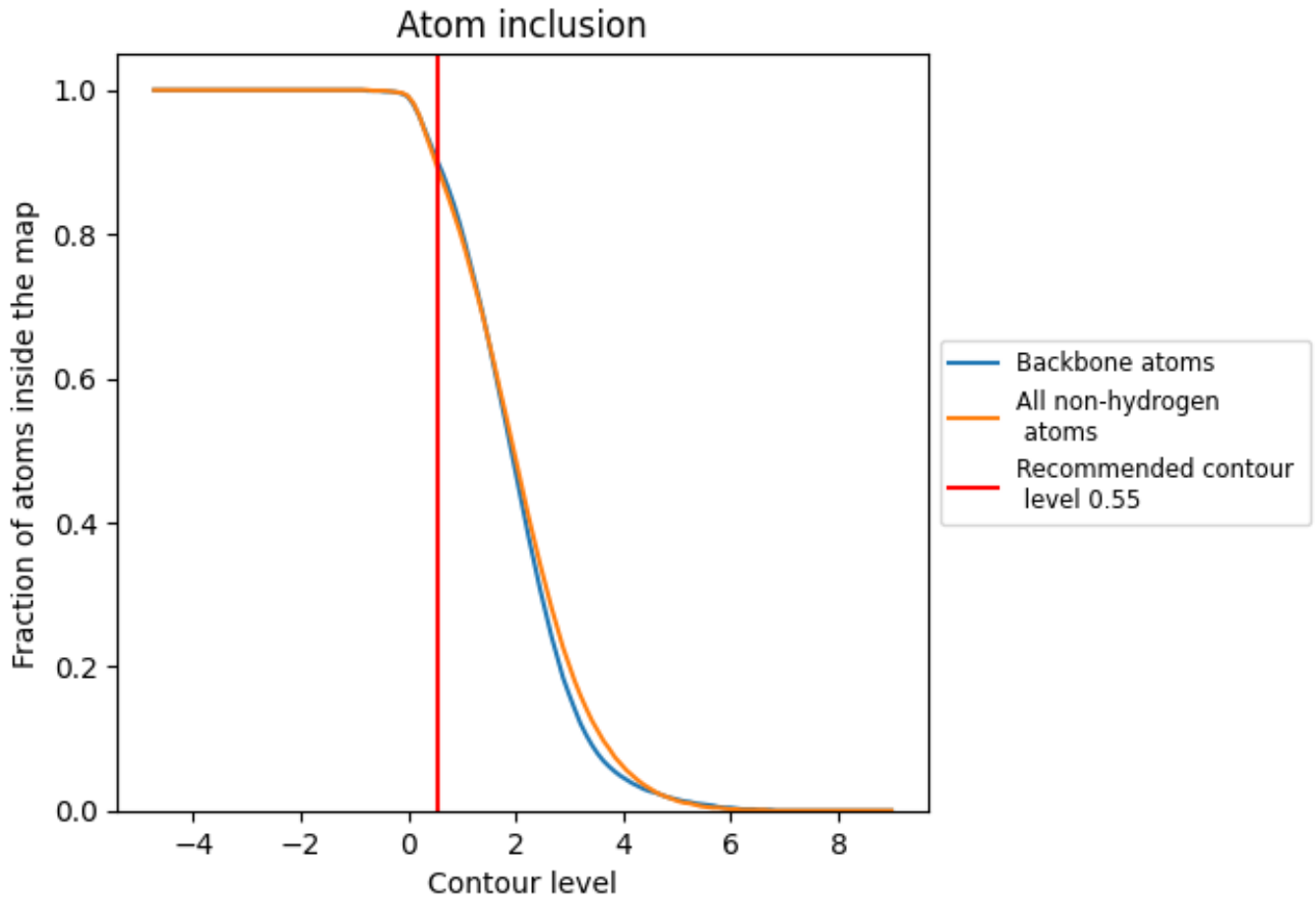
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8910	0.5770
A23S	0.9360	0.5940
A5S	0.9820	0.6060
AETN	0.5040	0.4280
AL1P	0.0250	0.1530
AL2P	0.9510	0.6200
AL3P	0.9220	0.5930
AL4P	0.9460	0.6100
AL5P	0.7910	0.5180
AL6P	0.8820	0.5680
ALX0	0.7660	0.4840
ARF1	0.3960	0.4770
L10E	0.8870	0.5850
L13P	0.8760	0.5720
L141	0.8480	0.5320
L142	0.8020	0.5170
L14P	0.9270	0.6070
L15E	0.9570	0.6260
L15P	0.9040	0.5890
L18E	0.9230	0.5960
L18P	0.8840	0.5550
L19E	0.9470	0.6210
L21E	0.9550	0.6240
L22P	0.9400	0.6160
L23P	0.8880	0.5850
L24E	0.9670	0.6360
L24P	0.9150	0.5910
L29P	0.8500	0.5520
L30E	0.8810	0.5790
L30P	0.7830	0.4880
L31E	0.9110	0.5830
L32E	0.8260	0.5650
L34E	0.7230	0.4090
L37A	0.9580	0.6190
L37E	0.9330	0.6160

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Chain	Atom inclusion	Q-score
L39E	0.8340	0.5290
L40E	0.6600	0.4210
L44E	0.9450	0.6210
L45A	0.8090	0.5390
L46A	0.8110	0.5590
L47A	0.5310	0.5420
L7A1	0.8740	0.5770
L7A2	0.6380	0.4730