



wwPDB EM Validation Summary Report ⓘ

Jun 9, 2025 – 07:18 PM JST

PDB ID : 8ZEJ / pdb_00008zej
EMDB ID : EMD-60034
Title : Structure of E.coli ribosome in complex with an engineered arrest peptide
Authors : Sriramoju, M.K.; Ko, T.P.; Draczkowski, P.; Hsu, S.T.D.
Deposited on : 2024-05-06
Resolution : 2.69 Å (reported)
Based on initial model : 3JBU

This is a wwPDB EM Validation Summary 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

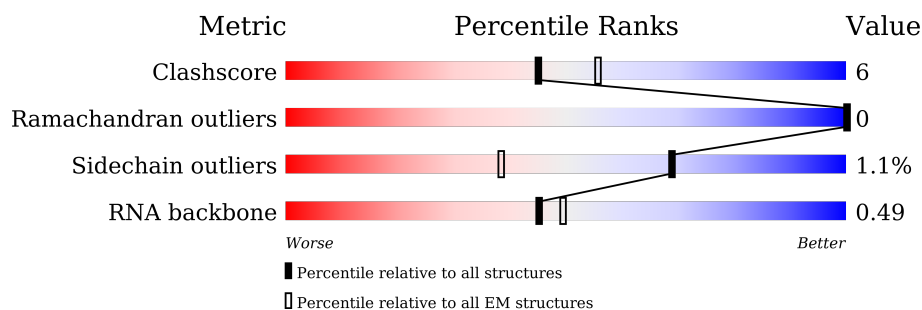
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.69 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	78	83% 15% .
2	1	63	86% 11% .
3	2	59	85% 14% .
4	4	57	77% 21% .
5	5	55	73% 22% 5%
6	6	46	93% 7%
7	7	65	88% 11% .









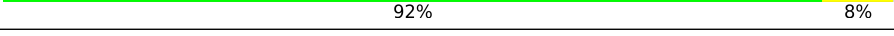
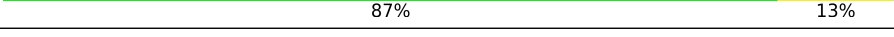
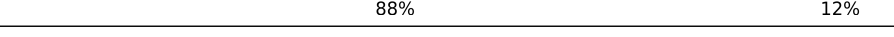

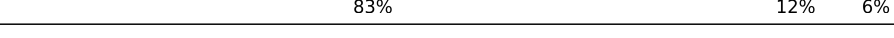
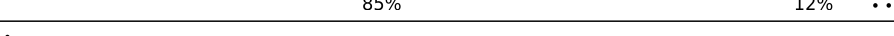
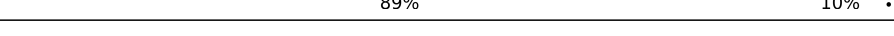
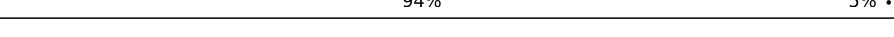

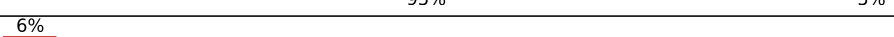
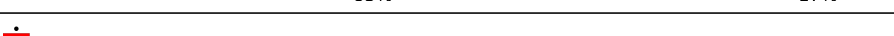

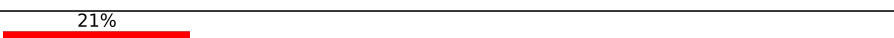


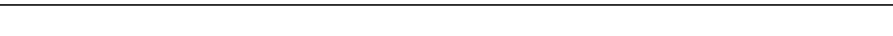
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Mol	Chain	Length	Quality of chain
8	8	38	
9	A	1533	
10	B	241	
11	C	233	
12	D	206	
13	E	167	
14	F	135	
15	G	179	
16	H	130	
17	I	130	
18	J	103	
19	K	129	
20	L	124	
21	M	118	
22	N	101	
23	O	89	
24	P	82	
25	Q	84	
26	R	75	
27	S	92	
28	T	87	
29	U	71	
30	X	76	
31	Y	77	
31	Z	77	

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Mol	Chain	Length	Quality of chain
32	a	120	
33	b	2904	
34	c	273	
35	d	209	
36	e	201	
37	f	179	
38	g	177	
39	h	149	
40	k	142	
41	l	123	
42	m	144	
43	n	136	
44	o	127	
45	p	117	
46	q	115	
47	r	118	
48	s	103	
49	t	110	
50	u	100	
51	v	104	
52	w	94	
53	x	14	
54	y	85	
55	z	28	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	PRO	Z	163	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 147438 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 4 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 5 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	5	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 6 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 8 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 9 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1533	Total	C	N	O	P	0	0
			32895	14671	6036	10655	1533		

- Molecule 10 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 11 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	207	Total	C	N	O	S	0	0
			1632	1034	306	289	3		

- Molecule 12 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 13 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 14 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 15 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 16 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 17 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 18 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	100	Total	C	N	O	S	0	0
			803	502	154	146	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	122	Total	C	N	O	S	0	0
			949	587	195	163	4		

- Molecule 21 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 22 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 23 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 24 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 25 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 26 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 27 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 28 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 29 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	64	Total	C	N	O	S	0	0
			529	329	110	89	1		

- Molecule 30 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	76	Total	C	N	O	P	0	0
			1621	722	287	536	76		

- Molecule 31 is a RNA chain called P-site tRNA (Chain Y), A-site tRNA-PRO (Chain Z).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		
31	Z	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		

- Molecule 32 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 33 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	2902	Total	C	N	O	P	0	0
			62297	27791	11462	20142	2902		

- Molecule 34 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 35 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 36 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 37 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	178	Total	C	N	O	S	0	0
			1419	905	251	257	6		

- Molecule 38 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 39 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	149	Total	C	N	O	S	0	0
			1108	699	197	211	1		

- Molecule 40 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 41 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 42 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 43 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 44 is a protein called 50S ribosomal protein L17.

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

- Molecule 45 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 46 is a protein called 50S ribosomal protein L19.

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

- Molecule 47 is a protein called 50S ribosomal protein L20.

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

- Molecule 48 is a protein called 50S ribosomal protein L21.

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

- Molecule 49 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	100	Total	C	N	O	S	0	0
			786	496	146	142	2		

- Molecule 51 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	v	103	Total	C	N	O	0	0
			788	498	148	142		

- Molecule 52 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	14	Total	C	N	O	P	0	0
			299	133	55	97	14		

- Molecule 54 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

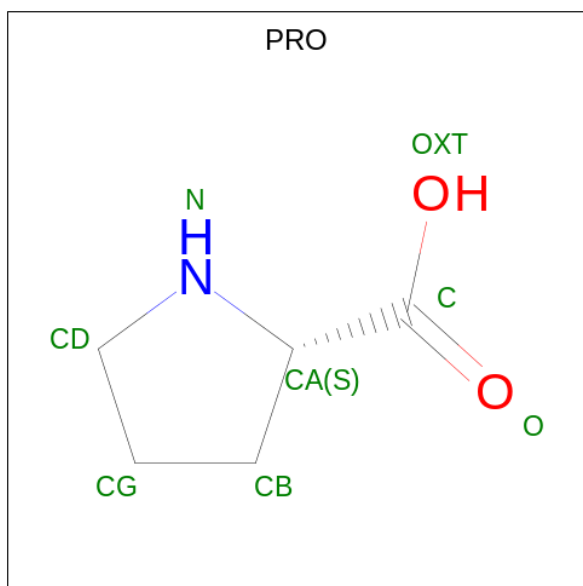
- Molecule 55 is a protein called eRAP.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	z	26	Total	C	N	O	8	0
			298	204	52	42		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	8	1	Total	Zn	0
			1	1	

- Molecule 57 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).




Mol	Chain	Residues	Atoms				AltConf
57	Z	1	Total	C	N	O	0
			7	5	1	1	

3 Residue-property plots [i](#)


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

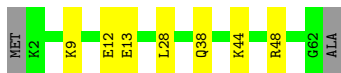
- Molecule 1: 50S ribosomal protein L28

Chain 0:  83% 15% .




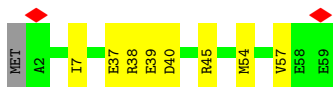
- Molecule 2: 50S ribosomal protein L29

Chain 1:  86% 11% .




- Molecule 3: 50S ribosomal protein L30

Chain 2:  85% 14% .



- Molecule 4: 50S ribosomal protein L32

Chain 4:  77% 21% .



- Molecule 5: 50S ribosomal protein L33

Chain 5:  73% 22% 5% .




- Molecule 6: 50S ribosomal protein L34

Chain 6:  93% 7%



- Molecule 7: 50S ribosomal protein L35

Chain 7:  88% 11%



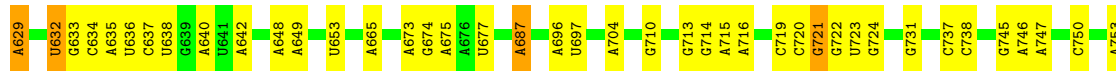
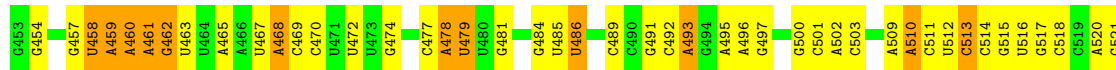
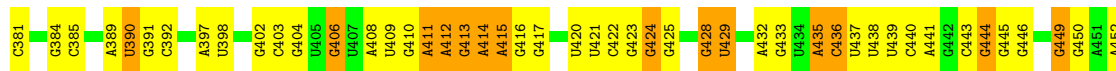
- Molecule 8: 50S ribosomal protein L36

Chain 8:  92% 8%



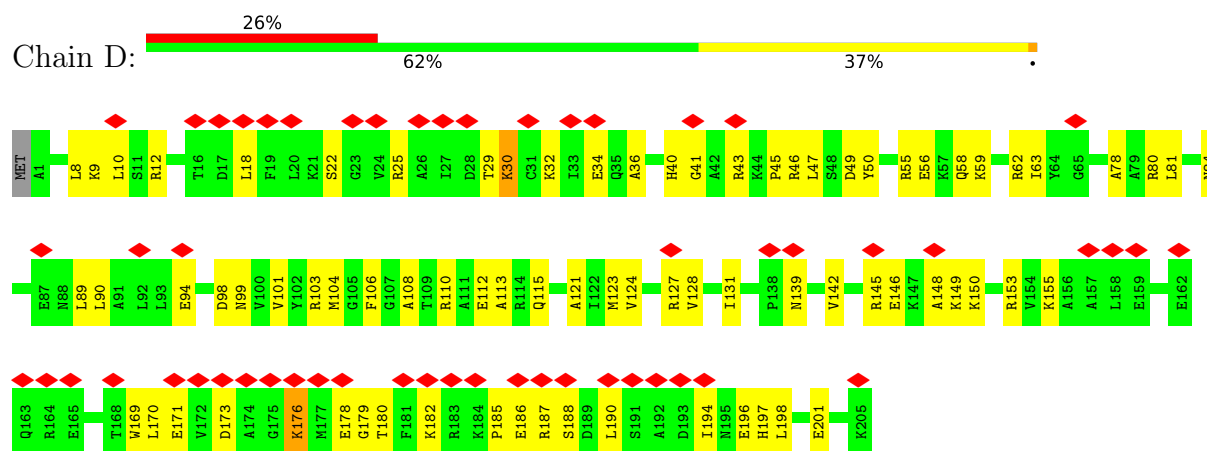
- Molecule 9: 16S rRNA

Chain A:  61% 31% 8%

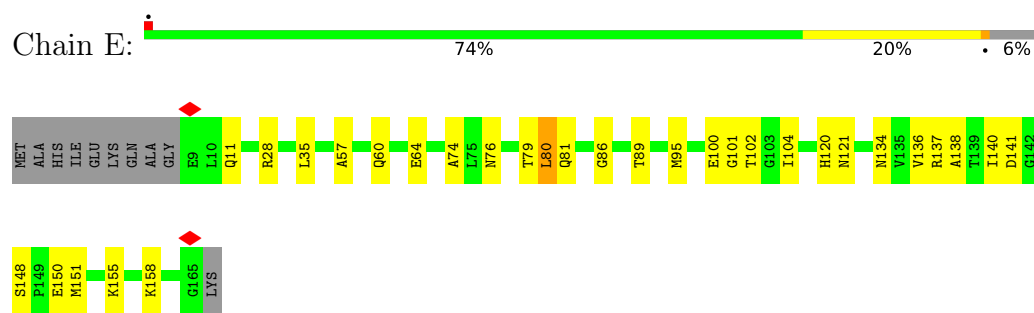




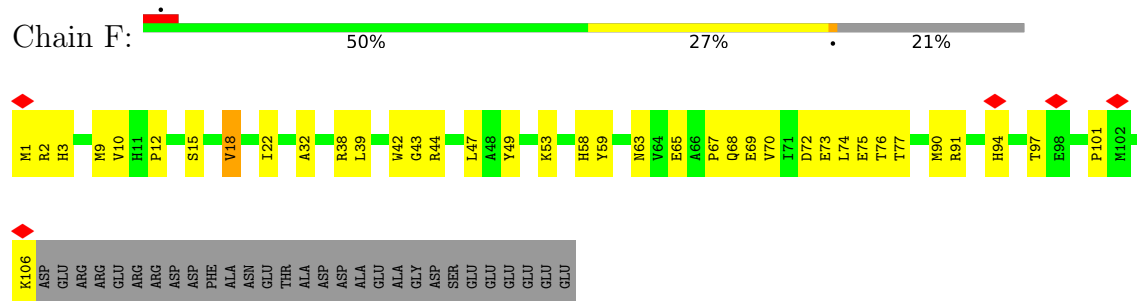
- Molecule 12: 30S ribosomal protein S4



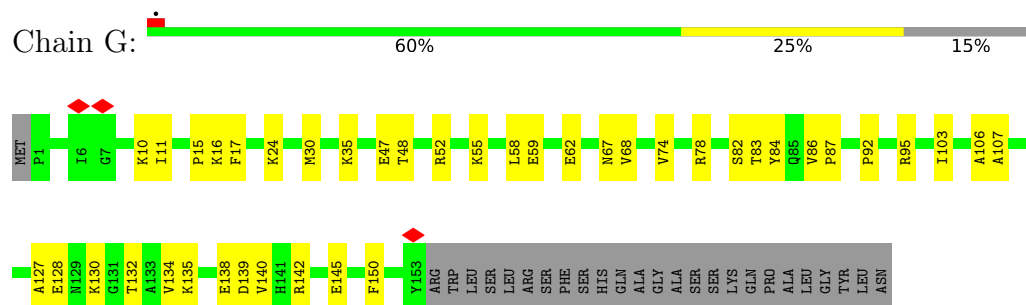
- Molecule 13: 30S ribosomal protein S5



- Molecule 14: 30S ribosomal protein S6, fully modified isoform

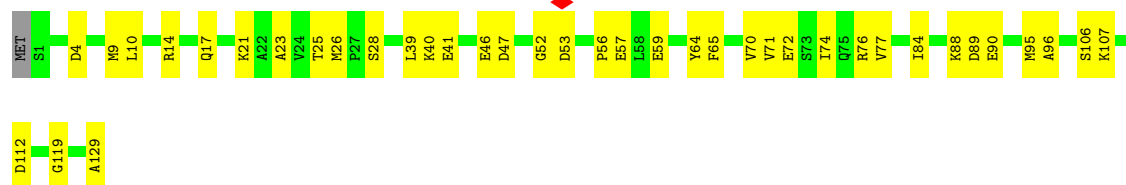


- Molecule 15: 30S ribosomal protein S7



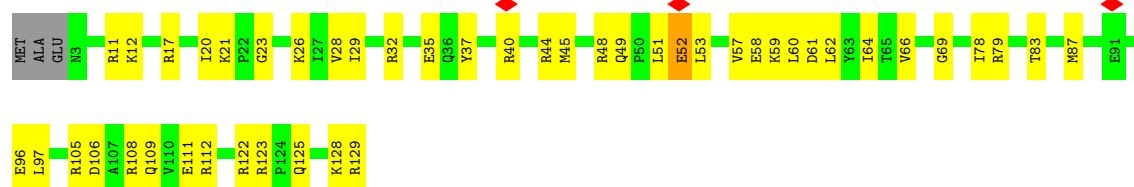
- Molecule 16: 30S ribosomal protein S8

Chain H: 



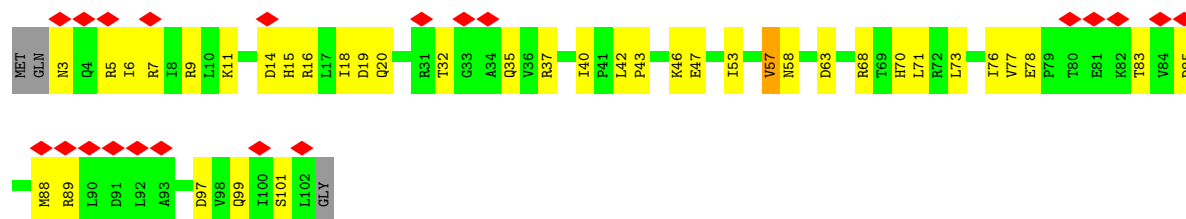
- Molecule 17: 30S ribosomal protein S9

Chain I: 



- Molecule 18: 30S ribosomal protein S10

Chain J: 




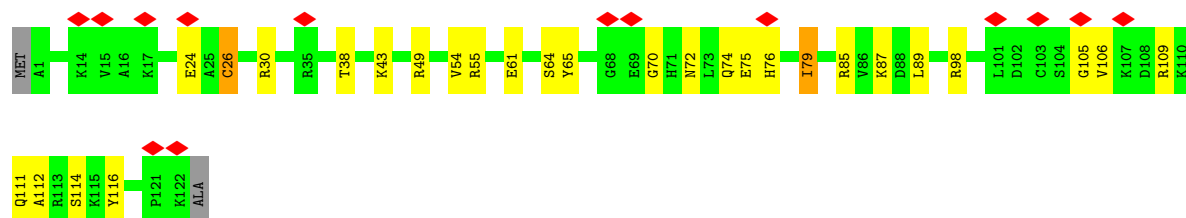
- Molecule 19: Small ribosomal subunit protein uS11

Chain K: 



- Molecule 20: Small ribosomal subunit protein uS12

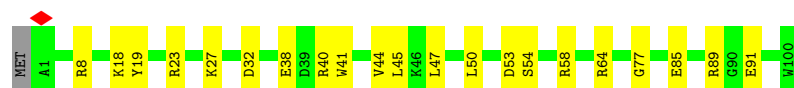
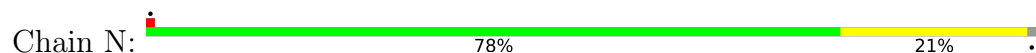
Chain L: 



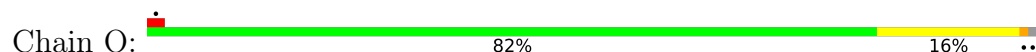
- Molecule 21: 30S ribosomal protein S13



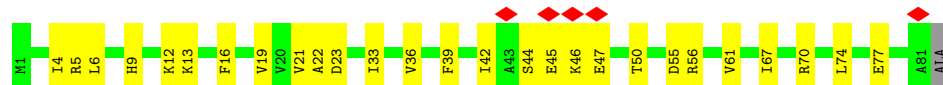
- Molecule 22: 30S ribosomal protein S14



- Molecule 23: 30S ribosomal protein S15



- Molecule 24: 30S ribosomal protein S16



- Molecule 25: 30S ribosomal protein S17



- Molecule 26: 30S ribosomal protein S18

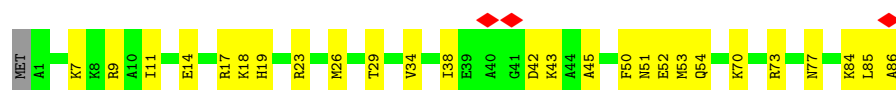


- Molecule 27: 30S ribosomal protein S19



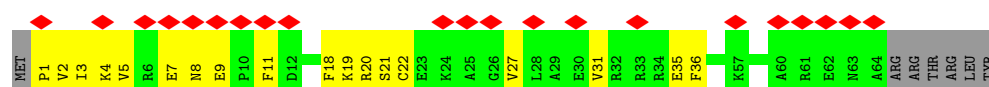
- Molecule 28: 30S ribosomal protein S20

Chain T: 



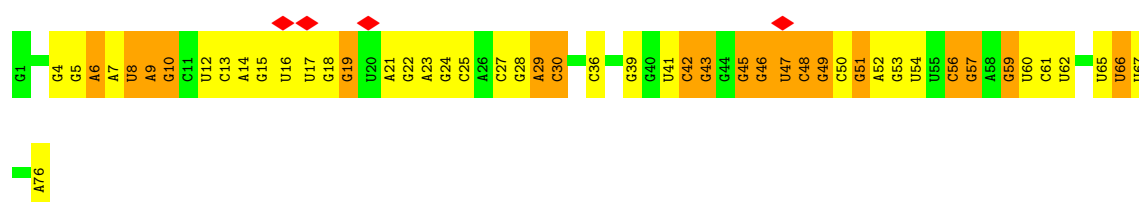
- Molecule 29: 30S ribosomal protein S21

Chain U: 



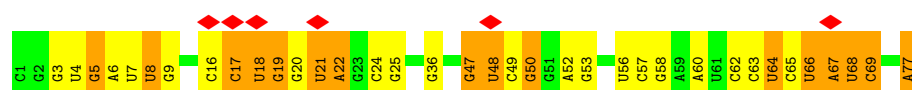
- Molecule 30: E-site tRNA

Chain X: 



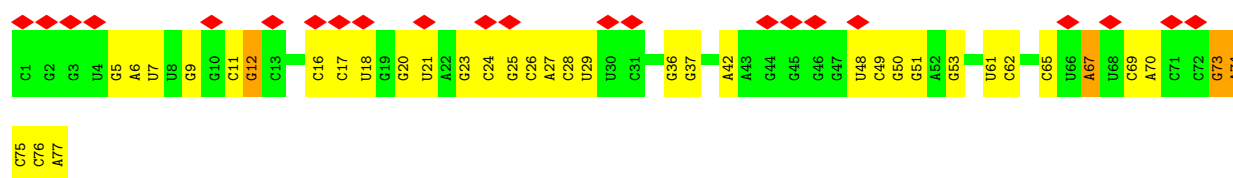
- Molecule 31: P-site tRNA (Chain Y), A-site tRNA-PRO (Chain Z)

Chain Y: 




- Molecule 31: P-site tRNA (Chain Y), A-site tRNA-PRO (Chain Z)

Chain Z: 



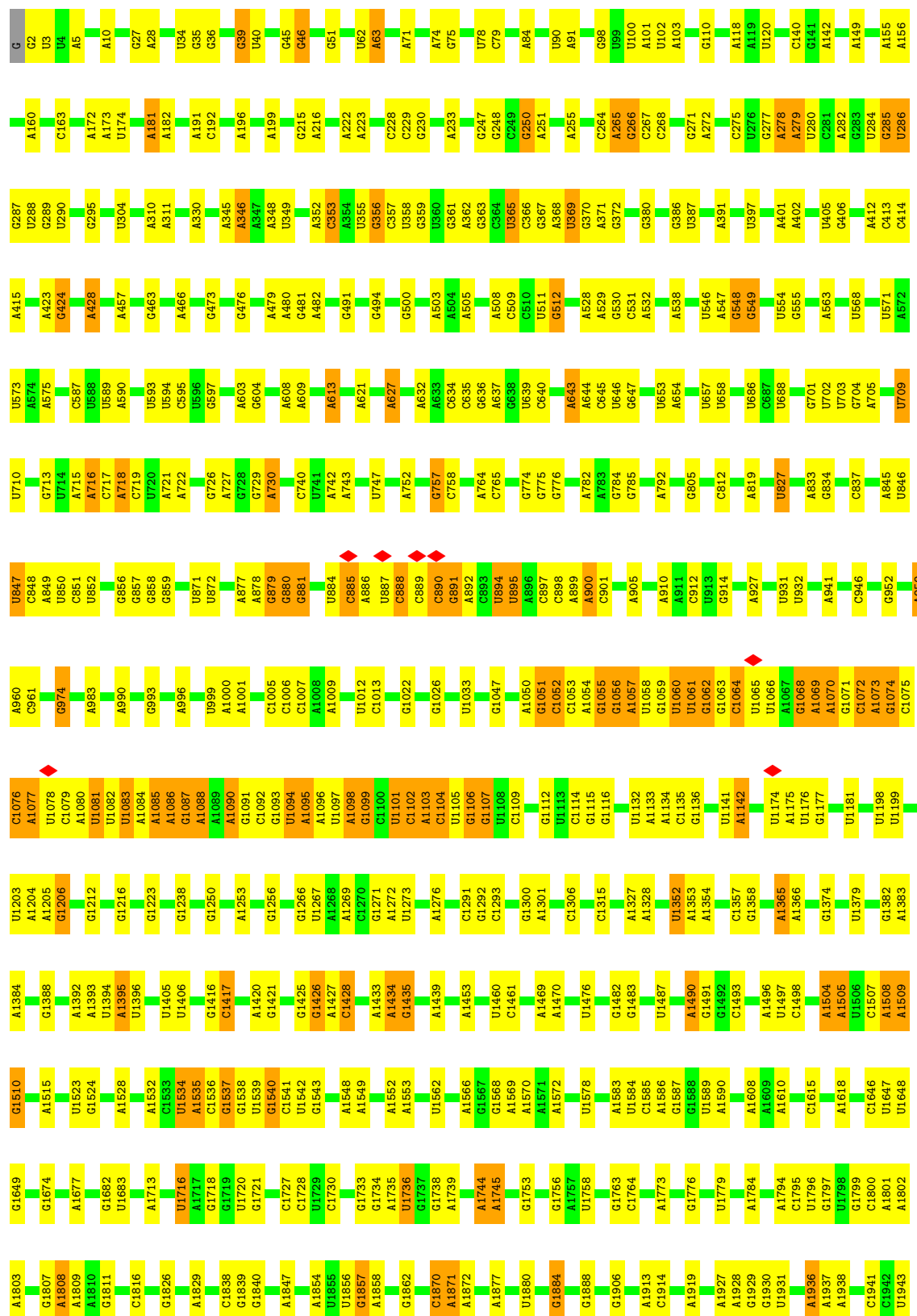
- Molecule 32: 5S rRNA

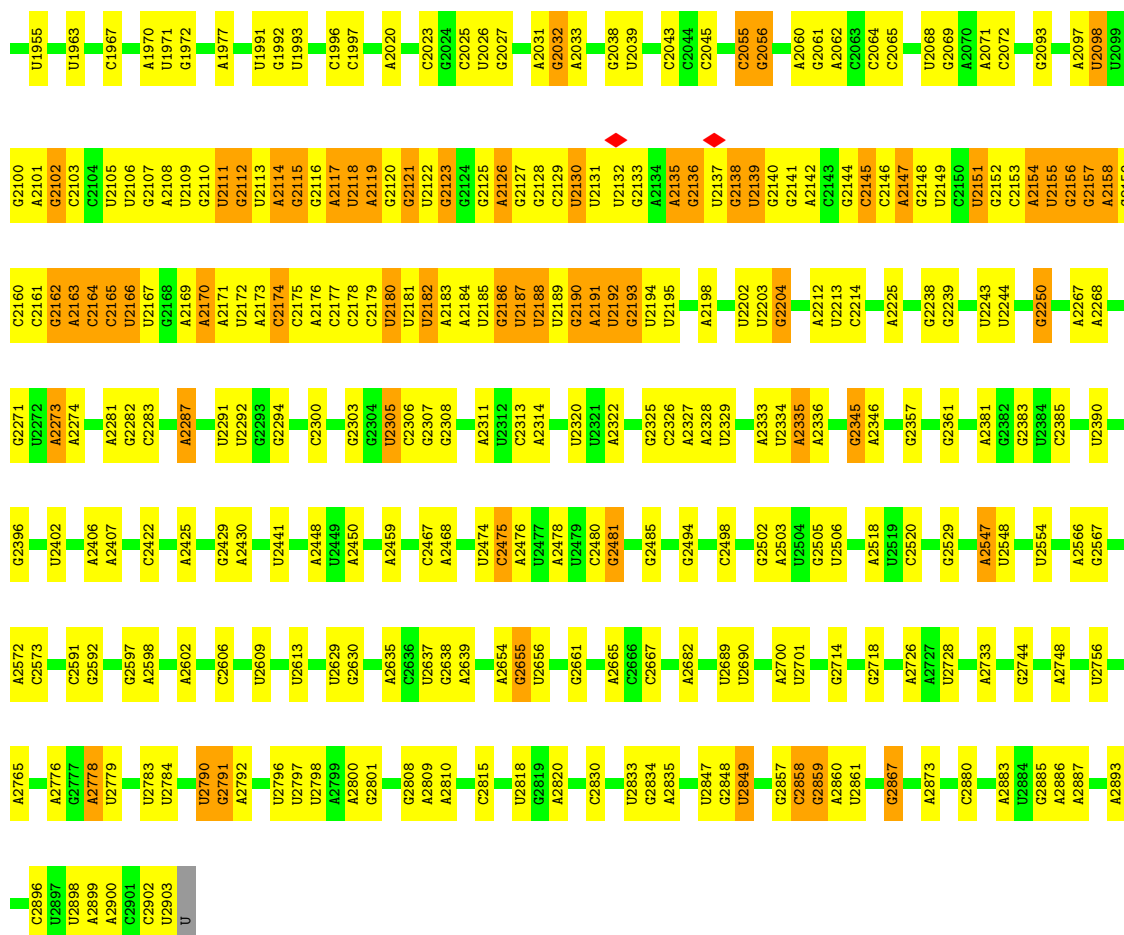
Chain a: 



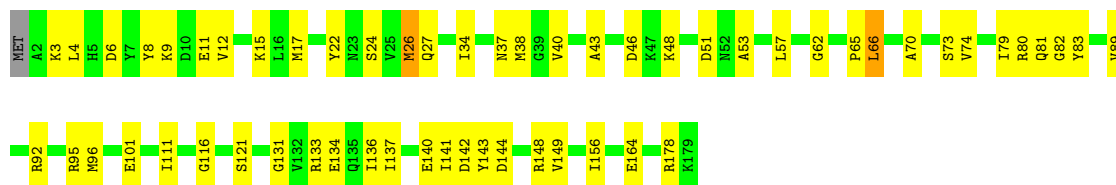
• Molecule 33: 23S rRNA

Chain b:  70% 24% 6%




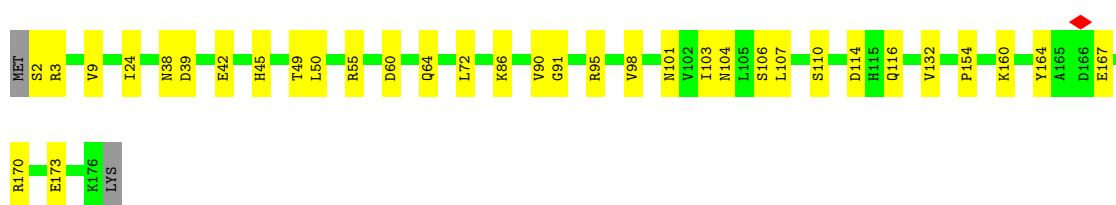


Chain f:  68% 31% ..




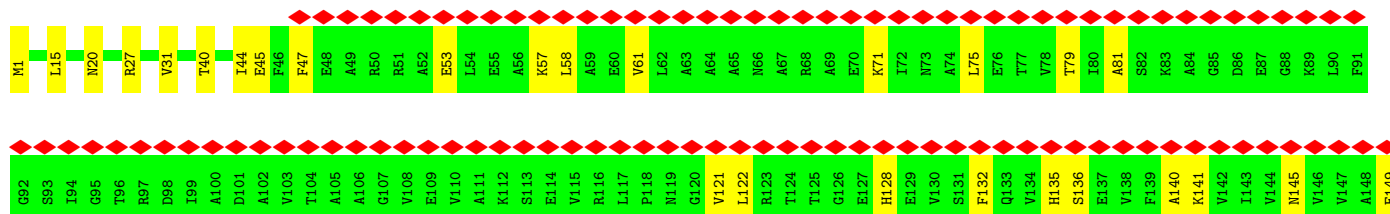
- Molecule 38: 50S ribosomal protein L6

Chain g:  80% 19% .




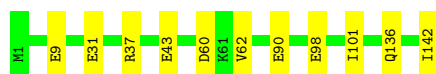
- Molecule 39: 50S ribosomal protein L9

Chain h:  69% 82% 18%




- Molecule 40: 50S ribosomal protein L13

Chain k:  92% 8%




- Molecule 41: 50S ribosomal protein L14

Chain l:  87% 13%

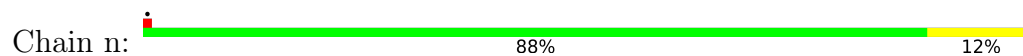


- Molecule 42: 50S ribosomal protein L15

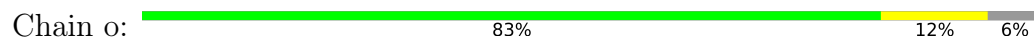
Chain m:  88% 12%



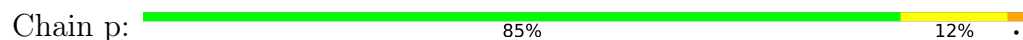
- Molecule 43: 50S ribosomal protein L16



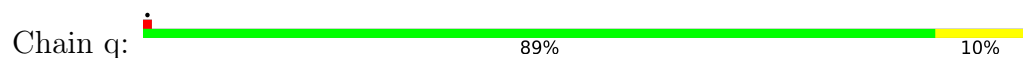
- Molecule 44: 50S ribosomal protein L17



- Molecule 45: 50S ribosomal protein L18



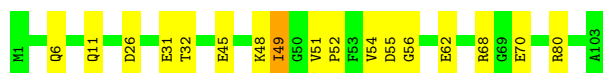
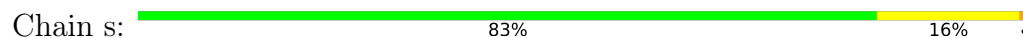
- Molecule 46: 50S ribosomal protein L19



- Molecule 47: 50S ribosomal protein L20



- Molecule 48: 50S ribosomal protein L21

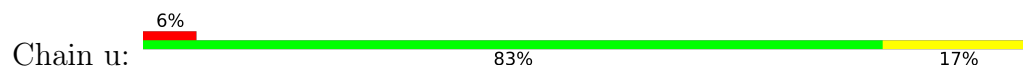


- Molecule 49: 50S ribosomal protein L22

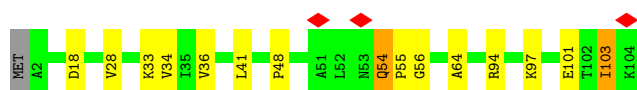
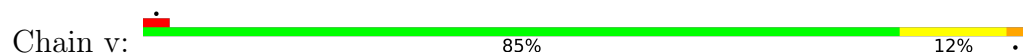




- Molecule 50: 50S ribosomal protein L23



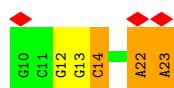
- Molecule 51: 50S ribosomal protein L24



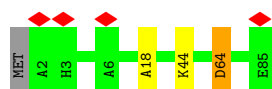
- Molecule 52: 50S ribosomal protein L25



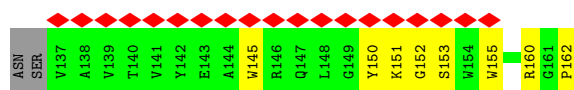
- Molecule 53: mRNA



- Molecule 54: 50S ribosomal protein L27



- Molecule 55: eRAP



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	152000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.638	Depositor
Minimum map value	-0.680	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	682.0, 682.0, 682.0	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.34	0/635	0.29	0/848
2	1	0.28	0/496	0.30	0/660
3	2	0.32	0/453	0.30	0/605
4	4	0.34	0/450	0.36	0/599
5	5	0.27	0/433	0.30	0/576
6	6	0.37	0/380	0.43	0/498
7	7	0.36	0/513	0.35	0/676
8	8	0.35	0/303	0.30	0/397
9	A	0.25	0/36834	0.28	0/57462
10	B	0.22	0/1735	0.34	0/2338
11	C	0.20	0/1659	0.30	0/2236
12	D	0.15	0/1665	0.33	0/2227
13	E	0.24	0/1169	0.36	0/1573
14	F	0.57	1/881 (0.1%)	0.43	0/1189
15	G	0.18	0/1219	0.29	0/1635
16	H	0.26	0/989	0.31	0/1326
17	I	0.20	0/1034	0.36	0/1375
18	J	0.20	0/813	0.43	0/1100
19	K	0.23	0/893	0.30	0/1205
20	L	0.19	0/963	0.34	0/1293
21	M	0.18	0/909	0.30	0/1215
22	N	0.20	0/817	0.31	0/1088
23	O	0.23	0/722	0.32	0/964
24	P	0.21	0/653	0.29	0/877
25	Q	0.21	0/657	0.31	0/881
26	R	0.24	0/553	0.31	0/742
27	S	0.17	0/680	0.34	0/915
28	T	0.22	0/676	0.33	0/895
29	U	0.16	0/536	0.29	0/711
30	X	0.16	0/1810	0.27	0/2820
31	Y	0.21	0/1839	0.33	0/2866
31	Z	0.16	0/1839	0.27	0/2866

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	a	0.29	0/2872	0.28	0/4478
33	b	0.37	0/69773	0.32	0/108851
34	c	0.35	0/2121	0.33	0/2852
35	d	0.34	0/1586	0.34	0/2134
36	e	0.32	0/1571	0.28	0/2113
37	f	0.23	0/1443	0.32	0/1937
38	g	0.22	0/1333	0.29	0/1805
39	h	0.53	1/1119 (0.1%)	0.32	0/1512
40	k	0.41	1/1152 (0.1%)	0.30	0/1551
41	l	0.32	0/955	0.38	0/1279
42	m	0.34	0/1062	0.35	0/1413
43	n	0.27	0/1093	0.32	0/1460
44	o	0.36	0/973	0.38	0/1301
45	p	0.27	0/902	0.31	0/1209
46	q	0.32	0/929	0.29	0/1242
47	r	0.39	0/960	0.34	0/1278
48	s	0.34	0/829	0.35	0/1107
49	t	0.35	0/864	0.35	0/1156
50	u	0.32	0/793	0.35	0/1060
51	v	0.61	1/796 (0.1%)	0.38	0/1062
52	w	0.26	0/766	0.31	0/1025
53	x	0.20	0/333	0.27	0/517
54	y	0.33	0/642	0.29	0/848
55	z	0.17	0/316	0.33	0/435
All	All	0.32	4/160391 (0.0%)	0.31	0/240283

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	h	31	VAL	CA-CB	16.57	1.63	1.54
14	F	18	VAL	CA-CB	14.55	1.62	1.54
51	v	54	GLN	C-O	13.48	1.30	1.23
40	k	136	GLN	C-O	-5.93	1.21	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	0	625	0	652	8	0
2	1	495	0	526	5	0
3	2	449	0	488	7	0
4	4	444	0	458	11	0
5	5	426	0	464	11	0
6	6	377	0	418	2	0
7	7	504	0	572	5	0
8	8	302	0	340	3	0
9	A	32895	0	16553	335	0
10	B	1704	0	1732	42	0
11	C	1632	0	1710	24	0
12	D	1643	0	1710	65	0
13	E	1156	0	1199	27	0
14	F	862	0	864	24	0
15	G	1203	0	1256	27	0
16	H	979	0	1034	29	0
17	I	1022	0	1070	42	0
18	J	803	0	842	34	0
19	K	877	0	887	18	0
20	L	949	0	1014	23	0
21	M	900	0	968	20	0
22	N	805	0	847	14	0
23	O	714	0	737	10	0
24	P	643	0	661	16	0
25	Q	648	0	691	16	0
26	R	544	0	565	12	0
27	S	663	0	690	15	0
28	T	670	0	722	18	0
29	U	529	0	565	10	0
30	X	1621	0	820	33	0
31	Y	1646	0	832	27	0
31	Z	1646	0	832	19	0
32	a	2569	0	1301	11	0
33	b	62297	0	31333	373	0
34	c	2082	0	2154	17	0
35	d	1565	0	1616	11	0
36	e	1552	0	1619	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	f	1419	0	1457	36	0
38	g	1313	0	1358	20	0
39	h	1108	0	1148	14	0
40	k	1129	0	1162	8	0
41	l	946	0	1023	13	0
42	m	1053	0	1129	12	0
43	n	1074	0	1157	10	0
44	o	960	0	1000	10	0
45	p	892	0	923	16	0
46	q	917	0	962	11	0
47	r	947	0	1019	5	0
48	s	816	0	839	14	0
49	t	857	0	922	3	0
50	u	786	0	846	11	0
51	v	788	0	844	9	0
52	w	753	0	780	8	0
53	x	299	0	154	3	0
54	y	634	0	653	2	0
55	z	298	0	273	9	0
56	8	1	0	0	0	0
57	Z	7	0	7	5	0
All	All	147438	0	98398	1453	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 6.

The worst 5 of 1453 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)
10:B:150:ILE:HD11	10:B:153:MET:SD	1.77	1.25
10:B:150:ILE:CD1	10:B:153:MET:SD	2.28	1.22
31:Z:77:A:O3'	57:Z:163:PRO:C	1.90	1.14
31:Y:77:A:O3'	55:z:162:PRO:C	1.90	1.14
31:Z:77:A:O3'	57:Z:163:PRO:O	1.76	1.03

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
2	1	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
3	2	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
4	4	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
5	5	50/55 (91%)	46 (92%)	4 (8%)	0	100	100
6	6	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
7	7	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
8	8	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
10	B	216/241 (90%)	197 (91%)	19 (9%)	0	100	100
11	C	205/233 (88%)	191 (93%)	14 (7%)	0	100	100
12	D	203/206 (98%)	179 (88%)	24 (12%)	0	100	100
13	E	155/167 (93%)	136 (88%)	19 (12%)	0	100	100
14	F	104/135 (77%)	94 (90%)	10 (10%)	0	100	100
15	G	151/179 (84%)	143 (95%)	8 (5%)	0	100	100
16	H	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
17	I	125/130 (96%)	109 (87%)	16 (13%)	0	100	100
18	J	98/103 (95%)	87 (89%)	11 (11%)	0	100	100
19	K	115/129 (89%)	105 (91%)	10 (9%)	0	100	100
20	L	120/124 (97%)	101 (84%)	19 (16%)	0	100	100
21	M	114/118 (97%)	103 (90%)	11 (10%)	0	100	100
22	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
23	O	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
24	P	79/82 (96%)	70 (89%)	9 (11%)	0	100	100
25	Q	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
26	R	64/75 (85%)	58 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	S	81/92 (88%)	75 (93%)	6 (7%)	0	100	100
28	T	84/87 (97%)	84 (100%)	0	0	100	100
29	U	62/71 (87%)	57 (92%)	5 (8%)	0	100	100
34	c	269/273 (98%)	253 (94%)	16 (6%)	0	100	100
35	d	207/209 (99%)	194 (94%)	13 (6%)	0	100	100
36	e	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
37	f	176/179 (98%)	165 (94%)	11 (6%)	0	100	100
38	g	173/177 (98%)	159 (92%)	14 (8%)	0	100	100
39	h	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
40	k	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
41	l	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
42	m	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
43	n	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
44	o	118/127 (93%)	112 (95%)	6 (5%)	0	100	100
45	p	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
46	q	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
47	r	115/118 (98%)	115 (100%)	0	0	100	100
48	s	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
49	t	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
50	u	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
51	v	101/104 (97%)	91 (90%)	10 (10%)	0	100	100
52	w	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
54	y	82/85 (96%)	80 (98%)	2 (2%)	0	100	100
55	z	32/28 (114%)	29 (91%)	3 (9%)	0	100	100
All	All	5582/5871 (95%)	5197 (93%)	385 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	67/68 (98%)	67 (100%)	0	100	100
2	1	54/55 (98%)	54 (100%)	0	100	100
3	2	48/49 (98%)	48 (100%)	0	100	100
4	4	47/48 (98%)	47 (100%)	0	100	100
5	5	47/49 (96%)	47 (100%)	0	100	100
6	6	38/38 (100%)	38 (100%)	0	100	100
7	7	51/52 (98%)	51 (100%)	0	100	100
8	8	34/34 (100%)	34 (100%)	0	100	100
10	B	180/199 (90%)	179 (99%)	1 (1%)	84	94
11	C	171/190 (90%)	170 (99%)	1 (1%)	84	94
12	D	172/173 (99%)	168 (98%)	4 (2%)	45	74
13	E	119/126 (94%)	117 (98%)	2 (2%)	56	81
14	F	92/116 (79%)	89 (97%)	3 (3%)	33	62
15	G	126/147 (86%)	126 (100%)	0	100	100
16	H	104/105 (99%)	104 (100%)	0	100	100
17	I	105/107 (98%)	103 (98%)	2 (2%)	52	79
18	J	88/90 (98%)	86 (98%)	2 (2%)	45	74
19	K	90/99 (91%)	89 (99%)	1 (1%)	70	87
20	L	103/104 (99%)	100 (97%)	3 (3%)	37	67
21	M	94/96 (98%)	93 (99%)	1 (1%)	70	87
22	N	83/84 (99%)	83 (100%)	0	100	100
23	O	76/77 (99%)	74 (97%)	2 (3%)	41	70
24	P	65/65 (100%)	62 (95%)	3 (5%)	23	49
25	Q	74/78 (95%)	72 (97%)	2 (3%)	40	69
26	R	57/65 (88%)	57 (100%)	0	100	100
27	S	72/79 (91%)	71 (99%)	1 (1%)	62	84
28	T	65/66 (98%)	65 (100%)	0	100	100
29	U	54/61 (88%)	52 (96%)	2 (4%)	29	58
34	c	216/218 (99%)	216 (100%)	0	100	100
35	d	164/164 (100%)	163 (99%)	1 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	e	165/165 (100%)	164 (99%)	1 (1%)	84	94
37	f	149/150 (99%)	147 (99%)	2 (1%)	65	85
38	g	136/138 (99%)	135 (99%)	1 (1%)	81	93
39	h	113/114 (99%)	111 (98%)	2 (2%)	54	80
40	k	116/116 (100%)	116 (100%)	0	100	100
41	l	104/104 (100%)	104 (100%)	0	100	100
42	m	103/103 (100%)	102 (99%)	1 (1%)	73	89
43	n	109/109 (100%)	109 (100%)	0	100	100
44	o	100/103 (97%)	98 (98%)	2 (2%)	50	78
45	p	86/87 (99%)	84 (98%)	2 (2%)	45	74
46	q	99/100 (99%)	98 (99%)	1 (1%)	73	89
47	r	89/90 (99%)	89 (100%)	0	100	100
48	s	84/84 (100%)	83 (99%)	1 (1%)	67	86
49	t	93/93 (100%)	93 (100%)	0	100	100
50	u	84/84 (100%)	84 (100%)	0	100	100
51	v	84/85 (99%)	82 (98%)	2 (2%)	44	73
52	w	78/78 (100%)	77 (99%)	1 (1%)	65	85
54	y	62/63 (98%)	60 (97%)	2 (3%)	34	63
55	z	26/23 (113%)	23 (88%)	3 (12%)	4	11
All	All	4636/4791 (97%)	4584 (99%)	52 (1%)	69	87

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	U	2	VAL
39	h	121	VAL
55	z	145	TRP
29	U	31	VAL
37	f	26	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
36	e	115	GLN

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Mol	Chain	Res	Type
47	r	44	GLN
36	e	195	GLN
41	l	82	ASN
49	t	31	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	X	75/76 (98%)	32 (42%)	1 (1%)
31	Y	76/77 (98%)	26 (34%)	3 (3%)
31	Z	76/77 (98%)	15 (19%)	2 (2%)
32	a	119/120 (99%)	20 (16%)	0
33	b	2901/2904 (99%)	562 (19%)	0
53	x	13/14 (92%)	3 (23%)	0
9	A	1532/1533 (99%)	336 (21%)	10 (0%)
All	All	4792/4801 (99%)	994 (20%)	16 (0%)

5 of 994 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	2	A
9	A	4	U
9	A	9	G
9	A	32	A
9	A	33	A

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	Z	20	G
31	Y	66	U
9	A	1357	A
31	Y	16	C
9	A	1255	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	PRO	Z	163	-	5,7,8	0.71	0	7,8,10	1.49	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PRO	Z	163	-	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	Z	163	PRO	O-C-CA	-2.86	117.28	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	Z	163	PRO	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

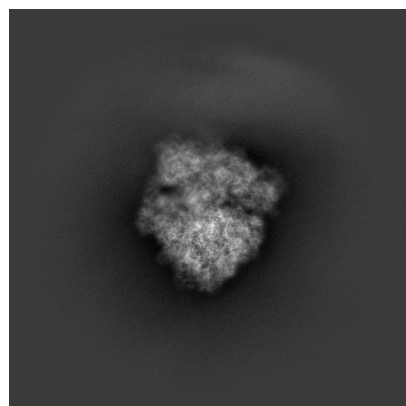
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60034. These allow visual inspection of the internal detail of the map and identification of artifacts.

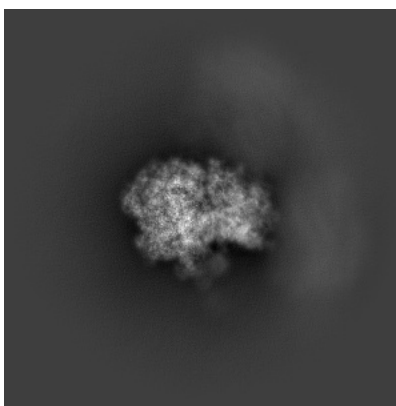
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

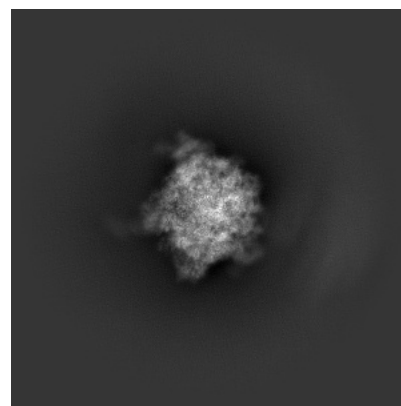
6.1.1 Primary map



X

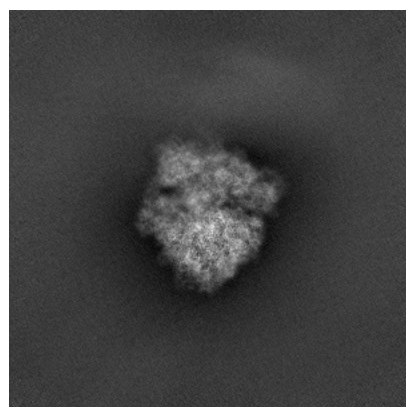


Y

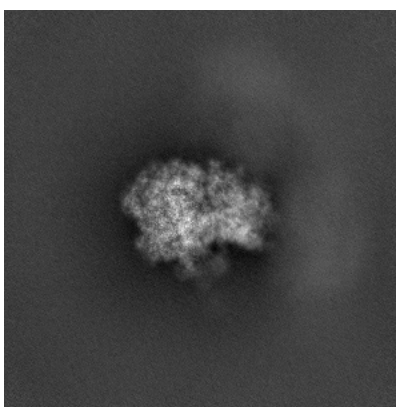


Z

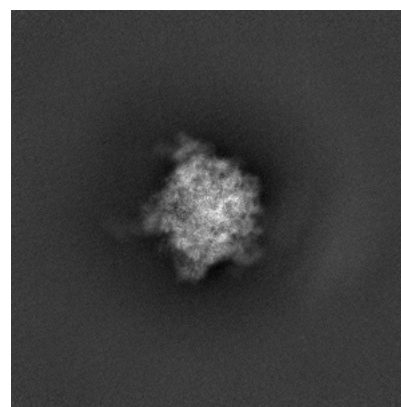
6.1.2 Raw map



X



Y

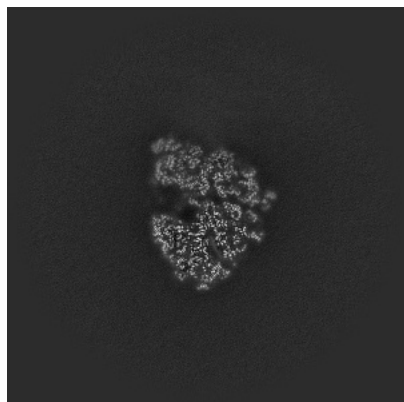


Z

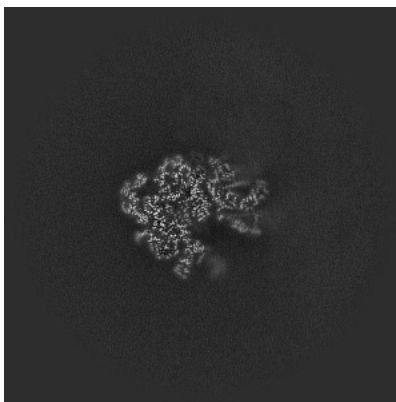
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

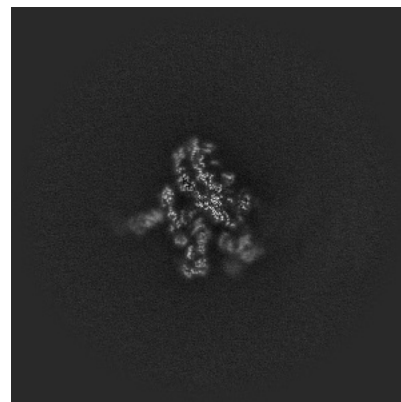
6.2.1 Primary map



X Index: 310

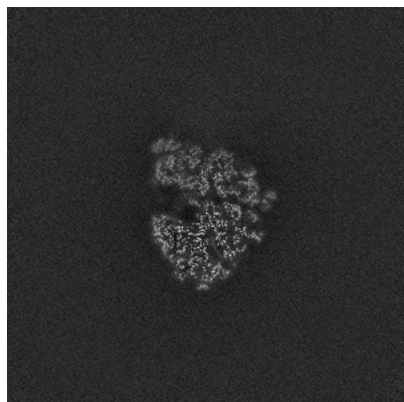


Y Index: 310

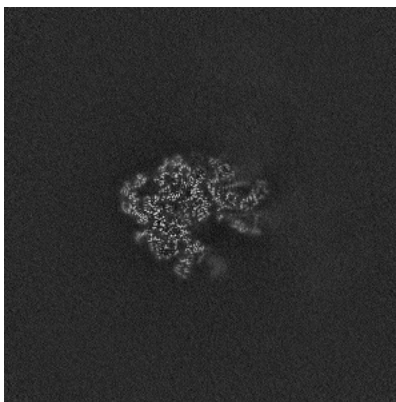


Z Index: 310

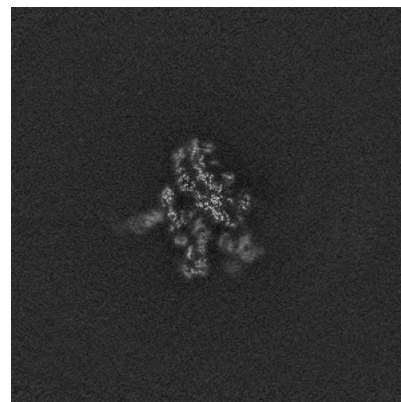
6.2.2 Raw map



X Index: 310



Y Index: 310

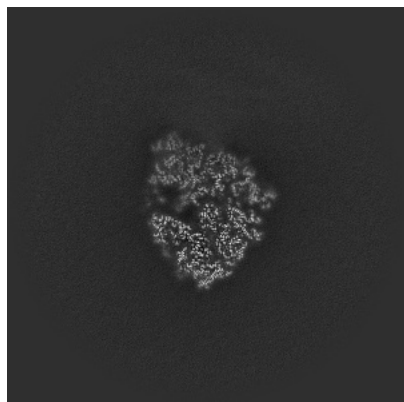


Z Index: 310

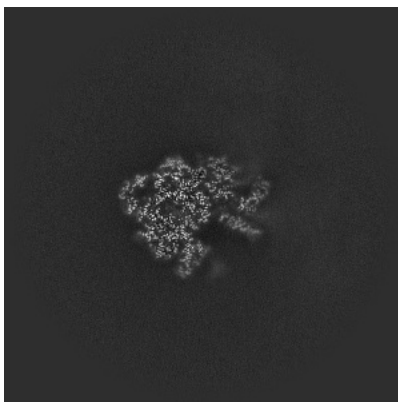
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

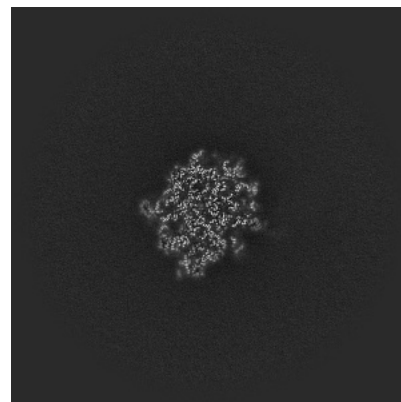
6.3.1 Primary map



X Index: 306

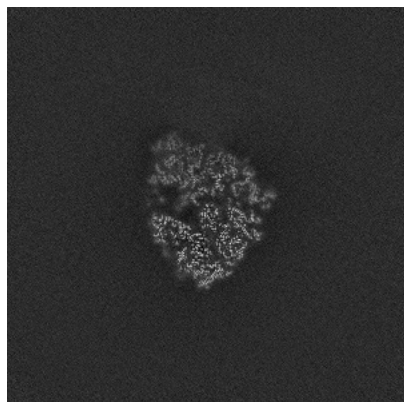


Y Index: 314

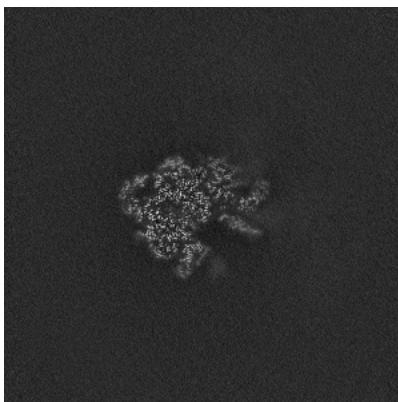


Z Index: 278

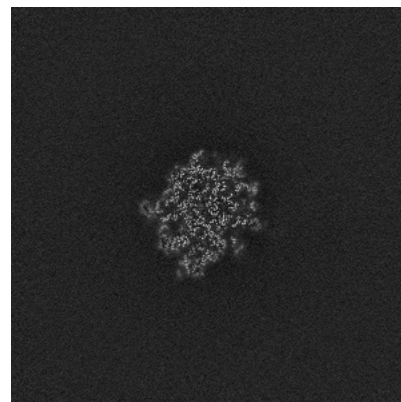
6.3.2 Raw map



X Index: 306



Y Index: 313

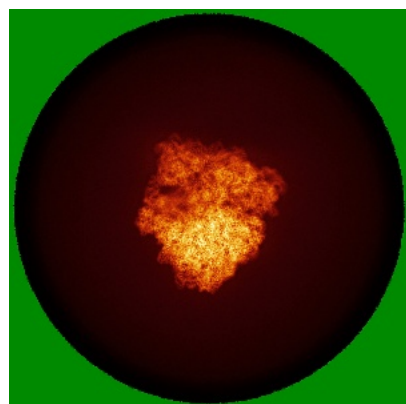


Z Index: 278

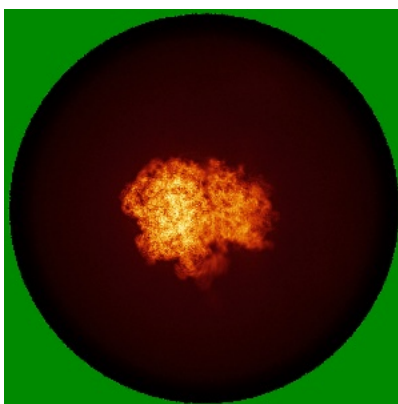
The images above show the largest variance slices of the map in three orthogonal directions.

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

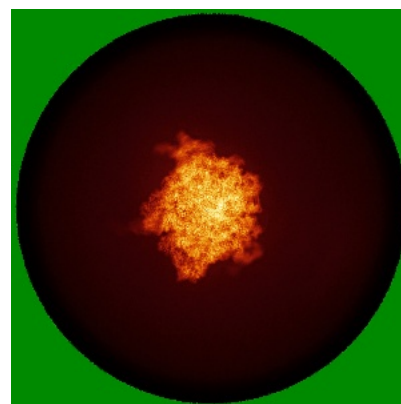
6.4.1 Primary map



X

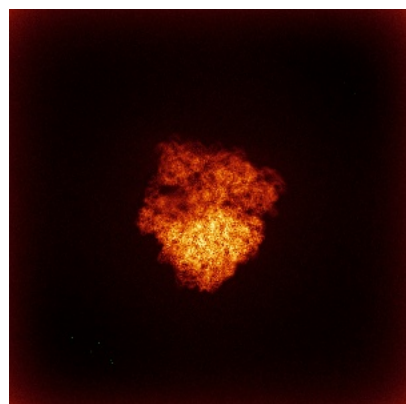


Y

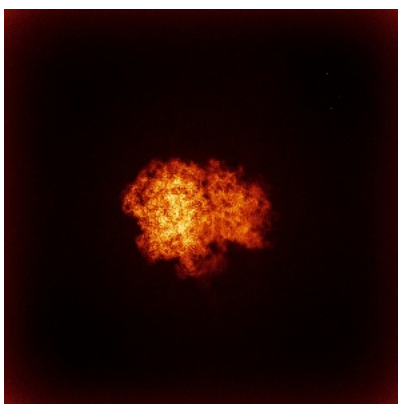


Z

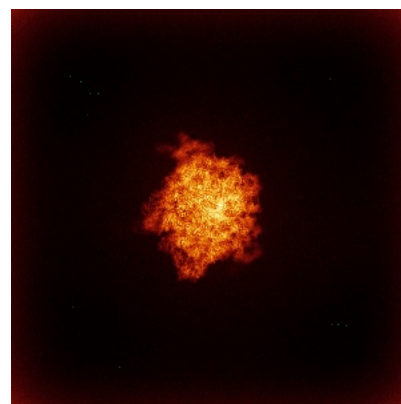
6.4.2 Raw map



X



Y

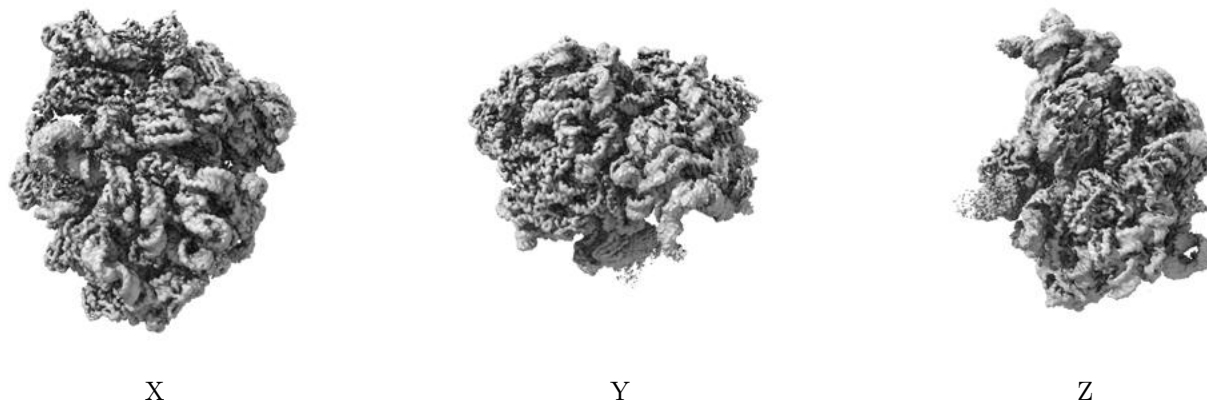


Z

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.

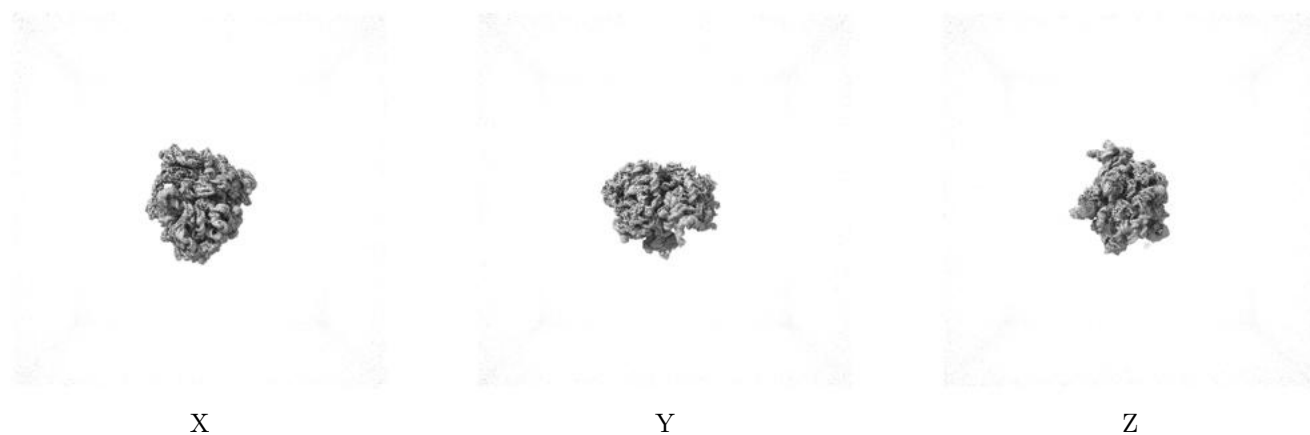
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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.

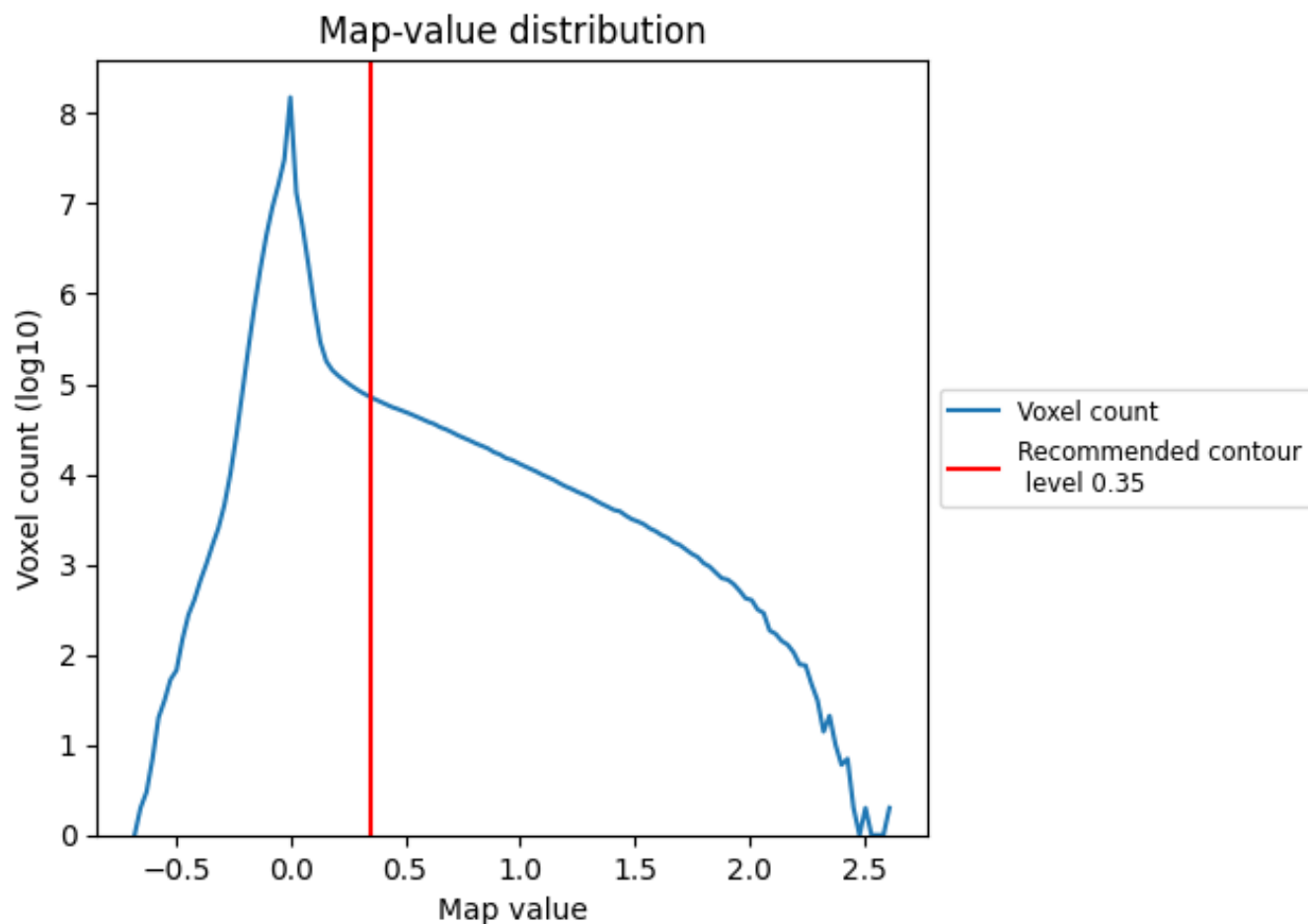
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

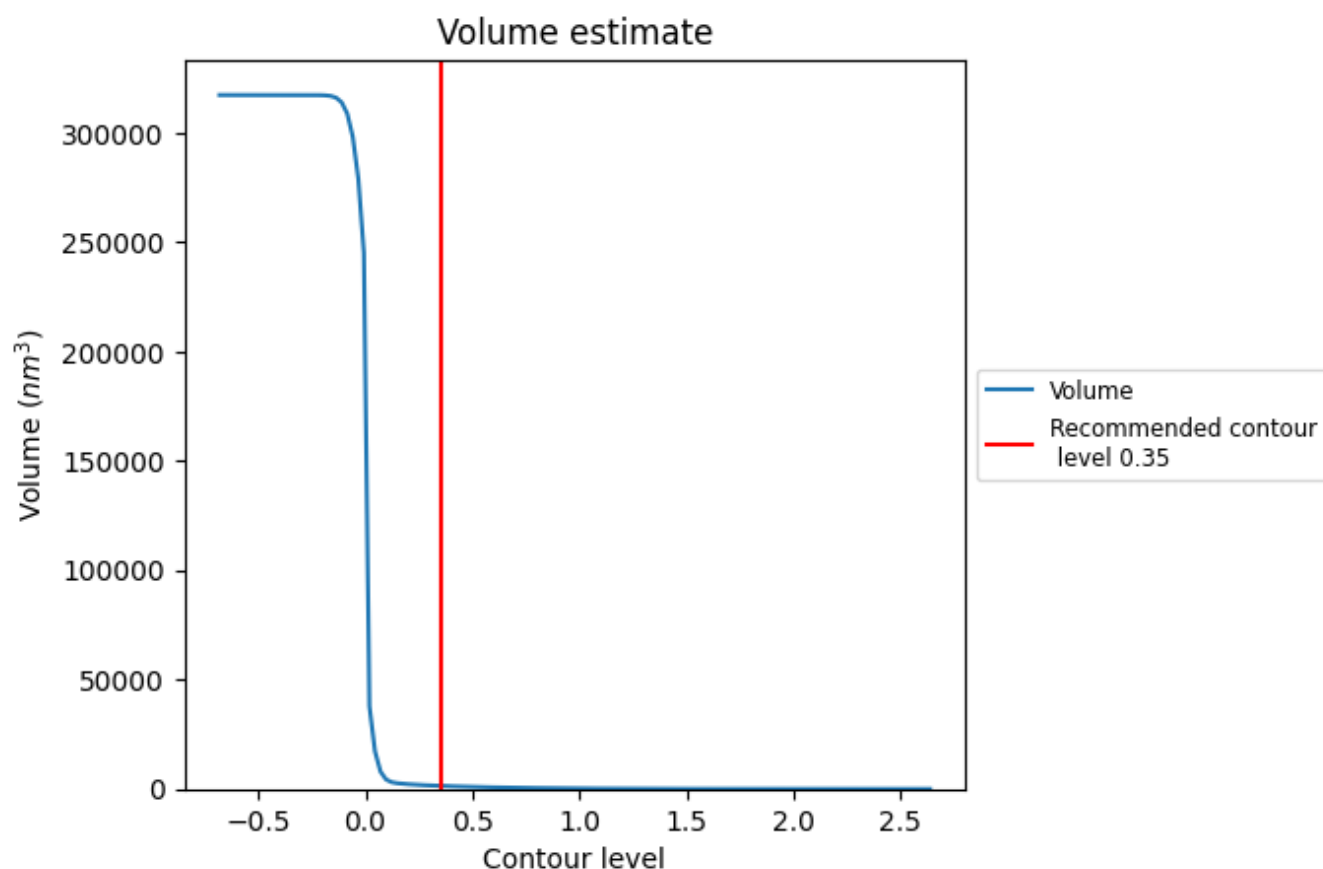
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

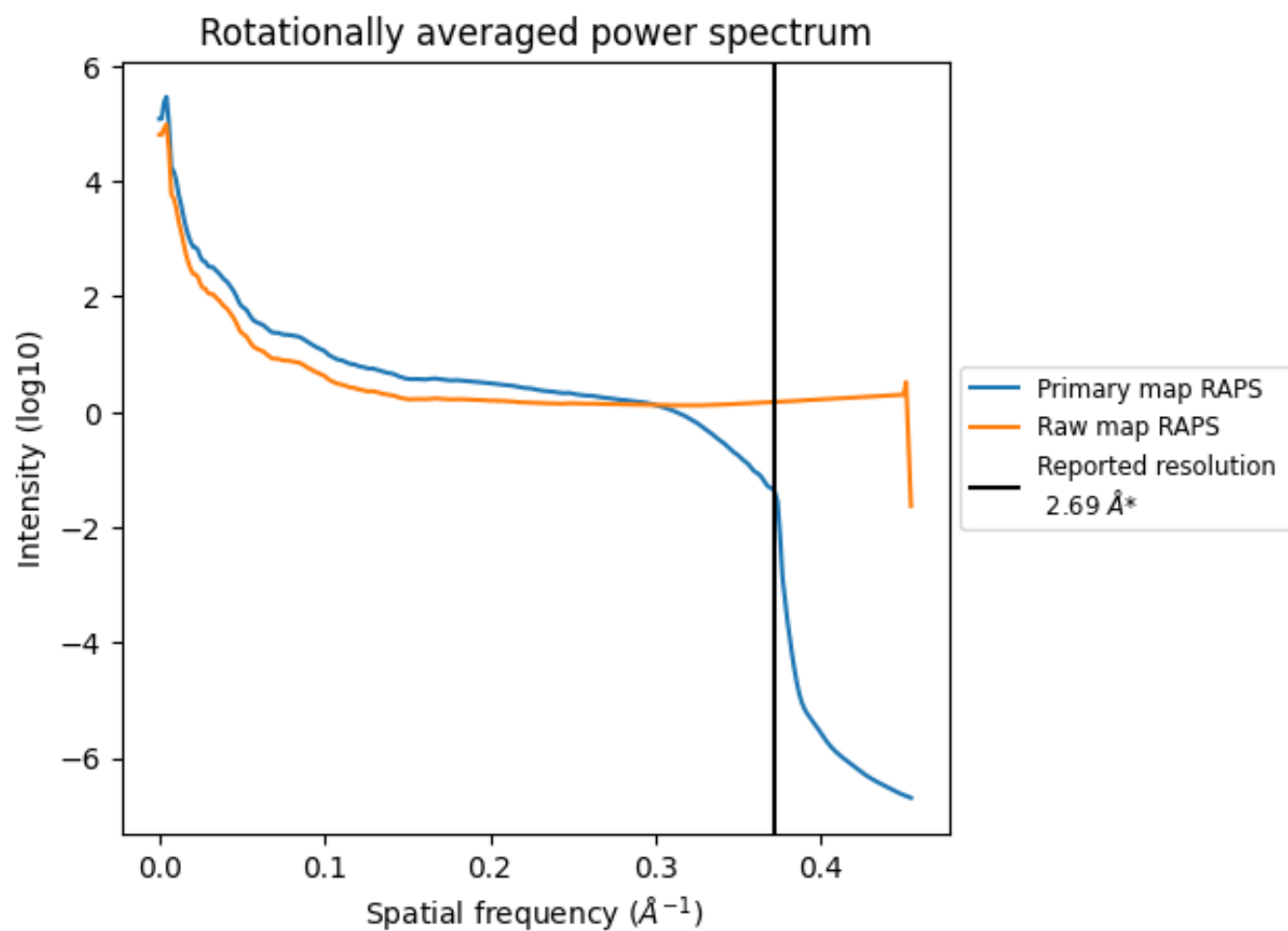
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1417 nm^3 ; this corresponds to an approximate mass of 1280 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 ⓘ

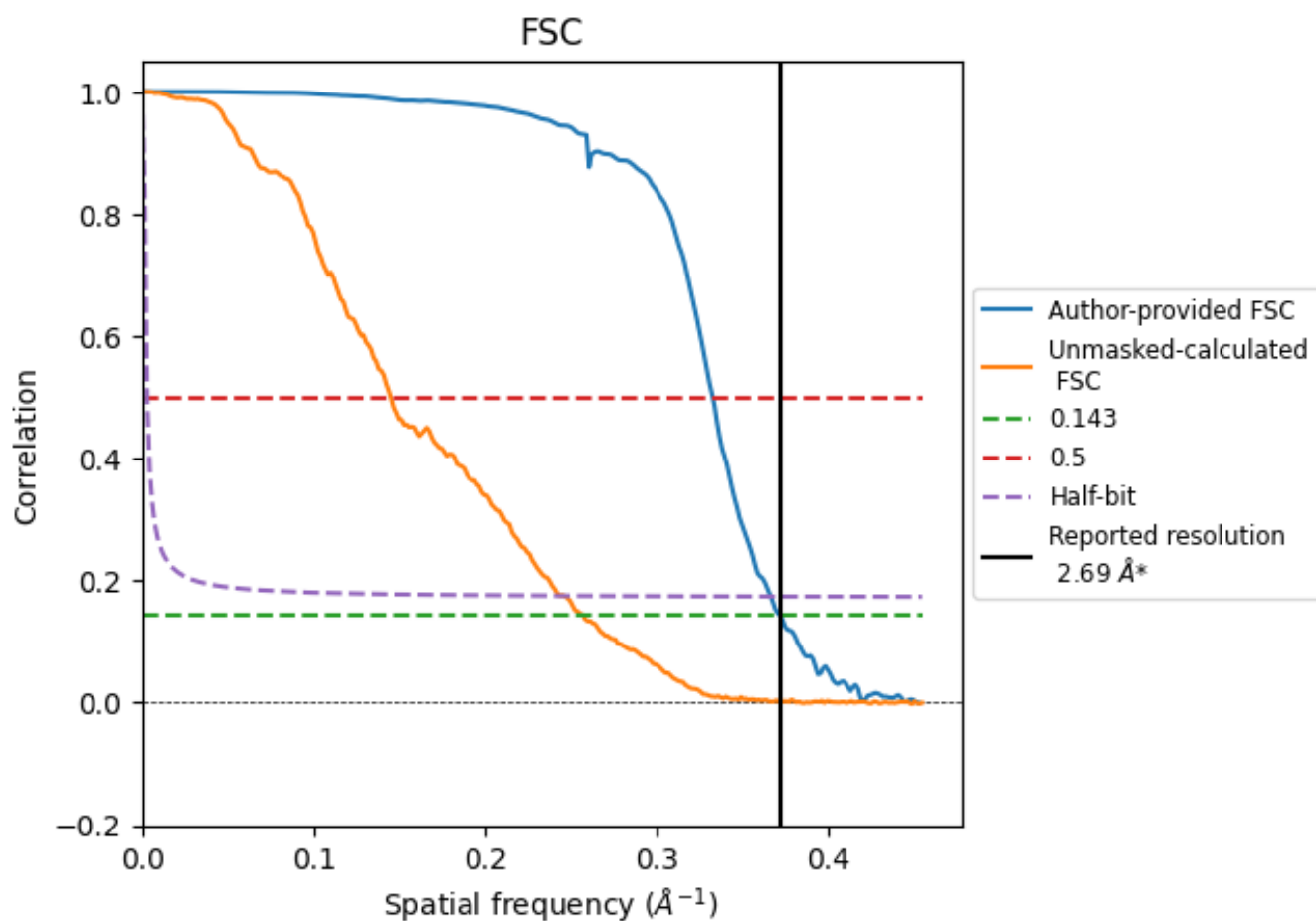


*Reported resolution corresponds to spatial frequency of 0.372 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.372 Å⁻¹

8.2 Resolution estimates [i](#)

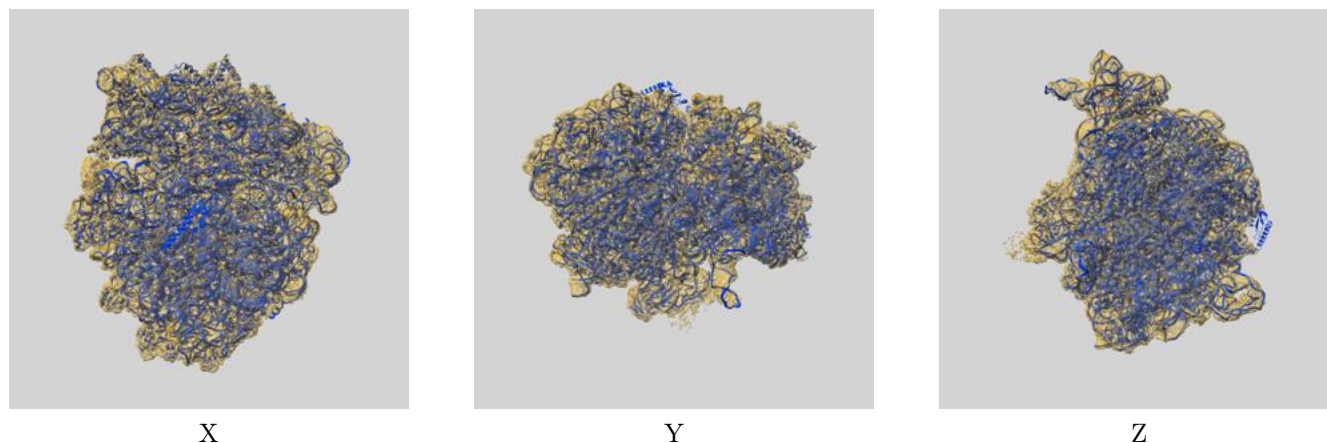
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.69	3.01	2.73
Unmasked-calculated*	3.89	6.91	4.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 2.69 by more than 10 %

9 Map-model fit [i](#)

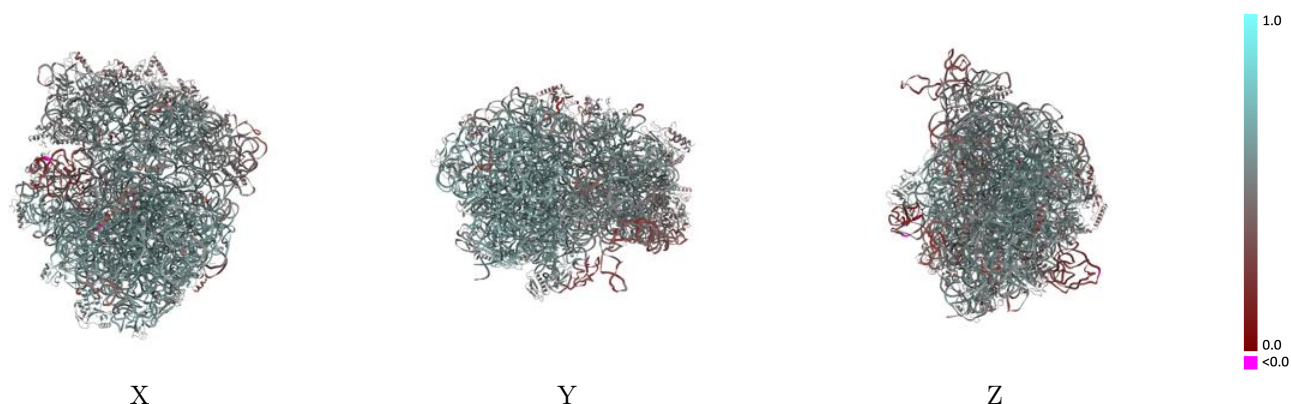
This section contains information regarding the fit between EMDB map EMD-60034 and PDB model 8ZEJ. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



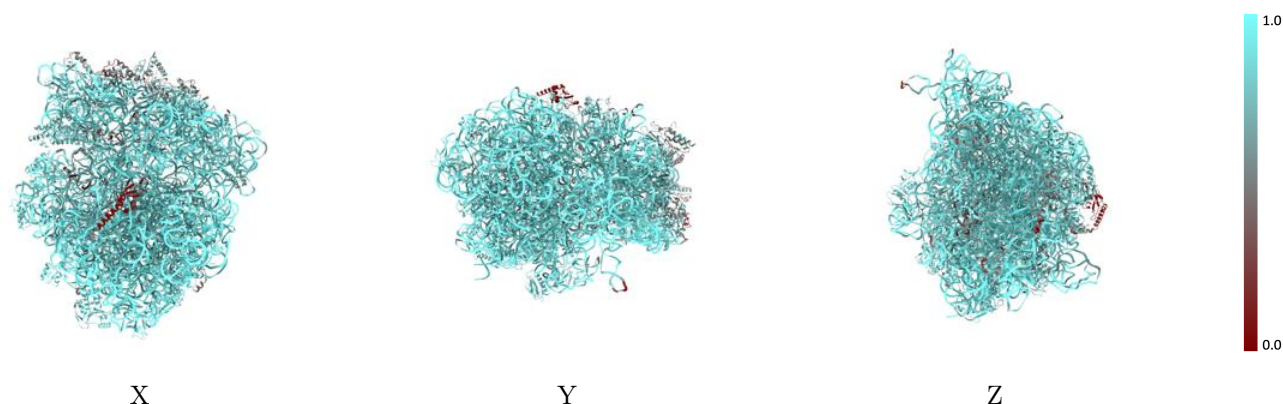
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



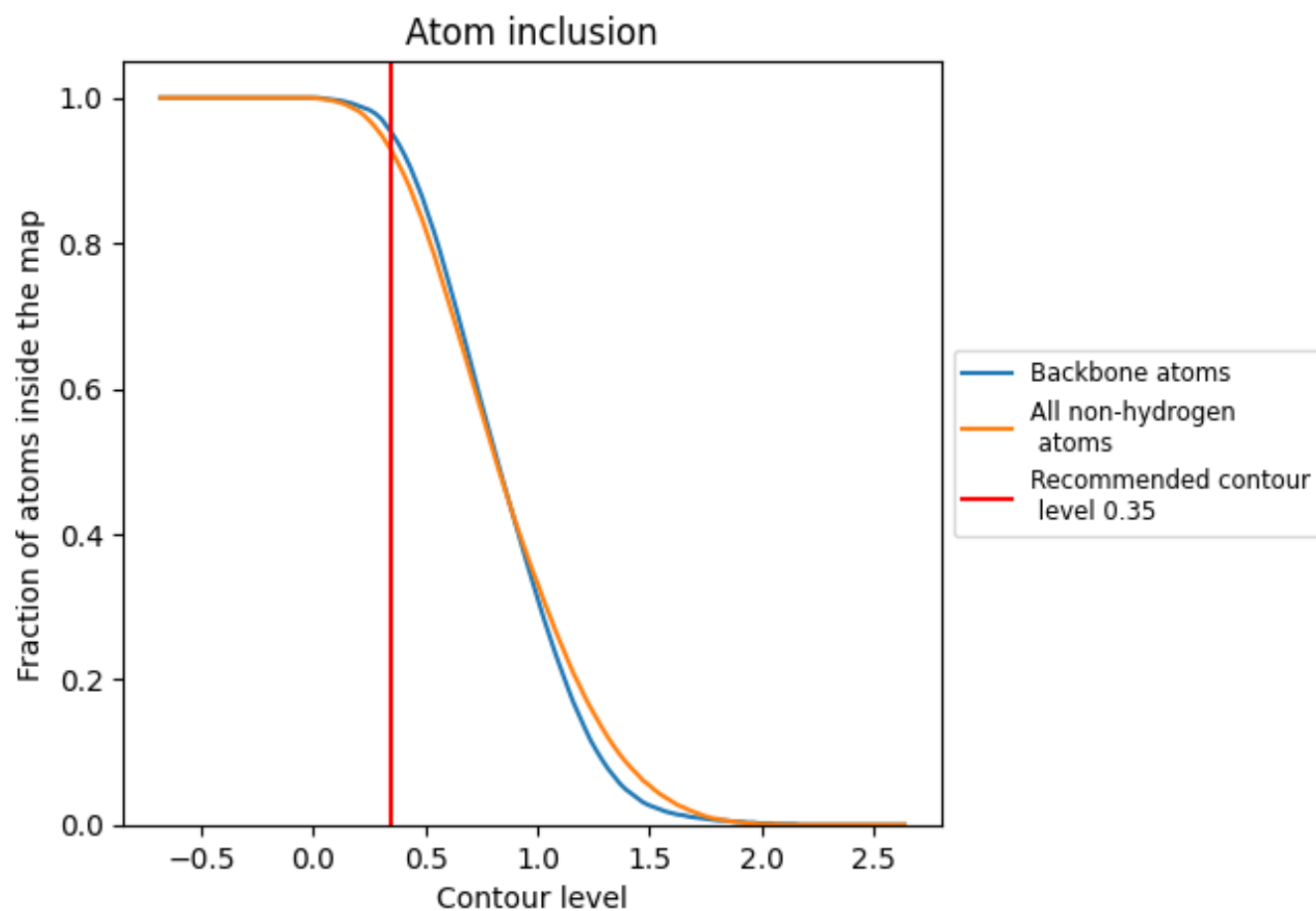
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ













































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

Chain	Atom inclusion	Q-score
All	 0.9270	 0.5400
0	 0.9380	 0.5710
1	 0.9300	 0.5200
2	 0.9110	 0.5630
4	 0.9110	 0.5720
5	 0.7920	 0.5470
6	 0.9490	 0.6100
7	 0.9490	 0.6070
8	 0.9450	 0.5900
A	 0.9720	 0.5170
B	 0.5120	 0.4410
C	 0.7230	 0.5060
D	 0.5990	 0.4090
E	 0.8140	 0.5190
F	 0.7860	 0.4690
G	 0.7440	 0.4750
H	 0.8770	 0.5230
I	 0.8390	 0.4900
J	 0.6440	 0.4380
K	 0.8420	 0.5250
L	 0.6800	 0.4540
M	 0.8090	 0.4820
N	 0.8330	 0.5110
O	 0.8840	 0.5170
P	 0.8310	 0.4720
Q	 0.8350	 0.4860
R	 0.8360	 0.5170
S	 0.7970	 0.4910
T	 0.8350	 0.4540
U	 0.5220	 0.4550
X	 0.8040	 0.3890
Y	 0.8680	 0.4840
Z	 0.6020	 0.5100
a	 0.9900	 0.5530
b	 0.9850	 0.5700



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Chain	Atom inclusion	Q-score
c	 0.9390	 0.5970
d	 0.9490	 0.5890
e	 0.9240	 0.5690
f	 0.8650	 0.4920
g	 0.8930	 0.5020
h	 0.2480	 0.3910
k	 0.9460	 0.5850
l	 0.9120	 0.5770
m	 0.9460	 0.5770
n	 0.8770	 0.5810
o	 0.9630	 0.5980
p	 0.9320	 0.5260
q	 0.9090	 0.5780
r	 0.9680	 0.5970
s	 0.9490	 0.5670
t	 0.9280	 0.5750
u	 0.8660	 0.5310
v	 0.9210	 0.5410
w	 0.9090	 0.5420
x	 0.7190	 0.4930
y	 0.8920	 0.5910
z	 0.2870	 0.4340