



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:57 AM UTC

PDB ID : 8K2B / pdb_00008k2b
EMDB ID : EMD-36837
Title : Cryo-EM structure of the human 39S mitoribosome with Tigecycline
Authors : Li, X.; Wang, M.; Cheng, J.
Deposited on : 2023-07-12
Resolution : 3.40 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:

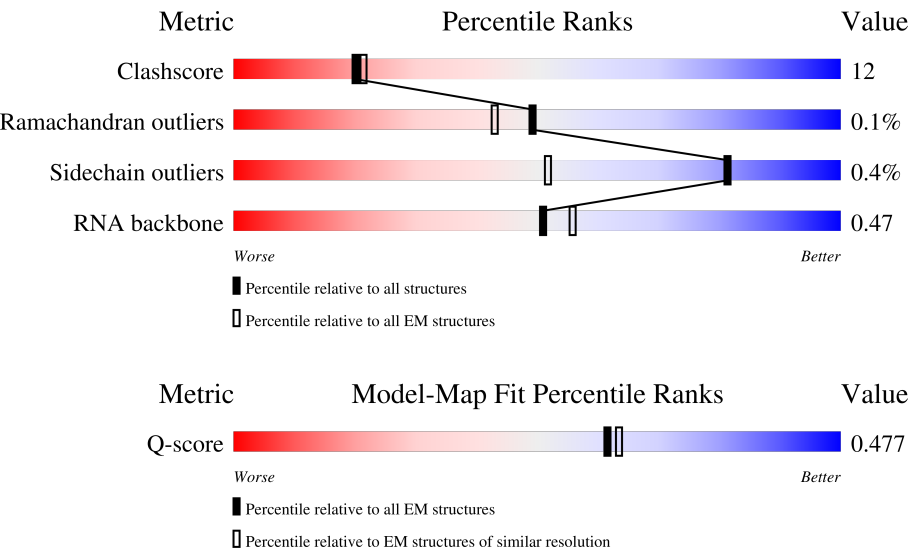
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	L1	1559	
2	L2	69	
3	LB	305	

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Mol	Chain	Length	Quality of chain
4	LC	348	
5	LD	311	
6	LI	267	
7	LJ	261	
8	LK	192	
9	LM	178	
10	LN	145	
11	LO	296	
12	LP	251	
13	LQ	175	
14	LR	179	
15	LS	292	
16	LT	149	
17	LU	205	
18	LV	212	
19	LW	153	
20	LX	216	
21	La	148	
22	Lb	256	
23	Lu	250	
24	Ld	161	
25	Lf	188	
26	Lg	65	
27	Lh	92	
28	Li	188	

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Mol	Chain	Length	Quality of chain
29	Lj	103	
30	Lk	423	
31	Ll	380	
32	Lm	338	
33	Ln	206	
34	Lo	137	
35	Lp	142	
36	Lq	215	
37	Lr	332	
38	Ls	306	
39	Lt	279	
40	Lv	212	
41	Lw	166	
42	Lx	158	
43	Ly	128	
44	Lz	123	
45	L3	112	
46	L4	138	
47	L5	128	
48	L6	102	
49	L7	206	
50	L8	222	
51	SR	196	
52	Sf	439	
53	u	234	

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Mol	Chain	Length	Quality of chain
54	v	70	99% 49% 50%
55	w	156	51% 24% 26% 49%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 102269 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 16s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L1	1500	Total	C	N	O	P	0	0
			31847	14290	5750	10307	1500		

- Molecule 2 is a RNA chain called Val tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L2	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LB	237	Total	C	N	O	S	0	0
			1851	1151	375	316	9		

- Molecule 4 is a protein called Large ribosomal subunit protein uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LC	304	Total	C	N	O	S	0	0
			2393	1538	415	429	11		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LD	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 6 is a protein called Large ribosomal subunit protein bL9m.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	LI	95	Total	C	N	O	0	0
			784	498	152	134		

- Molecule 7 is a protein called Large ribosomal subunit protein uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LJ	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 8 is a protein called Large ribosomal subunit protein uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LK	175	Total	C	N	O	S	0	0
			1330	847	237	244	2		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LM	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 10 is a protein called Large ribosomal subunit protein uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LN	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 11 is a protein called Large ribosomal subunit protein uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LO	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 12 is a protein called Large ribosomal subunit protein uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LP	221	Total	C	N	O	S	0	0
			1779	1138	325	306	10		

- Molecule 13 is a protein called Large ribosomal subunit protein bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LQ	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 14 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LR	146	Total	C	N	O	S	0	0
			1189	743	226	215	5		

- Molecule 15 is a protein called Large ribosomal subunit protein bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LS	219	Total	C	N	O	S	0	0
			1822	1168	322	323	9		

- Molecule 16 is a protein called Large ribosomal subunit protein bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LT	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 17 is a protein called Large ribosomal subunit protein bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LU	160	Total	C	N	O	S	0	0
			1284	829	226	225	4		

- Molecule 18 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LV	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 19 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LW	143	Total	C	N	O	S	0	0
			1188	752	224	208	4		

- Molecule 20 is a protein called Large ribosomal subunit protein uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LX	202	Total	C	N	O	S	0	0
			1652	1053	294	297	8		

- Molecule 21 is a protein called Large ribosomal subunit protein bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	La	111	Total	C	N	O	S	0	0
			871	558	164	146	3		

- Molecule 22 is a protein called Large ribosomal subunit protein bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Lb	243	Total	C	N	O	S	0	0
			2035	1317	351	362	5		

- Molecule 23 is a protein called Large ribosomal subunit protein uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Lu	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 24 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ld	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 25 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Lf	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 26 is a protein called Large ribosomal subunit protein bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Lg	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 27 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Lh	46	Total	C	N	O	S	0	0
			376	233	83	59	1		

- Molecule 28 is a protein called Large ribosomal subunit protein bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Li	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 29 is a protein called Large ribosomal subunit protein bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lj	38	Total	C	N	O	S	0	0
			341	217	72	48	4		

- Molecule 30 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lk	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 31 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ll	354	Total	C	N	O	S	0	0
			2947	1881	525	532	9		

- Molecule 32 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lm	293	Total	C	N	O	S	0	0
			2382	1525	404	435	18		

- Molecule 33 is a protein called Large ribosomal subunit protein mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ln	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 34 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lo	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 35 is a protein called Large ribosomal subunit protein mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lp	97	Total	C	N	O	S	0	0
			815	514	147	149	5		

- Molecule 36 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lq	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 37 is a protein called Large ribosomal subunit protein mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lr	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 38 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Ls	214	Total	C	N	O	S	0	0
			1754	1117	304	320	13		

- Molecule 39 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lt	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 40 is a protein called Large ribosomal subunit protein mL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lv	131	Total	C	N	O	S	0	0
			1039	663	169	203	4		

- Molecule 41 is a protein called Large ribosomal subunit protein mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lw	132	Total	C	N	O	S	0	0
			1097	710	191	194	2		

- Molecule 42 is a protein called Large ribosomal subunit protein mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lx	110	Total	C	N	O	S	0	0
			895	568	156	168	3		

- Molecule 43 is a protein called Large ribosomal subunit protein mL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ly	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 44 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lz	92	Total	C	N	O	S	0	0
			732	454	142	134	2		

- Molecule 45 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	L3	96	Total	C	N	O	S	0	0
			743	462	143	133	5		

- Molecule 46 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L4	83	Total	C	N	O	S	0	0
			703	446	124	130	3		

- Molecule 47 is a protein called Large ribosomal subunit protein mL55.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	L5	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 48 is a protein called Large ribosomal subunit protein mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L6	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 49 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	L7	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 50 is a protein called Large ribosomal subunit protein mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	L8	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 51 is a protein called Large ribosomal subunit protein mL66.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SR	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 52 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Sf	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 53 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	111	Total	C	N	O	S	0	0
			927	595	155	167	10		

- Molecule 54 is a protein called Mitochondrial ribosome and complex I assembly factor Alt-MIEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	69	Total	C	N	O	S	0	0
			588	372	116	100			

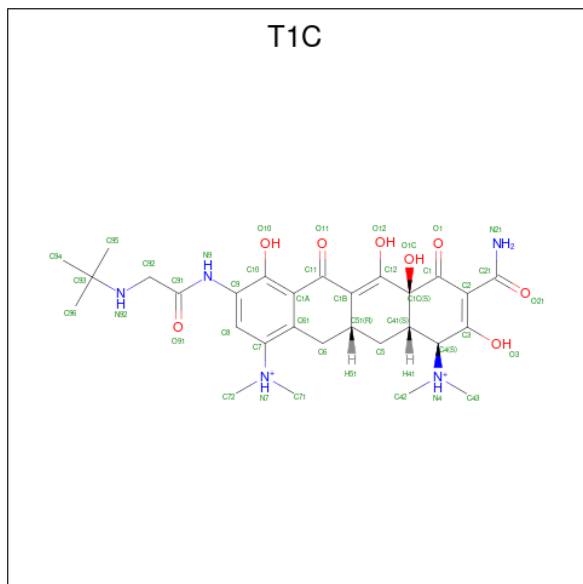
- Molecule 55 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	w	79	Total	C	N	O	S	0	0
			638	410	95	128	5		

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	L1	93	Total	Mg	0
			93	93	
56	LB	1	Total	Mg	0
			1	1	
56	Lw	1	Total	Mg	0
			1	1	

- Molecule 57 is TIGECYCLINE (CCD ID: T1C) (formula: $C_{29}H_{41}N_5O_8$).

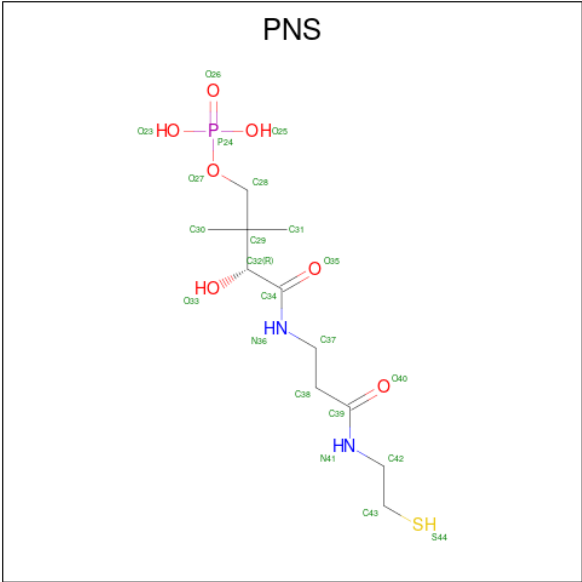


Mol	Chain	Residues	Atoms				AltConf
57	L1	1	Total	C	N	O	0
			42	29	5	8	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
58	Lf	1	Total	Zn	0
			1	1	
58	Lj	1	Total	Zn	0
			1	1	
58	SR	1	Total	Zn	0
			1	1	

- Molecule 59 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).

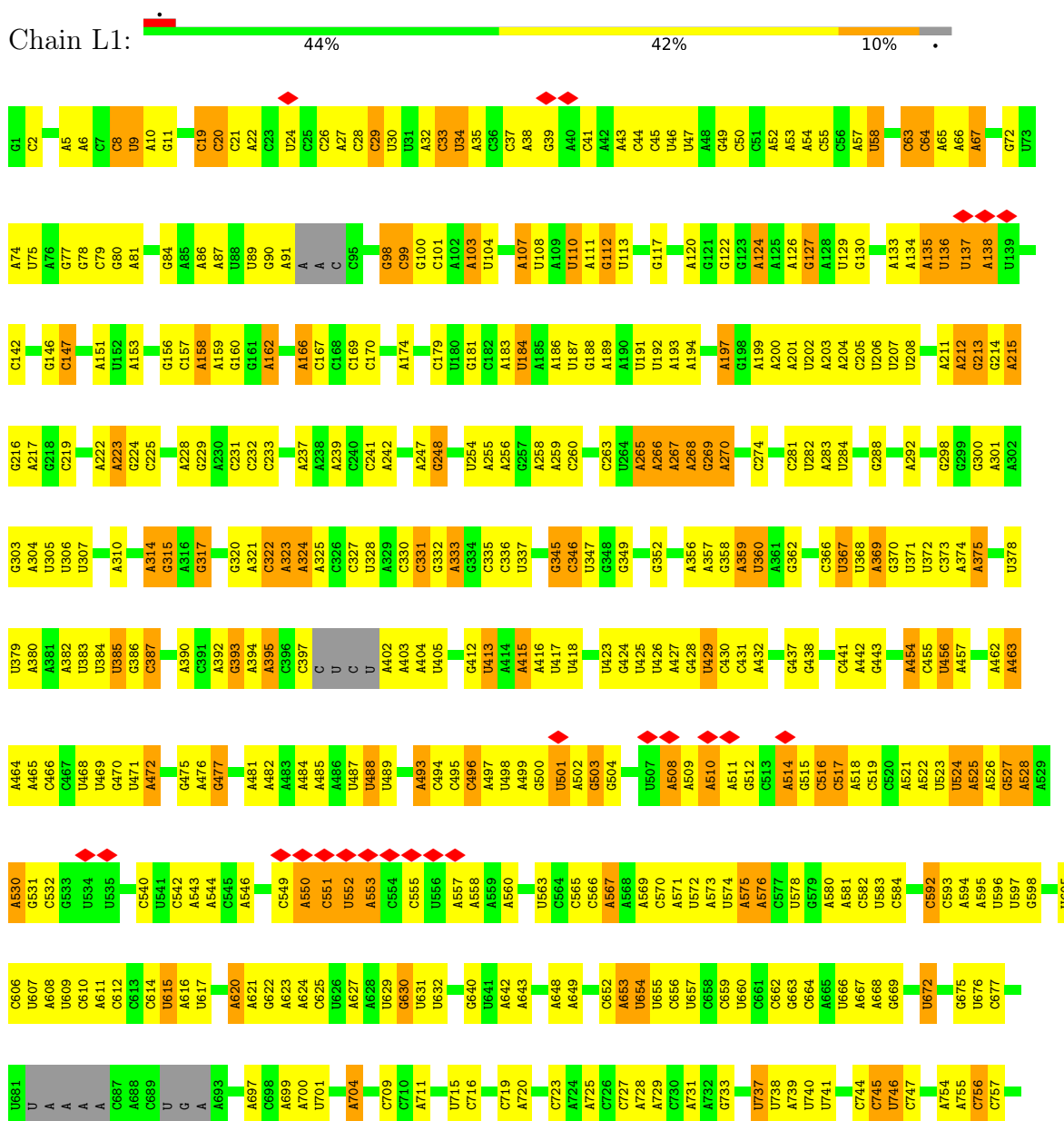


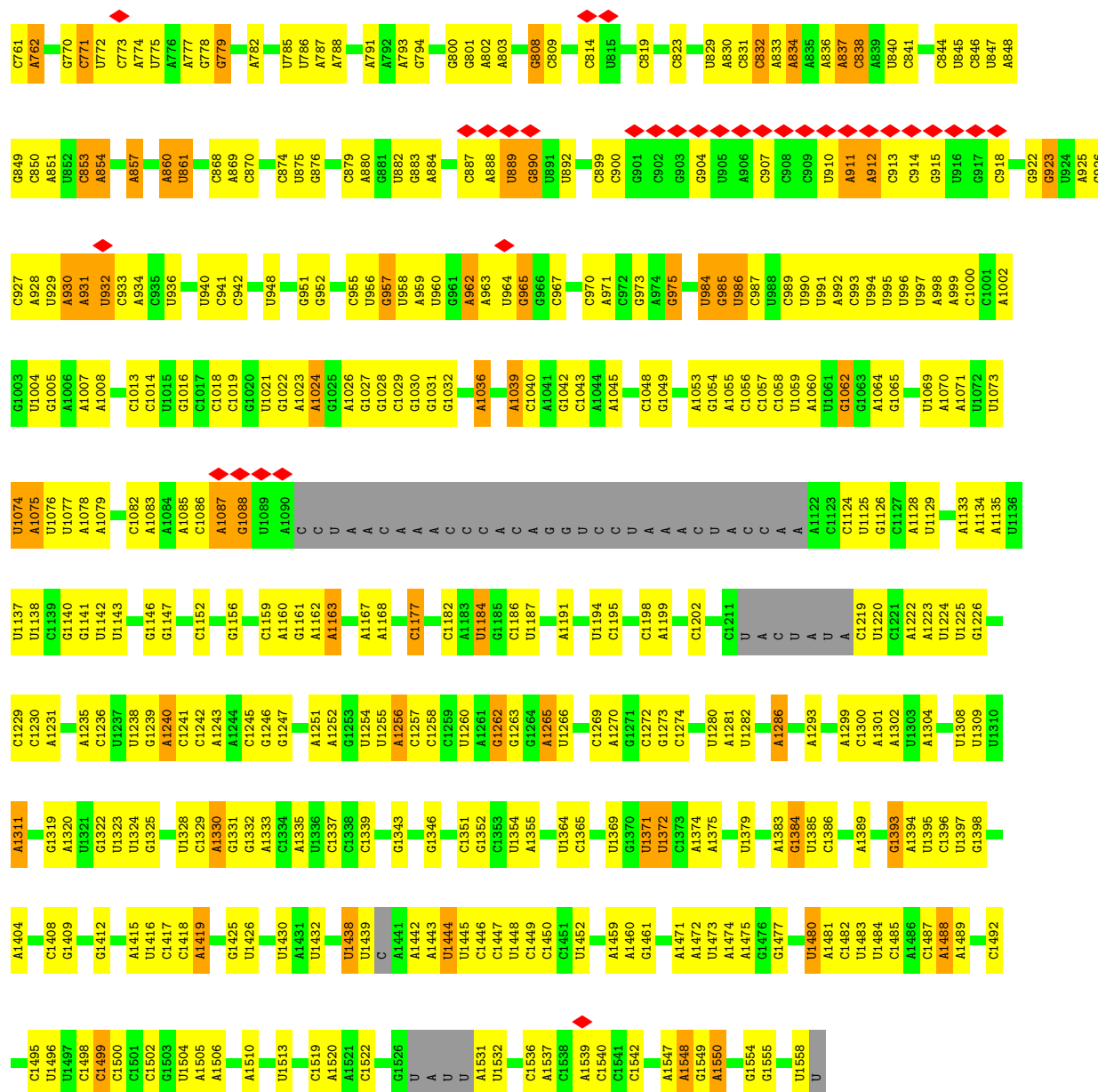
Mol	Chain	Residues	Atoms						AltConf
59	v	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

3 Residue-property plots

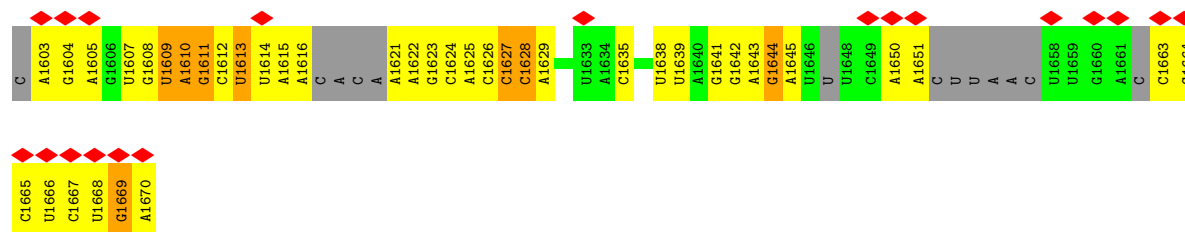
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16s rRNA



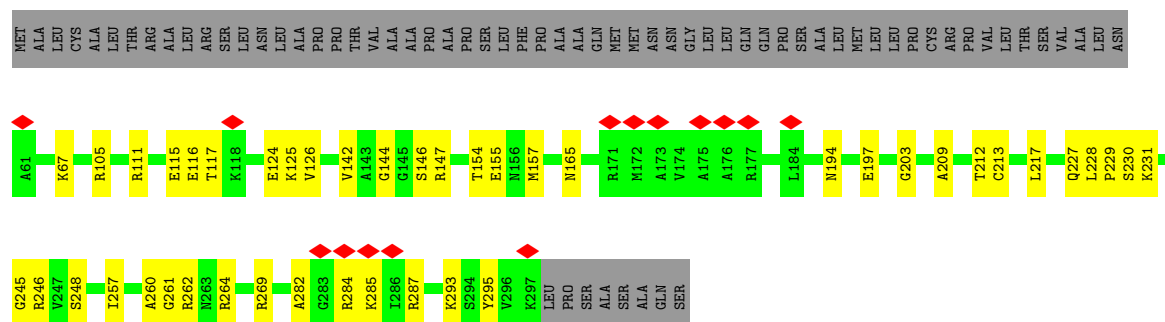


• Molecule 2: Val tRNA



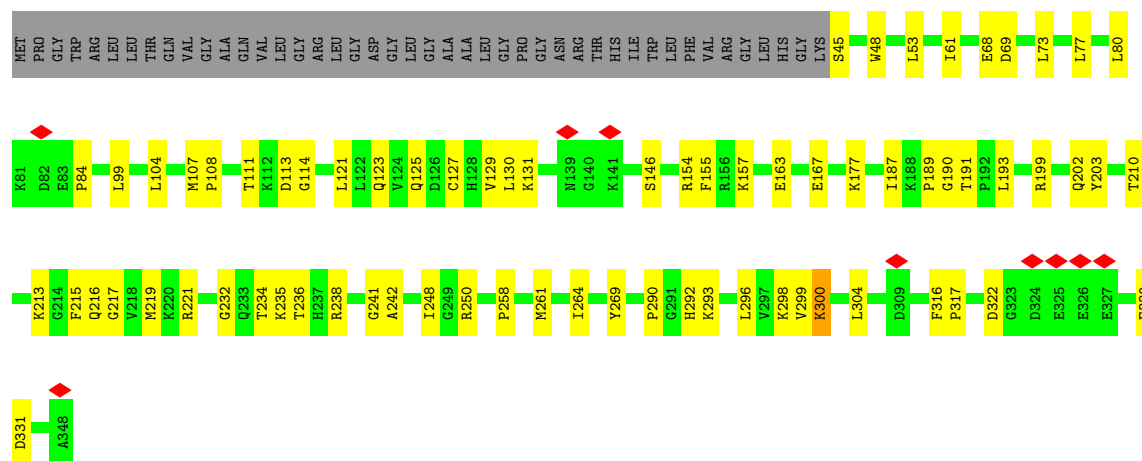
• Molecule 3: Large ribosomal subunit protein uL2m





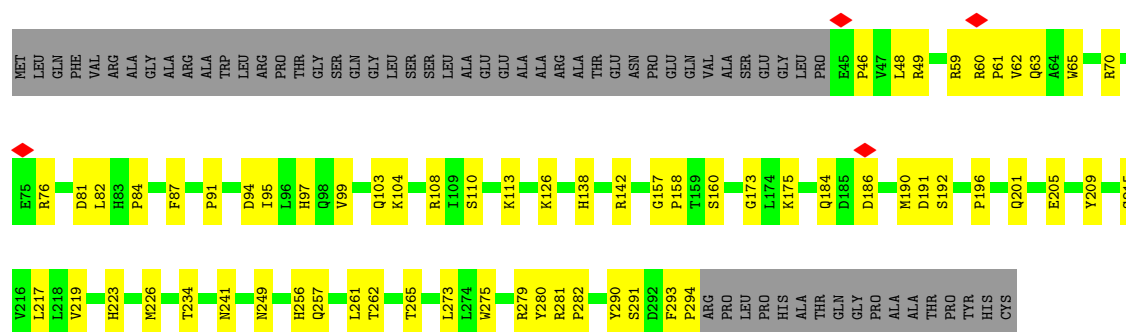
- Molecule 4: Large ribosomal subunit protein uL3m

Chain LC: 67% 20% 13%



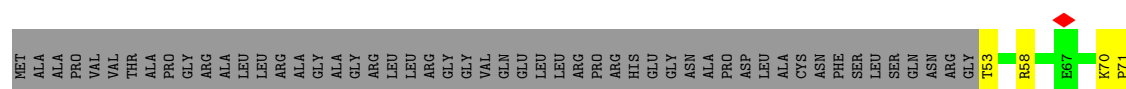
- Molecule 5: Large ribosomal subunit protein uL4m

Chain LD: 59% 21% 20%

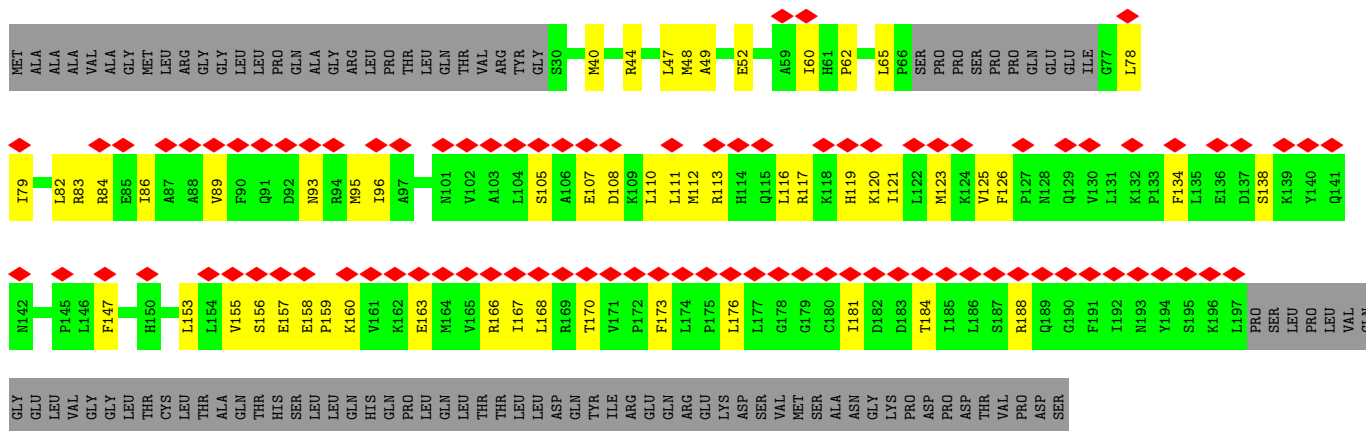


- Molecule 6: Large ribosomal subunit protein bL9m

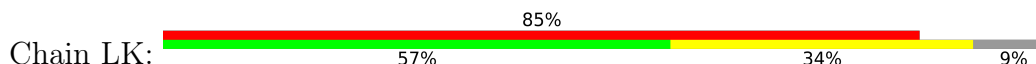
Chain LI: 7% 24% 12% 64%



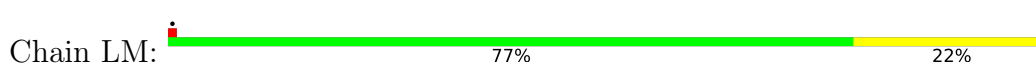
- Molecule 7: Large ribosomal subunit protein uL10m

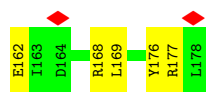


- Molecule 8: Large ribosomal subunit protein uL11m

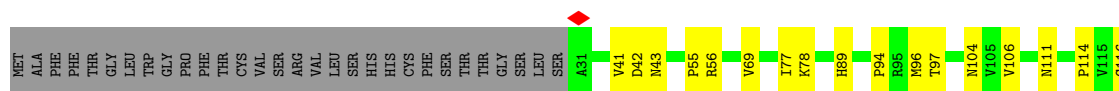


- Molecule 9: Large ribosomal subunit protein uL13m

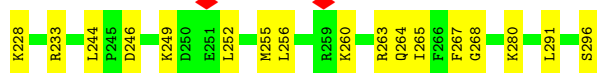




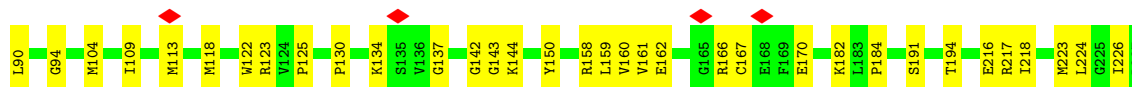
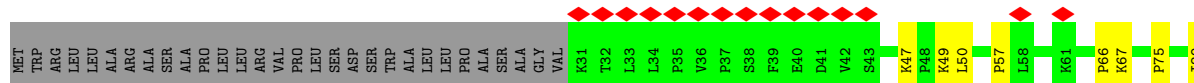
- Molecule 10: Large ribosomal subunit protein uL14m



- Molecule 11: Large ribosomal subunit protein uL15m

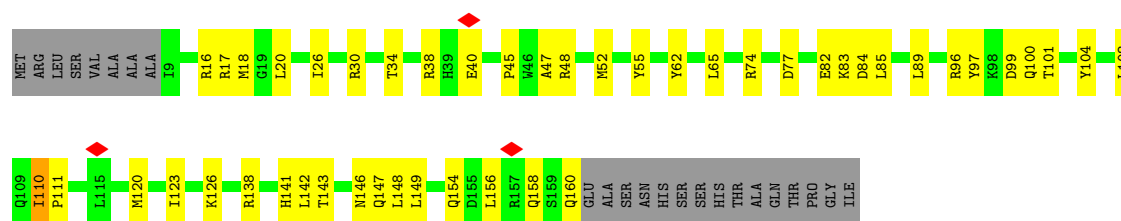


- Molecule 12: Large ribosomal subunit protein uL16m

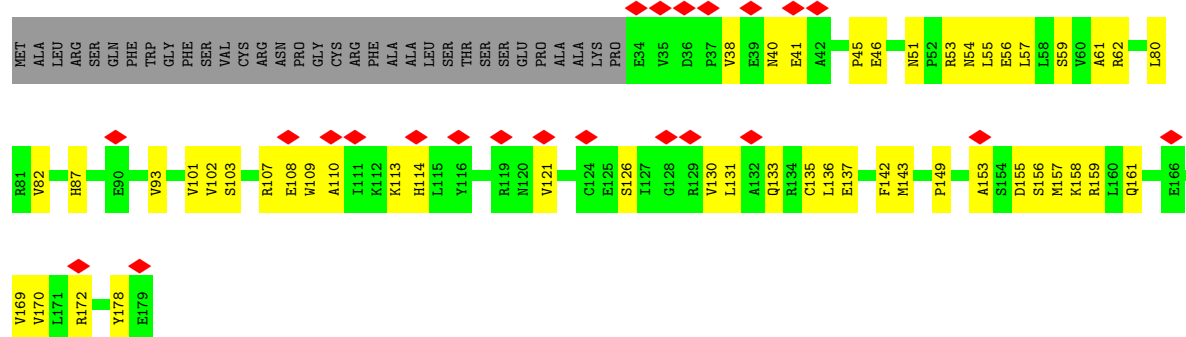


- Molecule 13: Large ribosomal subunit protein bL17m





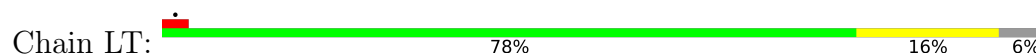
- Molecule 14: Mitochondrial ribosomal protein L18, isoform CRA_b



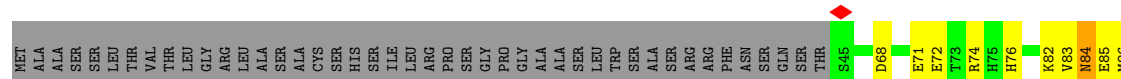
- Molecule 15: Large ribosomal subunit protein bL19m



- Molecule 16: Large ribosomal subunit protein bL20m

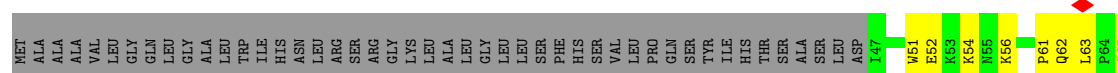


- Molecule 17: Large ribosomal subunit protein bL21m

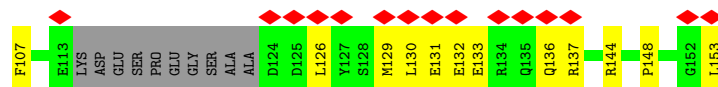
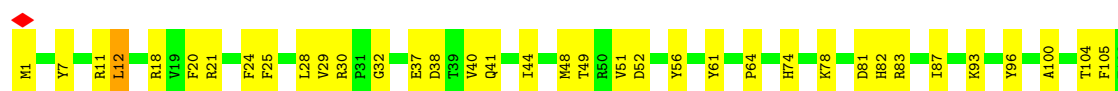




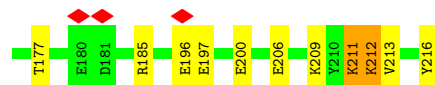
- Molecule 18: 39S ribosomal protein L22, mitochondrial



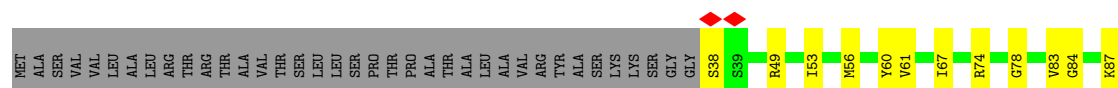
- Molecule 19: Large ribosomal subunit protein uL23m

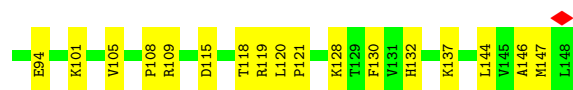


- Molecule 20: Large ribosomal subunit protein uL24m

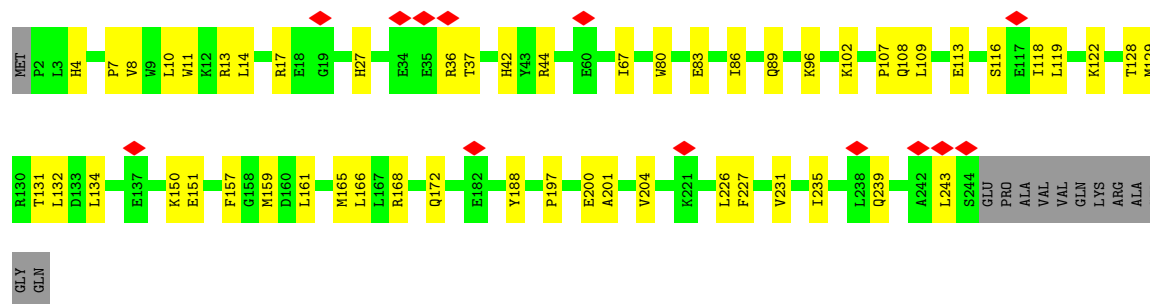
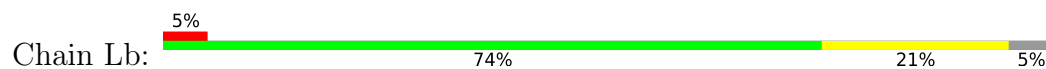


- Molecule 21: Large ribosomal subunit protein bL27m

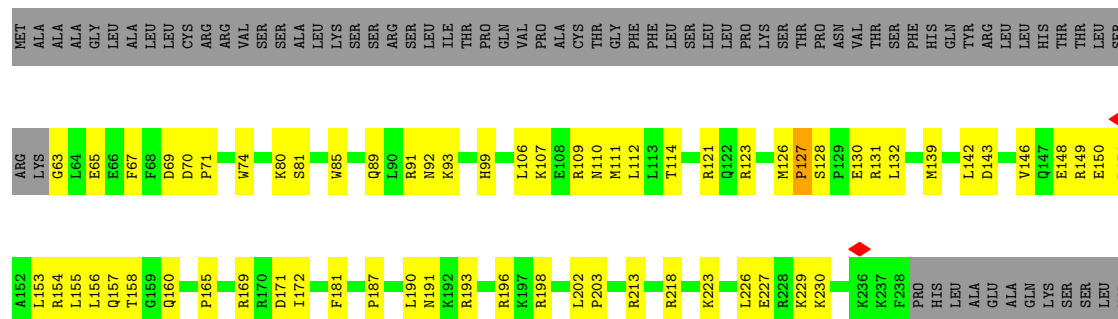




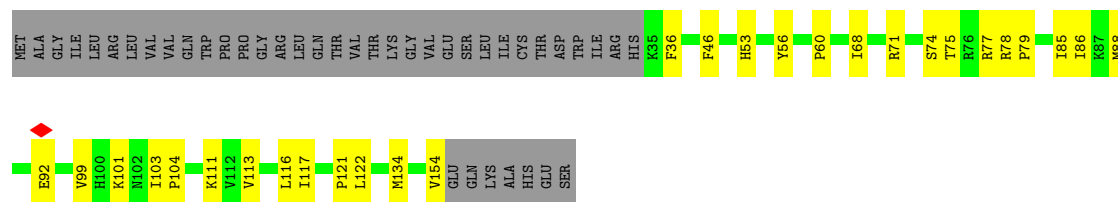
- Molecule 22: Large ribosomal subunit protein bL28m



- Molecule 23: Large ribosomal subunit protein uL29m



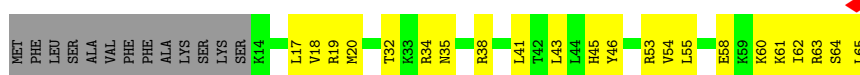
- Molecule 24: Large ribosomal subunit protein uL30m



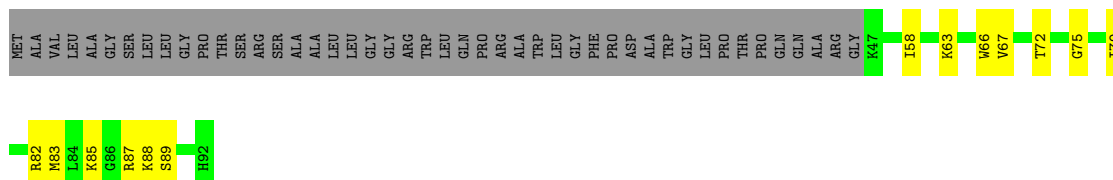
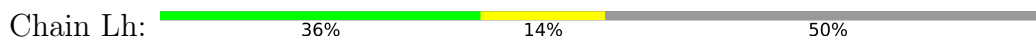
- Molecule 25: Large ribosomal subunit protein bL32m



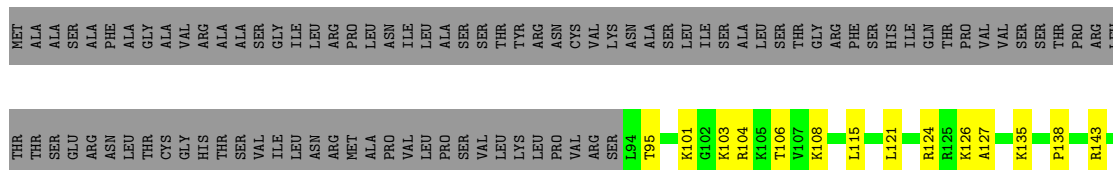
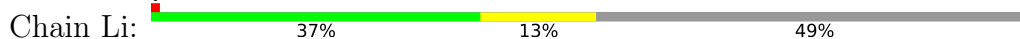
- Molecule 26: Large ribosomal subunit protein bL33m



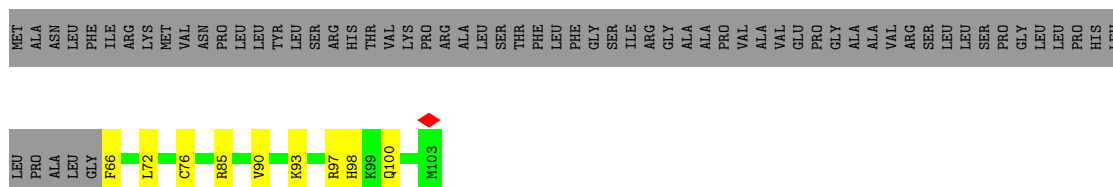
- Molecule 27: Large ribosomal subunit protein bL34m



- Molecule 28: Large ribosomal subunit protein bL35m

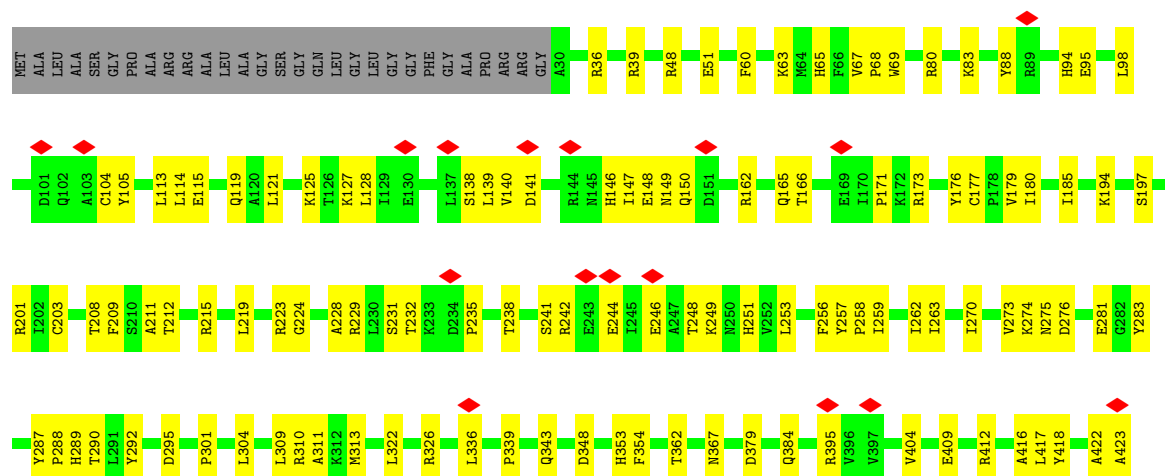


- Molecule 29: Large ribosomal subunit protein bL36m

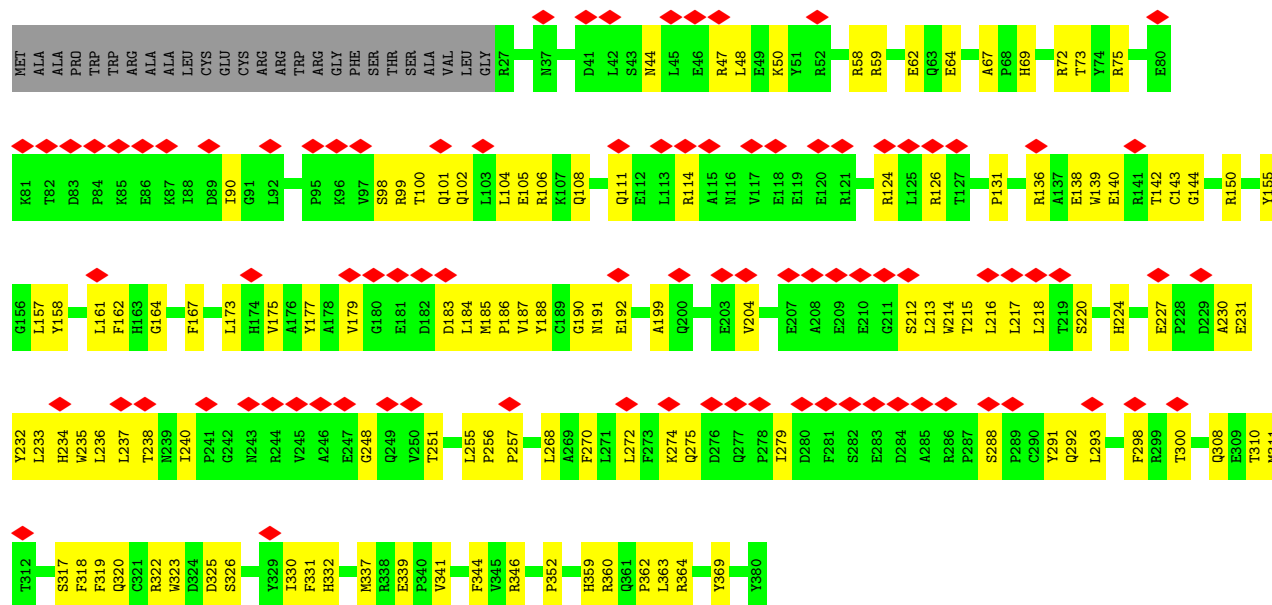


- Molecule 30: Large ribosomal subunit protein mL37

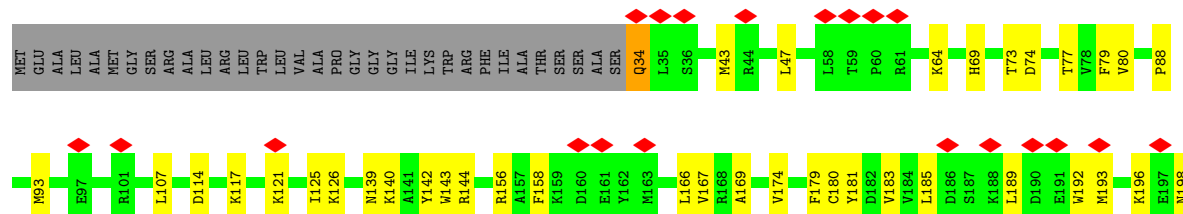


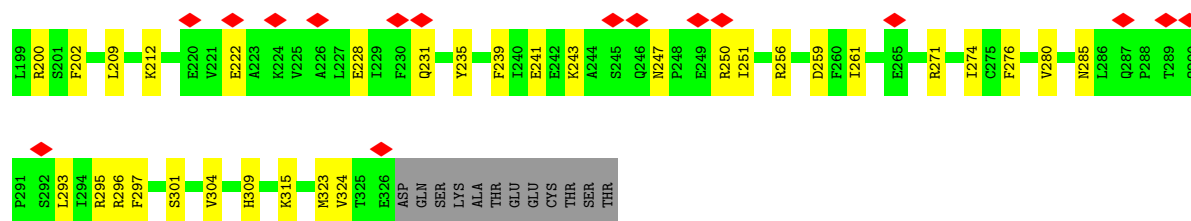


• Molecule 31: Large ribosomal subunit protein mL38

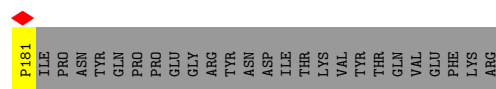
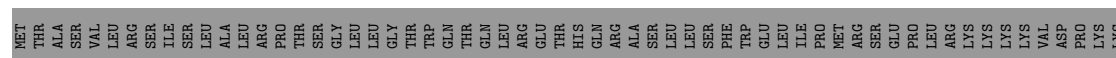
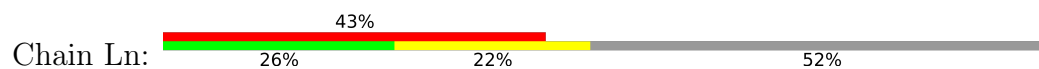


• Molecule 32: Large ribosomal subunit protein mL39

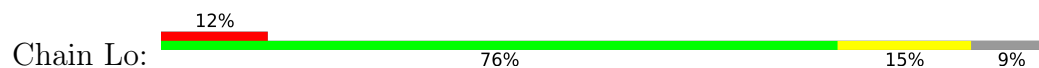




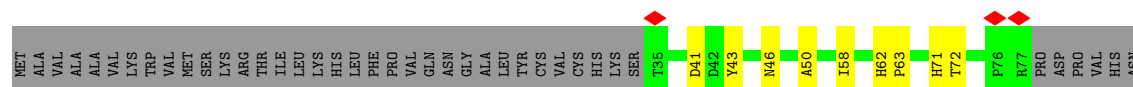
- Molecule 33: Large ribosomal subunit protein mL40



- Molecule 34: Large ribosomal subunit protein mL41

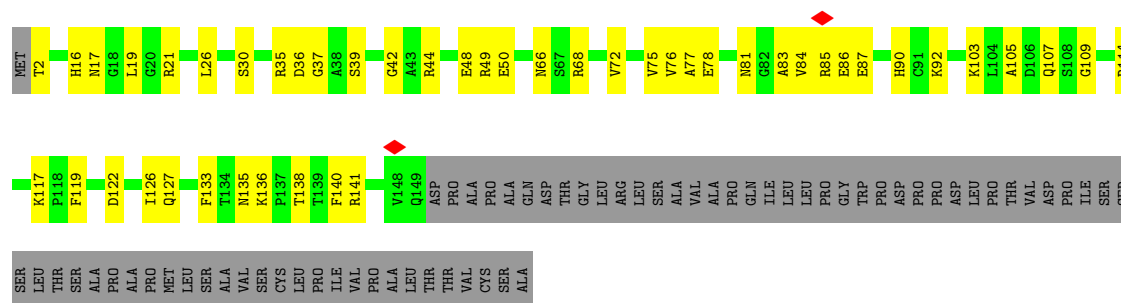


- Molecule 35: Large ribosomal subunit protein mL42

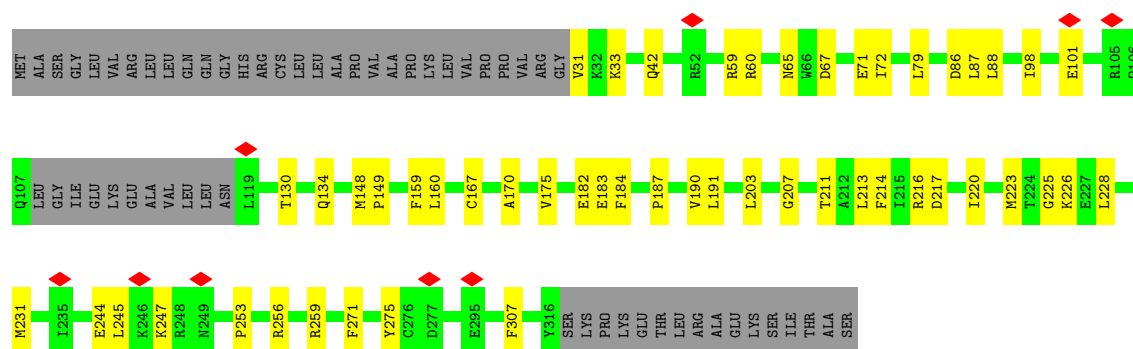


- Molecule 36: Large ribosomal subunit protein mL43

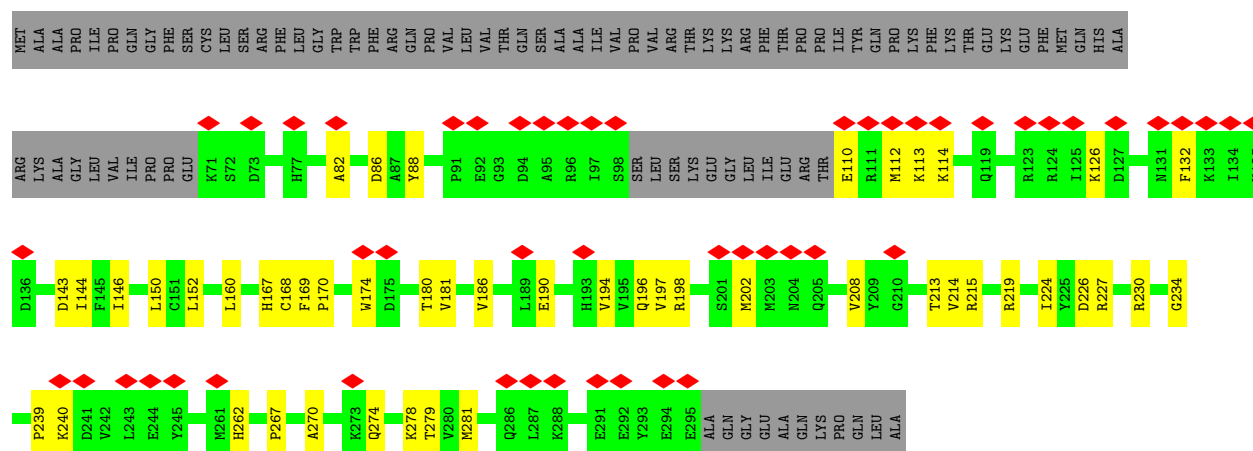




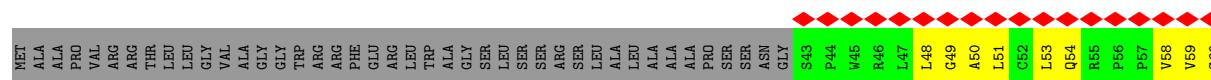
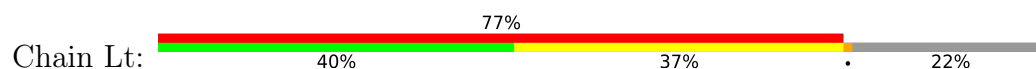
• Molecule 37: Large ribosomal subunit protein mL44



• Molecule 38: Large ribosomal subunit protein mL45

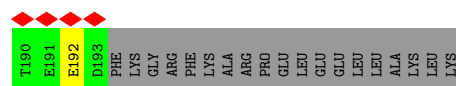
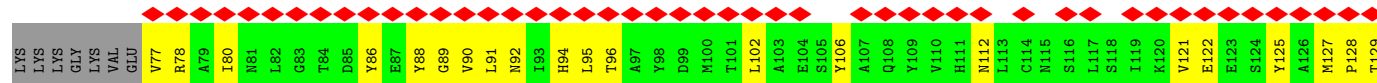
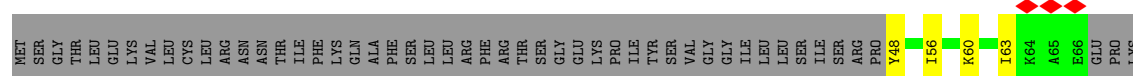


• Molecule 39: Large ribosomal subunit protein mL46

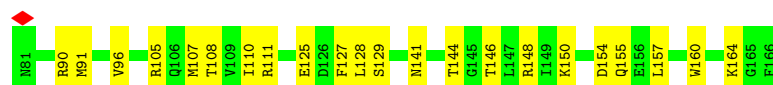
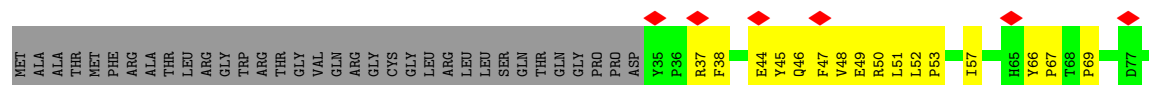




• Molecule 40: Large ribosomal subunit protein mL48

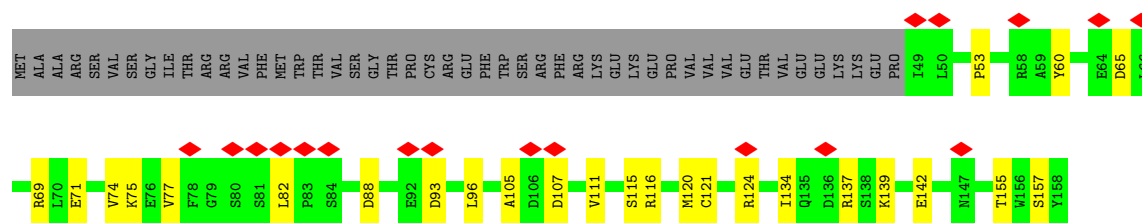


• Molecule 41: Large ribosomal subunit protein mL49

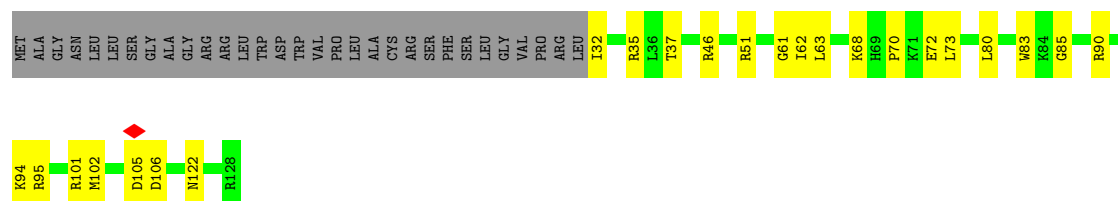


• Molecule 42: Large ribosomal subunit protein mL50

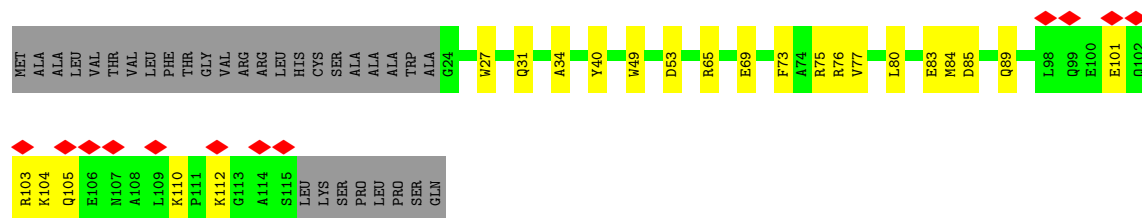




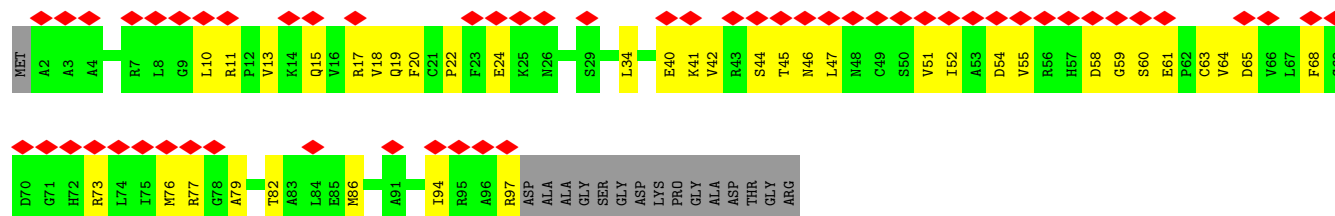
- Molecule 43: Large ribosomal subunit protein mL51



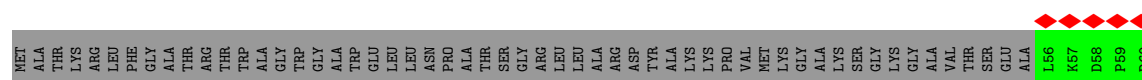
- Molecule 44: 39S ribosomal protein L52, mitochondrial

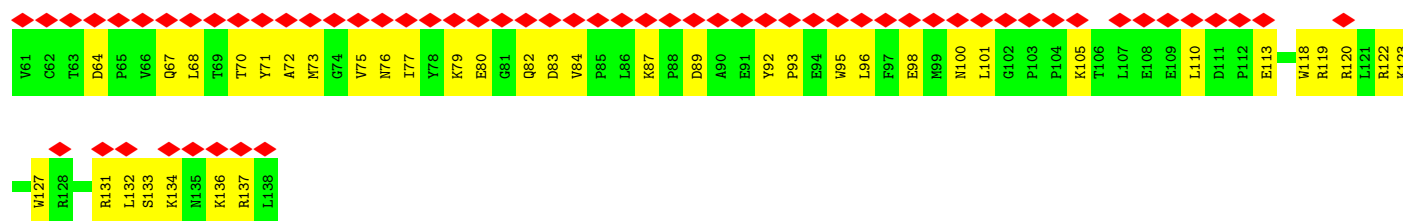


- Molecule 45: Large ribosomal subunit protein mL53

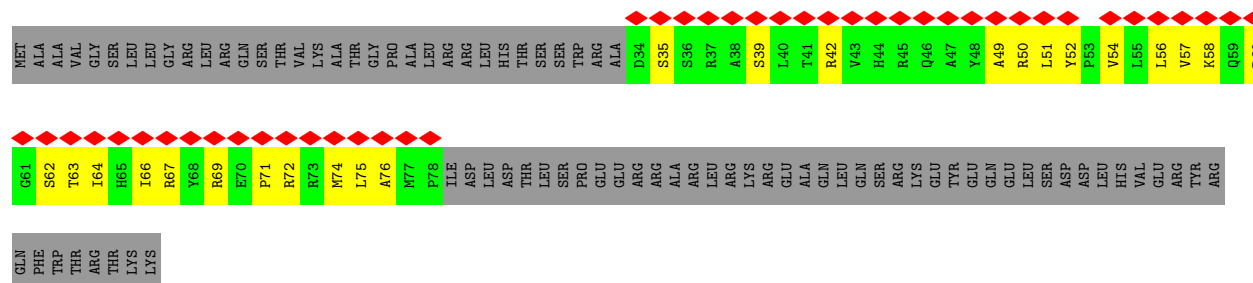


- Molecule 46: Large ribosomal subunit protein mL54

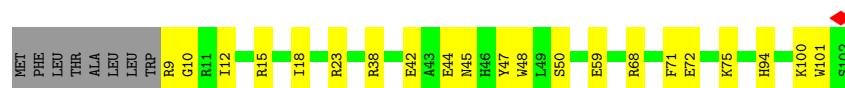




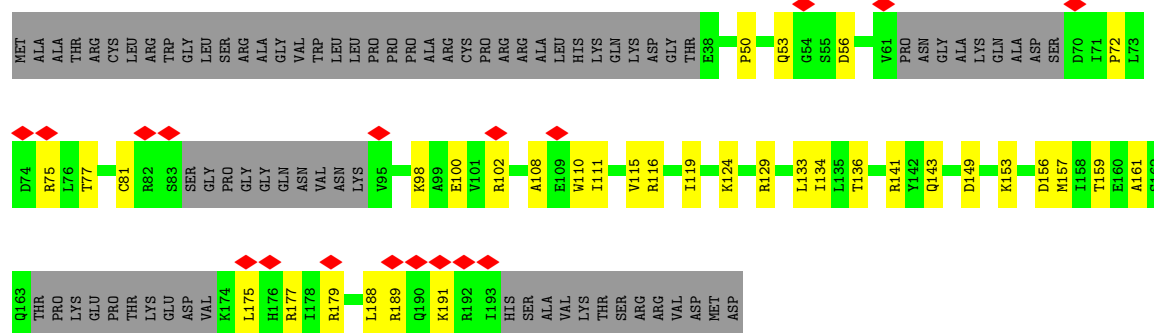
- Molecule 47: Large ribosomal subunit protein mL55



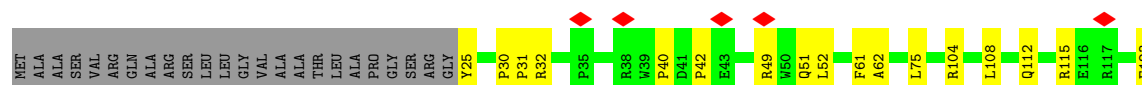
- Molecule 48: Large ribosomal subunit protein mL63



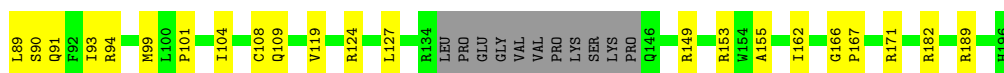
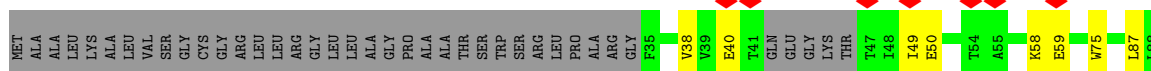
- Molecule 49: Large ribosomal subunit protein mL62



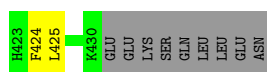
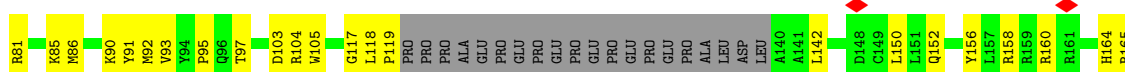
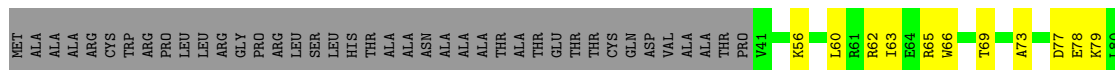
- Molecule 50: Large ribosomal subunit protein mL64



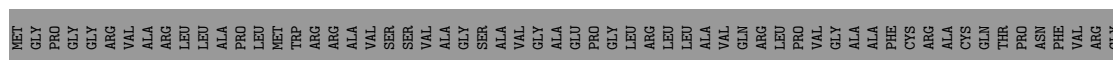
- Molecule 51: Large ribosomal subunit protein mL66

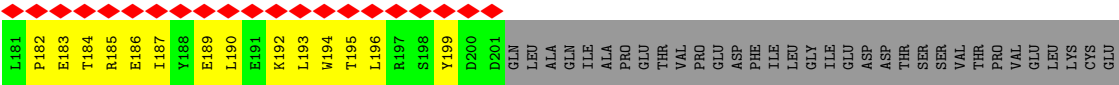


- Molecule 52: Large ribosomal subunit protein mL65

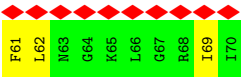
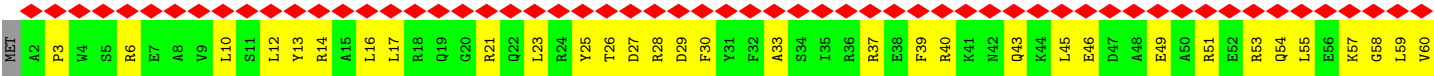


- Molecule 53: Mitochondrial assembly of ribosomal large subunit protein 1

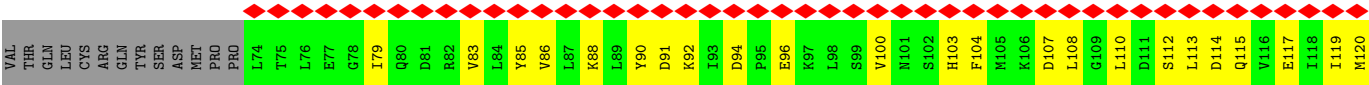
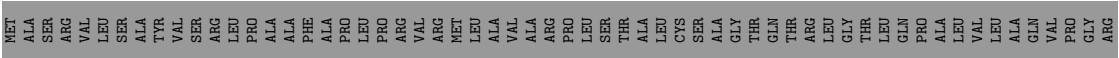
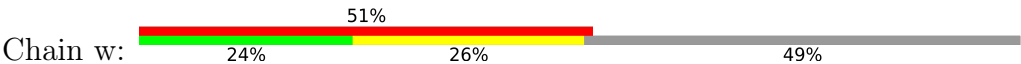




• Molecule 54: Mitochondrial ribosome and complex I assembly factor AltMIEF1



• Molecule 55: Acyl carrier protein, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12156	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	499.80002, 499.80002, 499.80002	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, T1C, ZN, PNS

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	L1	0.25	0/35628	0.36	1/55448 (0.0%)
2	L2	0.15	0/1328	0.28	0/2056
3	LB	0.23	0/1888	0.42	0/2538
4	LC	0.32	0/2462	0.57	0/3340
5	LD	0.27	0/2071	0.43	0/2817
6	LI	0.26	0/798	0.52	0/1073
7	LJ	0.26	0/1308	0.57	0/1761
8	LK	0.18	0/1348	0.41	0/1813
9	LM	0.28	0/1495	0.45	0/2029
10	LN	0.40	0/904	0.70	1/1218 (0.1%)
11	LO	0.26	0/2359	0.42	0/3185
12	LP	0.23	0/1826	0.41	0/2458
13	LQ	0.26	0/1269	0.46	0/1708
14	LR	0.35	0/1215	0.54	0/1645
15	LS	0.28	0/1863	0.47	0/2509
16	LT	0.39	0/1174	0.66	0/1572
17	LU	0.27	0/1311	0.47	0/1778
18	LV	0.27	0/1402	0.43	0/1886
19	LW	0.36	0/1217	0.54	0/1644
20	LX	0.28	0/1697	0.46	0/2302
21	La	0.29	0/893	0.41	0/1204
22	Lb	0.24	0/2090	0.41	0/2825
23	Lu	0.25	0/1552	0.44	2/2079 (0.1%)
24	Ld	0.27	0/1003	0.44	0/1354
25	Lf	0.33	0/895	0.48	0/1201
26	Lg	0.25	0/438	0.40	0/583
27	Lh	0.28	0/382	0.37	0/507
28	Li	0.28	0/852	0.42	0/1136
29	Lj	0.21	0/349	0.33	0/461
30	Lk	0.25	0/3305	0.41	0/4502
31	Ll	0.24	0/3042	0.48	0/4140
32	Lm	0.22	0/2439	0.41	0/3299

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ln	0.25	0/855	0.56	0/1152
34	Lo	0.25	0/1025	0.45	0/1379
35	Lp	0.24	0/839	0.45	0/1136
36	Lq	0.26	0/1202	0.43	0/1626
37	Lr	0.25	0/2264	0.43	0/3059
38	Ls	0.20	0/1800	0.40	0/2436
39	Lt	0.20	0/1797	0.54	0/2422
40	Lv	0.23	0/1055	0.47	0/1427
41	Lw	0.38	0/1134	0.66	1/1547 (0.1%)
42	Lx	0.23	0/918	0.37	0/1249
43	Ly	0.32	0/849	0.46	0/1135
44	Lz	0.26	0/747	0.44	0/1005
45	L3	0.22	0/754	0.48	0/1017
46	L4	0.23	0/722	0.56	0/978
47	L5	0.20	0/379	0.52	0/510
48	L6	0.28	0/818	0.43	0/1097
49	L7	0.22	0/1071	0.40	0/1433
50	L8	0.21	0/1107	0.40	0/1498
51	SR	0.37	0/1238	0.61	0/1676
52	Sf	0.26	0/3114	0.42	0/4225
53	u	0.29	0/949	0.61	0/1281
54	v	0.33	0/597	0.65	0/796
55	w	0.20	0/647	0.52	0/871
All	All	0.26	0/107684	0.43	5/153026 (0.0%)

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
13	LQ	0	1
31	Ll	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	LN	129	LYS	N-CA-C	-7.34	103.28	111.28
23	Lu	127	PRO	CA-C-N	-6.30	116.73	122.28
23	Lu	127	PRO	C-N-CA	-6.30	116.73	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L1	840	U	C4'-C3'-O3'	-6.00	104.00	113.00
41	Lw	67	PRO	N-CA-C	-5.32	101.52	112.47

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	LQ	110	ILE	Peptide
31	Ll	288	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L1	31847	0	16179	562	0
2	L2	1191	0	607	41	0
3	LB	1851	0	1909	32	0
4	LC	2393	0	2398	57	0
5	LD	2013	0	2044	52	0
6	LI	784	0	832	32	0
7	LJ	1283	0	1370	53	0
8	LK	1330	0	1407	58	0
9	LM	1451	0	1448	30	0
10	LN	889	0	941	31	0
11	LO	2305	0	2378	64	0
12	LP	1779	0	1808	37	0
13	LQ	1245	0	1283	40	0
14	LR	1189	0	1180	50	0
15	LS	1822	0	1859	42	0
16	LT	1153	0	1214	17	0
17	LU	1284	0	1354	44	0
18	LV	1368	0	1410	35	0
19	LW	1188	0	1180	46	0
20	LX	1652	0	1658	57	0
21	La	871	0	898	21	0
22	Lb	2035	0	2054	44	0
23	Lu	1517	0	1561	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Ld	978	0	1030	28	0
25	Lf	880	0	902	16	0
26	Lg	433	0	475	22	0
27	Lh	376	0	406	14	0
28	Li	831	0	883	22	0
29	Lj	341	0	361	8	0
30	Lk	3210	0	3206	83	0
31	Ll	2947	0	2841	108	0
32	Lm	2382	0	2393	57	0
33	Ln	836	0	844	70	0
34	Lo	997	0	987	22	0
35	Lp	815	0	792	24	0
36	Lq	1178	0	1180	48	0
37	Lr	2217	0	2220	37	0
38	Ls	1754	0	1732	39	0
39	Lt	1762	0	1767	94	0
40	Lv	1039	0	1044	65	0
41	Lw	1097	0	1085	37	0
42	Lx	895	0	881	25	0
43	Ly	827	0	857	18	0
44	Lz	732	0	730	17	0
45	L3	743	0	758	37	0
46	L4	703	0	693	44	0
47	L5	372	0	387	31	0
48	L6	797	0	804	21	0
49	L7	1058	0	1083	31	0
50	L8	1076	0	1049	26	0
51	SR	1203	0	1219	29	0
52	Sf	3036	0	3022	82	0
53	u	927	0	921	69	0
54	v	588	0	604	45	0
55	w	638	0	637	38	0
56	L1	93	0	0	0	0
56	LB	1	0	0	0	0
56	Lw	1	0	0	0	0
57	L1	42	0	38	1	0
58	Lf	1	0	0	0	0
58	Lj	1	0	0	0	0
58	SR	1	0	0	0	0
59	v	21	0	21	3	0
All	All	102269	0	86824	2316	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 12.

The worst 5 of 2316 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)
36:Lq:75:VAL:O	36:Lq:86:GLU:HA	1.38	1.19
9:LM:81:THR:O	9:LM:86:GLY:HA3	1.51	1.09
29:Lj:76:CYS:SG	29:Lj:98:HIS:CE1	2.45	1.09
35:Lp:71:HIS:HD1	36:Lq:138:THR:HG1	0.99	0.95
31:Ll:214:TRP:HB2	31:Ll:240:ILE:HB	1.51	0.91

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LB	235/305 (77%)	228 (97%)	7 (3%)	0	100	100
4	LC	302/348 (87%)	279 (92%)	23 (8%)	0	100	100
5	LD	248/311 (80%)	233 (94%)	15 (6%)	0	100	100
6	LI	93/267 (35%)	87 (94%)	6 (6%)	0	100	100
7	LJ	154/261 (59%)	134 (87%)	20 (13%)	0	100	100
8	LK	173/192 (90%)	165 (95%)	8 (5%)	0	100	100
9	LM	175/178 (98%)	164 (94%)	11 (6%)	0	100	100
10	LN	113/145 (78%)	106 (94%)	6 (5%)	1 (1%)	14	42
11	LO	285/296 (96%)	275 (96%)	10 (4%)	0	100	100
12	LP	219/251 (87%)	214 (98%)	5 (2%)	0	100	100
13	LQ	150/175 (86%)	142 (95%)	7 (5%)	1 (1%)	18	47
14	LR	144/179 (80%)	138 (96%)	6 (4%)	0	100	100
15	LS	217/292 (74%)	198 (91%)	19 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	LT	138/149 (93%)	134 (97%)	4 (3%)	0	100	100
17	LU	158/205 (77%)	151 (96%)	7 (4%)	0	100	100
18	LV	164/212 (77%)	151 (92%)	13 (8%)	0	100	100
19	LW	139/153 (91%)	137 (99%)	2 (1%)	0	100	100
20	LX	200/216 (93%)	182 (91%)	17 (8%)	1 (0%)	24	54
21	La	109/148 (74%)	103 (94%)	5 (5%)	1 (1%)	14	42
22	Lb	241/256 (94%)	233 (97%)	8 (3%)	0	100	100
23	Lu	174/250 (70%)	169 (97%)	5 (3%)	0	100	100
24	Ld	118/161 (73%)	116 (98%)	2 (2%)	0	100	100
25	Lf	106/188 (56%)	101 (95%)	5 (5%)	0	100	100
26	Lg	50/65 (77%)	50 (100%)	0	0	100	100
27	Lh	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
28	Li	93/188 (50%)	89 (96%)	4 (4%)	0	100	100
29	Lj	36/103 (35%)	36 (100%)	0	0	100	100
30	Lk	392/423 (93%)	383 (98%)	9 (2%)	0	100	100
31	Ll	352/380 (93%)	321 (91%)	31 (9%)	0	100	100
32	Lm	291/338 (86%)	280 (96%)	11 (4%)	0	100	100
33	Ln	97/206 (47%)	84 (87%)	13 (13%)	0	100	100
34	Lo	122/137 (89%)	116 (95%)	6 (5%)	0	100	100
35	Lp	93/142 (66%)	88 (95%)	5 (5%)	0	100	100
36	Lq	146/215 (68%)	133 (91%)	13 (9%)	0	100	100
37	Lr	271/332 (82%)	264 (97%)	7 (3%)	0	100	100
38	Ls	210/306 (69%)	204 (97%)	6 (3%)	0	100	100
39	Lt	211/279 (76%)	189 (90%)	20 (10%)	2 (1%)	14	42
40	Lv	125/212 (59%)	121 (97%)	4 (3%)	0	100	100
41	Lw	130/166 (78%)	119 (92%)	10 (8%)	1 (1%)	16	44
42	Lx	108/158 (68%)	105 (97%)	3 (3%)	0	100	100
43	Ly	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
44	Lz	90/123 (73%)	85 (94%)	5 (6%)	0	100	100
45	L3	94/112 (84%)	89 (95%)	5 (5%)	0	100	100
46	L4	81/138 (59%)	74 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	L5	43/128 (34%)	40 (93%)	3 (7%)	0	100	100
48	L6	92/102 (90%)	90 (98%)	2 (2%)	0	100	100
49	L7	119/206 (58%)	112 (94%)	7 (6%)	0	100	100
50	L8	126/222 (57%)	124 (98%)	2 (2%)	0	100	100
51	SR	140/196 (71%)	136 (97%)	4 (3%)	0	100	100
52	Sf	366/439 (83%)	350 (96%)	15 (4%)	1 (0%)	36	65
53	u	109/234 (47%)	103 (94%)	4 (4%)	2 (2%)	6	26
54	v	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
55	w	77/156 (49%)	71 (92%)	6 (8%)	0	100	100
All	All	8325/11134 (75%)	7894 (95%)	421 (5%)	10 (0%)	49	78

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	Lt	266	PRO
39	Lt	270	ALA
10	LN	132	GLY
52	Sf	260	GLU
53	u	120	TYR

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	
3	LB	191/245 (78%)	191 (100%)	0	100	100
4	LC	258/290 (89%)	253 (98%)	5 (2%)	50	66
5	LD	217/262 (83%)	217 (100%)	0	100	100
6	LI	86/228 (38%)	86 (100%)	0	100	100
7	LJ	145/232 (62%)	145 (100%)	0	100	100
8	LK	138/150 (92%)	138 (100%)	0	100	100
9	LM	155/156 (99%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	LN	98/124 (79%)	94 (96%)	4 (4%)	27	52
11	LO	245/249 (98%)	245 (100%)	0	100	100
12	LP	188/211 (89%)	188 (100%)	0	100	100
13	LQ	133/150 (89%)	133 (100%)	0	100	100
14	LR	128/154 (83%)	127 (99%)	1 (1%)	73	77
15	LS	201/256 (78%)	201 (100%)	0	100	100
16	LT	118/126 (94%)	115 (98%)	3 (2%)	42	62
17	LU	145/180 (81%)	143 (99%)	2 (1%)	59	70
18	LV	146/182 (80%)	146 (100%)	0	100	100
19	LW	128/135 (95%)	126 (98%)	2 (2%)	55	68
20	LX	180/191 (94%)	177 (98%)	3 (2%)	53	67
21	La	91/119 (76%)	90 (99%)	1 (1%)	65	74
22	Lb	219/229 (96%)	219 (100%)	0	100	100
23	Lu	159/223 (71%)	159 (100%)	0	100	100
24	Ld	111/147 (76%)	111 (100%)	0	100	100
25	Lf	97/164 (59%)	97 (100%)	0	100	100
26	Lg	49/60 (82%)	49 (100%)	0	100	100
27	Lh	40/72 (56%)	40 (100%)	0	100	100
28	Li	88/166 (53%)	88 (100%)	0	100	100
29	Lj	37/89 (42%)	37 (100%)	0	100	100
30	Lk	353/368 (96%)	353 (100%)	0	100	100
31	Ll	313/332 (94%)	313 (100%)	0	100	100
32	Lm	269/303 (89%)	268 (100%)	1 (0%)	84	83
33	Ln	91/190 (48%)	91 (100%)	0	100	100
34	Lo	104/112 (93%)	104 (100%)	0	100	100
35	Lp	93/133 (70%)	93 (100%)	0	100	100
36	Lq	130/186 (70%)	130 (100%)	0	100	100
37	Lr	241/288 (84%)	240 (100%)	1 (0%)	84	83
38	Ls	196/274 (72%)	196 (100%)	0	100	100
39	Lt	188/236 (80%)	188 (100%)	0	100	100
40	Lv	117/188 (62%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	Lw	122/148 (82%)	121 (99%)	1 (1%)	73	77
42	Lx	104/148 (70%)	104 (100%)	0	100	100
43	Ly	86/110 (78%)	83 (96%)	3 (4%)	32	56
44	Lz	73/97 (75%)	73 (100%)	0	100	100
45	L3	81/90 (90%)	81 (100%)	0	100	100
46	L4	78/116 (67%)	78 (100%)	0	100	100
47	L5	40/113 (35%)	40 (100%)	0	100	100
48	L6	80/87 (92%)	80 (100%)	0	100	100
49	L7	117/181 (65%)	117 (100%)	0	100	100
50	L8	110/178 (62%)	110 (100%)	0	100	100
51	SR	133/169 (79%)	133 (100%)	0	100	100
52	Sf	326/381 (86%)	325 (100%)	1 (0%)	86	84
53	u	105/200 (52%)	102 (97%)	3 (3%)	37	60
54	v	59/60 (98%)	59 (100%)	0	100	100
55	w	73/136 (54%)	73 (100%)	0	100	100
All	All	7473/9614 (78%)	7442 (100%)	31 (0%)	81	83

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	LU	118	ASN
52	Sf	408	ASN
20	LX	209	LYS
53	u	119	ARG
43	Ly	32	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
45	L3	35	GLN
53	u	178	HIS
49	L7	104	HIS
52	Sf	107	GLN
23	Lu	189	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1491/1559 (95%)	364 (24%)	19 (1%)
2	L2	51/69 (73%)	16 (31%)	0
All	All	1542/1628 (94%)	380 (24%)	19 (1%)

5 of 380 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	5	A
1	L1	6	A
1	L1	8	C
1	L1	9	U
1	L1	11	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	930	A
1	L1	1371	U
1	L1	1536	C
1	L1	1319	G
1	L1	551	C

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 100 ligands modelled in this entry, 98 are monoatomic - leaving 2 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	$\# Z > 2$
59	PNS	v	101	-	14,20,21	2.34	4 (28%)	18,26,29	3.01	7 (38%)
57	T1C	L1	1692	56	45,45,45	1.14	4 (8%)	56,72,72	1.04	5 (8%)

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
59	PNS	v	101	-	-	12/24/26/27	-
57	T1C	L1	1692	56	-	11/22/80/80	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	v	101	PNS	C39-N41	5.72	1.46	1.33
57	L1	1692	T1C	C21-N21	5.02	1.47	1.33
59	v	101	PNS	C34-N36	5.01	1.45	1.33
59	v	101	PNS	O40-C39	-2.78	1.17	1.23
57	L1	1692	T1C	C4-N4	2.30	1.52	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	v	101	PNS	C38-C39-N41	7.21	129.47	116.34
59	v	101	PNS	O40-C39-C38	-6.01	111.13	122.02
59	v	101	PNS	C42-N41-C39	4.24	130.72	122.82
59	v	101	PNS	C37-N36-C34	-3.92	115.51	122.55
59	v	101	PNS	C32-C34-N36	3.19	122.54	116.48

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	L1	1692	T1C	C92-C91-N9-C9
57	L1	1692	T1C	C41-C4-N4-C43
57	L1	1692	T1C	C3-C4-N4-C43
57	L1	1692	T1C	C3-C4-N4-C42

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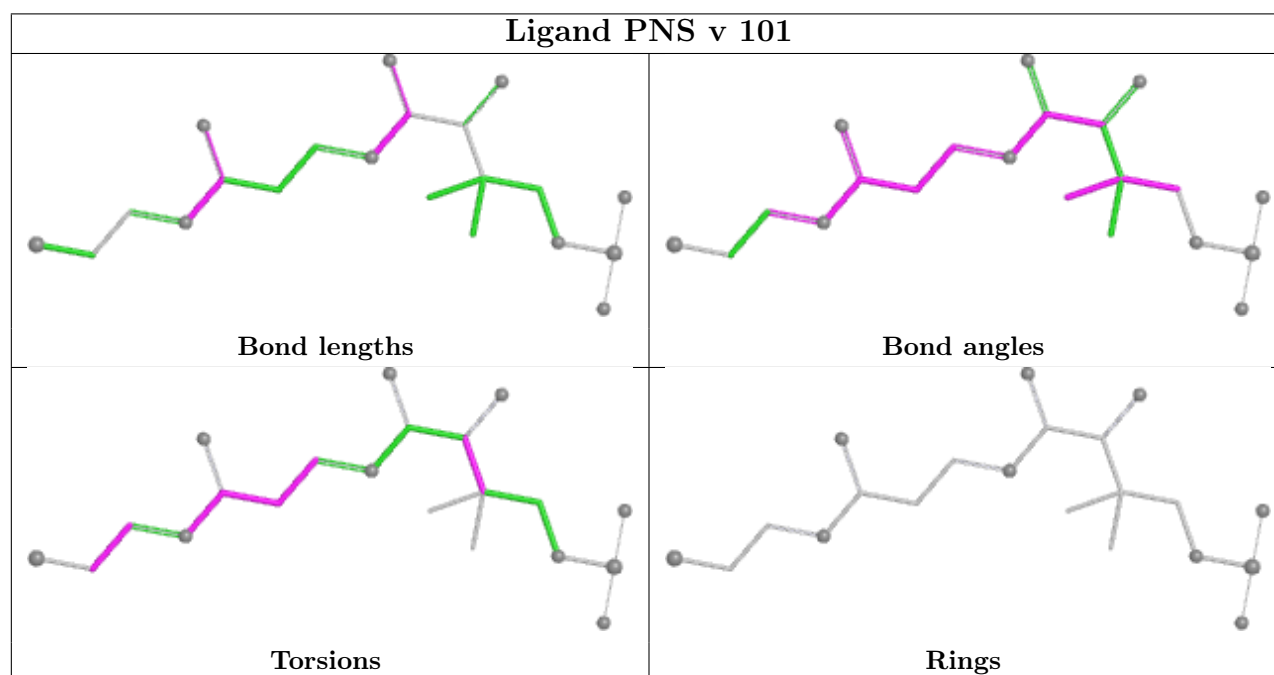
Mol	Chain	Res	Type	Atoms
57	L1	1692	T1C	C3-C2-C21-O21

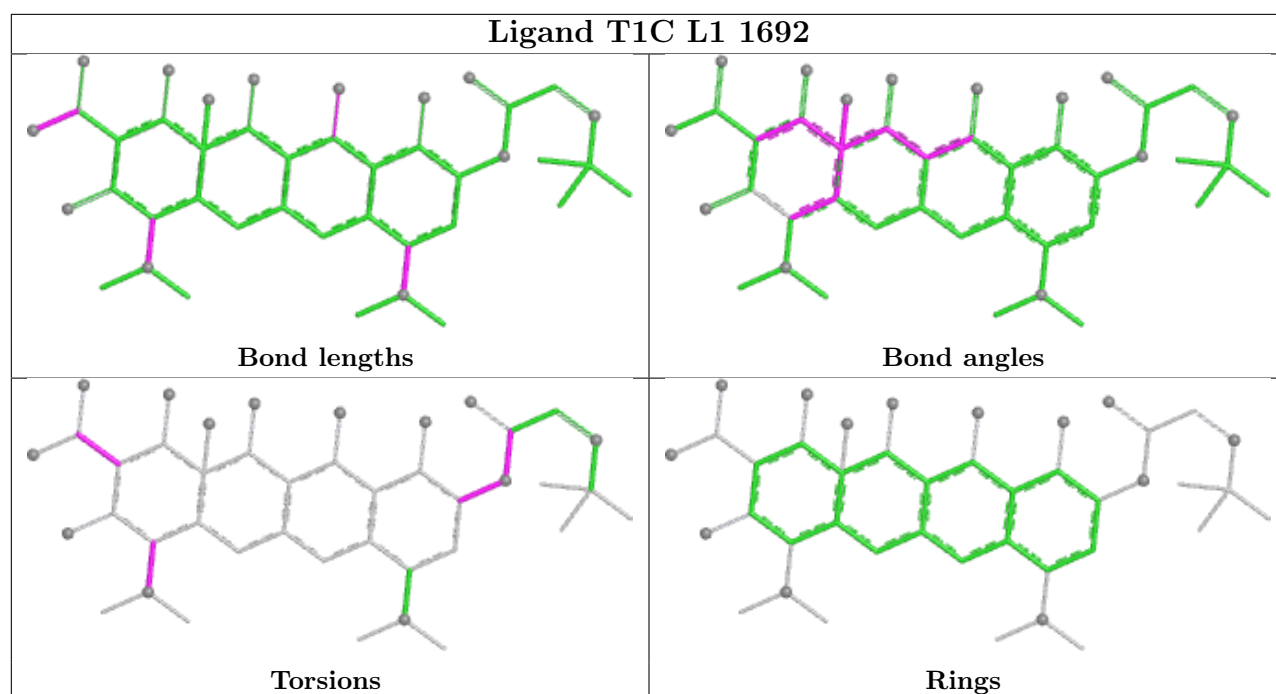
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	v	101	PNS	3	0
57	L1	1692	T1C	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

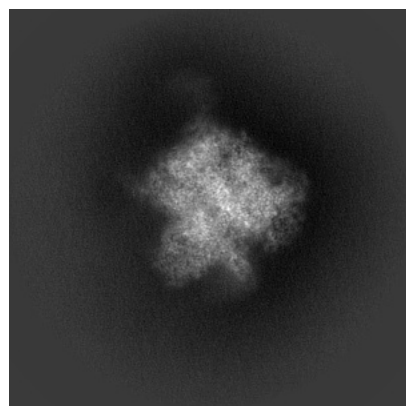
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36837. These allow visual inspection of the internal detail of the map and identification of artifacts.

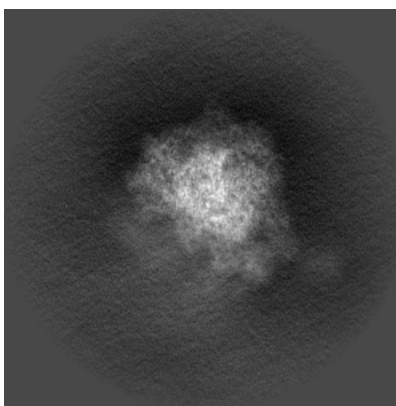
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

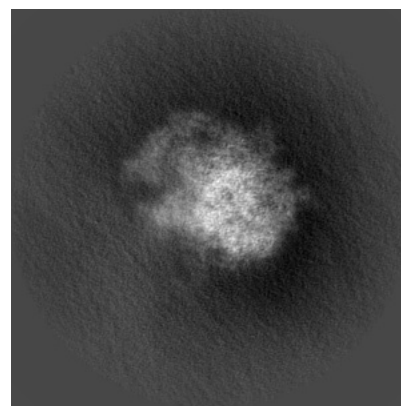
6.1.1 Primary map



X

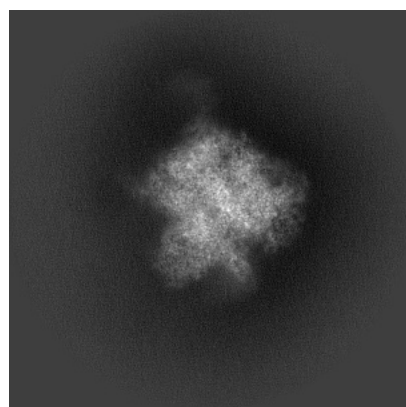


Y

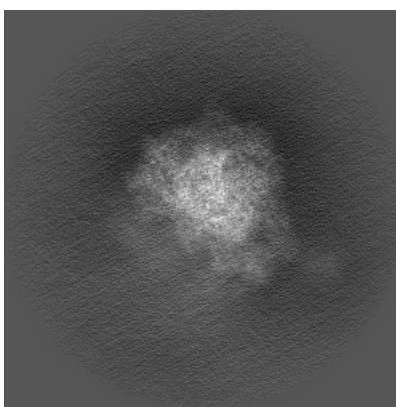


Z

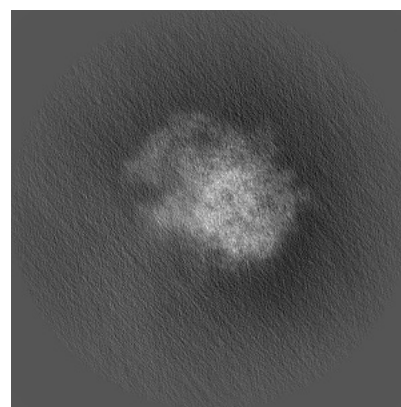
6.1.2 Raw map



X



Y

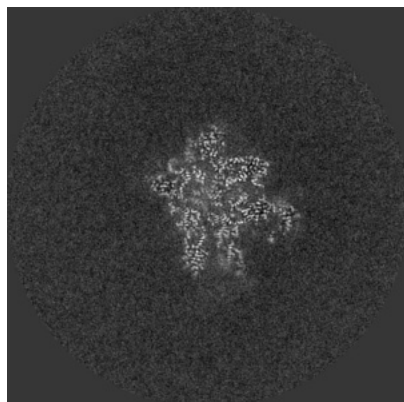


Z

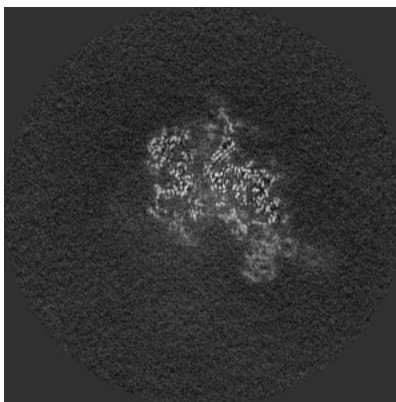
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

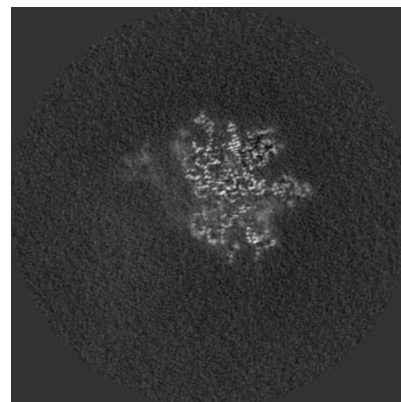
6.2.1 Primary map



X Index: 210

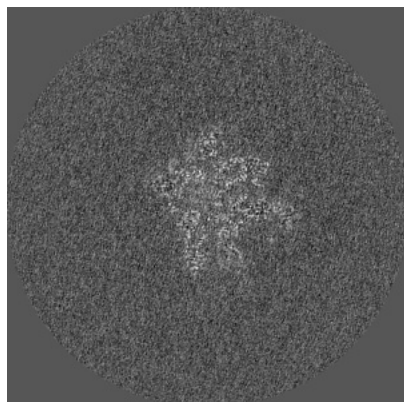


Y Index: 210

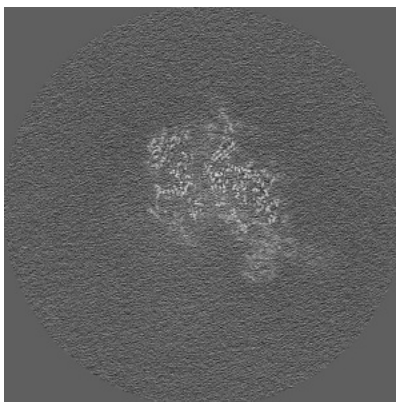


Z Index: 210

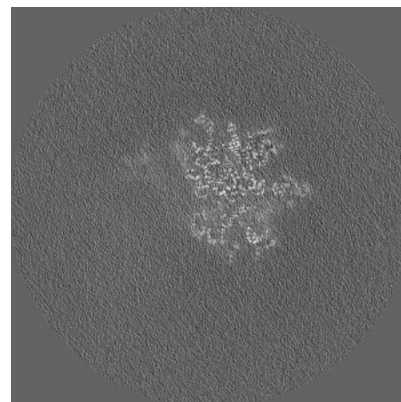
6.2.2 Raw map



X Index: 210



Y Index: 210

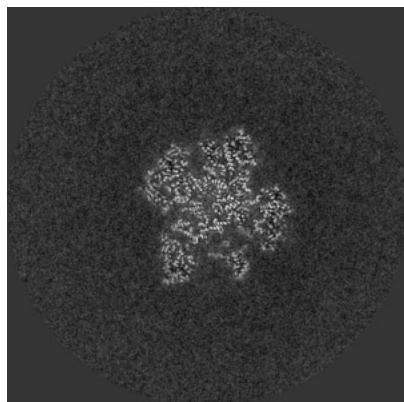


Z Index: 210

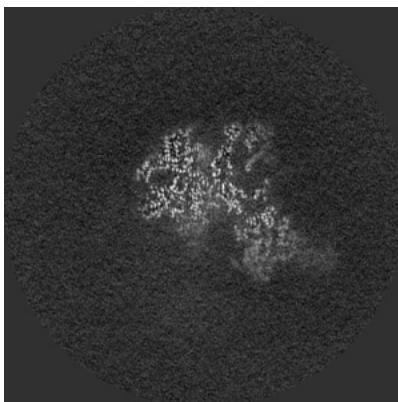
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

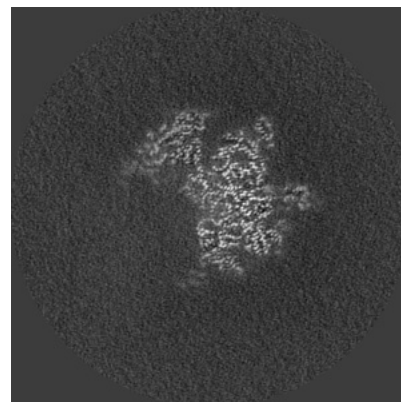
6.3.1 Primary map



X Index: 234

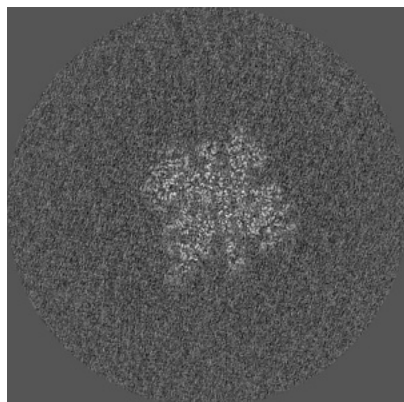


Y Index: 201

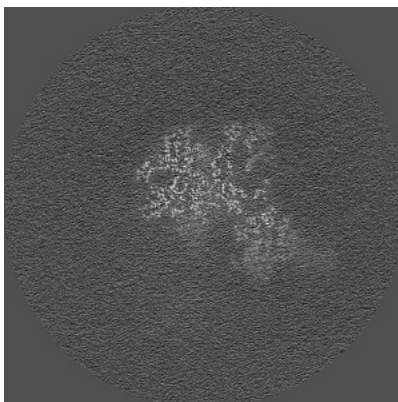


Z Index: 226

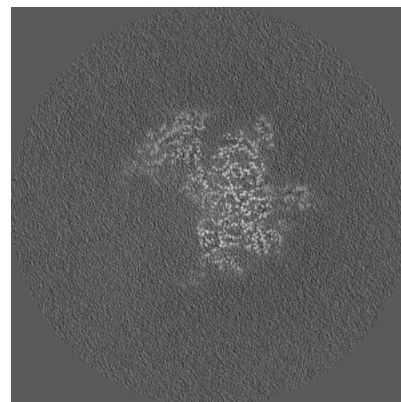
6.3.2 Raw map



X Index: 228



Y Index: 201

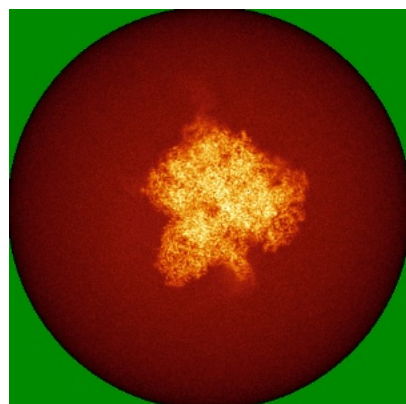


Z Index: 226

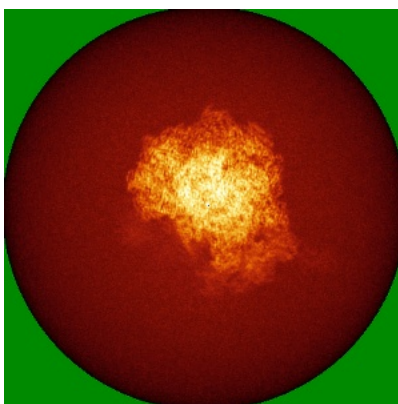
The images above show the largest variance slices of the map in three orthogonal directions.

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

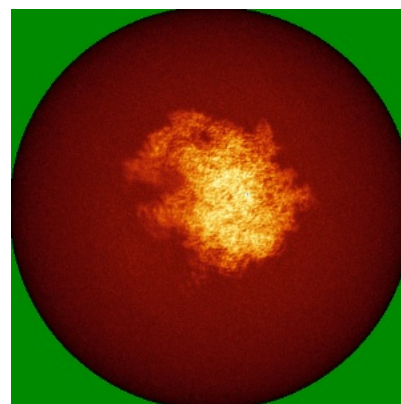
6.4.1 Primary map



X

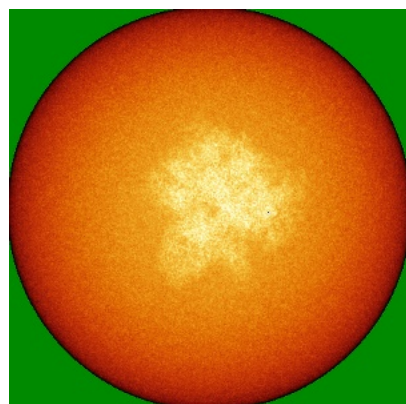


Y

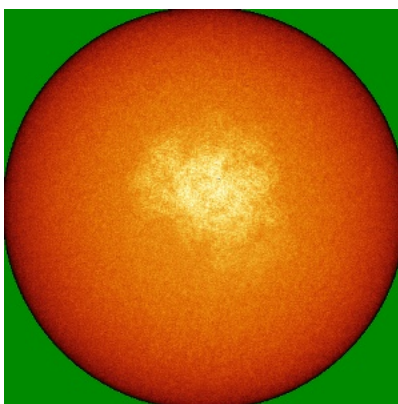


Z

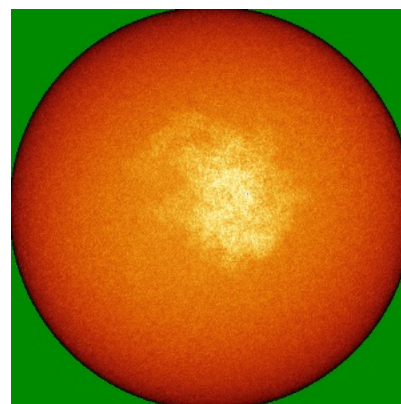
6.4.2 Raw map



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.

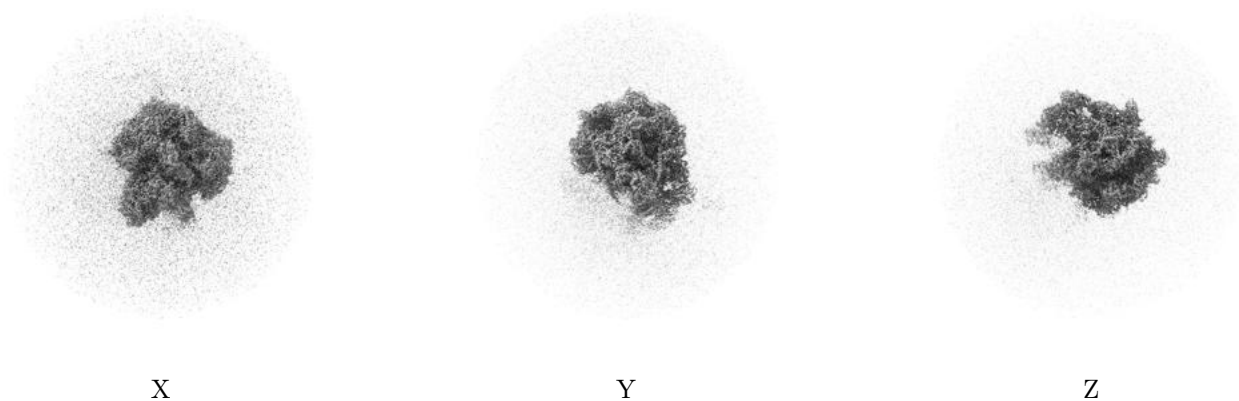
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

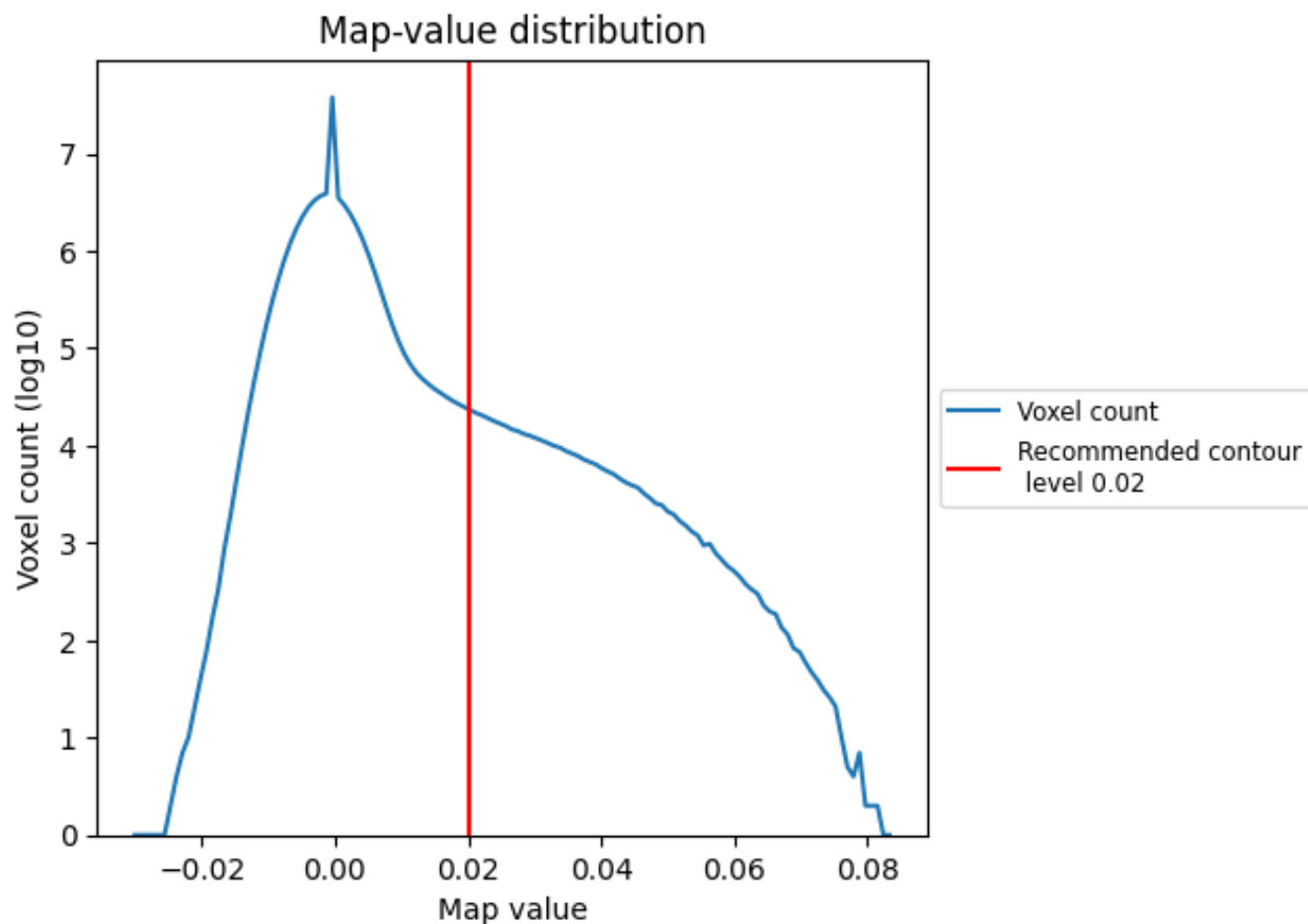
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

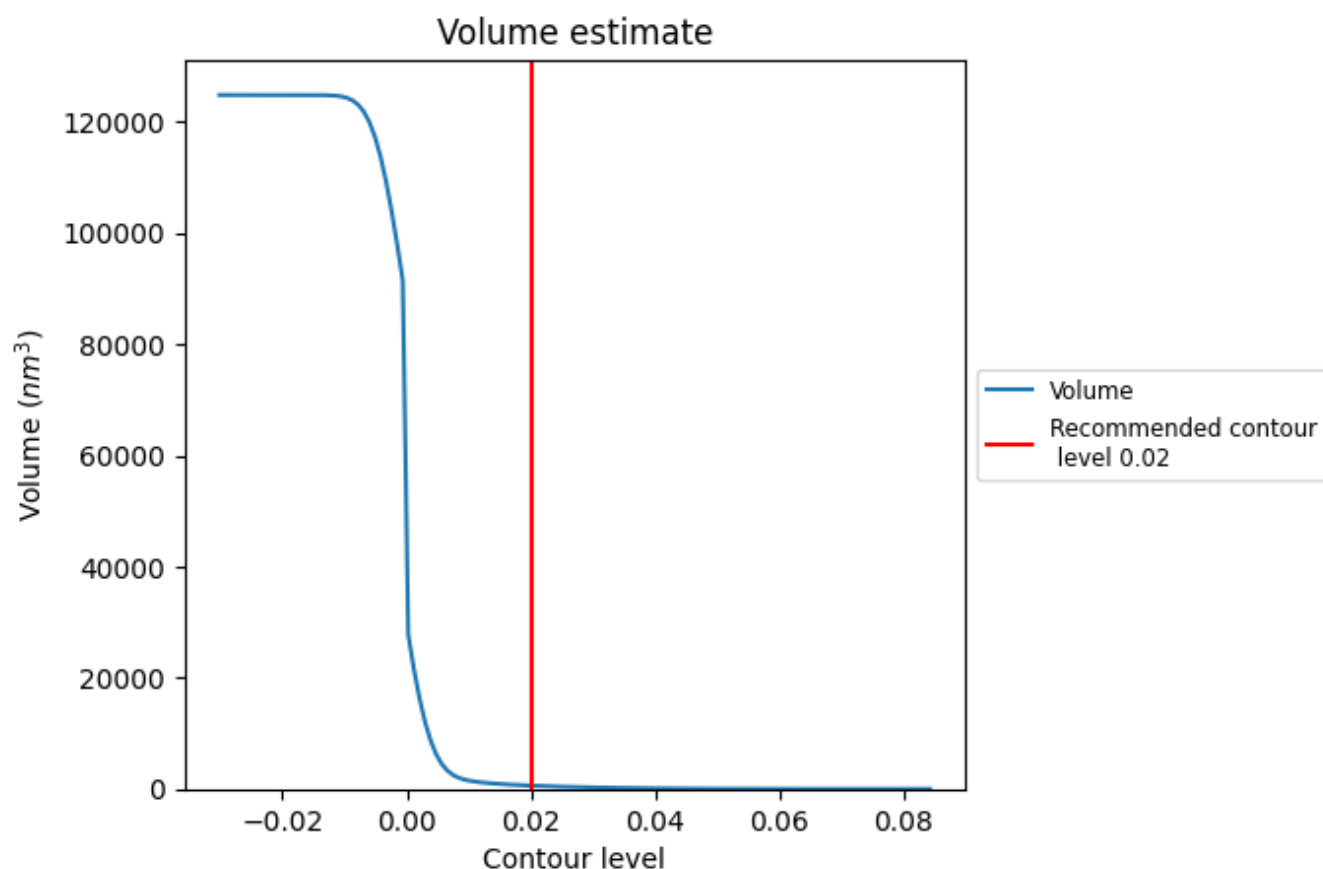
This section contains the results of statistical analysis of the map.

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.

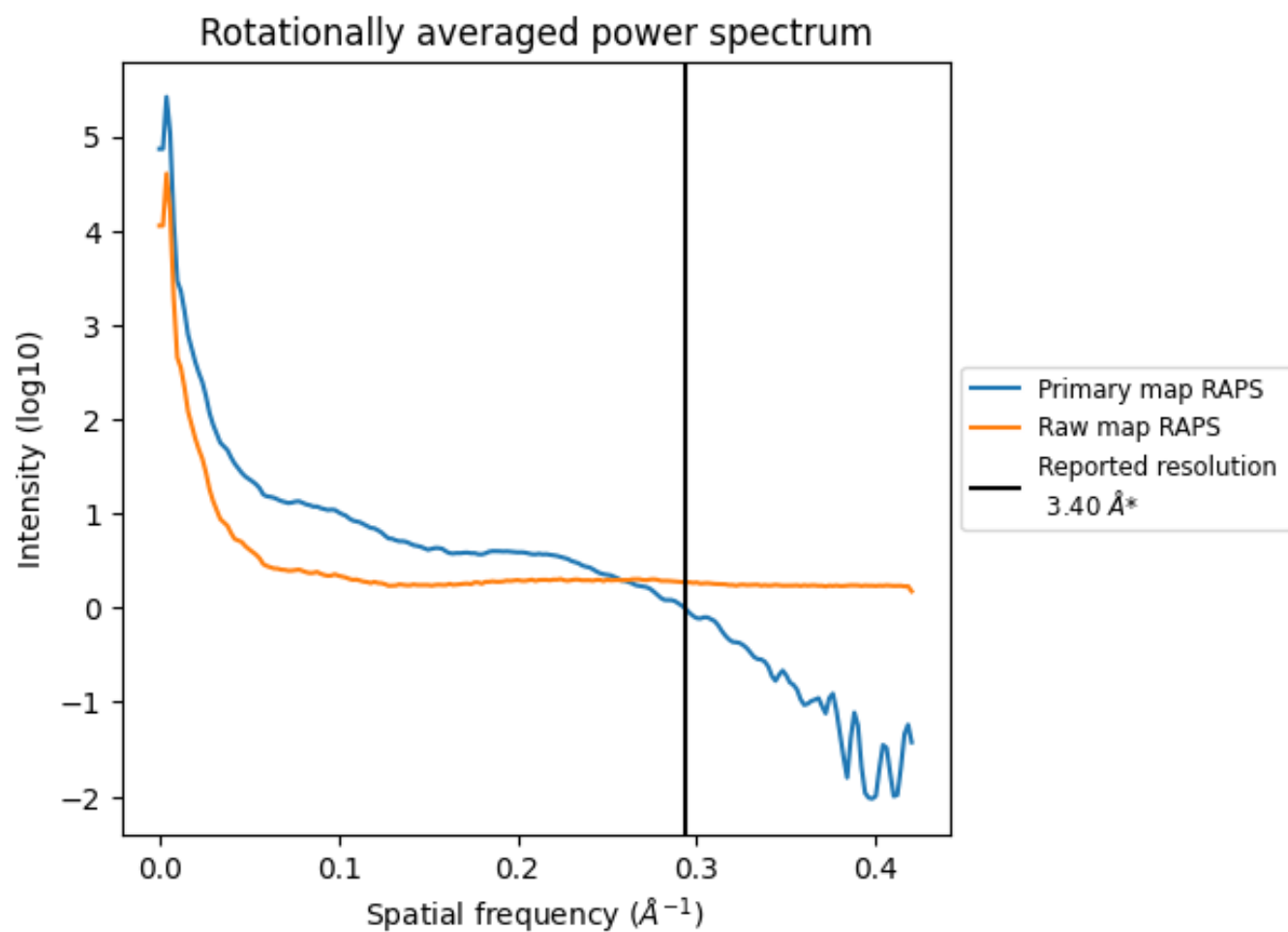
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 603 nm^3 ; this corresponds to an approximate mass of 544 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 ⓘ

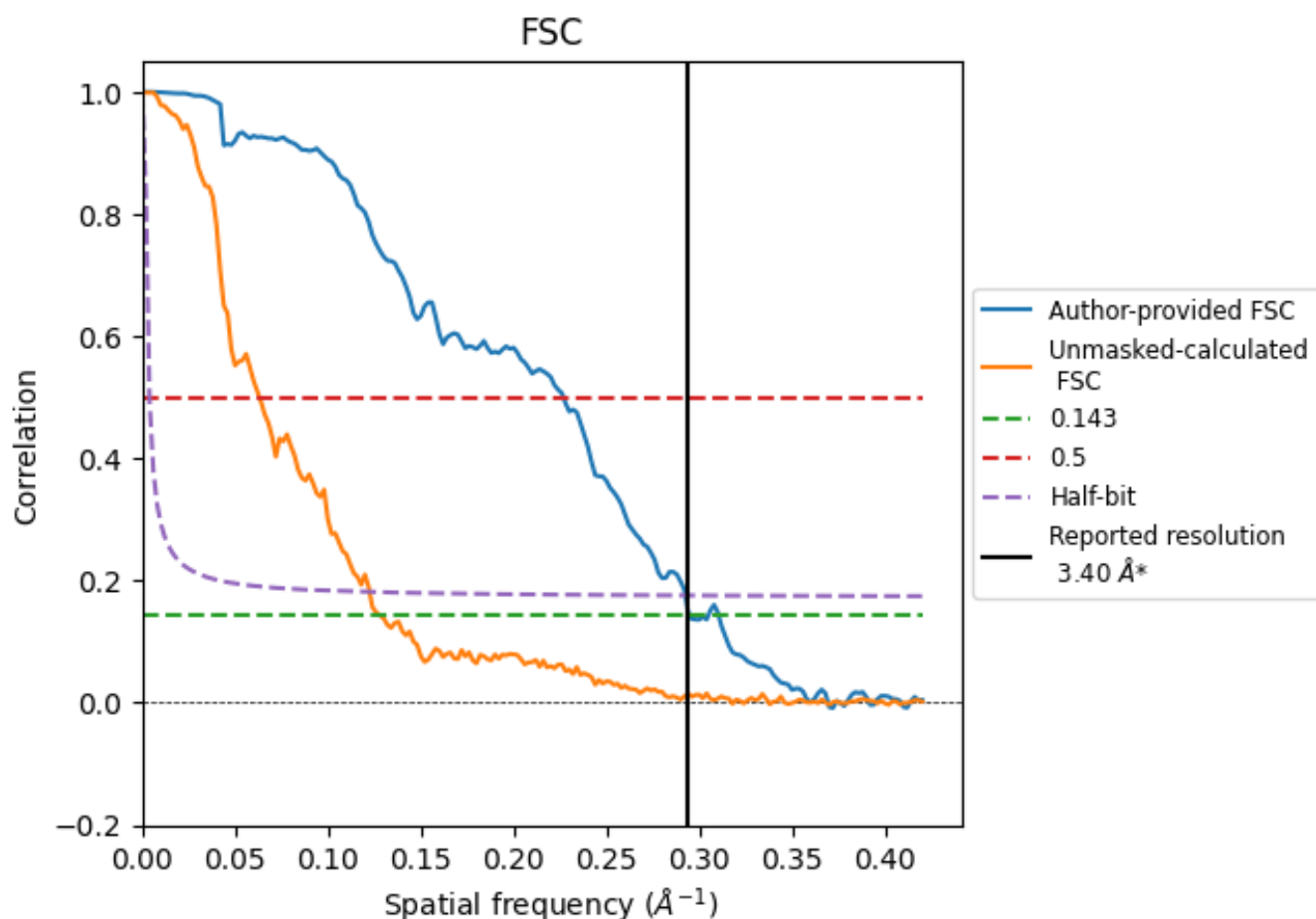


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

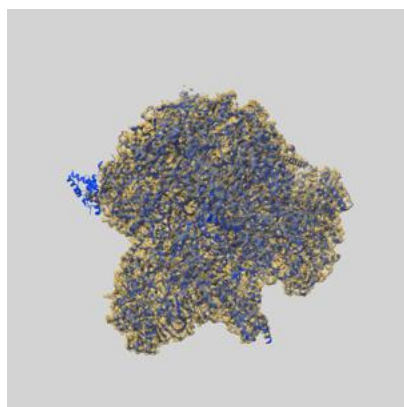
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	4.41	3.42
Unmasked-calculated*	7.81	15.82	8.16

*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 7.81 differs from the reported value 3.4 by more than 10 %

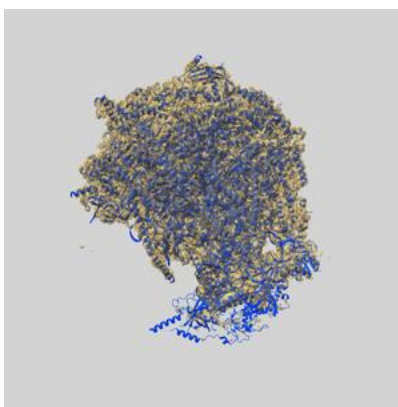
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36837 and PDB model 8K2B. Per-residue inclusion information can be found in section [3](#) on page [16](#).

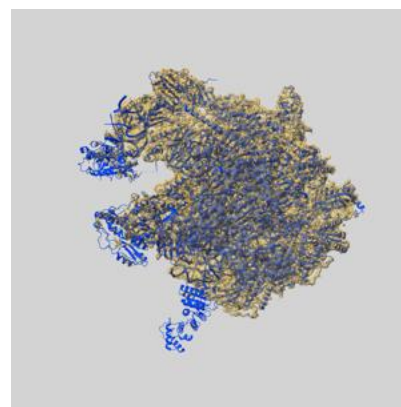
9.1 Map-model overlay [i](#)



X



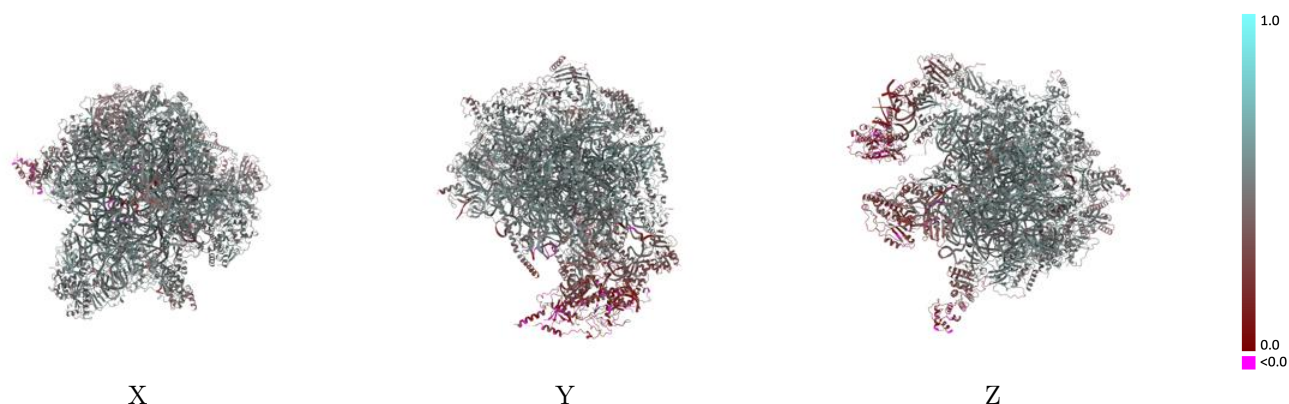
Y



Z

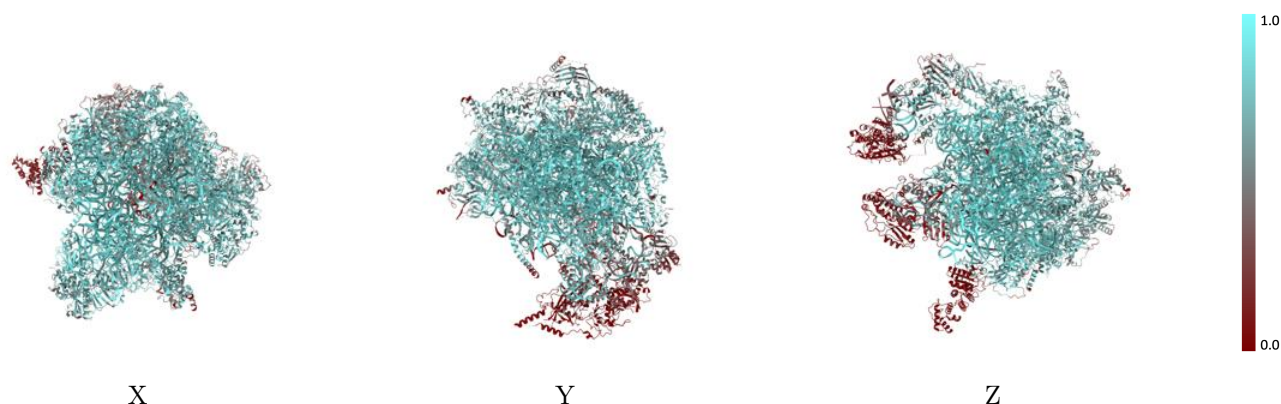
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



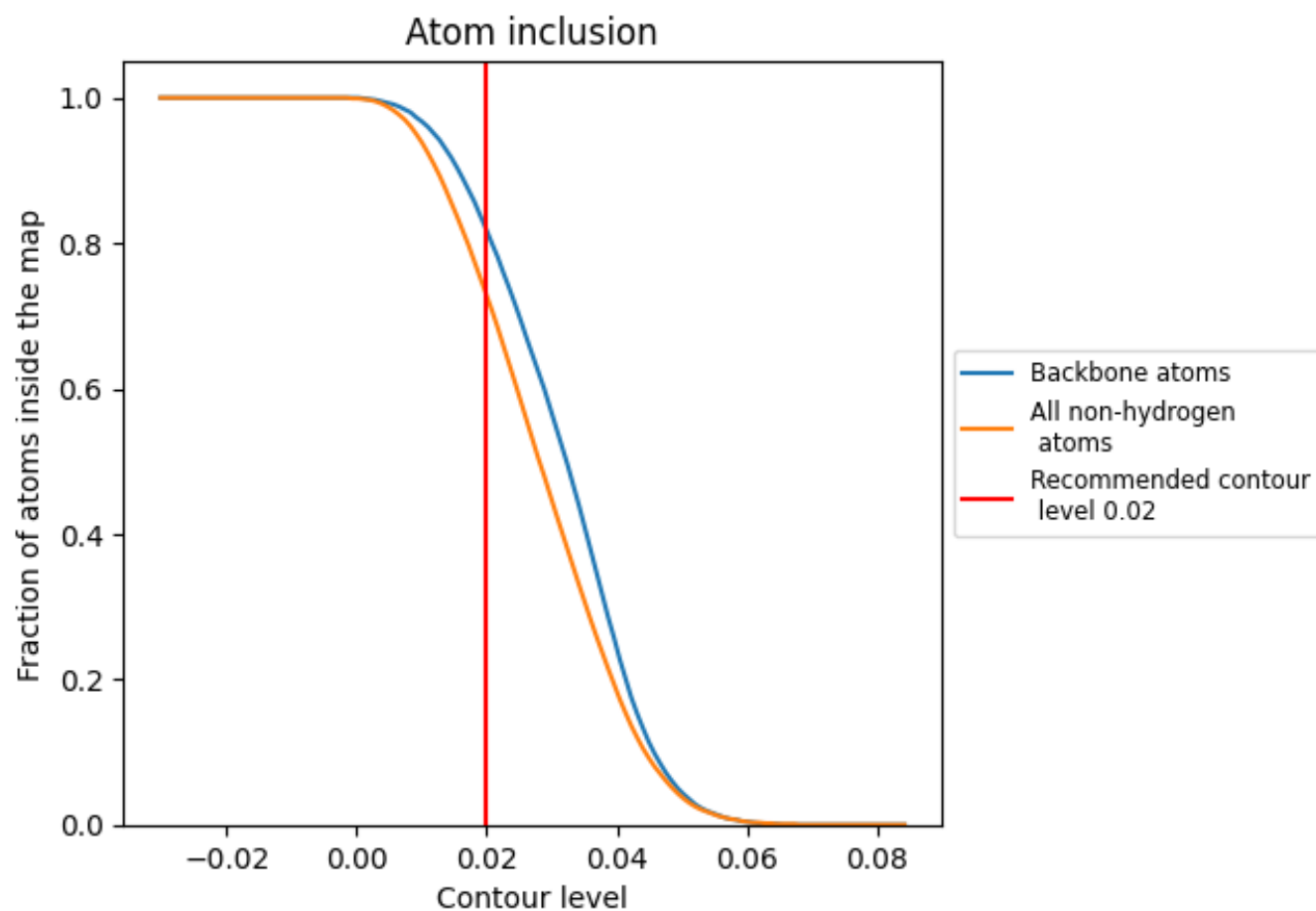
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 73% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7280	 0.4770
L1	 0.9020	 0.5070
L2	 0.5800	 0.2490
L3	 0.3620	 0.3780
L4	 0.1990	 0.2850
L5	 0.0170	 0.1300
L6	 0.8520	 0.5340
L7	 0.6160	 0.4660
L8	 0.6470	 0.4470
LB	 0.7580	 0.5260
LC	 0.7910	 0.5200
LD	 0.8090	 0.5400
LI	 0.6210	 0.4830
LJ	 0.4010	 0.3640
LK	 0.0920	 0.2550
LM	 0.8410	 0.5380
LN	 0.7400	 0.5080
LO	 0.8020	 0.5340
LP	 0.7110	 0.5020
LQ	 0.8140	 0.5250
LR	 0.6630	 0.4390
LS	 0.7280	 0.4940
LT	 0.8370	 0.5390
LU	 0.7760	 0.5290
LV	 0.8150	 0.5320
LW	 0.7460	 0.5160
LX	 0.6110	 0.4560
La	 0.8260	 0.5460
Lb	 0.7190	 0.5050
Ld	 0.8100	 0.5390
Lf	 0.7670	 0.5210
Lg	 0.7450	 0.5150
Lh	 0.9140	 0.5600
Li	 0.8680	 0.5580
Lj	 0.8130	 0.5440



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Chain	Atom inclusion	Q-score
Lk	 0.7370	 0.5060
Ll	 0.5870	 0.3940
Lm	 0.6430	 0.4750
Ln	 0.1080	 0.1920
Lo	 0.7060	 0.5000
Lp	 0.6960	 0.5030
Lq	 0.8240	 0.5470
Lr	 0.7280	 0.5100
Ls	 0.5500	 0.4530
Lt	 0.0310	 0.1460
Lu	 0.7720	 0.5110
Lv	 0.1820	 0.2530
Lw	 0.7670	 0.5210
Lx	 0.6200	 0.4770
Ly	 0.8470	 0.5480
Lz	 0.6980	 0.4890
SR	 0.7860	 0.5210
Sf	 0.7790	 0.5200
u	 0.0520	 0.3420
v	 0.0000	 0.2490
w	 0.0000	 0.1360