



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2023 – 10:58 AM JST

PDB ID : 8IE3
EMDB ID : EMD-35375
Title : human nuclear pre-60S ribosomal particle - State E
Authors : Zhang, Y.; Gao, N.
Deposited on : 2023-02-15
Resolution : 3.30 Å(reported)

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:

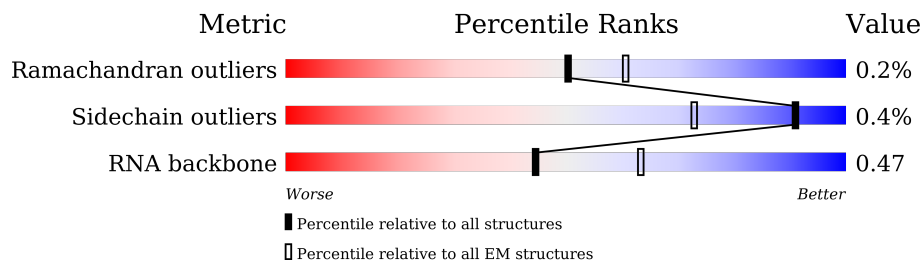
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	5	120	
2	6	245	
3	7	163	
4	8	156	
5	9	134	
6	B	403	
7	C	159	
8	D	427	


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Mol	Chain	Length	Quality of chain
9	E	115	58% 83% 15%
10	F	117	14% 93% 7%
11	G	266	21% 89% 9%
12	H	123	99%
13	I	192	9% 97%
14	K	105	6% 95%
15	L	148	88% 11%
16	M	97	89% 11%
17	O	70	27% 97%
18	P	51	94%
19	Q	211	8% 98%
20	S	215	62% 37%
21	U	204	6% 98%
22	V	203	98%
23	X	92	41% 99%
24	Z	188	80% 19%
25	a	196	21% 75% 24%
26	b	176	100%
27	c	160	12% 96%
28	e	140	6% 92% 6%
29	g	156	75% 24%
30	h	145	92% 8%
31	i	136	49% 96%
32	l	137	91% 9%
33	m	257	31% 96%

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Mol	Chain	Length	Quality of chain
34	n	110	 96%
35	o	288	 9% 80% 18%
36	p	248	 90% 9%
37	z	129	 36% 52% 48%
38	A	731	 42% 45% 54%
39	4	634	 50% 92%
40	R	260	 78% 84% 13%
41	2	5054	 10% 41% 24% 30%
42	r	297	 71% 95%
43	d	128	 9% 79% 19%
44	j	125	 9% 89% 11%
45	k	135	 95%
46	Y	184	 8% 90% 9%
47	J	239	 84% 84% 15%
48	T	178	 87% 91% 7%

2 Entry composition [i](#)

There are 48 unique types of molecules in this entry. The entry contains 145205 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 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	120	2558	1141	456	842	119	0	0

- Molecule 2 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	6	244	1852	1149	318	372	13	0	0

- Molecule 3 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	7	135	1159	737	225	187	10	0	0

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	8	156	3315	1481	585	1094	155	0	0

- Molecule 5 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	9	97	787	481	168	134	4	0	0

- Molecule 6 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	402	3244	2065	609	556	14	1	0

- Molecule 7 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	93	764	476	167	117	4	0	0

- Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	358	2853	1797	570	473	13	0	0

- Molecule 9 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	E	98	764	485	135	138	6	0	0

- Molecule 10 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	109	868	544	179	139	6	0	0

- Molecule 11 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	241	1935	1233	374	324	4	1	0

- Molecule 12 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	122	1015	641	205	168	1	0	0

- Molecule 13 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	190	1518	956	284	272	6	0	0

- Molecule 14 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 15 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	131	Total	C	N	O	S	0	0
			1043	666	205	169	3		

- Molecule 16 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 17 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 18 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 19 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 20 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 21 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	203	1701	1072	359	266	4	0	0

- Molecule 22 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	201	1650	1063	321	261	5	0	0

- Molecule 23 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	91	708	445	136	120	7	0	0

- Molecule 24 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Z	152	1227	770	248	204	5	0	0

- Molecule 25 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	a	148	1239	772	266	192	9	0	0

- Molecule 26 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	b	176	1461	930	284	236	11	0	0

- Molecule 27 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	c	155	1264	801	248	210	5	0	0

- Molecule 28 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 29 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	g	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 30 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 31 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 32 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	l	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 33 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 34 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	n	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 35 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	o	235	Total	C	N	O	S	0	0
			1897	1217	360	316	4		

- Molecule 36 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	p	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 37 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	z	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 38 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A	333	Total	C	N	O	S	0	0
			2672	1710	457	497	8		

- Molecule 39 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	4	608	Total	C	N	O	S	0	0
			4992	3138	912	915	27		

- Molecule 40 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	R	225	Total	C	N	O	S	0	0
			1843	1178	350	307	8		

- Molecule 41 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	2	3519	Total	C	N	O	P	0	0
			75565	33698	13833	24516	3518		

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	r	293	2382	1507	434	427	14	0	0

- Molecule 43 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	d	104	850	542	149	157	2	0	0

- Molecule 44 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	j	111	918	578	178	160	2	0	0

- Molecule 45 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	k	129	1064	673	220	166	5	0	0

- Molecule 46 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Y	167	1355	848	260	238	9	0	0

- Molecule 47 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	J	203	1658	1058	289	300	11	0	0

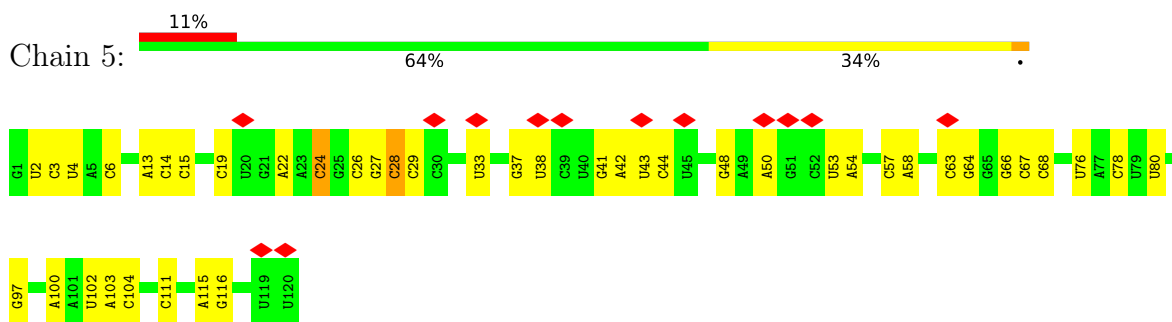
- Molecule 48 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	T	165	1319	836	245	233	5	0	0

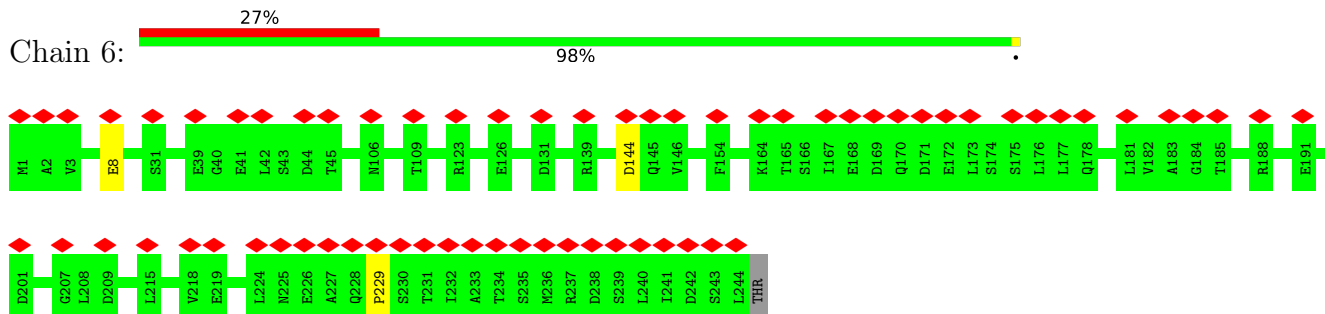
3 Residue-property plots [i](#)

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

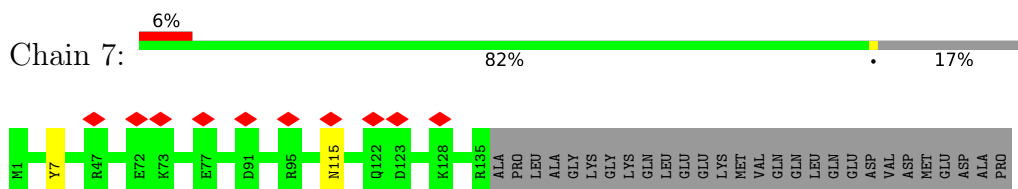
- Molecule 1: 5S rRNA



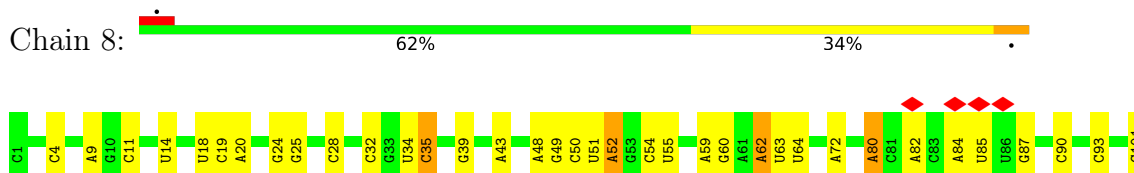
- Molecule 2: Eukaryotic translation initiation factor 6



- Molecule 3: Probable ribosome biogenesis protein RLP24

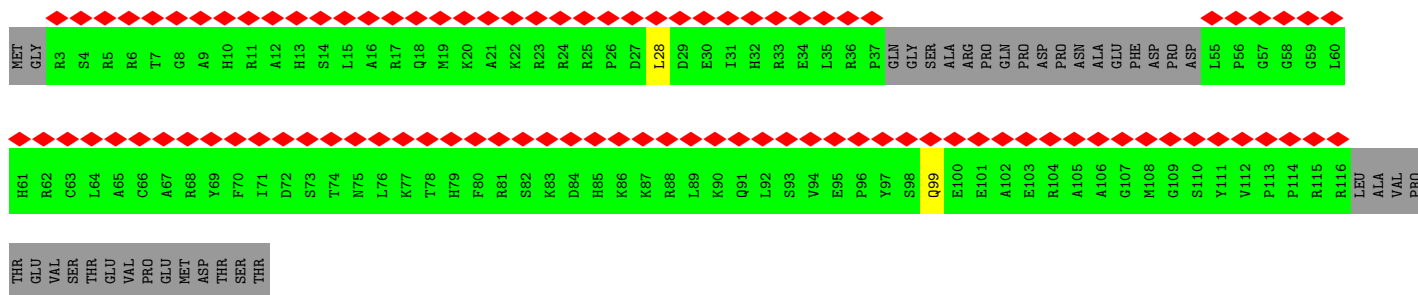


- Molecule 4: 5.8S rRNA

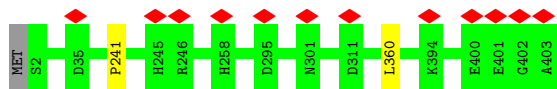




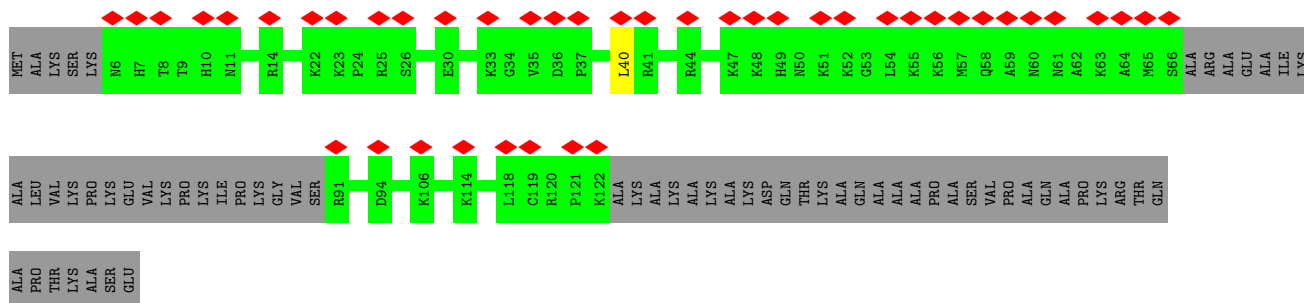
• Molecule 5: Zinc finger protein 593



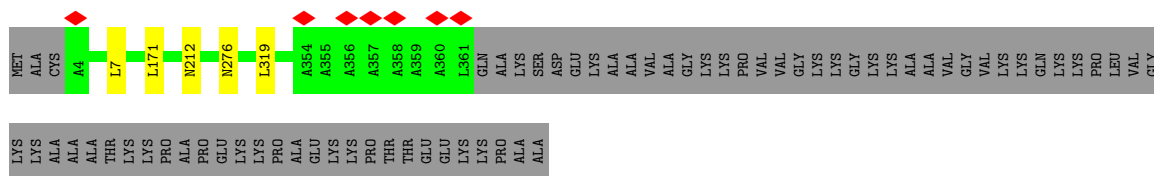
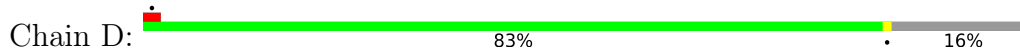
• Molecule 6: 60S ribosomal protein L3



• Molecule 7: 60S ribosomal protein L29

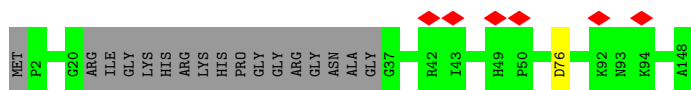
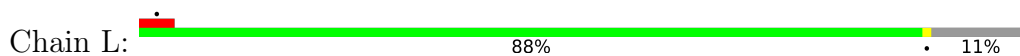


• Molecule 8: 60S ribosomal protein L4

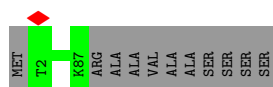


• Molecule 9: 60S ribosomal protein L30

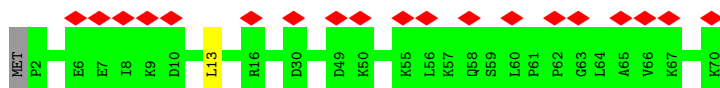
• Molecule 15: 60S ribosomal protein L27a



• Molecule 16: 60S ribosomal protein L37



• Molecule 17: 60S ribosomal protein L38



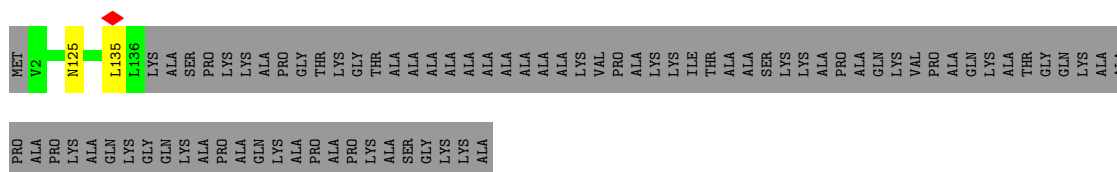
• Molecule 18: 60S ribosomal protein L39



• Molecule 19: 60S ribosomal protein L13

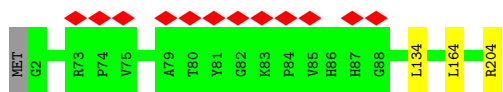


• Molecule 20: 60S ribosomal protein L14

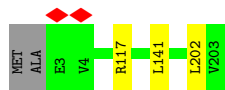


• Molecule 21: 60S ribosomal protein L15

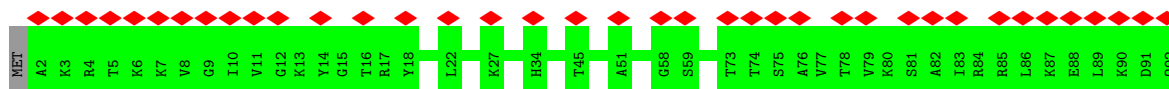
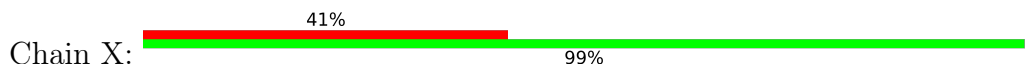




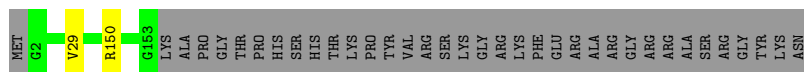
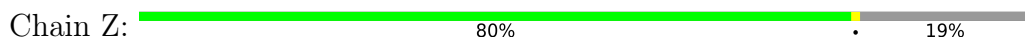
• Molecule 22: 60S ribosomal protein L13a



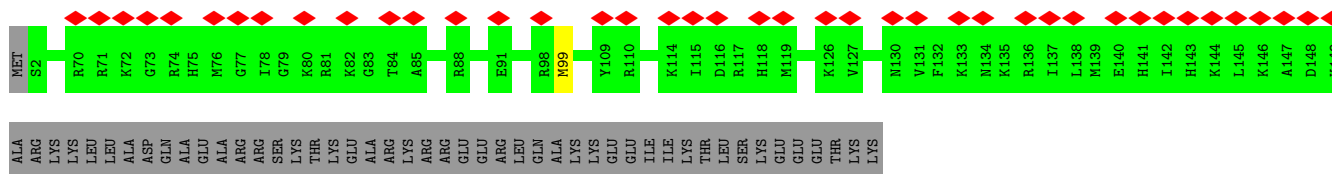
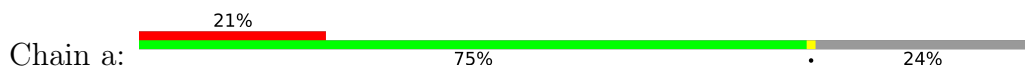
• Molecule 23: 60S ribosomal protein L37a



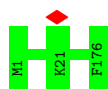
• Molecule 24: 60S ribosomal protein L18



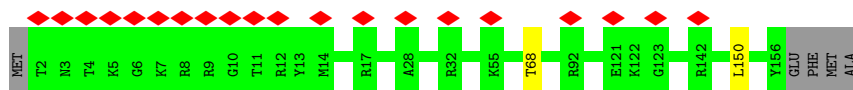
• Molecule 25: 60S ribosomal protein L19



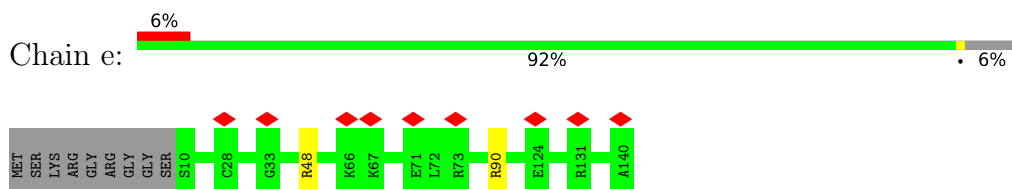
• Molecule 26: 60S ribosomal protein L18a



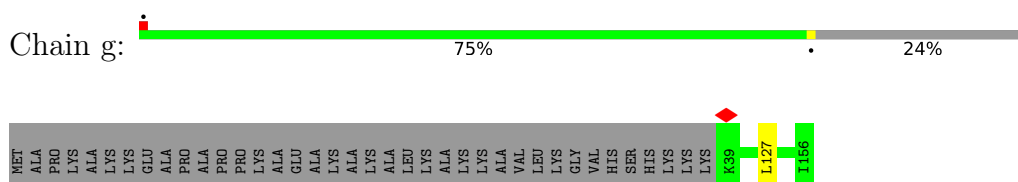
• Molecule 27: 60S ribosomal protein L21



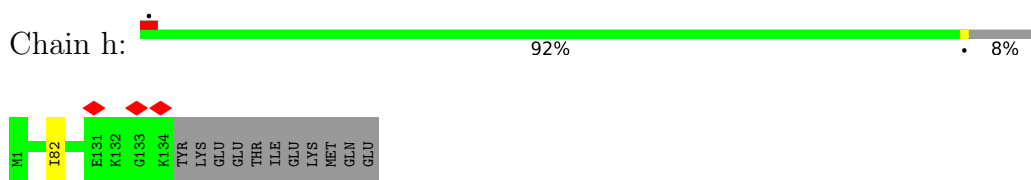
- Molecule 28: 60S ribosomal protein L23



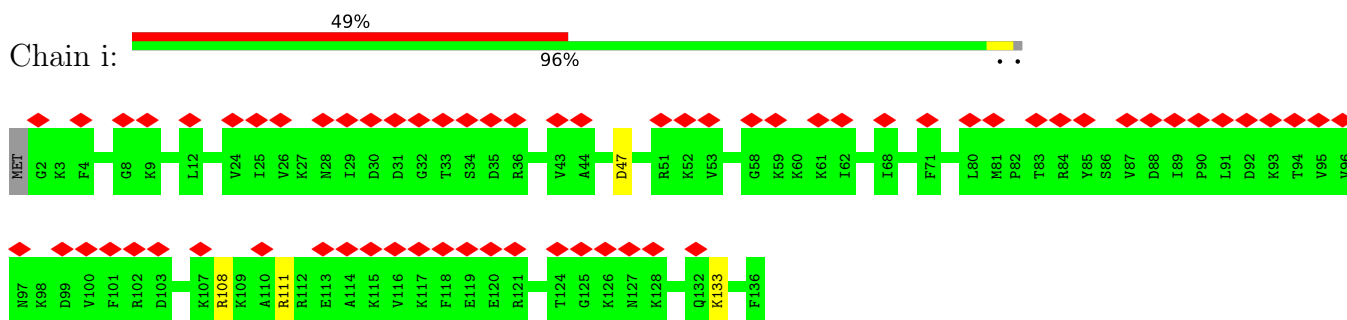
- Molecule 29: 60S ribosomal protein L23a



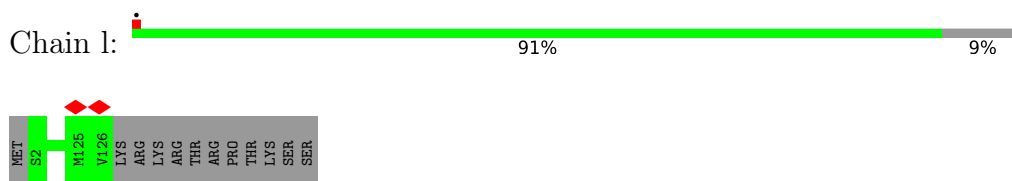
- Molecule 30: 60S ribosomal protein L26



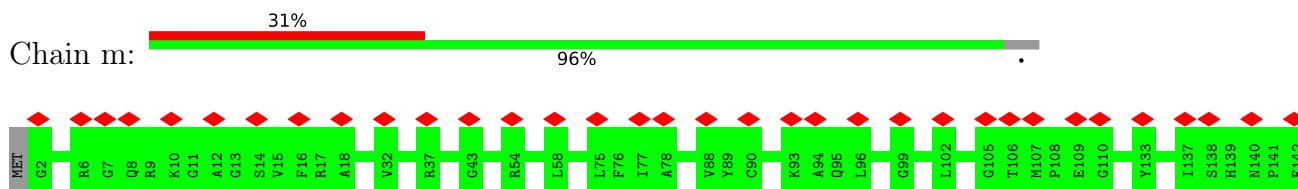
- Molecule 31: 60S ribosomal protein L27

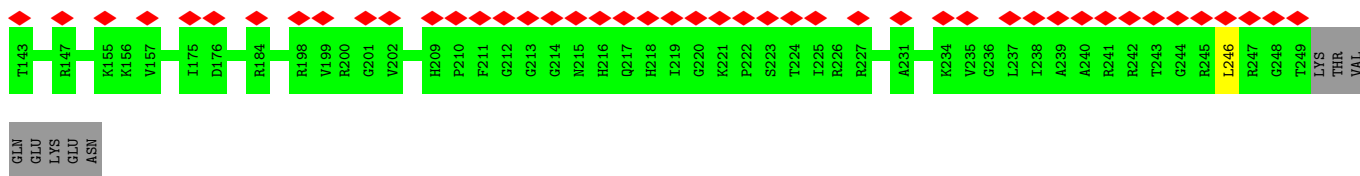


- Molecule 32: 60S ribosomal protein L28

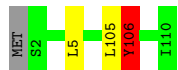


- Molecule 33: 60S ribosomal protein L8

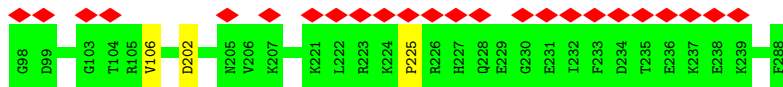
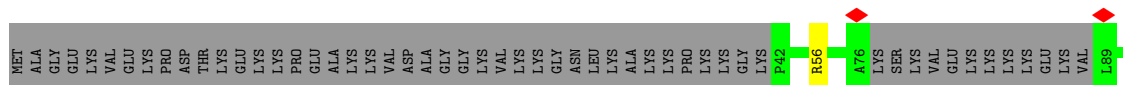
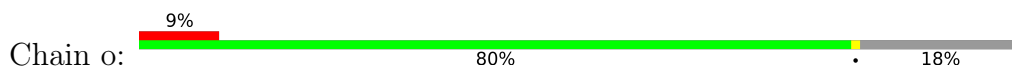




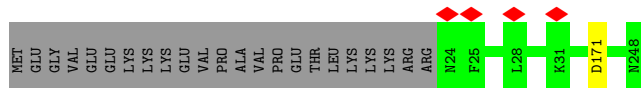
• Molecule 34: 60S ribosomal protein L35a



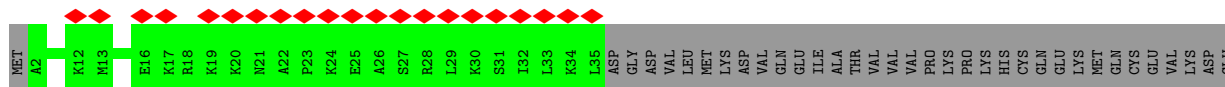
• Molecule 35: 60S ribosomal protein L6



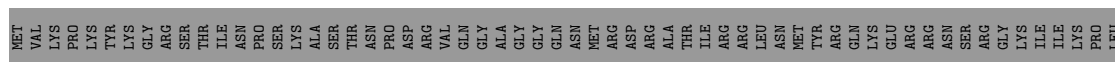
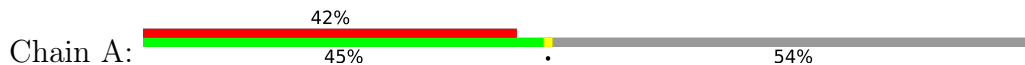
• Molecule 36: 60S ribosomal protein L7

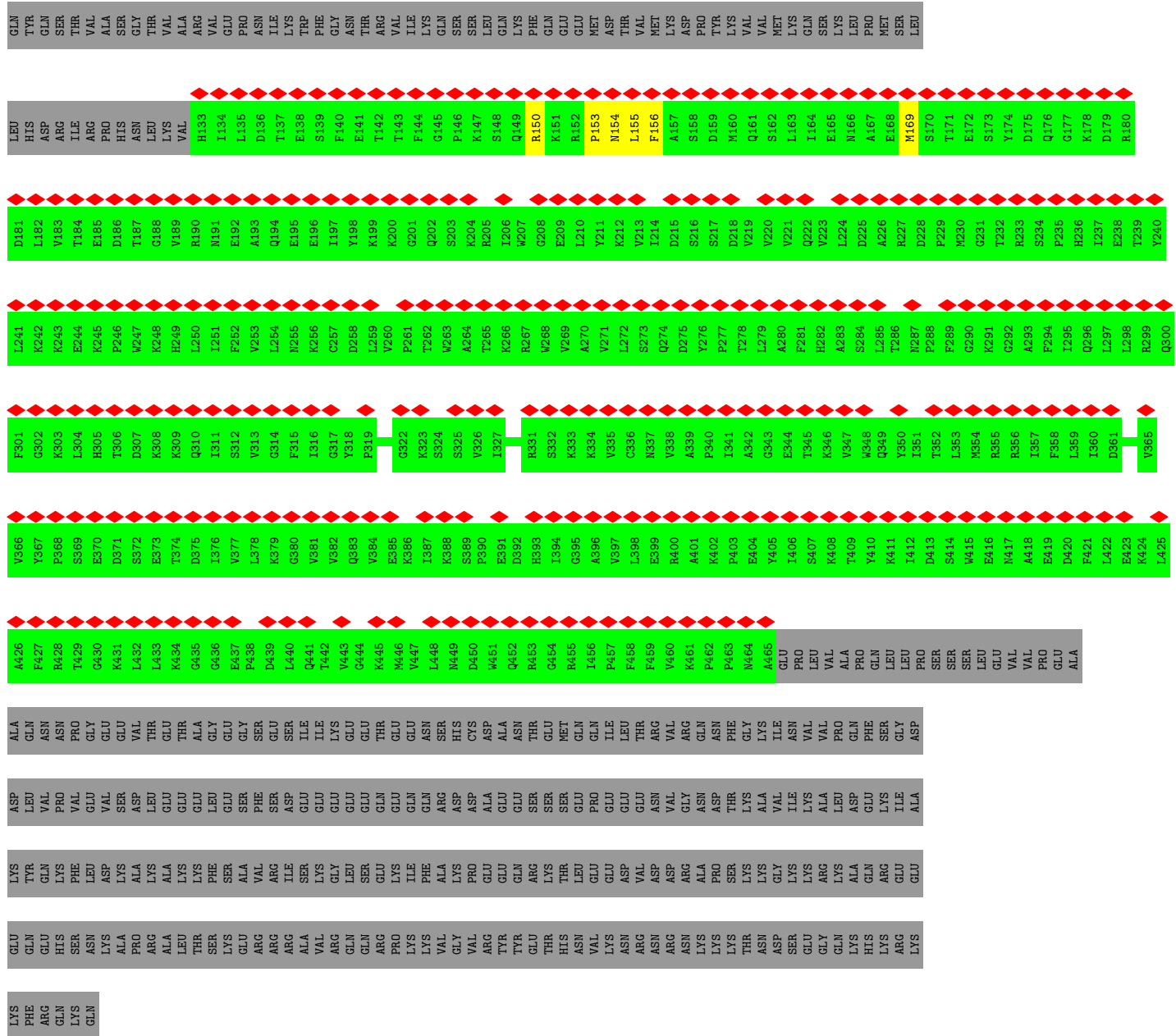


• Molecule 37: Protein LLP homolog

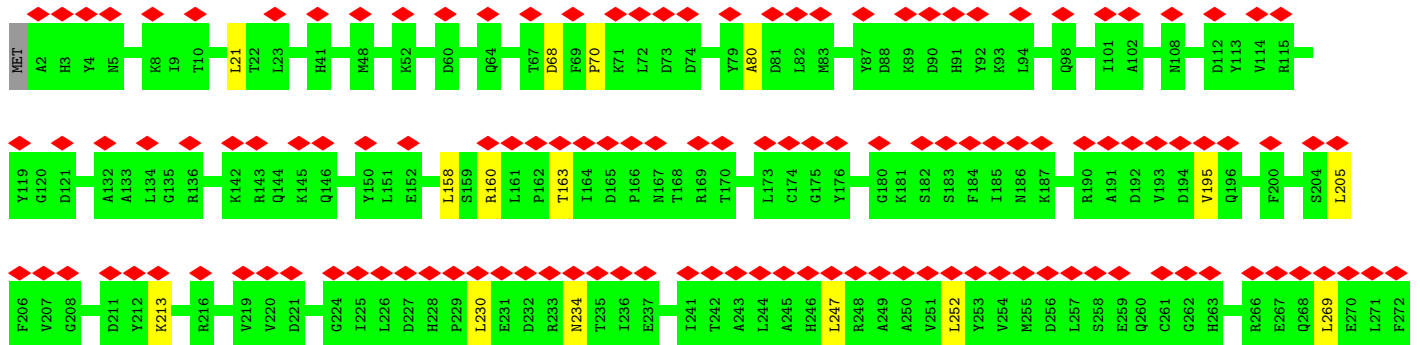
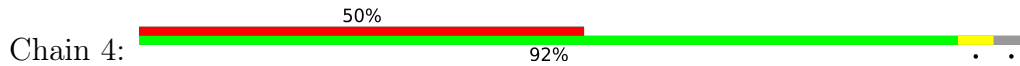


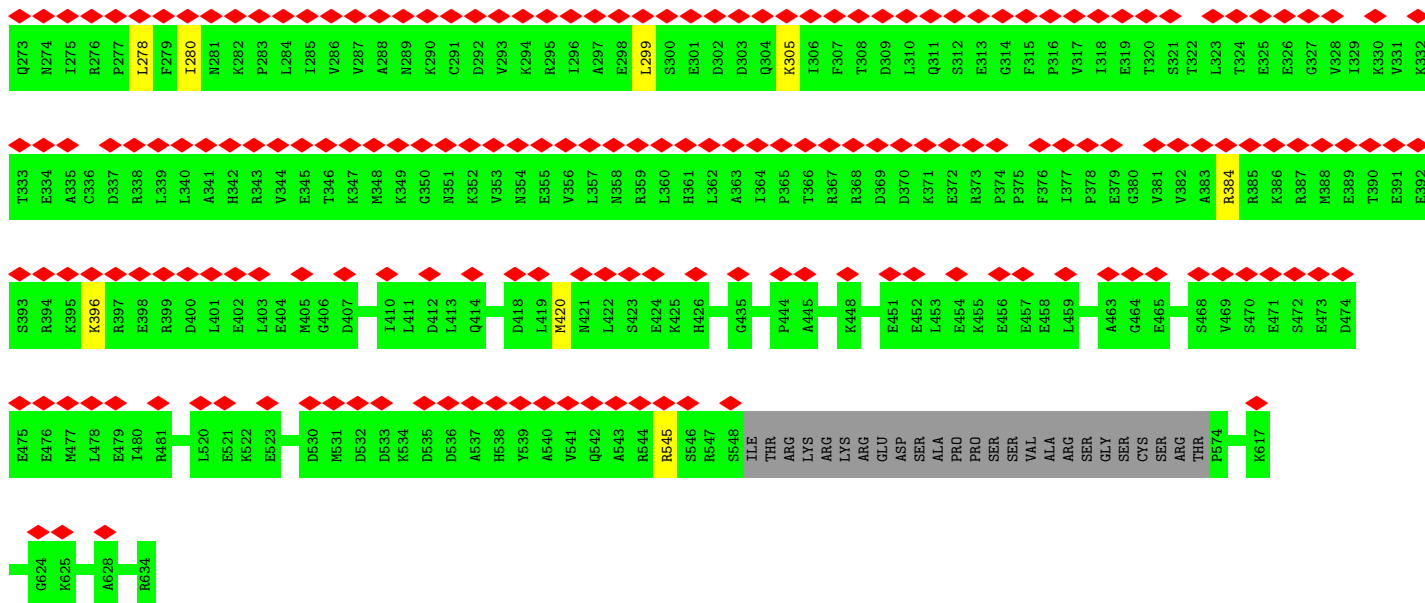
• Molecule 38: G Protein Nucleolar 2



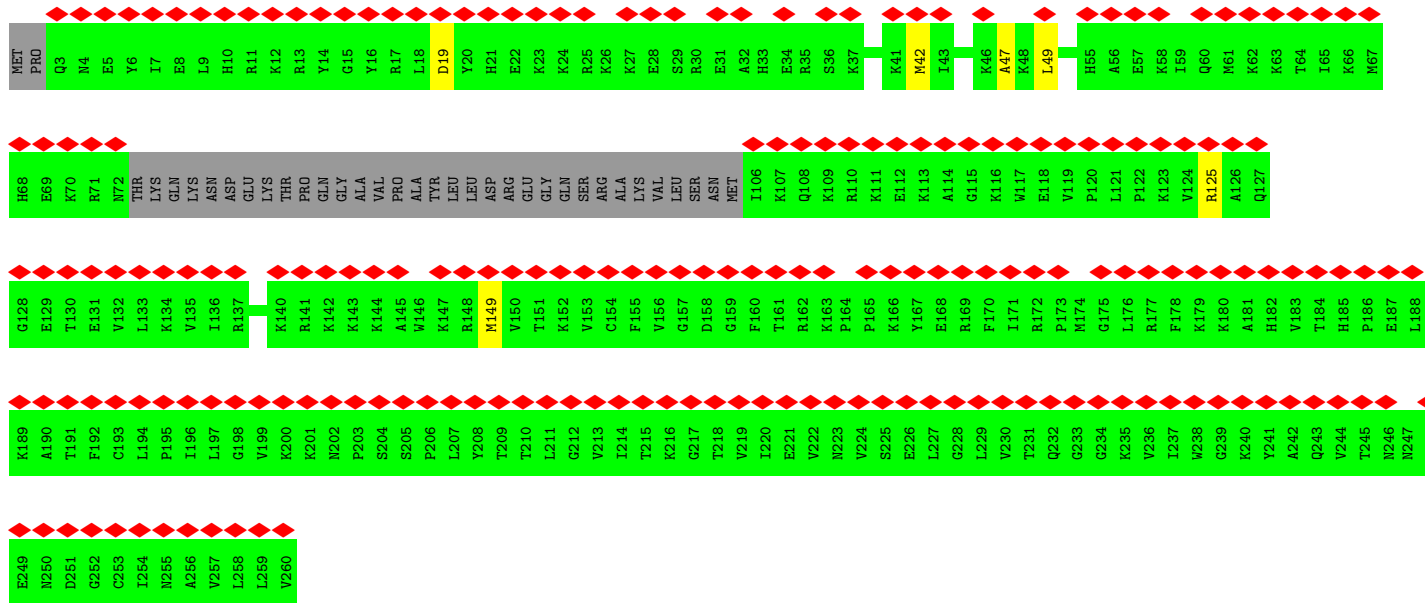
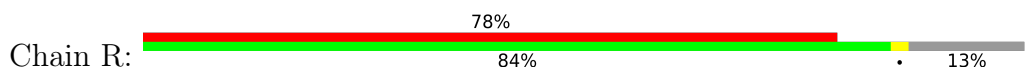


• Molecule 39: GTP-binding protein 4

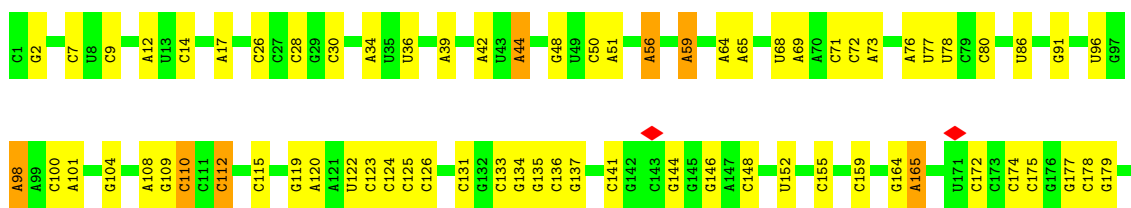


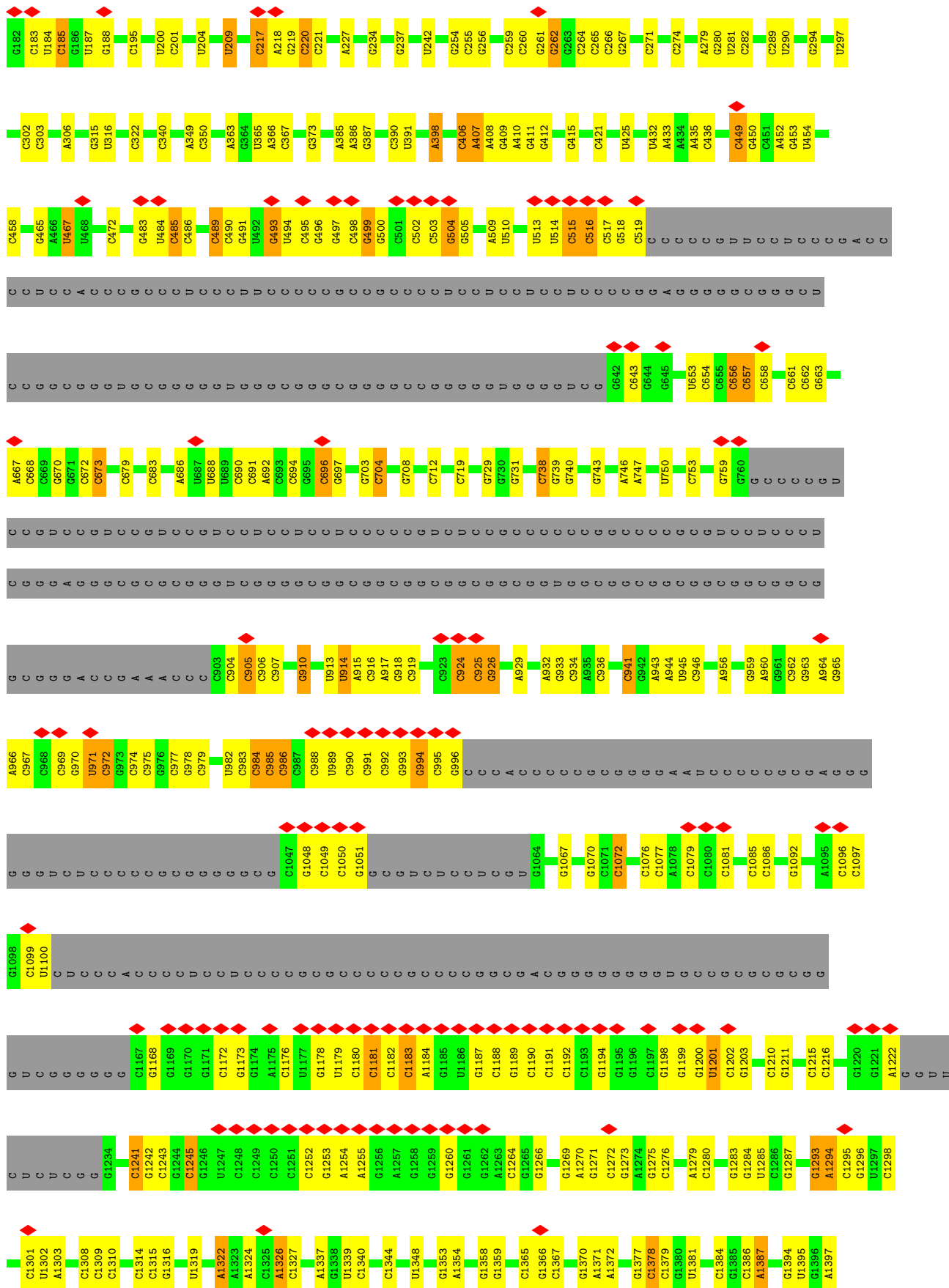


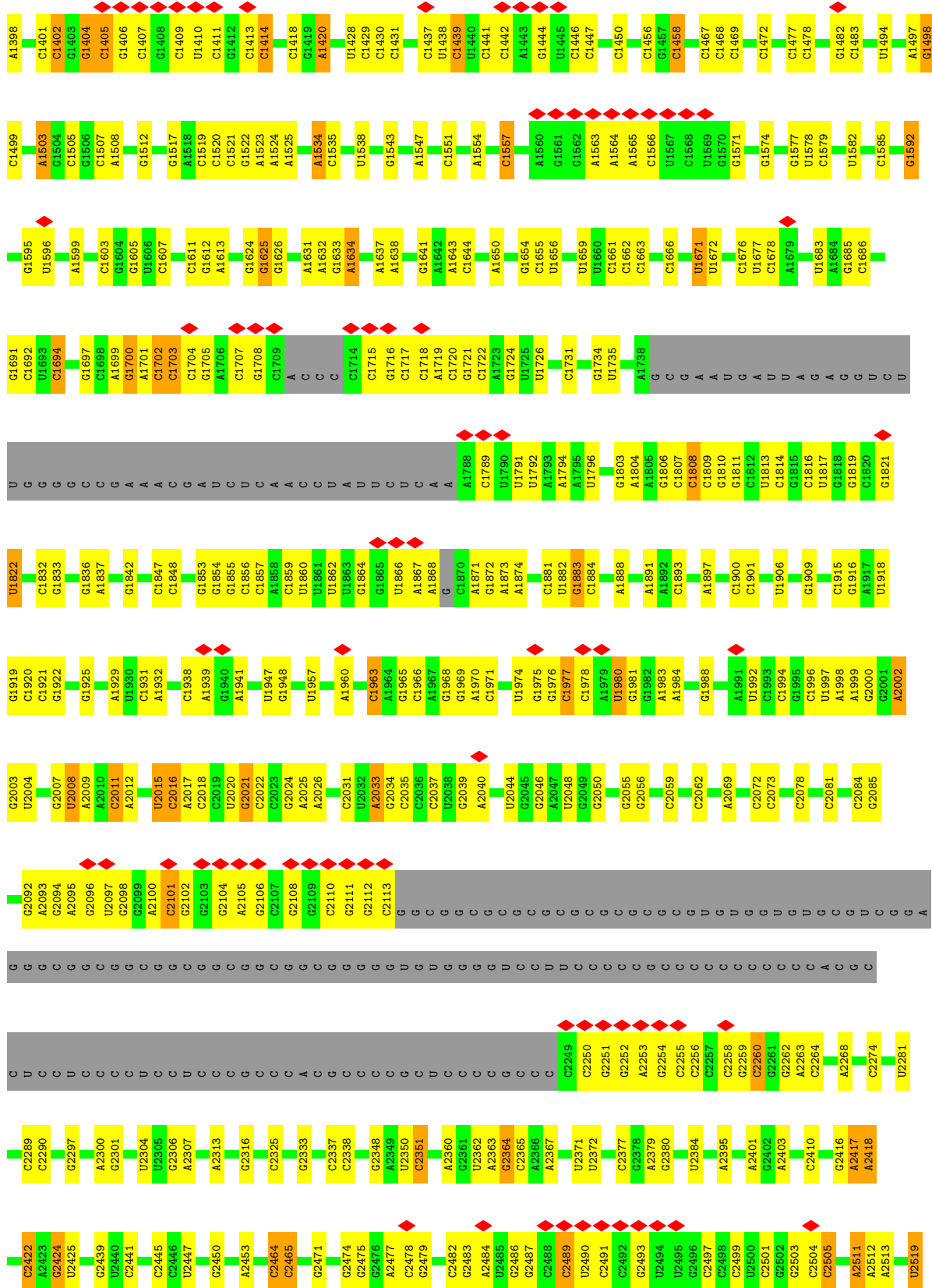
• Molecule 40: Ribosome biogenesis protein NSA2 homolog

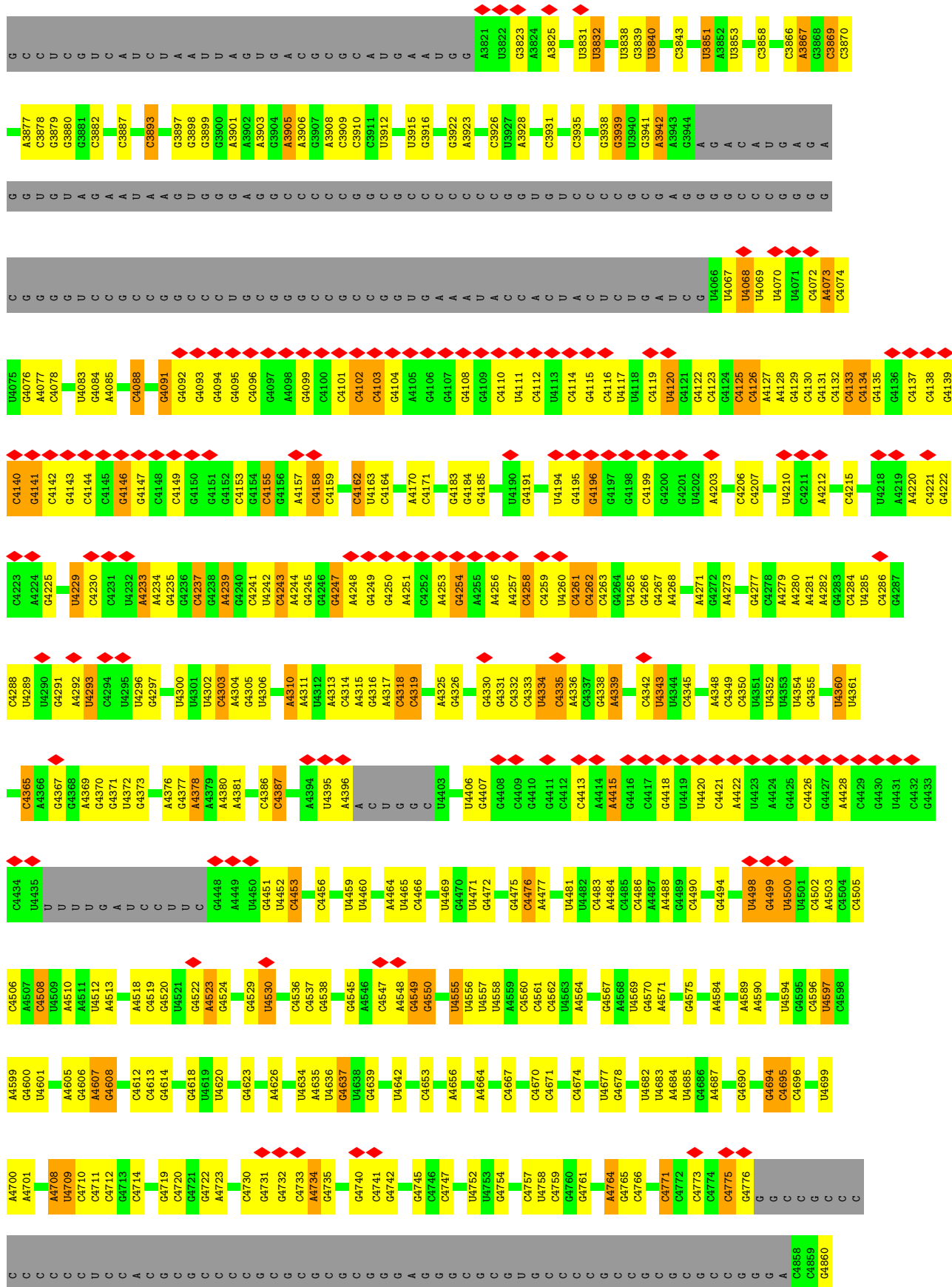


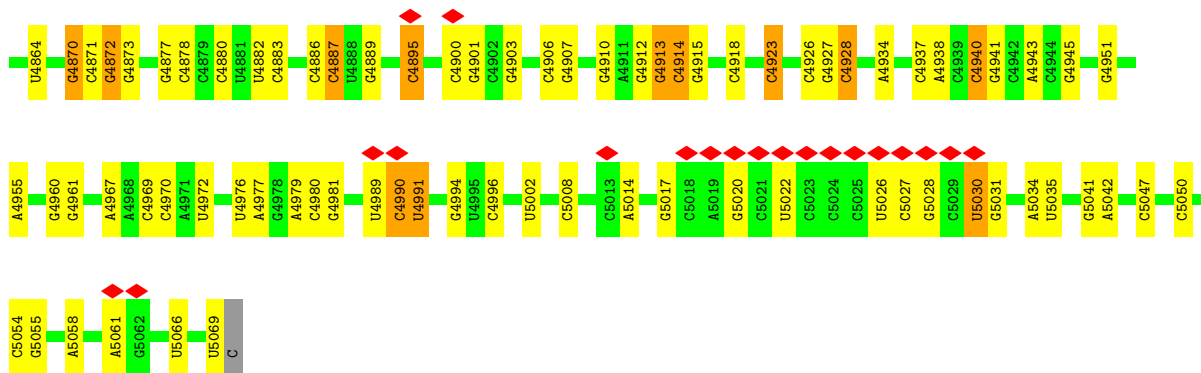
• Molecule 41: 28S rRNA



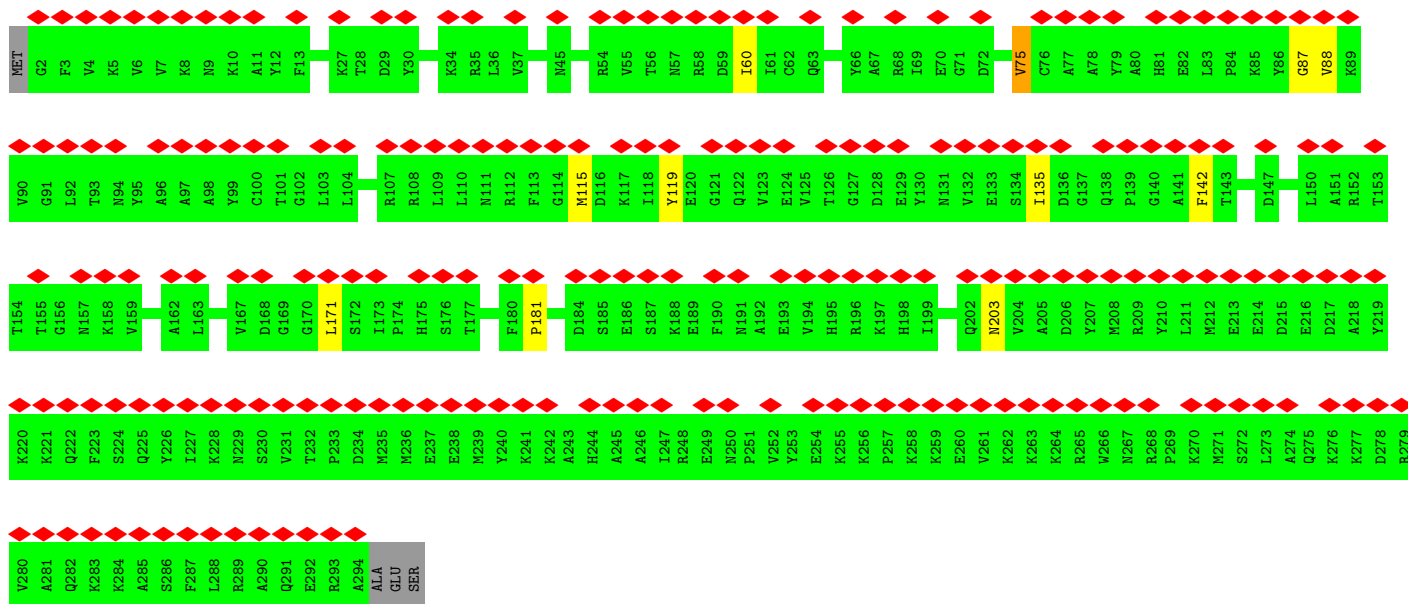




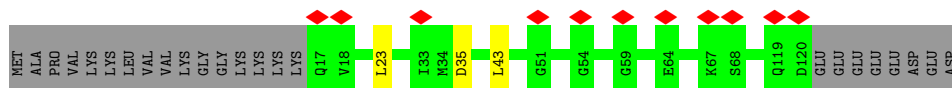
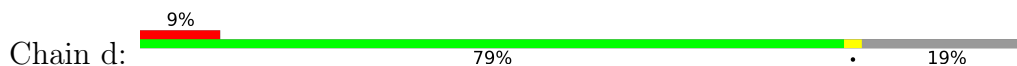




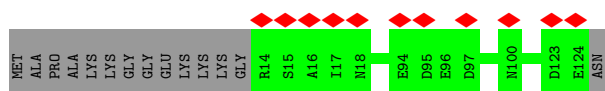
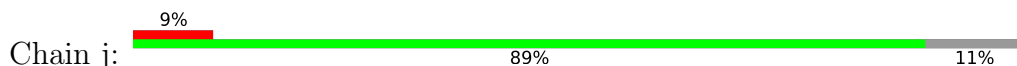
- Molecule 42: 60S ribosomal protein L5



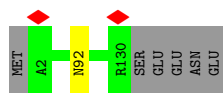
- Molecule 43: 60S ribosomal protein L22



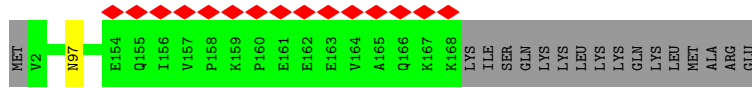
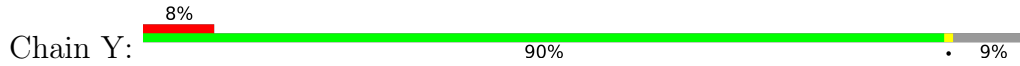
- Molecule 44: 60S ribosomal protein L31



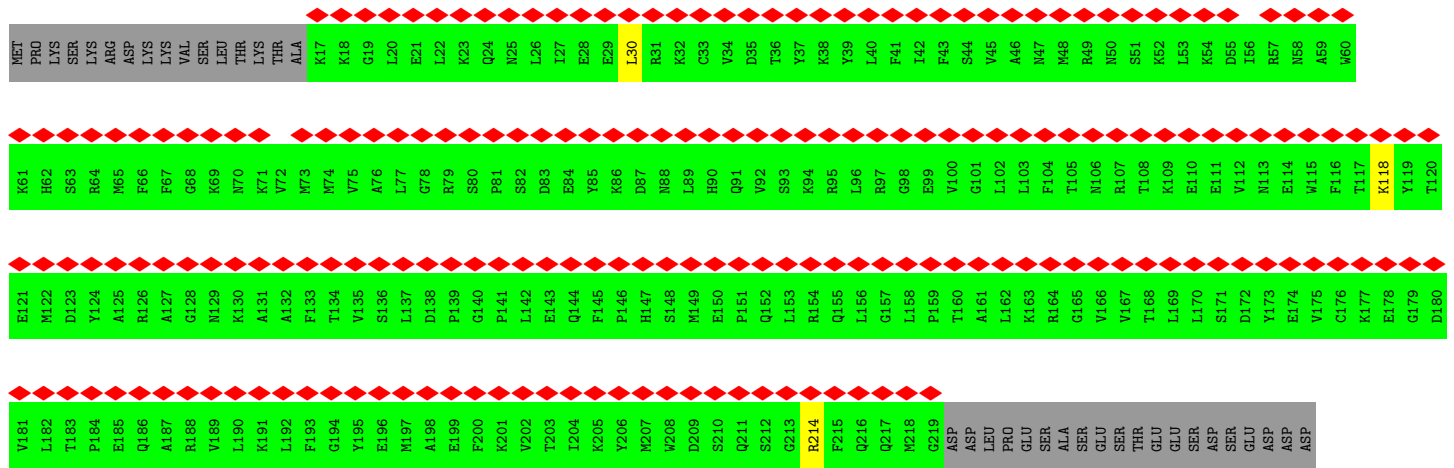
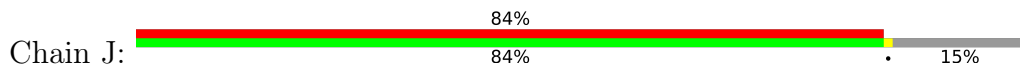
- Molecule 45: 60S ribosomal protein L32



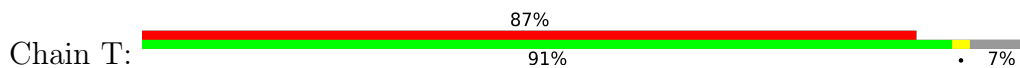
- Molecule 46: 60S ribosomal protein L17



- Molecule 47: mRNA turnover protein 4 homolog



- Molecule 48: 60S ribosomal protein L11



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34292	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 ($e^-/\text{\AA}^2$)	1.8	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	548.0, 548.0, 548.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	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: UR3, E7G, E6G, 5MU, B8Q, OMC, B9H, P7G, 6MZ, A2M, I4U, P4U, MHG, B8K, OMG, BGH, 1MA, 7MG, OMU, 2MG, B8T, B8W, M7A, B9B

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	5	0.47	0/2858	1.45	65/4455 (1.5%)
2	6	0.36	0/1877	0.78	2/2554 (0.1%)
3	7	0.39	0/1181	0.72	1/1563 (0.1%)
4	8	0.51	0/3679	1.45	68/5732 (1.2%)
5	9	0.31	0/802	0.82	1/1069 (0.1%)
6	B	0.33	0/3315	0.70	1/4435 (0.0%)
7	C	0.33	0/777	0.74	1/1026 (0.1%)
8	D	0.33	0/2907	0.75	3/3905 (0.1%)
9	E	0.35	0/774	0.76	2/1038 (0.2%)
10	F	0.32	0/878	0.78	0/1170
11	G	0.36	0/1971	0.73	2/2651 (0.1%)
12	H	0.34	0/1023	0.66	0/1351
13	I	0.37	0/1537	0.80	2/2066 (0.1%)
14	K	0.36	0/843	0.73	1/1115 (0.1%)
15	L	0.31	0/1068	0.69	1/1428 (0.1%)
16	M	0.33	0/720	0.74	0/952
17	O	0.39	0/575	0.78	1/761 (0.1%)
18	P	0.30	0/454	0.66	0/599
19	Q	0.35	0/1732	0.75	2/2315 (0.1%)
20	S	0.35	0/1133	0.70	1/1516 (0.1%)
21	U	0.32	0/1746	0.70	2/2338 (0.1%)
22	V	0.33	0/1682	0.68	2/2250 (0.1%)
23	X	0.32	0/718	0.66	0/953
24	Z	0.30	0/1243	0.69	1/1663 (0.1%)
25	a	0.36	0/1255	0.78	2/1662 (0.1%)
26	b	0.33	0/1501	0.65	0/2013
27	c	0.35	0/1291	0.74	2/1725 (0.1%)
28	e	0.31	0/993	0.72	1/1332 (0.1%)
29	g	0.32	0/984	0.64	1/1323 (0.1%)
30	h	0.34	0/1132	0.72	1/1504 (0.1%)
31	i	0.39	0/1130	0.80	1/1507 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	l	0.31	0/1017	0.69	0/1364
33	m	0.33	0/1936	0.74	1/2596 (0.0%)
34	n	0.32	0/895	0.78	4/1198 (0.3%)
35	o	0.33	0/1935	0.72	2/2596 (0.1%)
36	p	0.35	0/1916	0.70	1/2553 (0.0%)
37	z	0.32	0/587	0.73	0/767
38	A	0.34	0/2733	0.65	2/3697 (0.1%)
39	4	0.37	0/5075	0.82	10/6807 (0.1%)
40	R	0.34	0/1878	0.75	3/2503 (0.1%)
41	2	1.70	12/82657 (0.0%)	1.46	1519/128870 (1.2%)
42	r	0.40	0/2428	0.86	5/3252 (0.2%)
43	d	0.41	0/864	0.85	3/1160 (0.3%)
44	j	0.34	0/933	0.71	0/1256
45	k	0.33	0/1082	0.71	0/1443
46	Y	0.32	0/1383	0.64	0/1856
47	J	0.36	0/1692	0.70	2/2270 (0.1%)
48	T	0.37	0/1341	0.81	2/1793 (0.1%)
All	All	1.27	12/154131 (0.0%)	1.23	1721/225952 (0.8%)

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
2	6	0	1
6	B	0	1
19	Q	0	1
31	i	0	1
34	n	0	1
35	o	0	1
38	A	0	2
39	4	0	2
40	R	0	2
41	2	0	1
42	r	0	3
48	T	0	1
All	All	0	17

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	4605	A	N3-C4	250.96	2.85	1.34
41	2	4605	A	C6-N1	219.00	2.88	1.35
41	2	4605	A	C5-C4	181.40	2.65	1.38
41	2	4605	A	C2-N3	160.71	2.78	1.33
41	2	4605	A	N1-C2	159.34	2.77	1.34

The worst 5 of 1721 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	4335	C	O5'-P-OP1	-61.45	36.96	110.70
41	2	4605	A	C4-C5-N7	-47.80	86.80	110.70
41	2	4605	A	N7-C8-N9	46.34	136.97	113.80
41	2	4605	A	N9-C4-C5	-30.53	93.59	105.80
41	2	4605	A	N1-C2-N3	-25.97	116.32	129.30

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	6	8	GLU	Peptide
6	B	241	PRO	Peptide
19	Q	154	VAL	Peptide
31	i	133	LYS	Peptide
34	n	106	TYR	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	6	242/245 (99%)	221 (91%)	21 (9%)	0	100	100
3	7	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
5	9	93/134 (69%)	80 (86%)	12 (13%)	1 (1%)	14	45
6	B	401/403 (100%)	381 (95%)	20 (5%)	0	100	100
7	C	89/159 (56%)	85 (96%)	4 (4%)	0	100	100
8	D	356/427 (83%)	334 (94%)	22 (6%)	0	100	100
9	E	96/115 (84%)	92 (96%)	4 (4%)	0	100	100
10	F	107/117 (92%)	105 (98%)	2 (2%)	0	100	100
11	G	240/266 (90%)	229 (95%)	11 (5%)	0	100	100
12	H	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
13	I	188/192 (98%)	174 (93%)	14 (7%)	0	100	100
14	K	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
15	L	127/148 (86%)	120 (94%)	7 (6%)	0	100	100
16	M	84/97 (87%)	79 (94%)	5 (6%)	0	100	100
17	O	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
18	P	48/51 (94%)	48 (100%)	0	0	100	100
19	Q	208/211 (99%)	192 (92%)	16 (8%)	0	100	100
20	S	133/215 (62%)	125 (94%)	8 (6%)	0	100	100
21	U	201/204 (98%)	189 (94%)	12 (6%)	0	100	100
22	V	199/203 (98%)	195 (98%)	4 (2%)	0	100	100
23	X	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
24	Z	150/188 (80%)	148 (99%)	2 (1%)	0	100	100
25	a	146/196 (74%)	141 (97%)	5 (3%)	0	100	100
26	b	174/176 (99%)	168 (97%)	6 (3%)	0	100	100
27	c	153/160 (96%)	143 (94%)	10 (6%)	0	100	100
28	e	129/140 (92%)	118 (92%)	11 (8%)	0	100	100
29	g	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
30	h	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
31	i	133/136 (98%)	122 (92%)	11 (8%)	0	100	100
32	l	123/137 (90%)	114 (93%)	9 (7%)	0	100	100
33	m	246/257 (96%)	219 (89%)	27 (11%)	0	100	100
34	n	107/110 (97%)	100 (94%)	6 (6%)	1 (1%)	17	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	o	231/288 (80%)	215 (93%)	16 (7%)	0	100	100
36	p	224/248 (90%)	214 (96%)	10 (4%)	0	100	100
37	z	63/129 (49%)	60 (95%)	3 (5%)	0	100	100
38	A	331/731 (45%)	311 (94%)	18 (5%)	2 (1%)	25	57
39	4	604/634 (95%)	540 (89%)	57 (9%)	7 (1%)	13	42
40	R	221/260 (85%)	212 (96%)	9 (4%)	0	100	100
42	r	291/297 (98%)	251 (86%)	37 (13%)	3 (1%)	15	46
43	d	102/128 (80%)	98 (96%)	4 (4%)	0	100	100
44	j	109/125 (87%)	105 (96%)	4 (4%)	0	100	100
45	k	127/135 (94%)	120 (94%)	7 (6%)	0	100	100
46	Y	165/184 (90%)	154 (93%)	11 (7%)	0	100	100
47	J	201/239 (84%)	189 (94%)	12 (6%)	0	100	100
48	T	163/178 (92%)	147 (90%)	16 (10%)	0	100	100
All	All	7762/9117 (85%)	7267 (94%)	481 (6%)	14 (0%)	50	77

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	n	106	TYR
39	4	280	ILE
42	r	75	VAL
42	r	88	VAL
5	9	99	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	6	212/213 (100%)	212 (100%)	0	100	100
3	7	126/149 (85%)	125 (99%)	1 (1%)	81	89
5	9	81/114 (71%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	B	349/349 (100%)	349 (100%)	0	100	100
7	C	78/126 (62%)	78 (100%)	0	100	100
8	D	298/348 (86%)	296 (99%)	2 (1%)	84	90
9	E	83/97 (86%)	83 (100%)	0	100	100
10	F	94/100 (94%)	94 (100%)	0	100	100
11	G	204/223 (92%)	202 (99%)	2 (1%)	76	86
12	H	109/110 (99%)	109 (100%)	0	100	100
13	I	169/171 (99%)	168 (99%)	1 (1%)	86	91
14	K	86/89 (97%)	85 (99%)	1 (1%)	71	83
15	L	110/121 (91%)	110 (100%)	0	100	100
16	M	73/80 (91%)	73 (100%)	0	100	100
17	O	64/65 (98%)	64 (100%)	0	100	100
18	P	47/48 (98%)	45 (96%)	2 (4%)	29	59
19	Q	176/177 (99%)	176 (100%)	0	100	100
20	S	115/161 (71%)	114 (99%)	1 (1%)	78	87
21	U	171/172 (99%)	170 (99%)	1 (1%)	86	91
22	V	173/174 (99%)	172 (99%)	1 (1%)	86	91
23	X	74/75 (99%)	74 (100%)	0	100	100
24	Z	136/165 (82%)	135 (99%)	1 (1%)	84	90
25	a	133/175 (76%)	133 (100%)	0	100	100
26	b	157/157 (100%)	157 (100%)	0	100	100
27	c	136/140 (97%)	136 (100%)	0	100	100
28	e	101/107 (94%)	100 (99%)	1 (1%)	76	86
29	g	106/133 (80%)	106 (100%)	0	100	100
30	h	124/135 (92%)	124 (100%)	0	100	100
31	i	117/118 (99%)	115 (98%)	2 (2%)	60	78
32	l	109/121 (90%)	109 (100%)	0	100	100
33	m	190/199 (96%)	190 (100%)	0	100	100
34	n	88/89 (99%)	88 (100%)	0	100	100
35	o	208/252 (82%)	207 (100%)	1 (0%)	88	93
36	p	195/215 (91%)	195 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	z	61/115 (53%)	61 (100%)	0	100	100
38	A	296/654 (45%)	296 (100%)	0	100	100
39	4	551/574 (96%)	547 (99%)	4 (1%)	84	90
40	R	198/228 (87%)	197 (100%)	1 (0%)	88	93
42	r	246/250 (98%)	245 (100%)	1 (0%)	91	95
43	d	94/115 (82%)	94 (100%)	0	100	100
44	j	101/110 (92%)	101 (100%)	0	100	100
45	k	115/121 (95%)	114 (99%)	1 (1%)	78	87
46	Y	147/163 (90%)	146 (99%)	1 (1%)	84	90
47	J	180/214 (84%)	178 (99%)	2 (1%)	73	85
48	T	138/149 (93%)	138 (100%)	0	100	100
All	All	6819/7861 (87%)	6792 (100%)	27 (0%)	91	95

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	i	108	ARG
39	4	160	ARG
46	Y	97	ASN
35	o	56	ARG
39	4	305	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
47	J	50	ASN
48	T	110	GLN
30	h	43	ASN
30	h	127	GLN
39	4	76	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	119/120 (99%)	20 (16%)	0
4	8	155/156 (99%)	32 (20%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
41	2	3478/5054 (68%)	955 (27%)	21 (0%)
All	All	3752/5330 (70%)	1007 (26%)	21 (0%)

5 of 1007 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	13	A
1	5	22	A
1	5	24	C
1	5	27	G
1	5	28	C

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
41	2	4130	C
41	2	4334	U
41	2	4913	G
41	2	4335	C
41	2	4333	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A2M	2	1534	41	18,25,26	3.62	8 (44%)	18,36,39	3.60	5 (27%)
41	OMG	2	4196	41	18,26,27	2.93	7 (38%)	19,38,41	1.62	5 (26%)
41	MHG	2	4371	41	29,32,33	4.00	12 (41%)	34,46,49	2.30	12 (35%)
41	A2M	2	2401	41	18,25,26	3.65	8 (44%)	18,36,39	3.37	3 (16%)
41	B9B	2	1574	41	21,28,29	1.99	3 (14%)	23,40,43	6.60	5 (21%)
41	B8K	2	3897	41	24,28,29	3.41	11 (45%)	30,42,45	2.50	11 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	OMG	2	1316	41	18,26,27	2.84	8 (44%)	19,38,41	1.54	5 (26%)
41	E7G	2	2297	41	24,27,28	4.01	11 (45%)	30,40,43	2.19	11 (36%)
41	B8T	2	4671	41	19,22,23	3.58	8 (42%)	26,31,34	0.95	1 (3%)
41	A2M	2	4571	41	18,25,26	3.58	8 (44%)	18,36,39	3.40	4 (22%)
41	BGH	2	3899	41	25,29,30	4.64	17 (68%)	31,43,46	2.60	11 (35%)
41	OMC	2	3869	41	19,22,23	3.07	8 (42%)	26,31,34	1.41	4 (15%)
41	A2M	2	3718	41	18,25,26	3.57	8 (44%)	18,36,39	3.39	4 (22%)
41	B8Q	2	1456	41	17,22,23	2.95	5 (29%)	22,32,35	2.36	6 (27%)
41	UR3	2	4530	41	19,22,23	2.93	6 (31%)	26,32,35	1.32	2 (7%)
41	OMC	2	2804	41	19,22,23	2.91	8 (42%)	26,31,34	1.31	3 (11%)
41	OMU	2	4620	41	19,22,23	2.96	8 (42%)	26,31,34	1.68	5 (19%)
41	5MU	2	4083	41	19,22,23	7.18	8 (42%)	28,32,35	3.45	10 (35%)
41	P7G	2	1909	41	24,28,29	4.01	11 (45%)	27,41,44	1.51	3 (11%)
41	B8W	2	2380	41	18,26,27	2.09	2 (11%)	21,38,41	2.42	7 (33%)
41	OMC	2	2422	46,41	19,22,23	3.00	8 (42%)	26,31,34	1.16	3 (11%)
41	2MG	2	1517	41	18,26,27	2.67	6 (33%)	16,38,41	1.45	3 (18%)
41	I4U	2	1659	41	21,24,25	3.53	9 (42%)	27,34,37	1.19	2 (7%)
41	B8K	2	4690	41	24,28,29	3.36	11 (45%)	30,42,45	2.64	12 (40%)
41	OMC	2	4536	41	19,22,23	3.04	8 (42%)	26,31,34	1.19	3 (11%)
41	OMG	2	2364	41	18,26,27	2.80	8 (44%)	19,38,41	1.56	5 (26%)
41	OMC	2	3887	41	19,22,23	3.04	8 (42%)	26,31,34	0.84	1 (3%)
41	2MG	2	978	41	18,26,27	2.70	6 (33%)	16,38,41	1.41	3 (18%)
41	B8T	2	4483	41	19,22,23	3.67	8 (42%)	26,31,34	1.23	3 (11%)
41	A2M	2	4523	41	18,25,26	3.57	8 (44%)	18,36,39	3.40	4 (22%)
41	OMG	2	2773	41	18,26,27	2.87	7 (38%)	19,38,41	1.33	3 (15%)
41	B9B	2	237	41	21,28,29	2.02	3 (14%)	23,40,43	6.54	5 (21%)
41	OMG	2	2050	41	18,26,27	2.81	8 (44%)	19,38,41	1.52	5 (26%)
41	OMG	2	373	41	18,26,27	2.83	8 (44%)	19,38,41	1.61	5 (26%)
41	P7G	2	3880	41	24,28,29	4.18	11 (45%)	27,41,44	1.40	3 (11%)
41	OMG	2	4370	41	18,26,27	2.92	8 (44%)	19,38,41	1.55	4 (21%)
41	B8W	2	4529	41	18,26,27	2.13	2 (11%)	21,38,41	2.72	7 (33%)
41	OMG	2	4637	41	18,26,27	2.85	8 (44%)	19,38,41	1.52	4 (21%)
41	A2M	2	3825	41	18,25,26	3.58	8 (44%)	18,36,39	3.39	4 (22%)
41	A2M	2	3867	41	18,25,26	3.55	8 (44%)	18,36,39	3.46	4 (22%)
41	OMC	2	2365	41	19,22,23	2.90	8 (42%)	26,31,34	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	E6G	2	4355	41	20,27,28	2.81	3 (15%)	22,39,42	3.07	7 (31%)
41	B8W	2	4185	41	18,26,27	2.13	2 (11%)	21,38,41	2.50	7 (33%)
41	1MA	2	1322	41	16,25,26	4.40	5 (31%)	18,37,40	1.68	3 (16%)
41	2MG	2	4872	41	18,26,27	2.52	6 (33%)	16,38,41	1.73	4 (25%)
41	B8W	2	4472	41	18,26,27	2.14	2 (11%)	21,38,41	2.56	7 (33%)
41	A2M	2	3723	41	18,25,26	3.59	8 (44%)	18,36,39	3.43	3 (16%)
41	OMG	2	1522	41	18,26,27	2.79	8 (44%)	19,38,41	1.45	4 (21%)
41	UR3	2	4597	41	19,22,23	2.82	7 (36%)	26,32,35	1.91	3 (11%)
41	OMG	2	2424	41	18,26,27	2.87	8 (44%)	19,38,41	1.52	4 (21%)
41	M7A	2	4564	41	20,25,26	2.02	3 (15%)	28,37,40	3.92	8 (28%)
41	B9H	2	2786	41	20,25,26	3.36	4 (20%)	22,35,38	2.67	7 (31%)
4	OMU	8	14	4,41	19,22,23	2.97	8 (42%)	26,31,34	1.87	6 (23%)
41	7MG	2	4550	41	22,26,27	3.83	10 (45%)	29,39,42	1.92	8 (27%)
41	A2M	2	1524	41	18,25,26	3.59	8 (44%)	18,36,39	3.48	4 (22%)
41	A2M	2	2363	41	18,25,26	3.62	8 (44%)	18,36,39	3.42	4 (22%)
41	2MG	2	729	41	18,26,27	2.66	6 (33%)	16,38,41	1.35	3 (18%)
41	P4U	2	1348	41	21,24,25	3.50	8 (38%)	27,33,36	1.07	2 (7%)
41	6MZ	2	4220	41	18,25,26	1.85	3 (16%)	16,36,39	3.73	3 (18%)
41	OMG	2	4623	41	18,26,27	2.83	8 (44%)	19,38,41	1.51	5 (26%)
41	OMG	2	4494	41	18,26,27	2.91	8 (44%)	19,38,41	1.49	4 (21%)
41	1MA	2	4415	41	16,25,26	4.36	5 (31%)	18,37,40	1.72	3 (16%)
41	A2M	2	398	41	18,25,26	3.59	8 (44%)	18,36,39	3.49	4 (22%)
41	OMG	2	1625	41	18,26,27	2.94	7 (38%)	19,38,41	1.49	4 (21%)
41	OMG	2	1883	41	18,26,27	2.87	8 (44%)	19,38,41	1.61	4 (21%)
41	OMG	2	4870	41	18,26,27	2.89	8 (44%)	19,38,41	1.52	4 (21%)
41	I4U	2	4194	41	21,24,25	3.61	9 (42%)	27,34,37	0.96	1 (3%)
41	OMC	2	3701	41	19,22,23	3.03	8 (42%)	26,31,34	0.78	0
41	7MG	2	2522	41	22,26,27	3.72	10 (45%)	29,39,42	1.95	8 (27%)
41	7MG	2	1605	41	22,26,27	3.82	10 (45%)	29,39,42	1.96	9 (31%)
41	A2M	2	1326	41	18,25,26	3.55	8 (44%)	18,36,39	3.52	4 (22%)

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
41	A2M	2	1534	41	-	3/5/27/28	0/3/3/3
41	OMG	2	4196	41	-	4/5/27/28	0/3/3/3
41	MHG	2	4371	41	-	8/16/46/47	0/3/3/3
41	A2M	2	2401	41	-	3/5/27/28	0/3/3/3
41	B9B	2	1574	41	-	5/7/29/30	0/3/3/3
41	B8K	2	3897	41	-	3/11/41/42	0/3/3/3
41	OMG	2	1316	41	-	0/5/27/28	0/3/3/3
41	E7G	2	2297	41	-	1/9/39/40	0/3/3/3
41	B8T	2	4671	41	-	0/7/27/28	0/2/2/2
41	A2M	2	4571	41	-	1/5/27/28	0/3/3/3
41	BGH	2	3899	41	-	0/13/43/44	0/3/3/3
41	OMC	2	3869	41	-	5/9/27/28	0/2/2/2
41	A2M	2	3718	41	-	3/5/27/28	0/3/3/3
41	B8Q	2	1456	41	-	0/7/42/43	0/2/2/2
41	UR3	2	4530	41	-	0/7/25/26	0/2/2/2
41	OMC	2	2804	41	-	0/9/27/28	0/2/2/2
41	OMU	2	4620	41	-	1/9/27/28	0/2/2/2
41	5MU	2	4083	41	-	0/7/25/26	0/2/2/2
41	P7G	2	1909	41	-	2/10/40/41	0/3/3/3
41	B8W	2	2380	41	-	2/5/27/28	0/3/3/3
41	OMC	2	2422	46,41	-	1/9/27/28	0/2/2/2
41	2MG	2	1517	41	-	1/5/27/28	0/3/3/3
41	I4U	2	1659	41	-	1/9/29/30	0/2/2/2
41	B8K	2	4690	41	-	0/11/41/42	0/3/3/3
41	OMC	2	4536	41	-	0/9/27/28	0/2/2/2
41	OMG	2	2364	41	-	2/5/27/28	0/3/3/3
41	OMC	2	3887	41	-	1/9/27/28	0/2/2/2
41	2MG	2	978	41	-	0/5/27/28	0/3/3/3
41	B8T	2	4483	41	-	0/7/27/28	0/2/2/2
41	A2M	2	4523	41	-	4/5/27/28	0/3/3/3
41	OMG	2	2773	41	-	0/5/27/28	0/3/3/3
41	B9B	2	237	41	-	4/7/29/30	0/3/3/3
41	OMG	2	2050	41	-	0/5/27/28	0/3/3/3
41	OMG	2	373	41	-	1/5/27/28	0/3/3/3
41	P7G	2	3880	41	-	4/10/40/41	0/3/3/3
41	OMG	2	4370	41	-	0/5/27/28	0/3/3/3
41	B8W	2	4529	41	-	0/5/27/28	0/3/3/3
41	OMG	2	4637	41	-	3/5/27/28	0/3/3/3
41	A2M	2	3825	41	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A2M	2	3867	41	-	3/5/27/28	0/3/3/3
41	OMC	2	2365	41	-	0/9/27/28	0/2/2/2
41	E6G	2	4355	41	-	2/6/28/29	0/3/3/3
41	B8W	2	4185	41	-	2/5/27/28	0/3/3/3
41	1MA	2	1322	41	-	0/3/25/26	0/3/3/3
41	2MG	2	4872	41	-	2/5/27/28	0/3/3/3
41	B8W	2	4472	41	-	2/5/27/28	0/3/3/3
41	A2M	2	3723	41	-	1/5/27/28	0/3/3/3
41	OMG	2	1522	41	-	0/5/27/28	0/3/3/3
41	UR3	2	4597	41	-	2/7/25/26	0/2/2/2
41	OMG	2	2424	41	-	2/5/27/28	0/3/3/3
41	M7A	2	4564	41	-	0/7/37/38	0/3/3/3
41	B9H	2	2786	41	-	1/12/47/48	0/2/2/2
4	OMU	8	14	4,41	-	1/9/27/28	0/2/2/2
41	7MG	2	4550	41	-	2/7/37/38	0/3/3/3
41	A2M	2	1524	41	-	1/5/27/28	0/3/3/3
41	A2M	2	2363	41	-	0/5/27/28	0/3/3/3
41	2MG	2	729	41	-	2/5/27/28	0/3/3/3
41	P4U	2	1348	41	-	1/10/29/30	0/2/2/2
41	6MZ	2	4220	41	-	1/5/27/28	0/3/3/3
41	OMG	2	4623	41	-	0/5/27/28	0/3/3/3
41	OMG	2	4494	41	-	0/5/27/28	0/3/3/3
41	1MA	2	4415	41	-	2/3/25/26	0/3/3/3
41	A2M	2	398	41	-	2/5/27/28	0/3/3/3
41	OMG	2	1625	41	-	3/5/27/28	0/3/3/3
41	OMG	2	1883	41	-	2/5/27/28	0/3/3/3
41	OMG	2	4870	41	-	3/5/27/28	0/3/3/3
41	I4U	2	4194	41	-	8/9/29/30	0/2/2/2
41	OMC	2	3701	41	-	4/9/27/28	0/2/2/2
41	7MG	2	2522	41	-	0/7/37/38	0/3/3/3
41	7MG	2	1605	41	-	0/7/37/38	0/3/3/3
41	A2M	2	1326	41	-	1/5/27/28	0/3/3/3

The worst 5 of 528 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	4083	5MU	C4-C5	20.75	1.79	1.44
41	2	1322	1MA	C2-N3	16.28	1.48	1.29
41	2	4415	1MA	C2-N3	16.08	1.48	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2	4083	5MU	C6-N1	15.72	1.64	1.38
41	2	4083	5MU	C6-C5	-11.53	1.15	1.34

The worst 5 of 337 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2	1574	B9B	O6-C6-N1	-30.26	94.01	120.12
41	2	237	B9B	O6-C6-N1	-29.95	94.27	120.12
41	2	4564	M7A	C5-C6-N6	13.81	147.33	123.74
41	2	4220	6MZ	C1'-N9-C4	-12.57	104.56	126.64
41	2	4564	M7A	N6-C6-N1	-11.85	92.41	118.35

There are no chirality outliers.

5 of 113 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	8	14	OMU	C1'-C2'-O2'-CM2
41	2	237	B9B	C5-C6-O6-C61
41	2	237	B9B	N1-C6-O6-C61
41	2	237	B9B	C3'-C4'-C5'-O5'
41	2	237	B9B	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

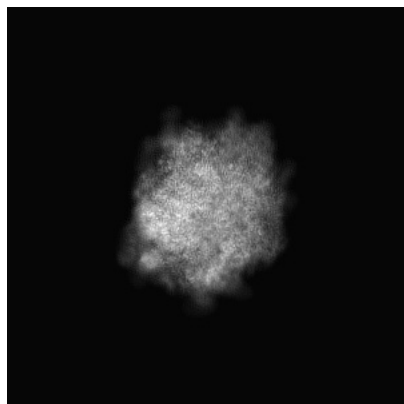
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35375. These allow visual inspection of the internal detail of the map and identification of artifacts.

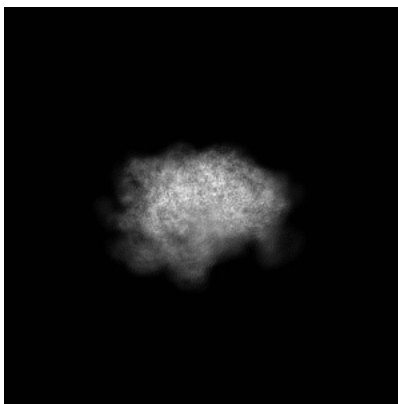
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

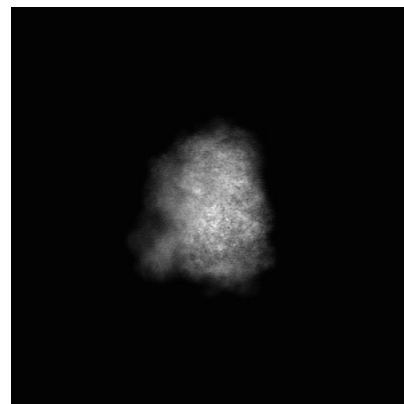
6.1.1 Primary map



X

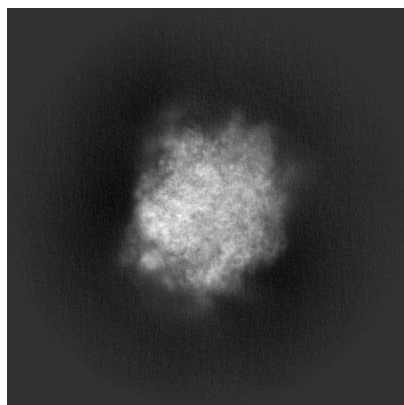


Y

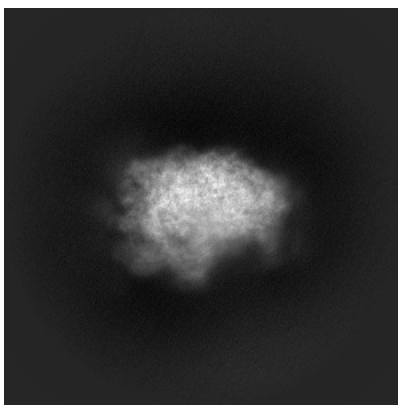


Z

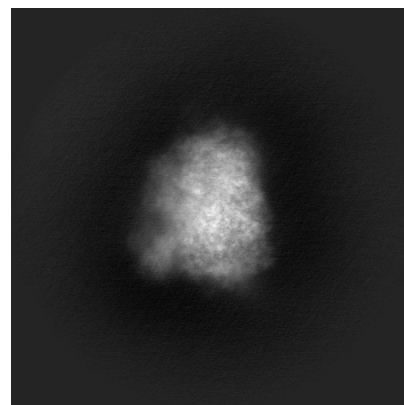
6.1.2 Raw map



X



Y

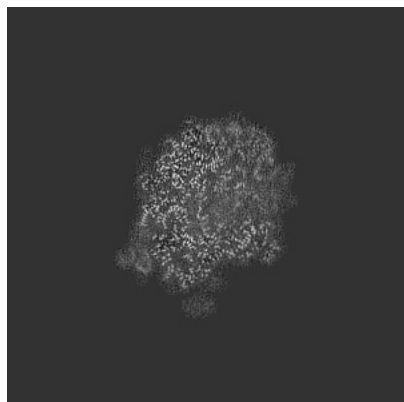


Z

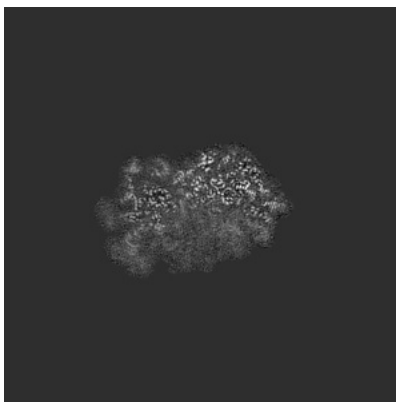
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

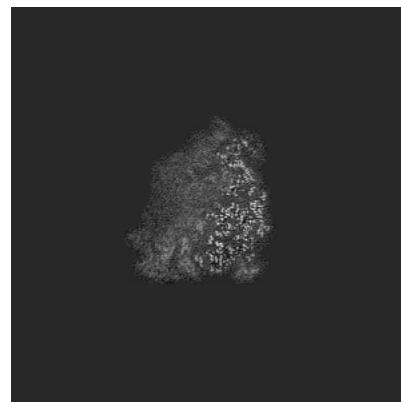
6.2.1 Primary map



X Index: 200

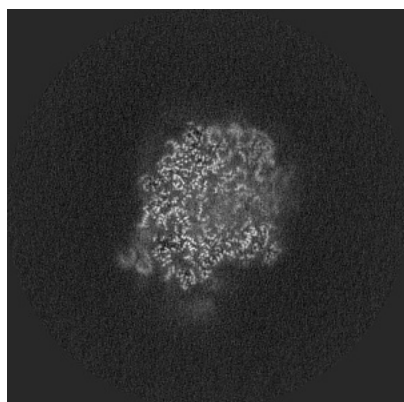


Y Index: 200

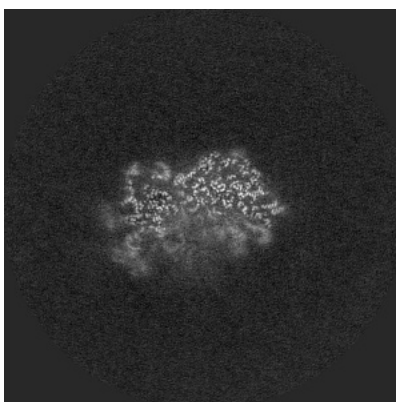


Z Index: 200

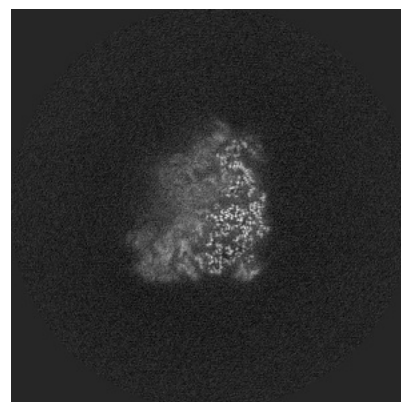
6.2.2 Raw map



X Index: 200



Y Index: 200

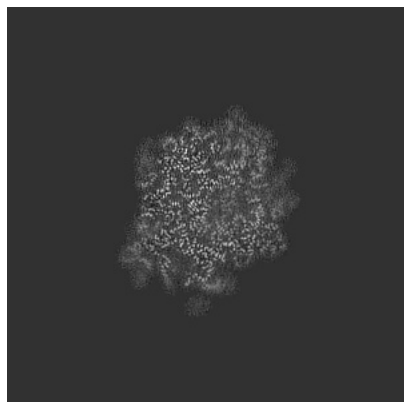


Z Index: 200

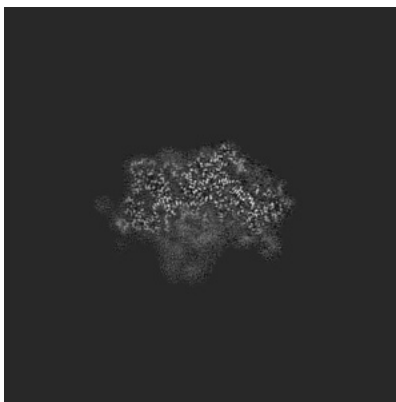
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

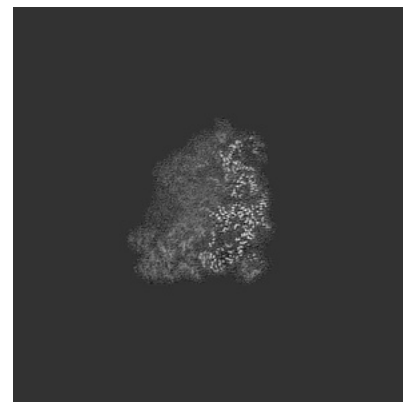
6.3.1 Primary map



X Index: 207

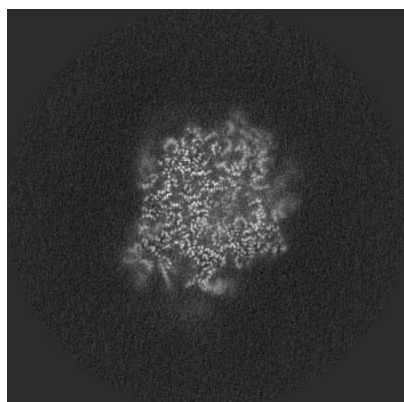


Y Index: 181

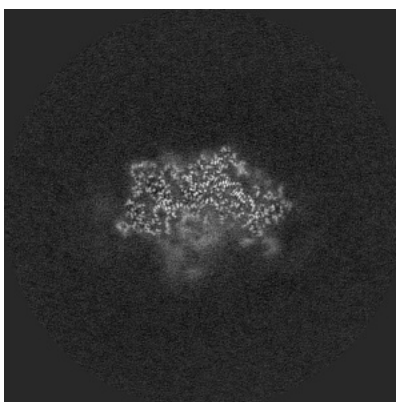


Z Index: 198

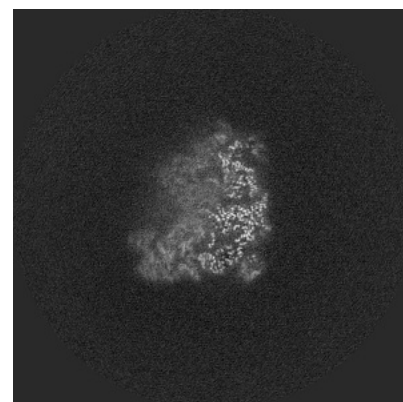
6.3.2 Raw map



X Index: 207



Y Index: 182

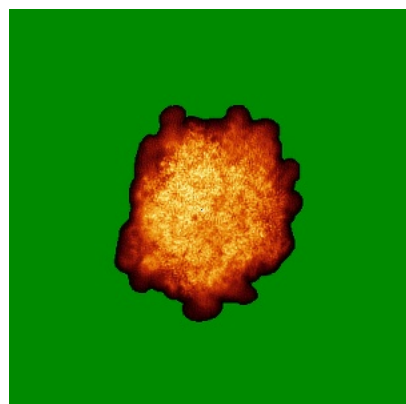


Z Index: 199

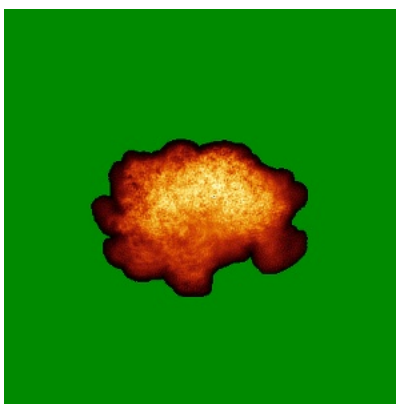
The images above show the largest variance slices of the map in three orthogonal directions.

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

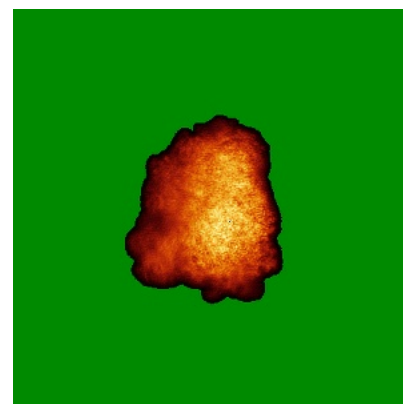
6.4.1 Primary map



X

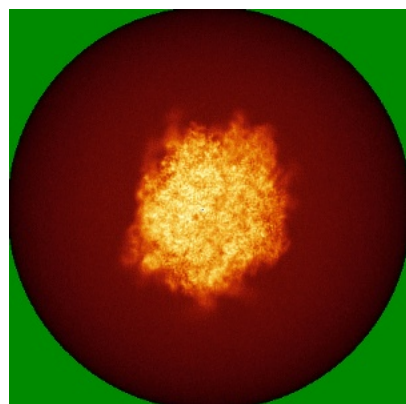


Y

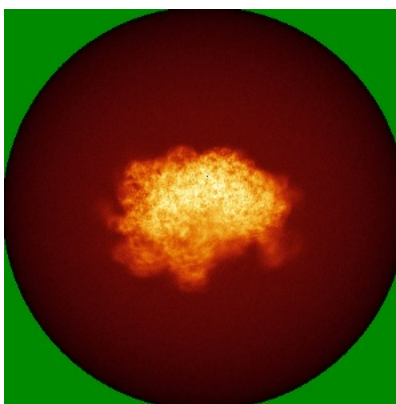


Z

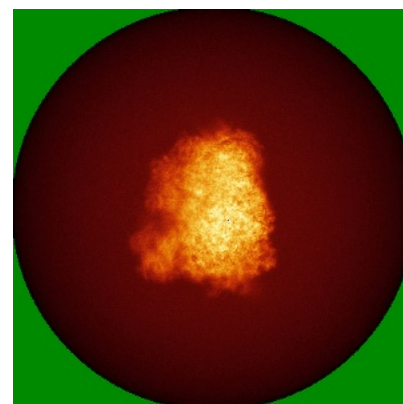
6.4.2 Raw map



X



Y

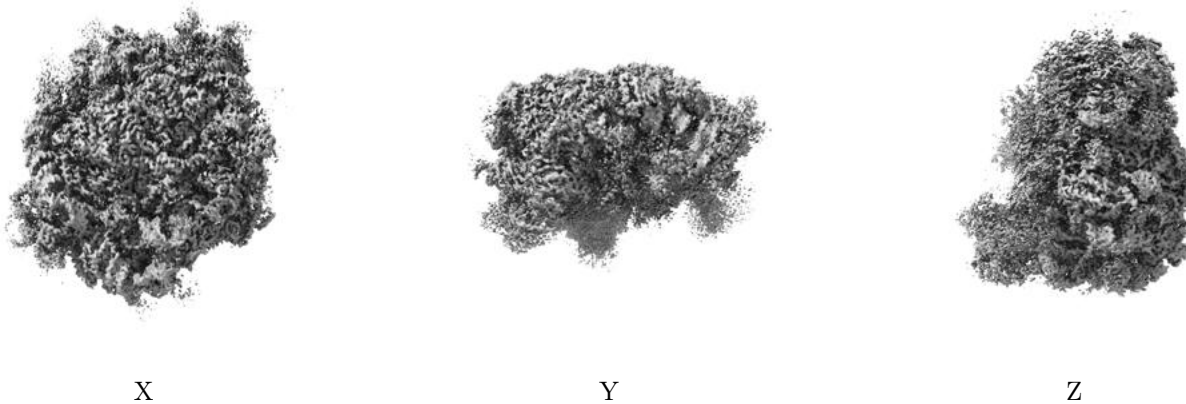


Z

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 0.035. 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.

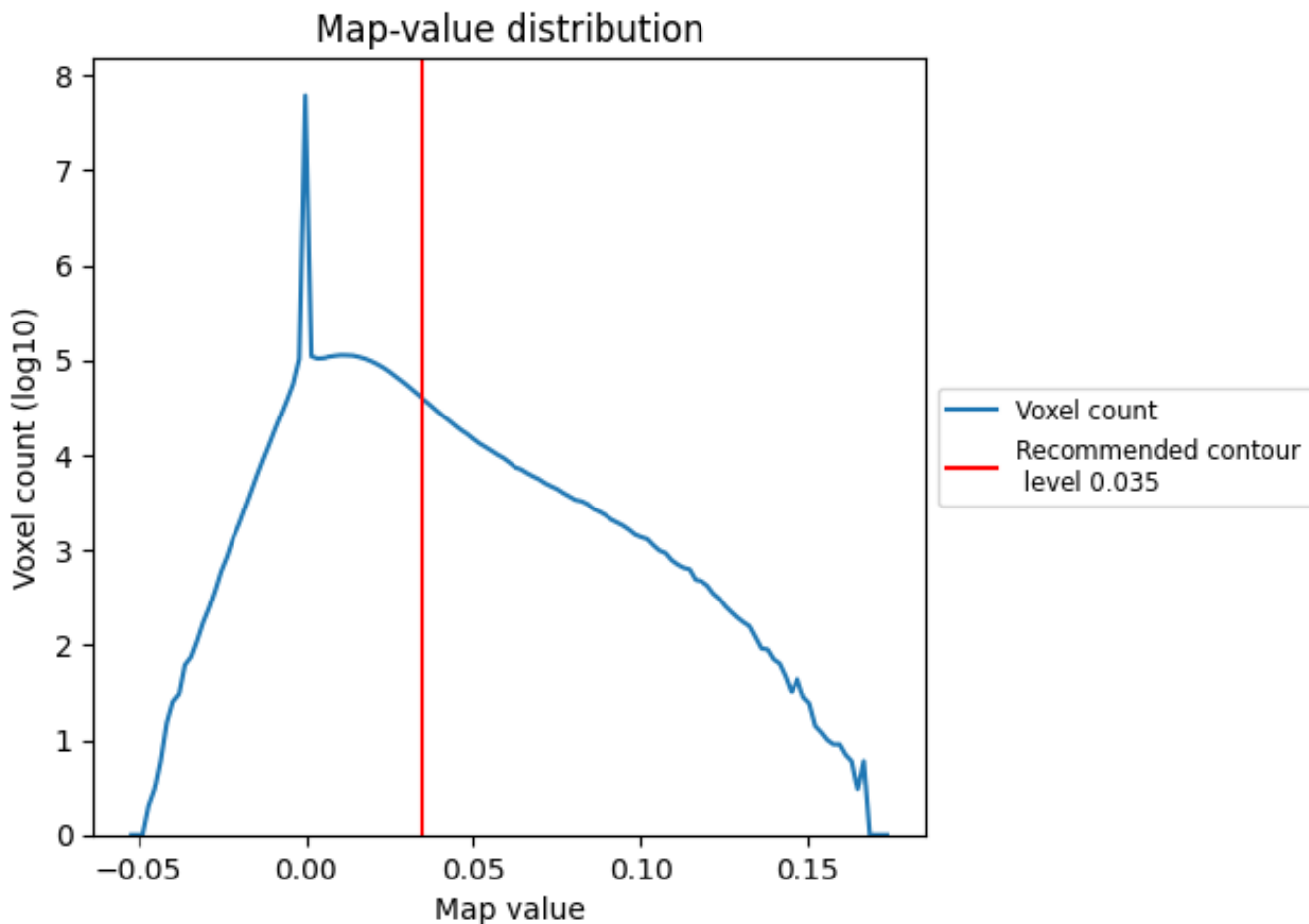
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

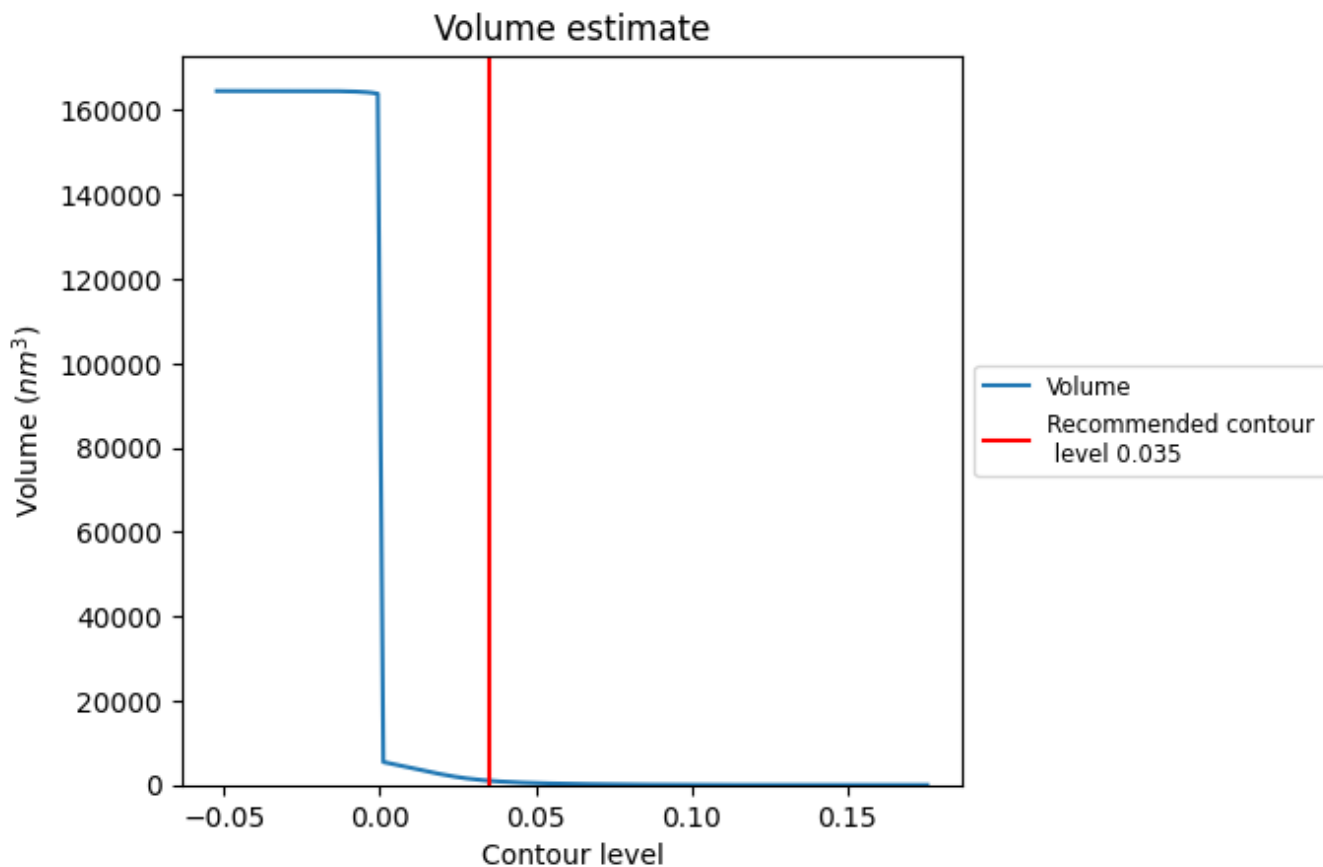
This section contains the results of statistical analysis of the map.

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.

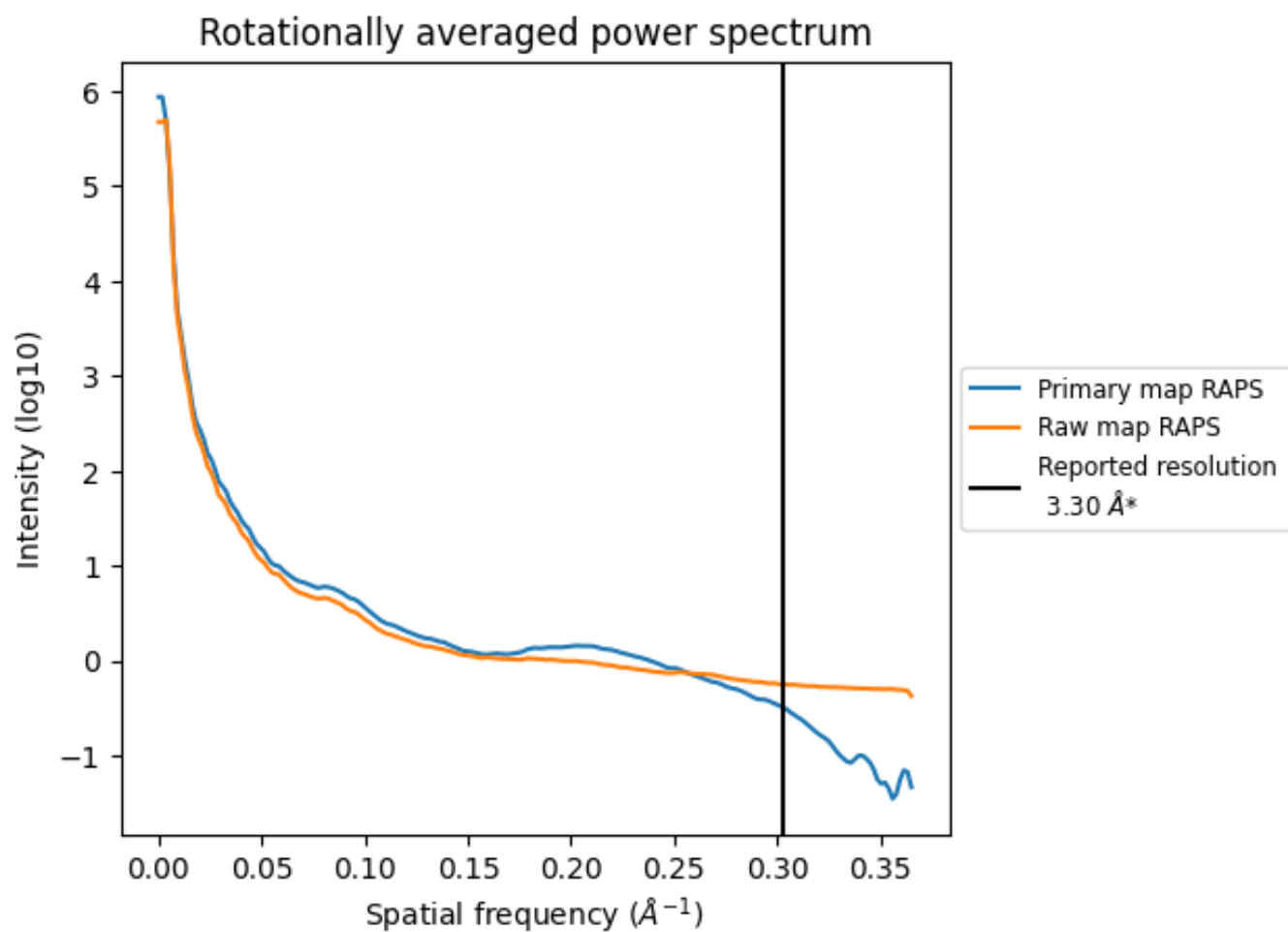
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1007 nm³; this corresponds to an approximate mass of 910 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

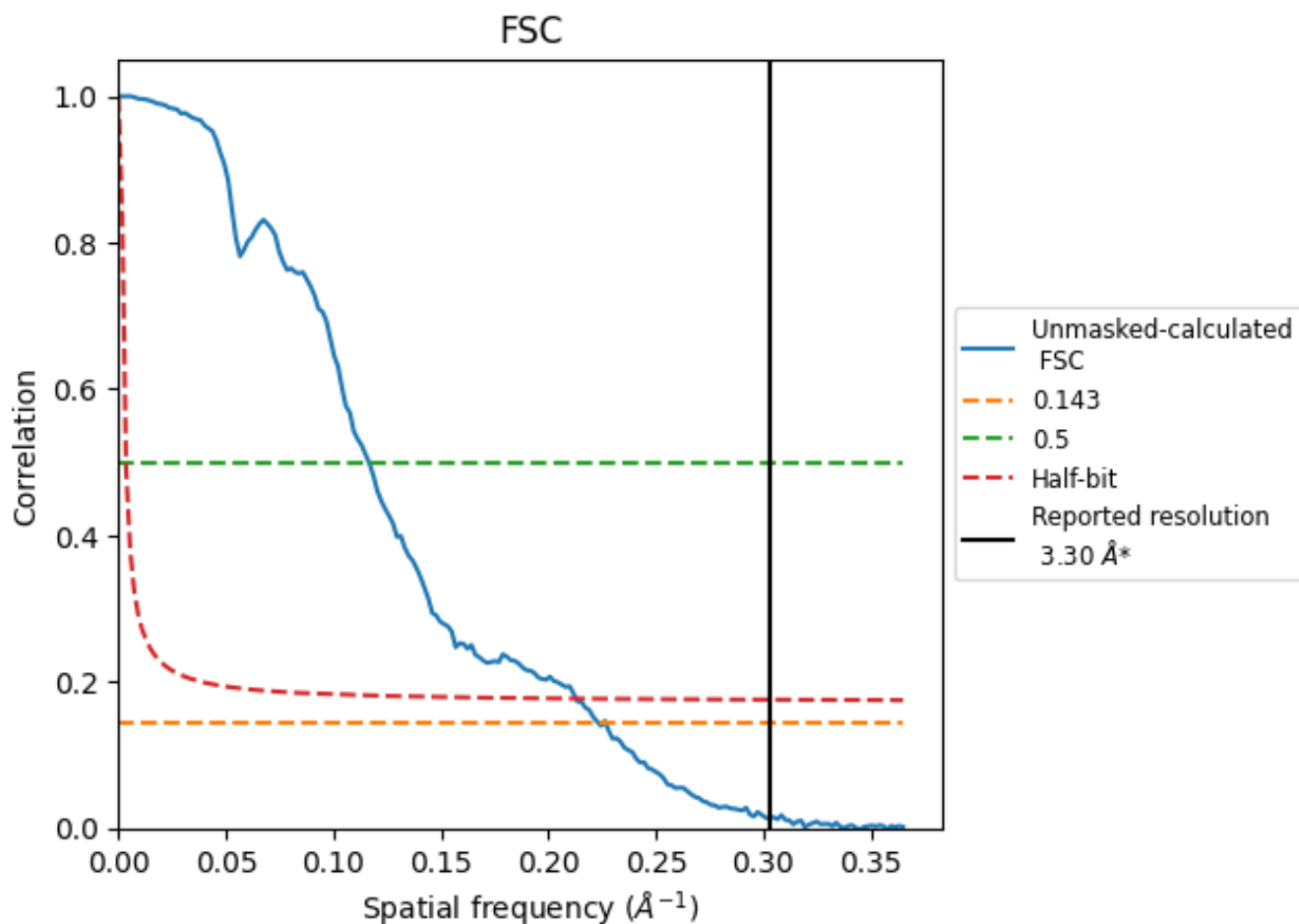


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

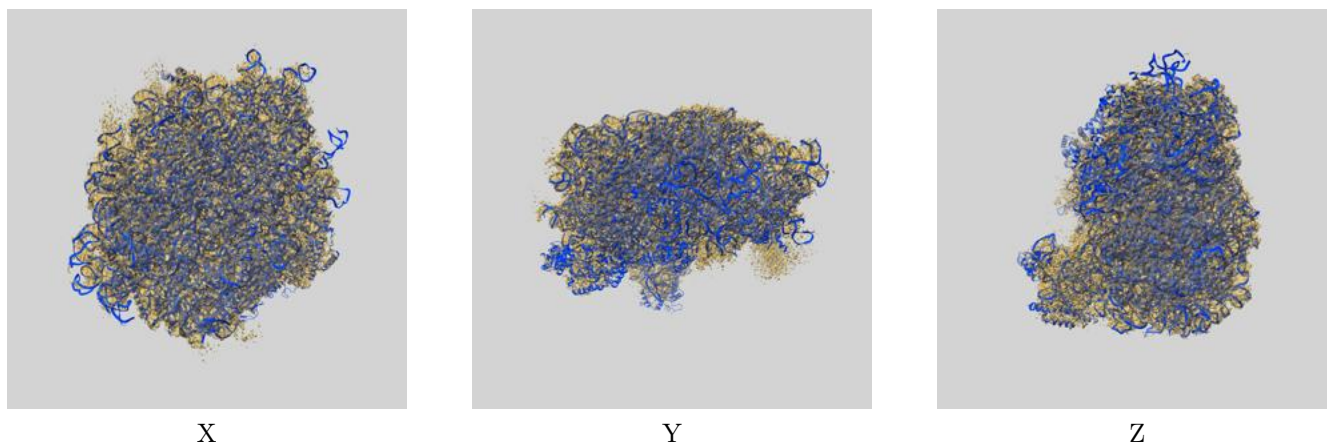
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.48	8.58	4.70

*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 4.48 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

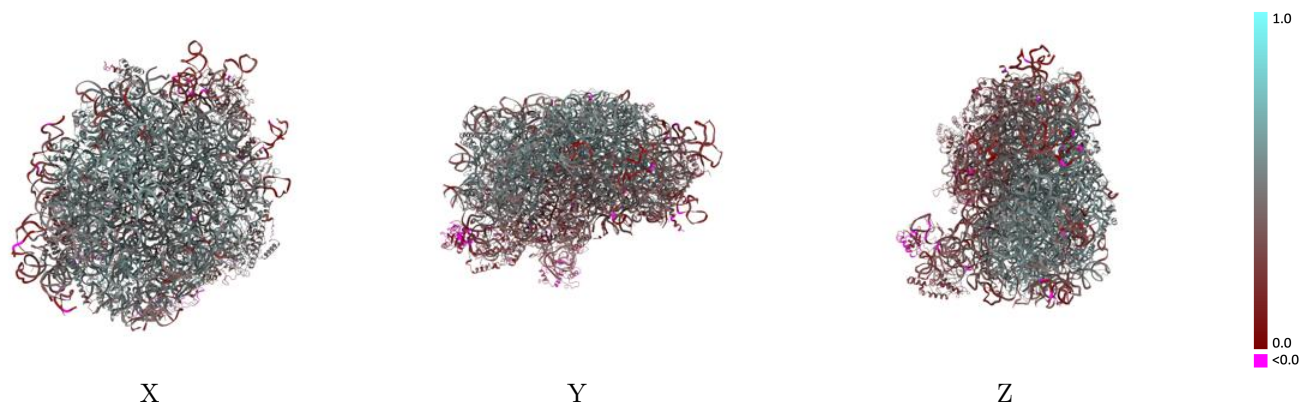
This section contains information regarding the fit between EMDB map EMD-35375 and PDB model 8IE3. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



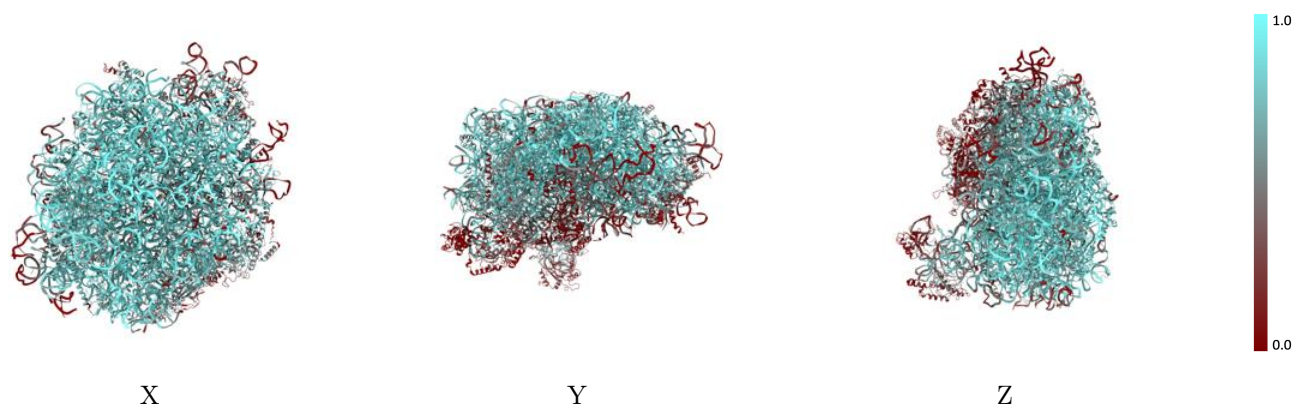
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



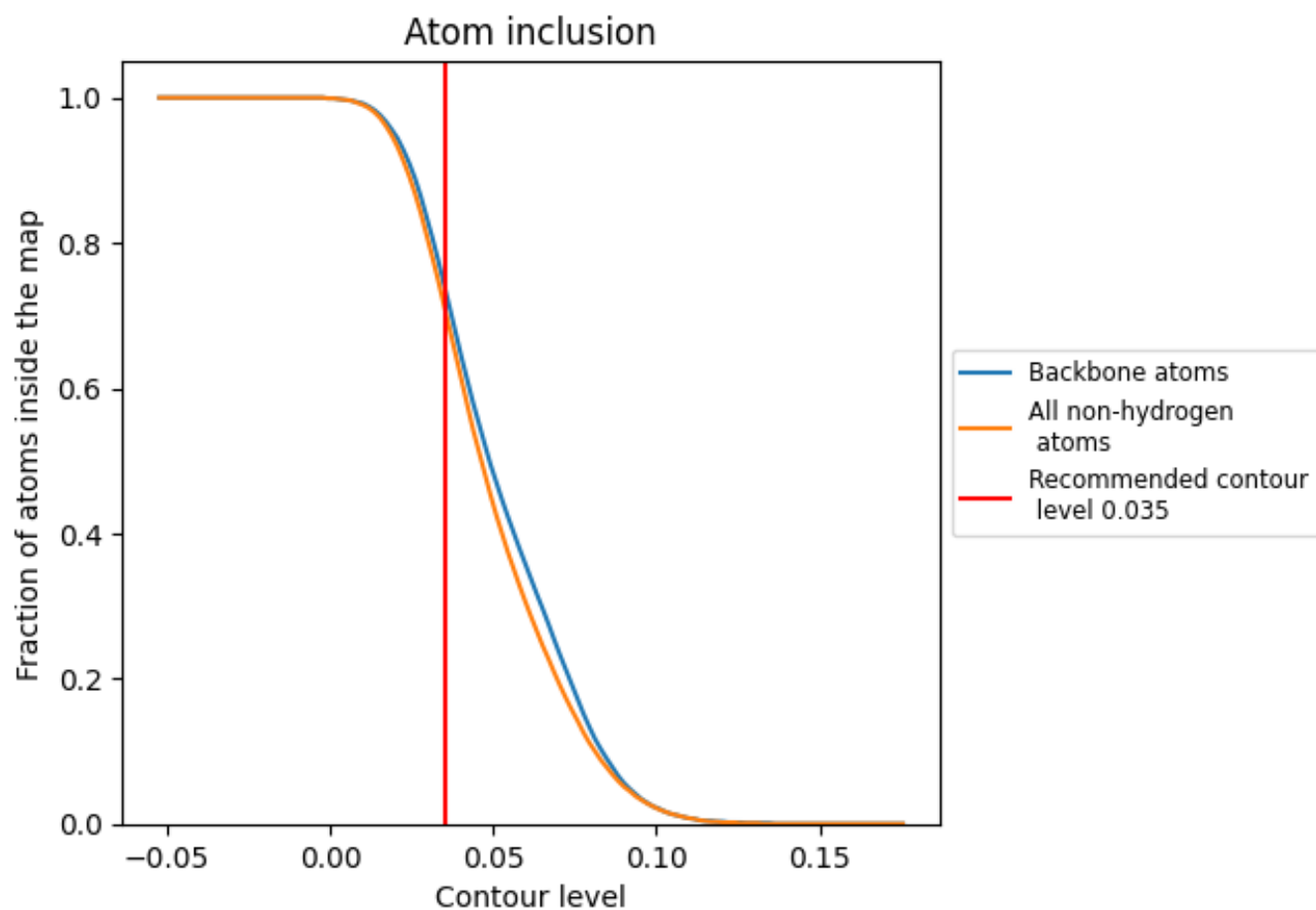
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 71% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7130	 0.4330
2	 0.7830	 0.4280
4	 0.3960	 0.3700
5	 0.7430	 0.3490
6	 0.5140	 0.4200
7	 0.7080	 0.4940
8	 0.9370	 0.5170
9	 0.0190	 0.2760
A	 0.1270	 0.3110
B	 0.8080	 0.5250
C	 0.4950	 0.3610
D	 0.8990	 0.5500
E	 0.2820	 0.3360
F	 0.7150	 0.4470
G	 0.6350	 0.4250
H	 0.8490	 0.5390
I	 0.6680	 0.4800
J	 0.0340	 0.0670
K	 0.7980	 0.4970
L	 0.8500	 0.5450
M	 0.9200	 0.5440
O	 0.5820	 0.4330
P	 0.9290	 0.5490
Q	 0.7920	 0.5080
R	 0.1550	 0.2590
S	 0.8340	 0.5220
T	 0.1020	 0.0780
U	 0.8880	 0.5480
V	 0.8570	 0.5340
X	 0.4810	 0.3740
Y	 0.8070	 0.5250
Z	 0.9000	 0.5710
a	 0.6220	 0.4370
b	 0.8690	 0.5470
c	 0.6460	 0.4150



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Chain	Atom inclusion	Q-score
d	 0.6810	 0.4720
e	 0.6840	 0.4720
g	 0.8460	 0.5310
h	 0.8610	 0.5440
i	 0.4390	 0.3340
j	 0.7830	 0.5170
k	 0.9110	 0.5640
l	 0.8740	 0.5510
m	 0.5320	 0.4030
n	 0.9250	 0.5660
o	 0.7080	 0.4820
p	 0.8440	 0.5390
r	 0.2790	 0.2800
z	 0.3000	 0.4130