wwPDB EM Validation Summary Report ⓘ

Jul 2, 2024 – 07:37 PM JST

PDB ID	:	8XT3
EMDB ID	:	EMD-38635
Title	:	Cryo-EM structure of the human 39S mitoribosome with 10uM Tigecycline
Authors	:	Li, X.; Wang, M.; Cheng, J.
Deposited on	:	2024-01-10
Resolution	:	3.10 Å(reported)
Based on initial model	:	7A5I

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

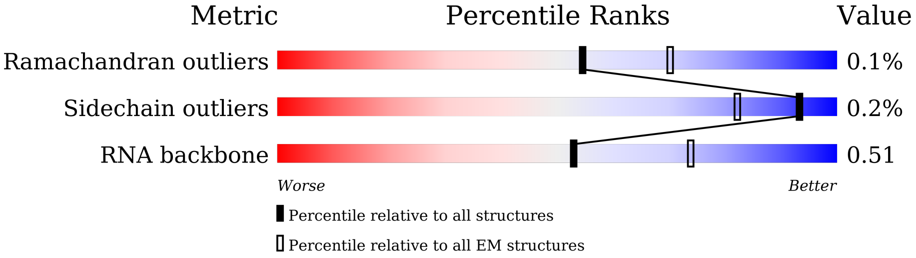
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance ⓘ

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

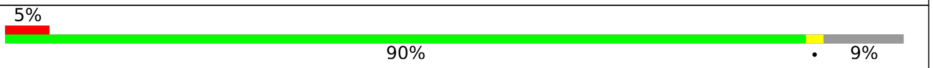
The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	L1	1559	
2	L2	69	
3	LB	305	
4	LC	348	
5	LD	311	
6	LI	267	
7	LJ	261	
8	LK	192	

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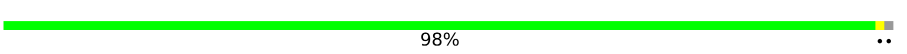
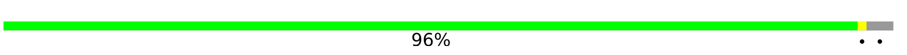
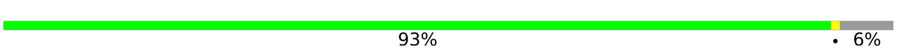
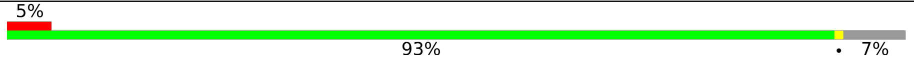
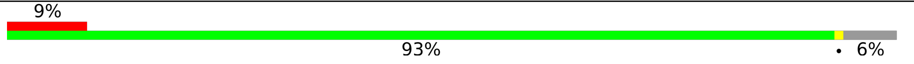
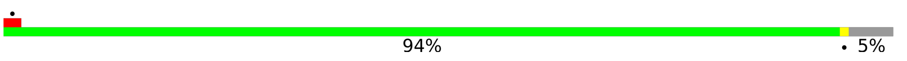
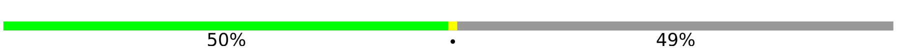
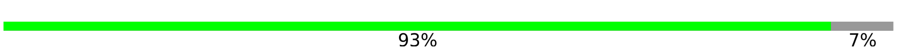
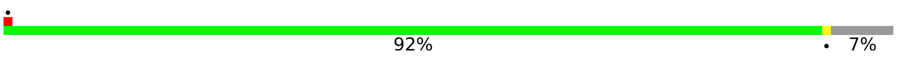
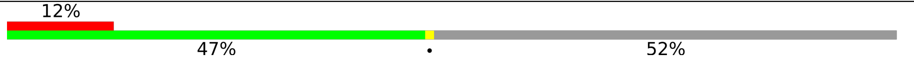
Mol	Chain	Length	Quality of chain
9	LM	178	
10	LN	145	
11	LO	296	
12	LP	251	
13	LQ	175	
14	LR	179	
15	LS	292	
16	LT	149	
17	LU	205	
18	LV	212	
19	LW	153	
20	LX	216	
21	La	148	
22	Lb	256	
23	Lu	250	
24	Ld	161	
25	Lf	188	
26	Lg	65	
27	Lh	92	
28	Li	188	
29	Lj	103	
30	Lk	423	
31	Ll	380	
32	Lm	338	
33	Ln	206	

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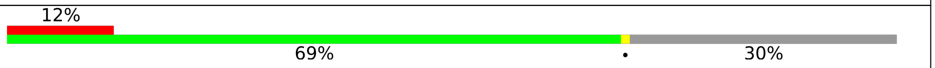
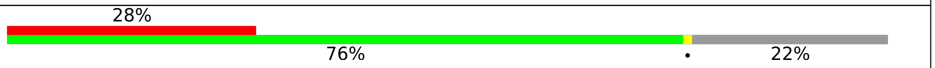
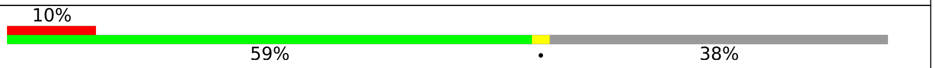
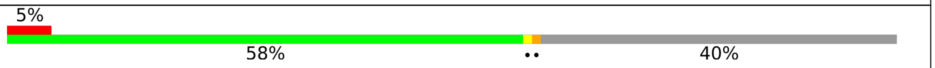
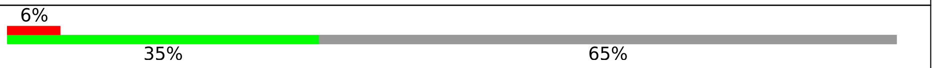
Mol	Chain	Length	Quality of chain
34	Lo	137	
35	Lp	142	
36	Lq	215	
37	Lr	332	
38	Ls	306	
39	Lt	279	
40	Lv	212	
41	Lw	166	
42	Lx	158	
43	Ly	128	
44	Lz	123	
45	L3	112	
46	L4	138	
47	L5	128	
48	L6	102	
49	L7	206	
50	L8	222	
51	SR	196	
52	Sf	439	

2 Entry composition ⓘ

There are 55 unique types of molecules in this entry. The entry contains 100095 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
			Total	C	N	O	P		
1	L1	1500	31847	14290	5750	10307	1500	0	0

- Molecule 2 is a RNA chain called Val tRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

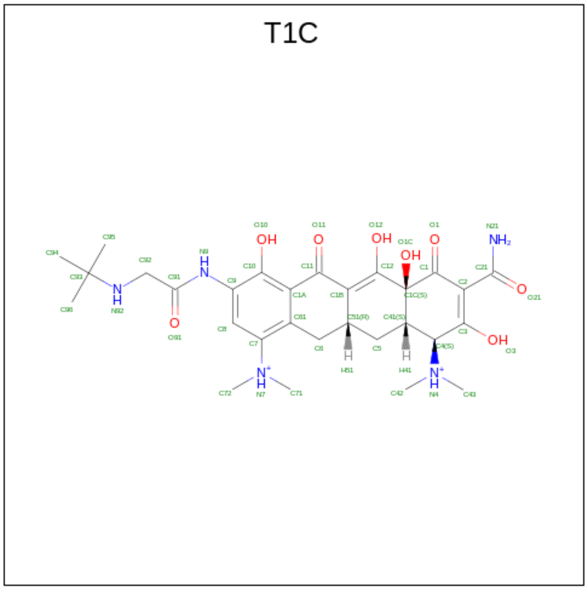
- Molecule 52 is a protein called Large ribosomal subunit protein mL65.

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

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	L1	91	Total 91	Mg 91	0
53	LB	1	Total 1	Mg 1	0
53	La	1	Total 1	Mg 1	0
53	Lw	1	Total 1	Mg 1	0
53	L6	1	Total 1	Mg 1	0

- Molecule 54 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$) (labeled as "Ligand of Interest" by depositor).



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

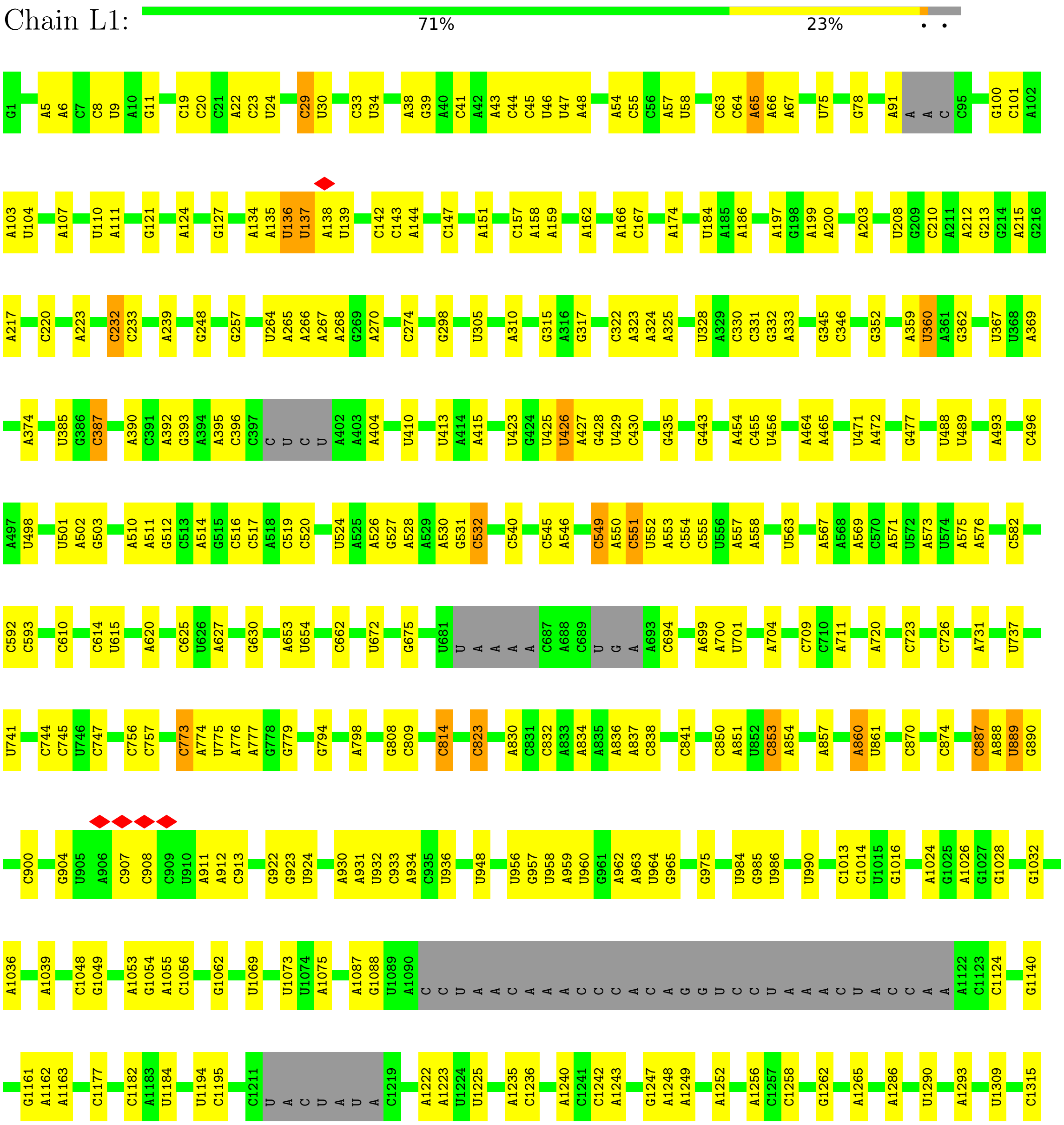
- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

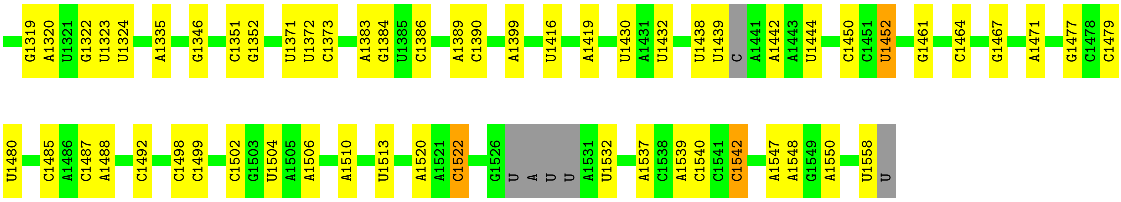
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	Lf	1	1	1	0
			Total	Zn	
55	Lj	1	1	1	0
			Total	Zn	
55	SR	1	1	1	0

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.

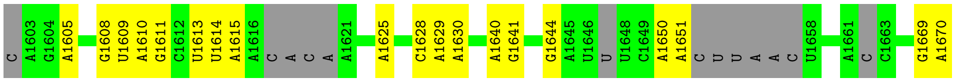
- Molecule 1: 16s rRNA





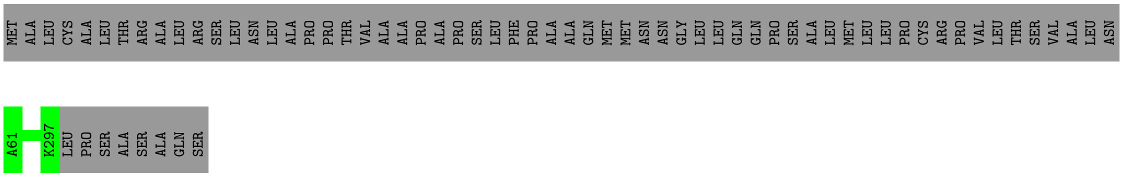
- Molecule 2: Val tRNA

Chain L2:



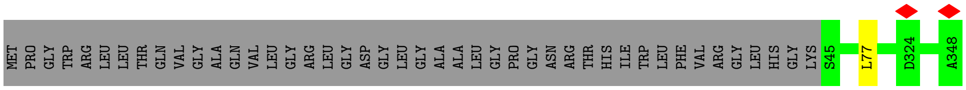
- Molecule 3: Large ribosomal subunit protein uL2m

Chain LB:



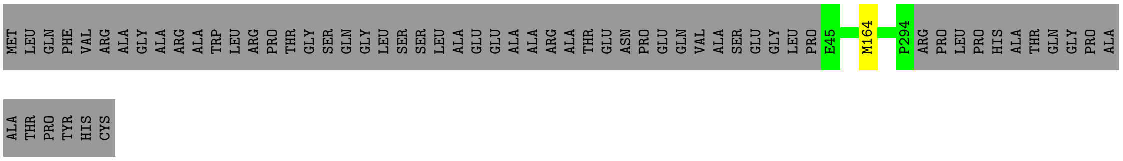
- Molecule 4: Large ribosomal subunit protein uL3m

Chain LC:



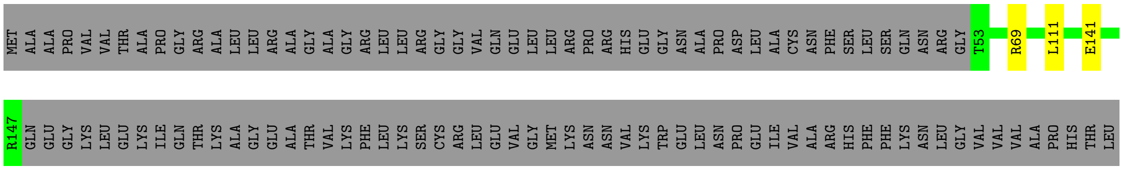
- Molecule 5: Large ribosomal subunit protein uL4m

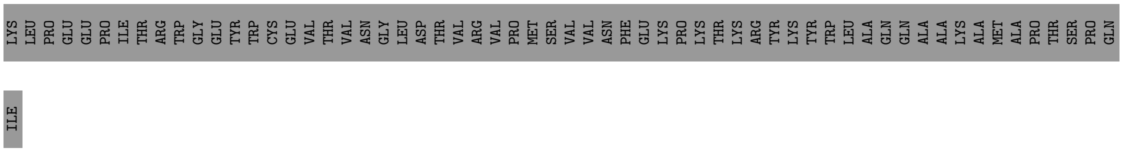
Chain LD:



- Molecule 6: Large ribosomal subunit protein bL9m

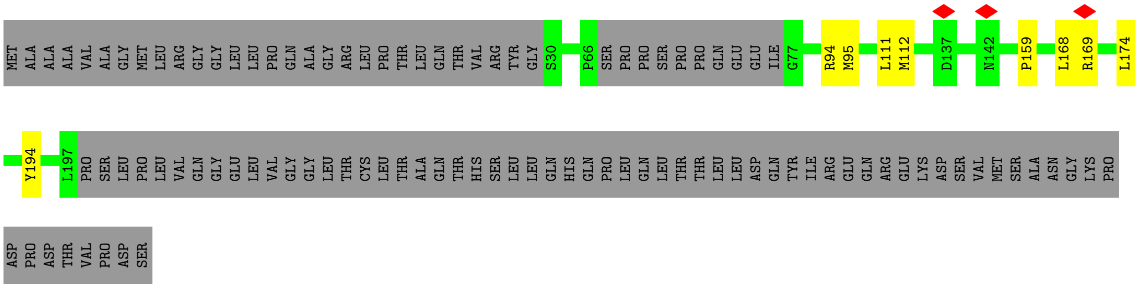
Chain LI:





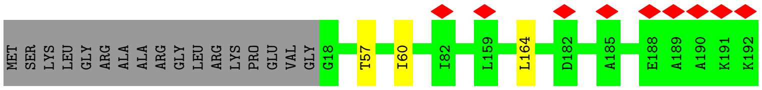
- Molecule 7: Large ribosomal subunit protein uL10m

Chain LJ:



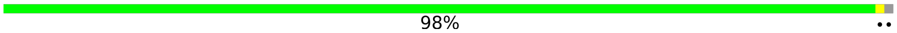
- Molecule 8: Large ribosomal subunit protein uL11m

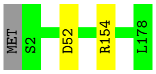
Chain LK:



- Molecule 9: Large ribosomal subunit protein uL13m

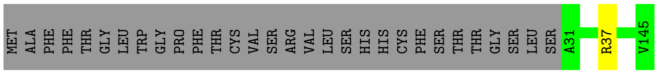
Chain LM:





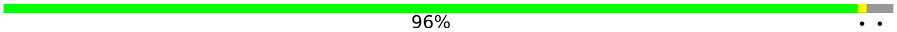
- Molecule 10: Large ribosomal subunit protein uL14m

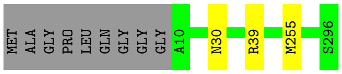
Chain LN:



- Molecule 11: Large ribosomal subunit protein uL15m

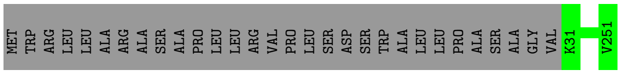
Chain LO:





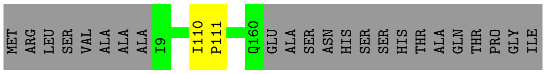
- Molecule 12: Large ribosomal subunit protein uL16m

Chain LP:



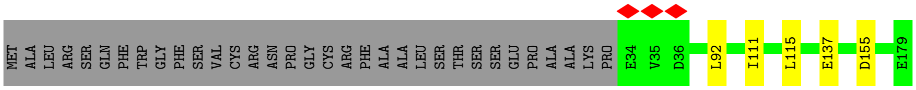
- Molecule 13: Large ribosomal subunit protein bL17m

Chain LQ:



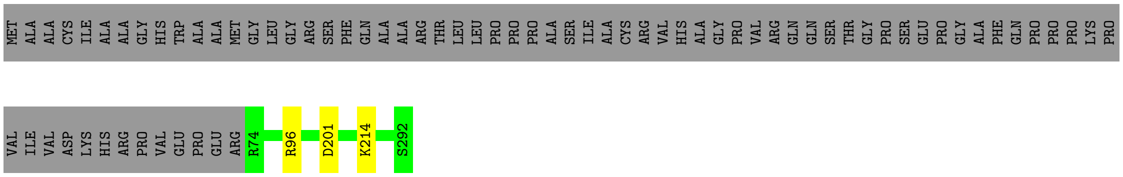
- Molecule 14: Mitochondrial ribosomal protein L18, isoform CRA_b

Chain LR:



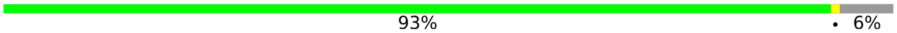
- Molecule 15: Large ribosomal subunit protein bL19m

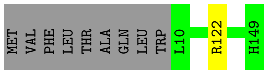
Chain LS:



- Molecule 16: Large ribosomal subunit protein bL20m

Chain LT:



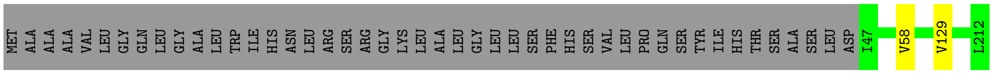


- Molecule 17: Large ribosomal subunit protein bL21m

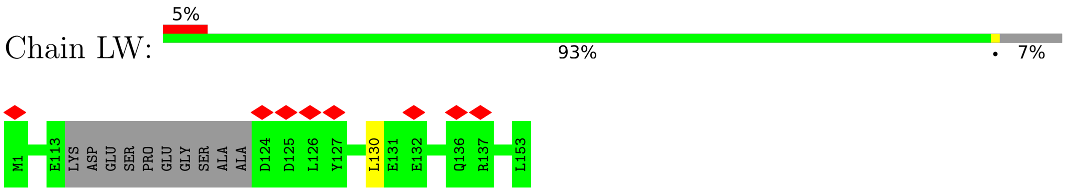
Chain LU:

- Molecule 18: 39S ribosomal protein L22, mitochondrial

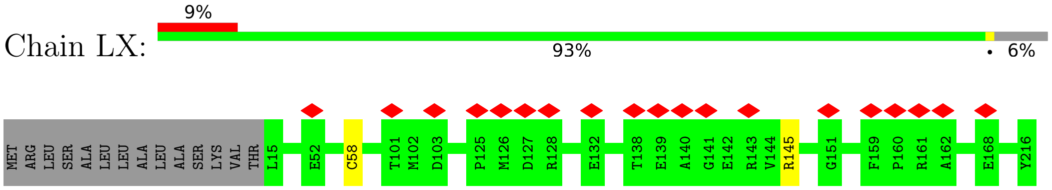
Chain LV:



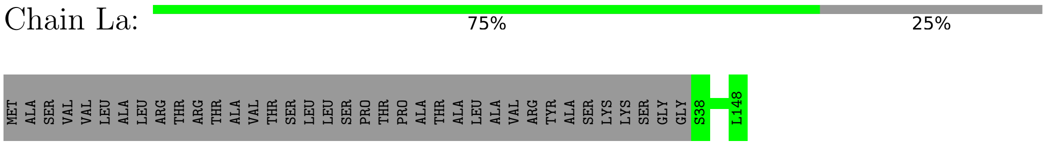
- Molecule 19: Large ribosomal subunit protein uL23m



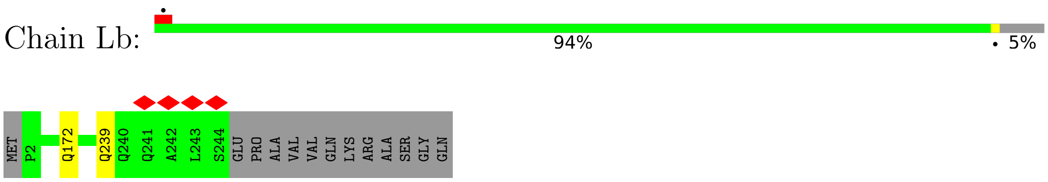
- Molecule 20: Large ribosomal subunit protein uL24m



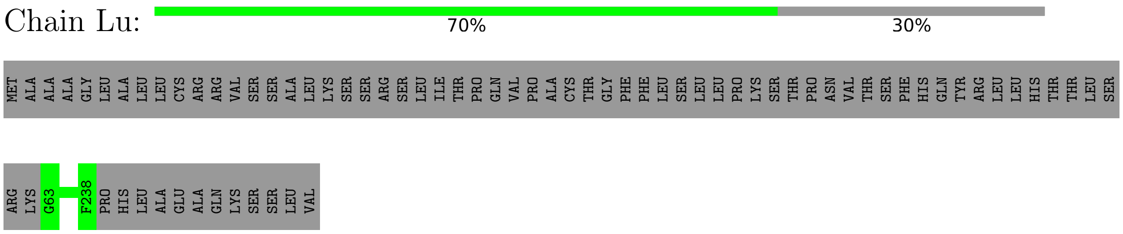
- Molecule 21: Large ribosomal subunit protein bL27m



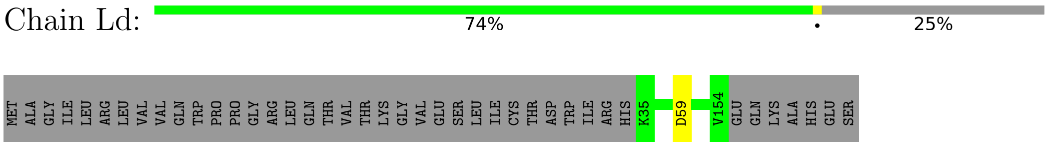
- Molecule 22: Large ribosomal subunit protein bL28m



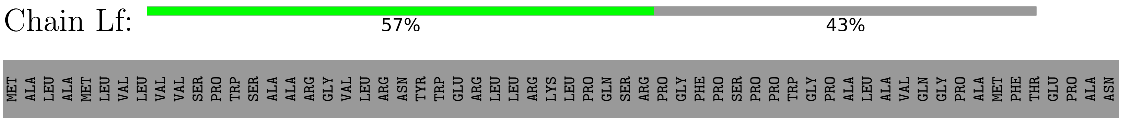
- Molecule 23: Large ribosomal subunit protein uL29m

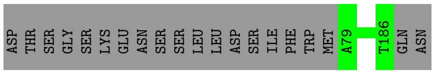


- Molecule 24: Large ribosomal subunit protein uL30m



- Molecule 25: Large ribosomal subunit protein bL32m



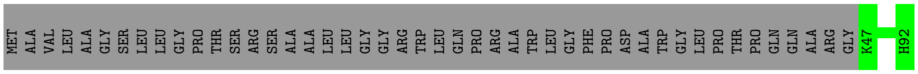


- Molecule 26: Large ribosomal subunit protein bL33m

Chain Lg:

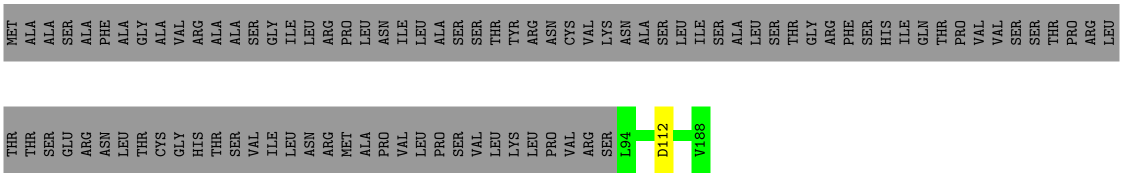
- Molecule 27: Large ribosomal subunit protein bL34m

Chain Lh:



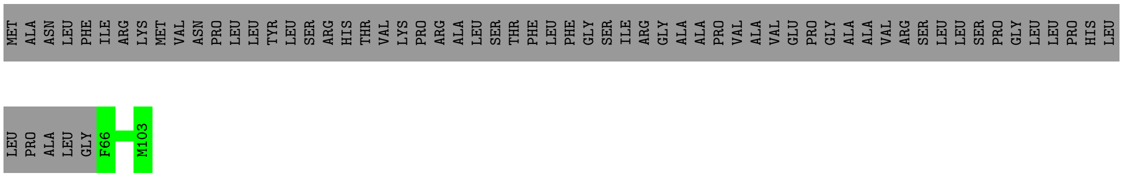
- Molecule 28: Large ribosomal subunit protein bL35m

Chain Li:



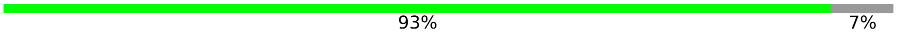
- Molecule 29: Large ribosomal subunit protein bL36m

Chain Lj:



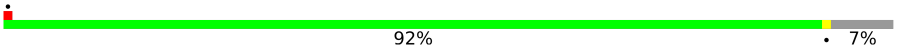
- Molecule 30: Large ribosomal subunit protein mL37

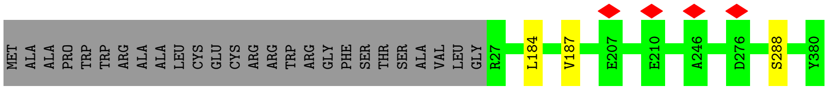
Chain Lk:



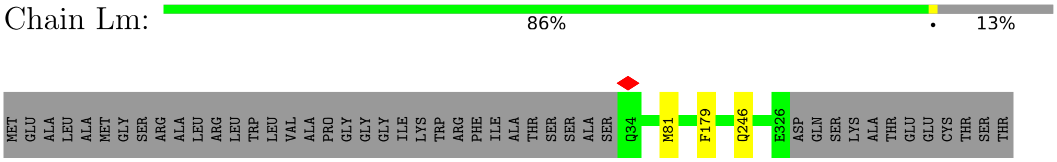
- Molecule 31: Large ribosomal subunit protein mL38

Chain Ll:

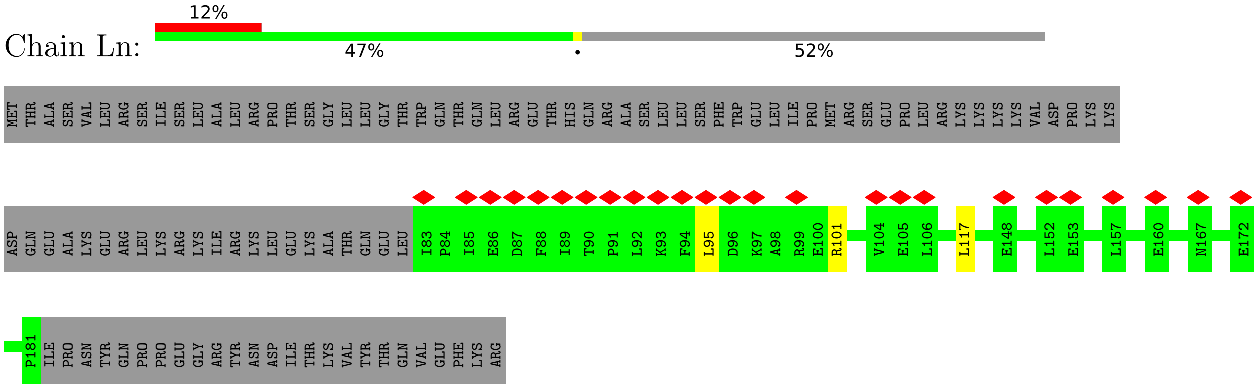




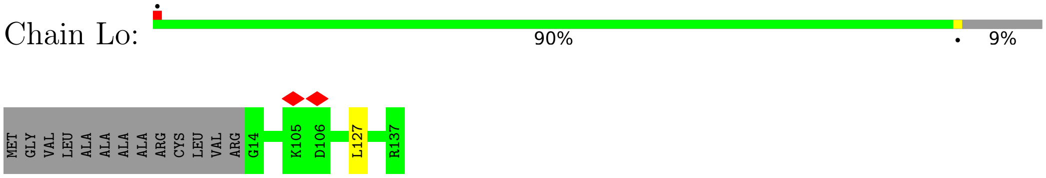
- Molecule 32: Large ribosomal subunit protein mL39



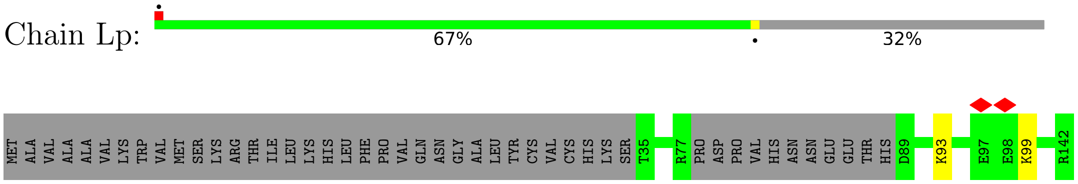
- Molecule 33: Large ribosomal subunit protein mL40



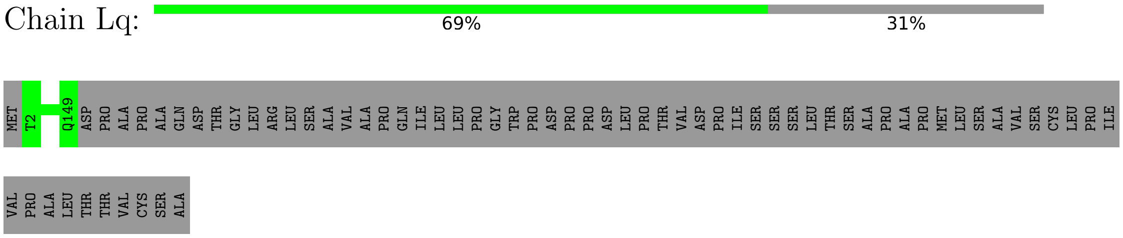
- Molecule 34: Large ribosomal subunit protein mL41



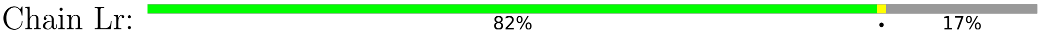
- Molecule 35: Large ribosomal subunit protein mL42

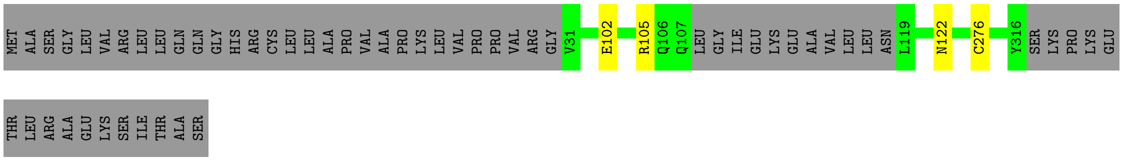


- Molecule 36: Large ribosomal subunit protein mL43



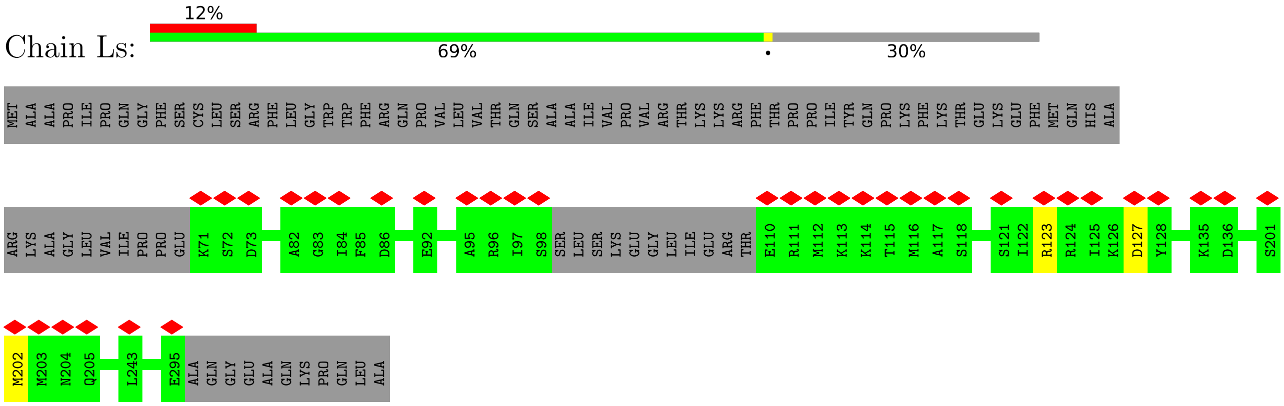
- Molecule 37: Large ribosomal subunit protein mL44





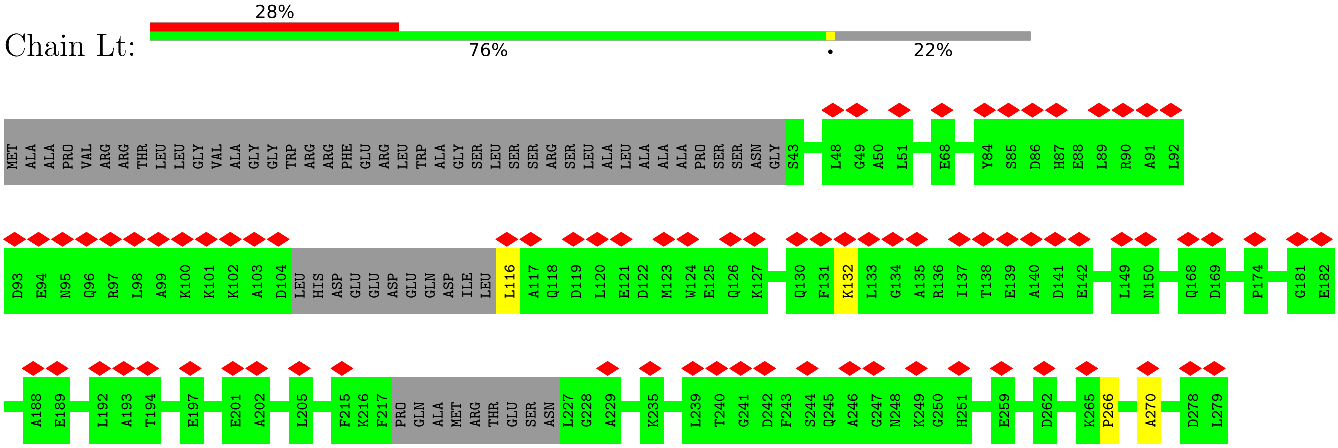
- Molecule 38: Large ribosomal subunit protein mL45

Chain Ls:



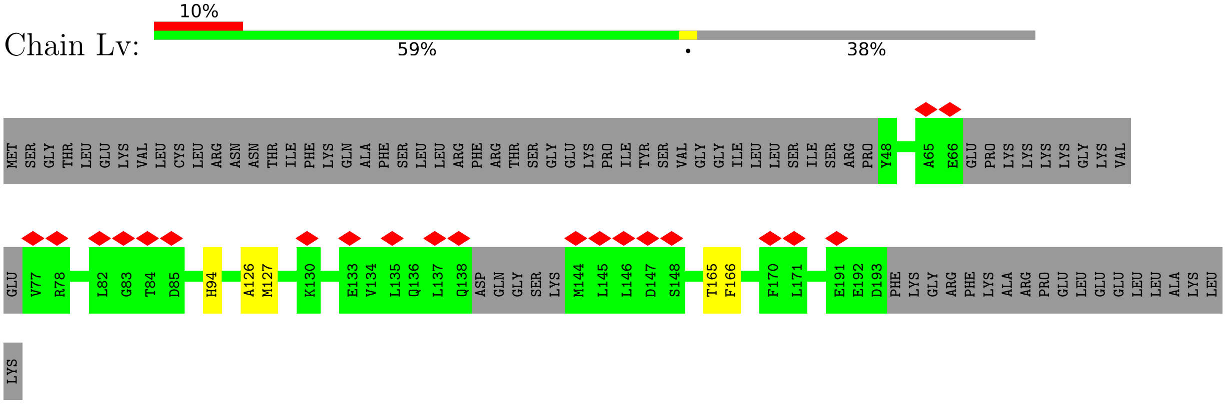
- Molecule 39: Large ribosomal subunit protein mL46

Chain Lt:

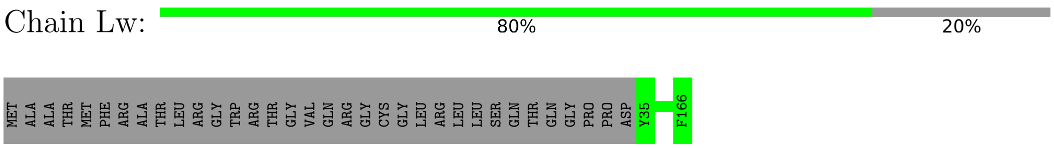


- Molecule 40: Large ribosomal subunit protein mL48

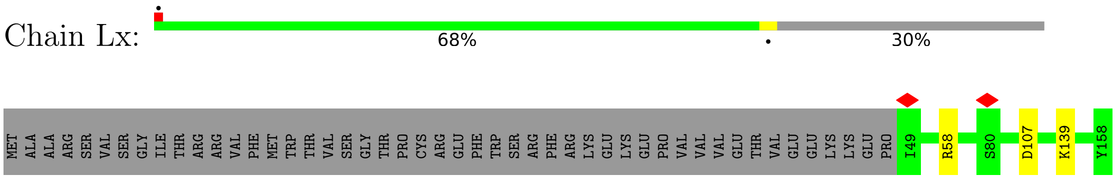
Chain Lv:



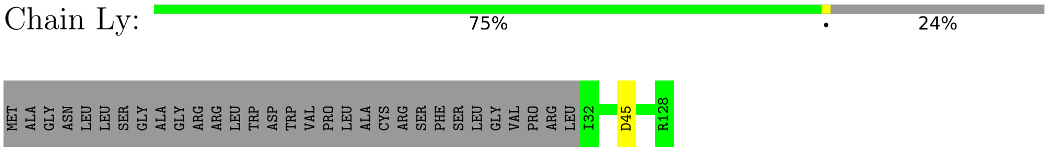
- Molecule 41: Large ribosomal subunit protein mL49



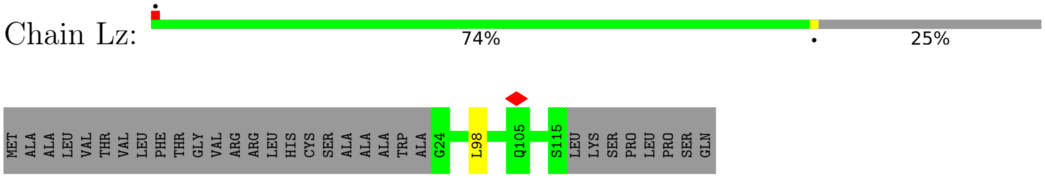
- Molecule 42: Large ribosomal subunit protein mL50



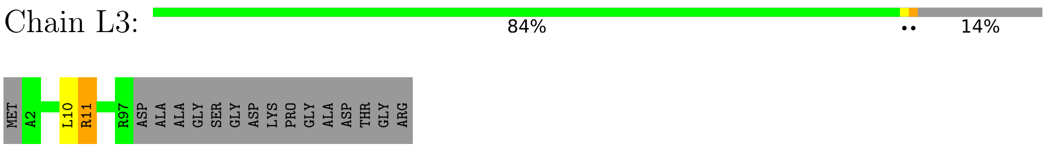
- Molecule 43: Large ribosomal subunit protein mL51



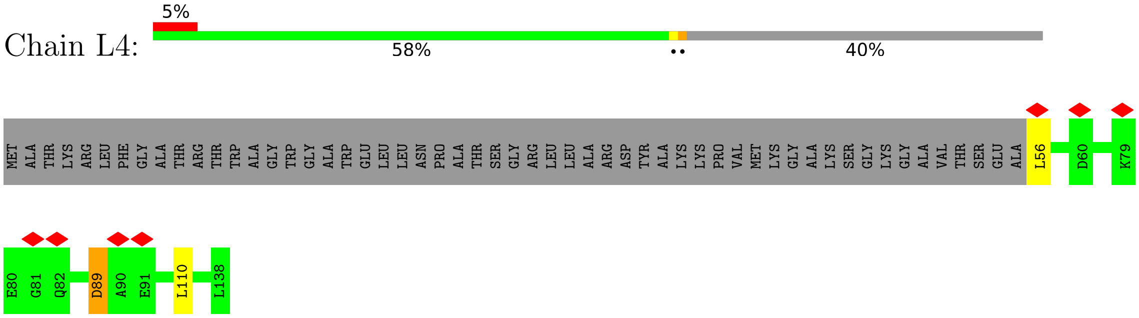
- Molecule 44: 39S ribosomal protein L52, mitochondrial



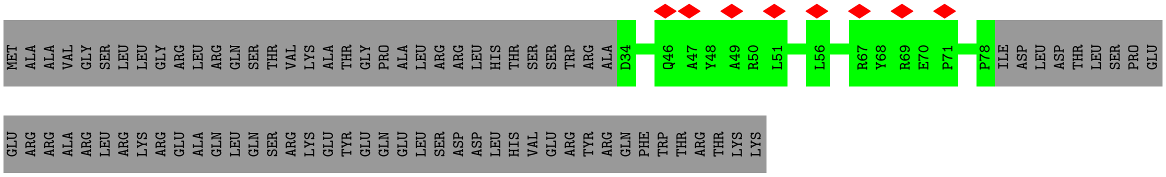
- Molecule 45: Large ribosomal subunit protein mL53



- Molecule 46: Large ribosomal subunit protein mL54

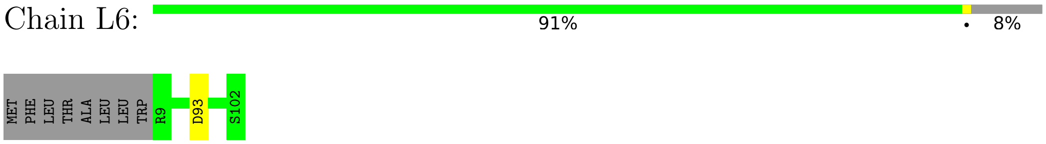


- Molecule 47: Large ribosomal subunit protein mL55



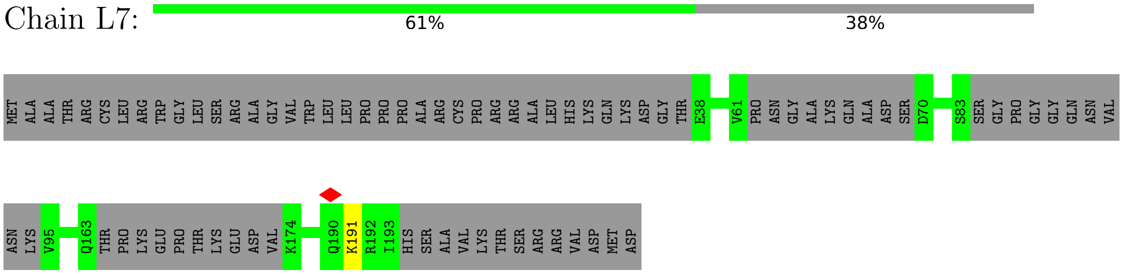
- Molecule 48: Large ribosomal subunit protein mL63

Chain L6:



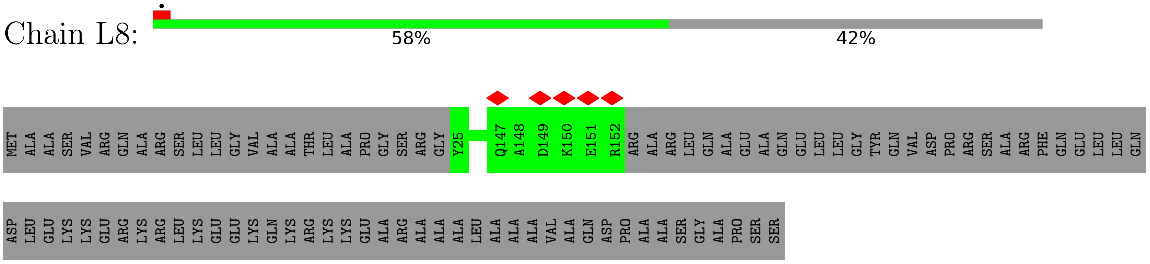
- Molecule 49: Large ribosomal subunit protein mL62

Chain L7:



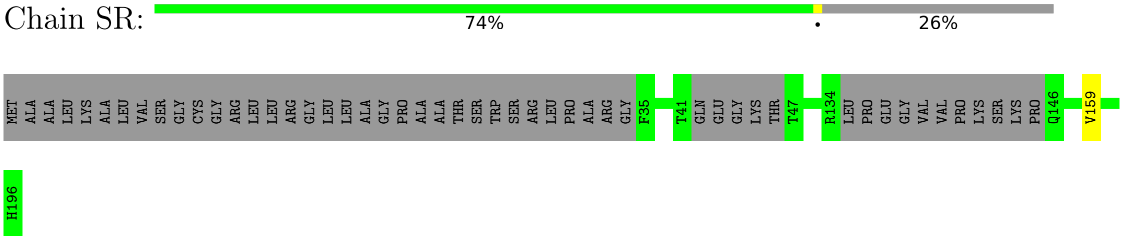
- Molecule 50: Large ribosomal subunit protein mL64

Chain L8:



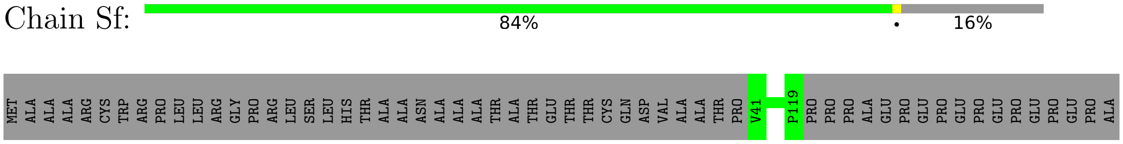
- Molecule 51: Large ribosomal subunit protein mL66

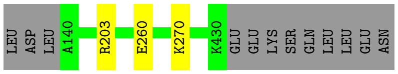
Chain SR:



- Molecule 52: Large ribosomal subunit protein mL65

Chain Sf:




LEU
ASP
LEU
A140
R203
E260
K270
K430
GLU
GLU
LYS
SER
GLN
LEU
LEU
GLU
ASN

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52961	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 ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.018	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	446.88, 446.88, 446.88	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.31	0/35628	1.01	111/55448 (0.2%)
2	L2	0.27	0/1328	0.98	0/2056
3	LB	0.30	0/1888	0.63	0/2538
4	LC	0.29	0/2462	0.59	1/3340 (0.0%)
5	LD	0.31	0/2071	0.62	1/2817 (0.0%)
6	LI	0.34	0/798	0.73	2/1073 (0.2%)
7	LJ	0.51	1/1308 (0.1%)	1.06	7/1761 (0.4%)
8	LK	0.35	0/1348	0.66	1/1813 (0.1%)
9	LM	0.34	0/1495	0.66	1/2029 (0.0%)
10	LN	0.27	0/904	0.57	0/1218
11	LO	0.32	0/2359	0.64	1/3185 (0.0%)
12	LP	0.29	0/1826	0.59	0/2458
13	LQ	0.35	0/1269	0.67	0/1708
14	LR	0.41	1/1215 (0.1%)	0.80	6/1645 (0.4%)
15	LS	0.33	0/1863	0.64	1/2509 (0.0%)
16	LT	0.33	0/1174	0.62	0/1572
17	LU	0.30	0/1311	0.64	0/1778
18	LV	0.35	1/1402 (0.1%)	0.59	0/1886
19	LW	0.31	0/1217	0.65	1/1644 (0.1%)
20	LX	0.32	0/1697	0.65	1/2302 (0.0%)
21	La	0.34	0/893	0.57	0/1204
22	Lb	0.31	0/2090	0.60	1/2825 (0.0%)
23	Lu	0.32	0/1552	0.58	0/2079
24	Ld	0.31	0/1003	0.64	1/1354 (0.1%)
25	Lf	0.32	0/895	0.59	0/1201
26	Lg	0.33	0/438	0.74	0/583
27	Lh	0.30	0/382	0.69	0/507
28	Li	0.30	0/852	0.64	1/1136 (0.1%)
29	Lj	0.28	0/349	0.62	0/461
30	Lk	0.29	0/3305	0.57	0/4502
31	Ll	0.34	0/3042	0.68	2/4140 (0.0%)
32	Lm	0.36	0/2439	0.62	3/3299 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Ln	0.36	0/855	0.75	2/1152 (0.2%)
34	Lo	0.33	0/1025	0.63	1/1379 (0.1%)
35	Lp	0.30	0/839	0.65	1/1136 (0.1%)
36	Lq	0.29	0/1202	0.62	0/1626
37	Lr	0.36	1/2264 (0.0%)	0.59	2/3059 (0.1%)
38	Ls	0.37	0/1800	0.66	3/2436 (0.1%)
39	Lt	0.29	0/1797	0.67	1/2422 (0.0%)
40	Lv	0.34	0/1055	0.70	2/1427 (0.1%)
41	Lw	0.38	0/1134	0.70	0/1547
42	Lx	0.41	0/918	0.77	2/1249 (0.2%)
43	Ly	0.29	0/849	0.63	1/1135 (0.1%)
44	Lz	0.32	0/747	0.74	2/1005 (0.2%)
45	L3	0.41	0/754	0.80	3/1017 (0.3%)
46	L4	0.43	0/722	0.89	4/978 (0.4%)
47	L5	0.27	0/379	0.69	0/510
48	L6	0.38	0/818	0.71	1/1097 (0.1%)
49	L7	0.29	0/1071	0.63	0/1433
50	L8	0.30	0/1107	0.60	0/1498
51	SR	0.32	0/1238	0.64	1/1676 (0.1%)
52	Sf	0.31	0/3114	0.59	1/4225 (0.0%)
All	All	0.32	4/105491 (0.0%)	0.81	169/150078 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	LI	0	1
7	LJ	0	2
8	LK	0	2
11	LO	0	1
13	LQ	0	1
16	LT	0	1
18	LV	0	1
22	Lb	0	1
31	Ll	0	1
37	Lr	0	1
40	Lv	0	2
46	L4	0	1
52	Sf	0	1
All	All	0	16

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	LR	115	LEU	CG-CD1	-6.64	1.27	1.51
37	Lr	276	CYS	CB-SG	-5.50	1.72	1.81
18	LV	58	VAL	C-N	5.46	1.46	1.34
7	LJ	194	TYR	CD2-CE2	-5.11	1.31	1.39

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	LJ	168	LEU	CB-CG-CD2	-13.90	87.38	111.00
46	L4	110	LEU	CB-CG-CD2	-11.22	91.92	111.00
1	L1	328	U	N3-C2-O2	-11.18	114.37	122.20
7	LJ	112	MET	CA-CB-CG	9.48	129.41	113.30
14	LR	155	ASP	CB-CG-OD1	9.25	126.63	118.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	LI	69	ARG	Sidechain
7	LJ	159	PRO	Peptide
7	LJ	169	ARG	Sidechain
8	LK	57	THR	Peptide
8	LK	60	ILE	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LB	235/305 (77%)	228 (97%)	7 (3%)	0	100	100
4	LC	302/348 (87%)	281 (93%)	21 (7%)	0	100	100
5	LD	248/311 (80%)	237 (96%)	11 (4%)	0	100	100
6	LI	93/267 (35%)	88 (95%)	5 (5%)	0	100	100
7	LJ	154/261 (59%)	138 (90%)	16 (10%)	0	100	100
8	LK	173/192 (90%)	165 (95%)	8 (5%)	0	100	100
9	LM	175/178 (98%)	164 (94%)	10 (6%)	1 (1%)	25	59
10	LN	113/145 (78%)	107 (95%)	6 (5%)	0	100	100
11	LO	285/296 (96%)	270 (95%)	15 (5%)	0	100	100
12	LP	219/251 (87%)	216 (99%)	3 (1%)	0	100	100
13	LQ	150/175 (86%)	141 (94%)	8 (5%)	1 (1%)	22	57
14	LR	144/179 (80%)	140 (97%)	4 (3%)	0	100	100
15	LS	217/292 (74%)	202 (93%)	15 (7%)	0	100	100
16	LT	138/149 (93%)	134 (97%)	4 (3%)	0	100	100
17	LU	158/205 (77%)	148 (94%)	10 (6%)	0	100	100
18	LV	164/212 (77%)	157 (96%)	7 (4%)	0	100	100
19	LW	139/153 (91%)	138 (99%)	1 (1%)	0	100	100
20	LX	200/216 (93%)	189 (94%)	11 (6%)	0	100	100
21	La	109/148 (74%)	106 (97%)	3 (3%)	0	100	100
22	Lb	241/256 (94%)	233 (97%)	8 (3%)	0	100	100
23	Lu	174/250 (70%)	172 (99%)	2 (1%)	0	100	100
24	Ld	118/161 (73%)	113 (96%)	5 (4%)	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%)	91 (98%)	2 (2%)	0	100	100
29	Lj	36/103 (35%)	36 (100%)	0	0	100	100
30	Lk	392/423 (93%)	382 (97%)	10 (3%)	0	100	100
31	Ll	352/380 (93%)	330 (94%)	22 (6%)	0	100	100
32	Lm	291/338 (86%)	279 (96%)	12 (4%)	0	100	100
33	Ln	97/206 (47%)	88 (91%)	9 (9%)	0	100	100
34	Lo	122/137 (89%)	118 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	Lp	93/142 (66%)	90 (97%)	3 (3%)	0	100	100
36	Lq	146/215 (68%)	135 (92%)	11 (8%)	0	100	100
37	Lr	271/332 (82%)	266 (98%)	5 (2%)	0	100	100
38	Ls	210/306 (69%)	202 (96%)	8 (4%)	0	100	100
39	Lt	211/279 (76%)	187 (89%)	22 (10%)	2 (1%)	17	52
40	Lv	125/212 (59%)	119 (95%)	6 (5%)	0	100	100
41	Lw	130/166 (78%)	123 (95%)	7 (5%)	0	100	100
42	Lx	108/158 (68%)	104 (96%)	4 (4%)	0	100	100
43	Ly	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
44	Lz	90/123 (73%)	83 (92%)	7 (8%)	0	100	100
45	L3	94/112 (84%)	90 (96%)	4 (4%)	0	100	100
46	L4	81/138 (59%)	74 (91%)	7 (9%)	0	100	100
47	L5	43/128 (34%)	40 (93%)	3 (7%)	0	100	100
48	L6	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
49	L7	119/206 (58%)	116 (98%)	3 (2%)	0	100	100
50	L8	126/222 (57%)	123 (98%)	3 (2%)	0	100	100
51	SR	140/196 (71%)	137 (98%)	3 (2%)	0	100	100
52	Sf	366/439 (83%)	354 (97%)	11 (3%)	1 (0%)	41	73
All	All	8072/10674 (76%)	7708 (96%)	359 (4%)	5 (0%)	54	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	Lt	266	PRO
39	Lt	270	ALA
9	LM	154	ARG
52	Sf	260	GLU
13	LQ	111	PRO

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%)	258 (100%)	0	100	100
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%)	144 (99%)	1 (1%)	84	93
8	LK	138/150 (92%)	138 (100%)	0	100	100
9	LM	155/156 (99%)	155 (100%)	0	100	100
10	LN	98/124 (79%)	97 (99%)	1 (1%)	76	90
11	LO	245/249 (98%)	244 (100%)	1 (0%)	91	96
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%)	128 (100%)	0	100	100
15	LS	201/256 (78%)	199 (99%)	2 (1%)	76	90
16	LT	118/126 (94%)	118 (100%)	0	100	100
17	LU	145/180 (81%)	145 (100%)	0	100	100
18	LV	146/182 (80%)	146 (100%)	0	100	100
19	LW	128/135 (95%)	128 (100%)	0	100	100
20	LX	180/191 (94%)	179 (99%)	1 (1%)	86	94
21	La	91/119 (76%)	91 (100%)	0	100	100
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%)	269 (100%)	0	100	100
33	Ln	91/190 (48%)	90 (99%)	1 (1%)	73	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	Lo	104/112 (93%)	104 (100%)	0	100	100
35	Lp	93/133 (70%)	92 (99%)	1 (1%)	73	89
36	Lq	130/186 (70%)	130 (100%)	0	100	100
37	Lr	241/288 (84%)	240 (100%)	1 (0%)	91	96
38	Ls	196/274 (72%)	196 (100%)	0	100	100
39	Lt	188/236 (80%)	187 (100%)	1 (0%)	88	94
40	Lv	117/188 (62%)	116 (99%)	1 (1%)	78	91
41	Lw	122/148 (82%)	122 (100%)	0	100	100
42	Lx	104/148 (70%)	103 (99%)	1 (1%)	76	90
43	Ly	86/110 (78%)	86 (100%)	0	100	100
44	Lz	73/97 (75%)	73 (100%)	0	100	100
45	L3	81/90 (90%)	80 (99%)	1 (1%)	71	88
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%)	116 (99%)	1 (1%)	78	91
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%)	326 (100%)	0	100	100
All	All	7236/9218 (78%)	7222 (100%)	14 (0%)	93	97

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	Lp	99	LYS
37	Lr	105	ARG
49	L7	191	LYS
42	Lx	58	ARG
45	L3	11	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	LC	57	ASN

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Mol	Chain	Res	Type
16	LT	77	GLN
40	Lv	94	HIS
46	L4	76	ASN
49	L7	123	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1491/1559 (95%)	351 (23%)	16 (1%)
2	L2	51/69 (73%)	19 (37%)	0
All	All	1542/1628 (94%)	370 (23%)	16 (1%)

5 of 370 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 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	1319	G
1	L1	1235	A
1	L1	575	A
1	L1	930	A
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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 99 ligands modelled in this entry, 98 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	T1C	L1	1691	53	44,45,45	1.18	4 (9%)	53,72,72	1.08	5 (9%)

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
54	T1C	L1	1691	53	-	11/22/80/80	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	L1	1691	T1C	C21-N21	5.43	1.47	1.33
54	L1	1691	T1C	O11-C11	2.23	1.28	1.23
54	L1	1691	T1C	C4-N4	2.18	1.52	1.47
54	L1	1691	T1C	C7-N7	2.13	1.48	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	L1	1691	T1C	C1-C1C-C12	3.14	113.56	109.88
54	L1	1691	T1C	C11-C1B-C12	2.95	121.13	118.80
54	L1	1691	T1C	O1C-C1C-C12	-2.74	105.77	110.14
54	L1	1691	T1C	C1C-C41-C4	2.70	115.32	111.64
54	L1	1691	T1C	C1C-C1-C2	2.13	119.14	115.75

There are no chirality outliers.

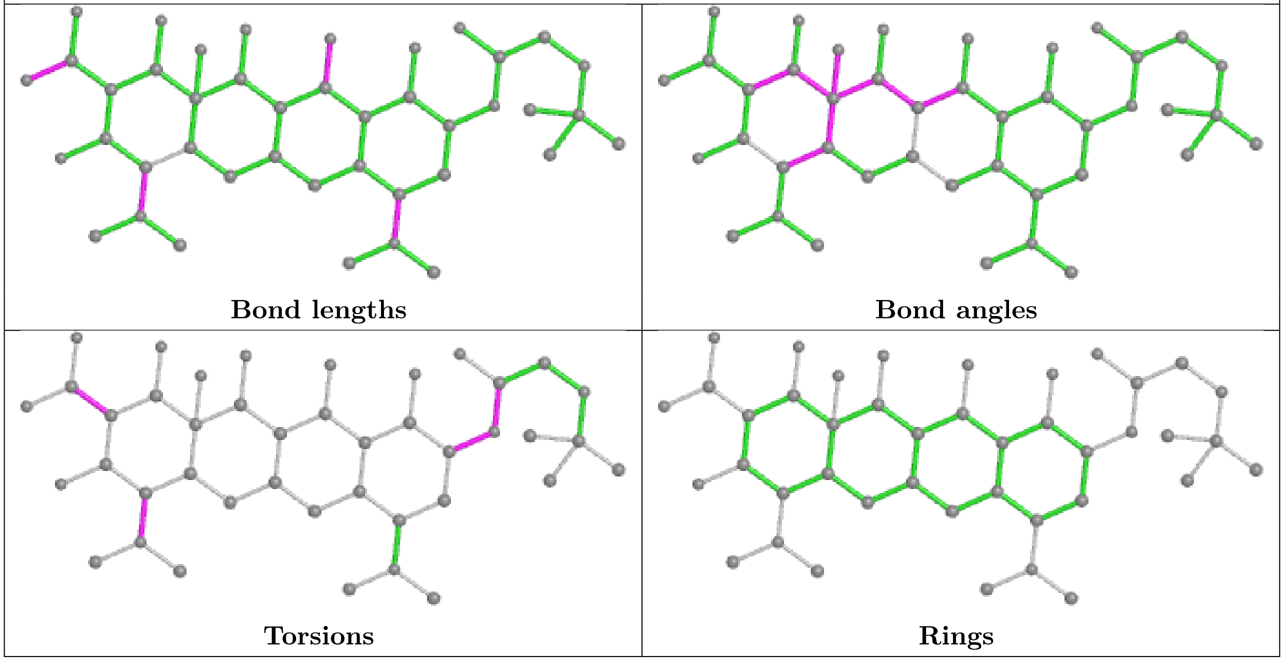
5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	L1	1691	T1C	C92-C91-N9-C9
54	L1	1691	T1C	C41-C4-N4-C43
54	L1	1691	T1C	C3-C4-N4-C43
54	L1	1691	T1C	C3-C4-N4-C42
54	L1	1691	T1C	C3-C2-C21-O21

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.


Ligand T1C L1 1691

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

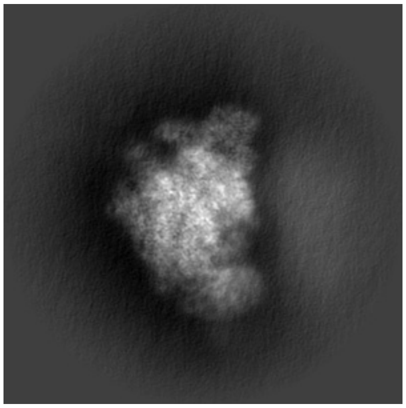
6 Map visualisation

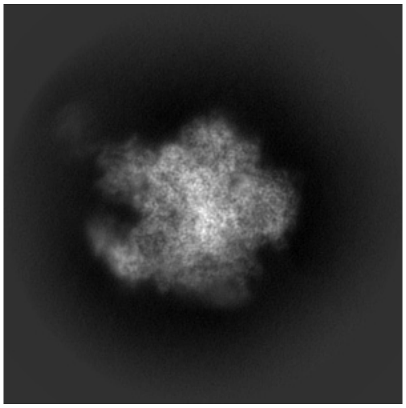
This section contains visualisations of the EMDB entry EMD-38635. These allow visual inspection of the internal detail of the map and identification of artifacts.

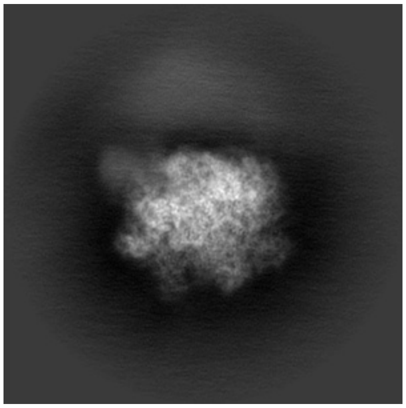
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

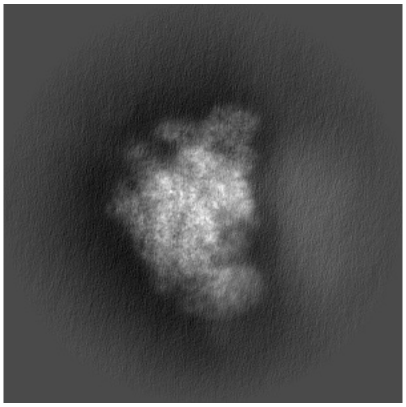
6.1.1 Primary map

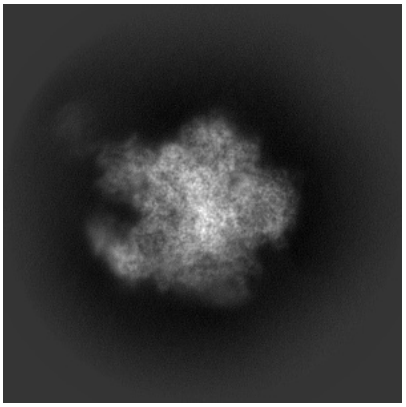

X

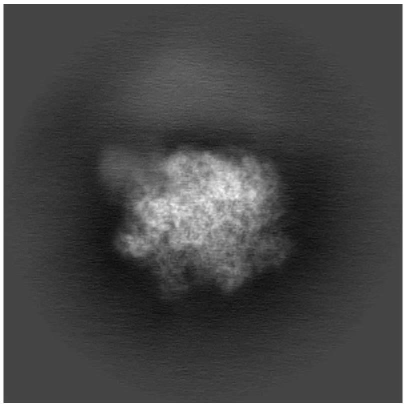

Y


Z

6.1.2 Raw map


X

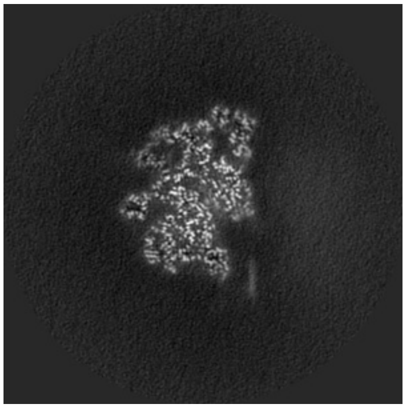

Y


Z

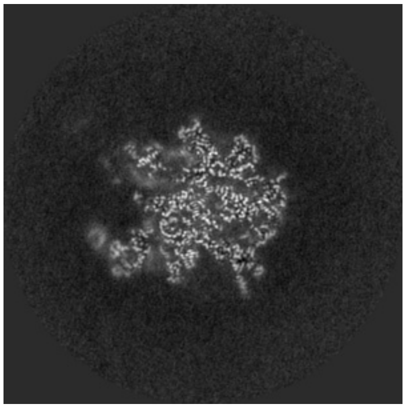
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

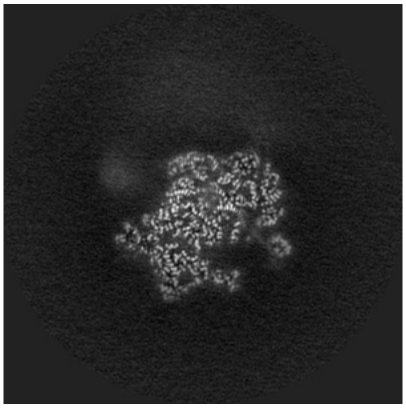
6.2.1 Primary map



X Index: 210

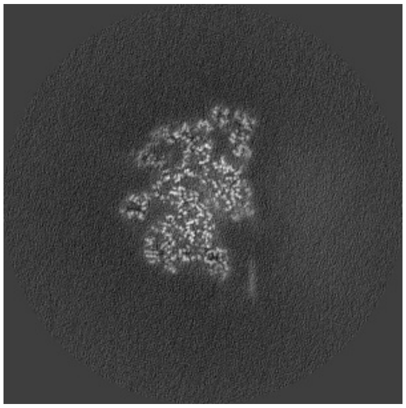


Y Index: 210

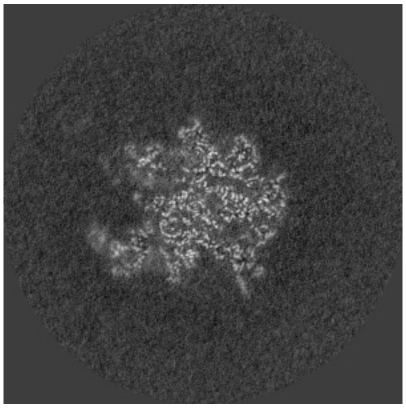


Z Index: 210

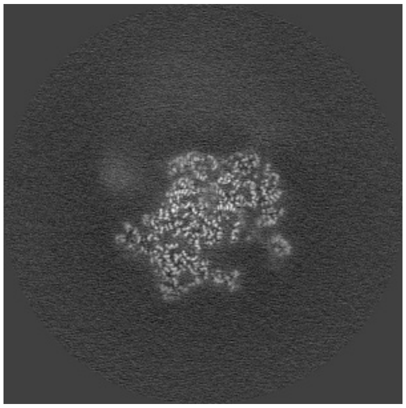
6.2.2 Raw map



X Index: 210



Y Index: 210

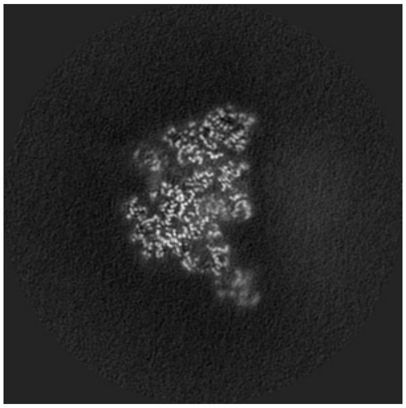


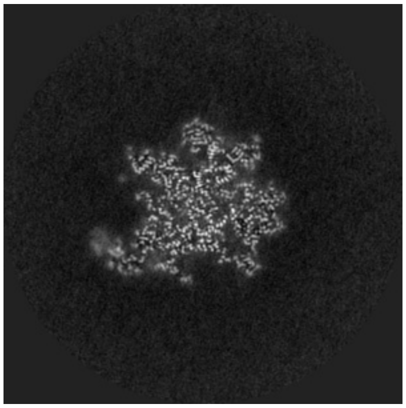
Z Index: 210

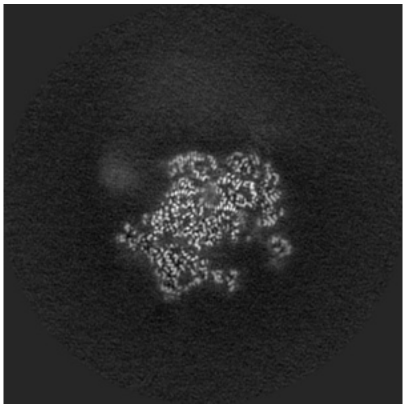
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

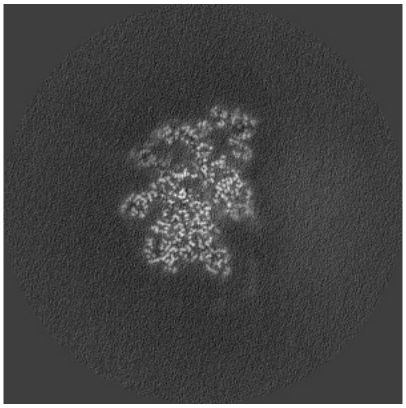
6.3.1 Primary map

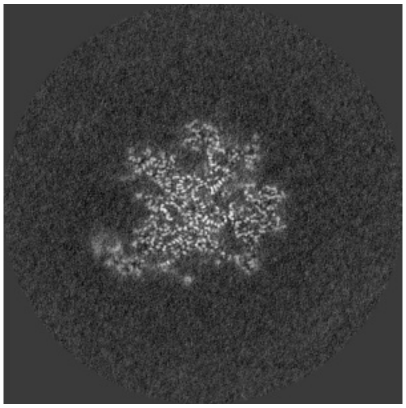

X Index: 221

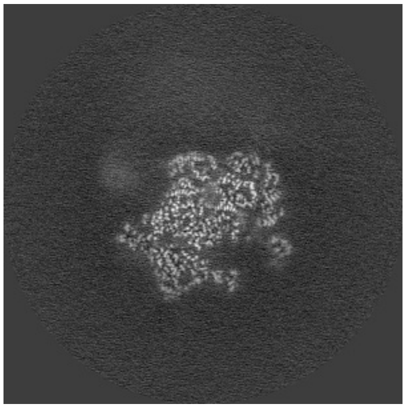

Y Index: 201


Z Index: 211

6.3.2 Raw map


X Index: 208

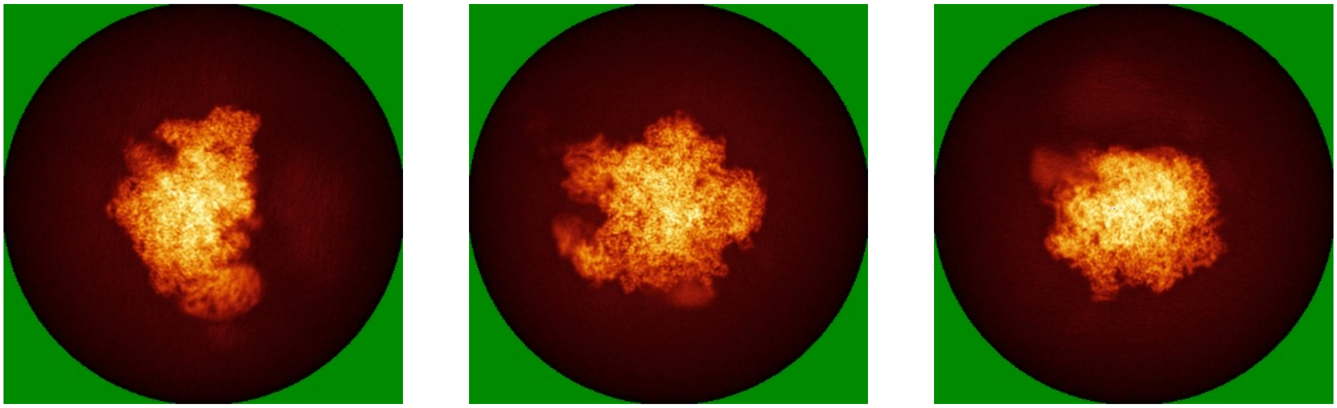

Y Index: 199


Z Index: 211

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

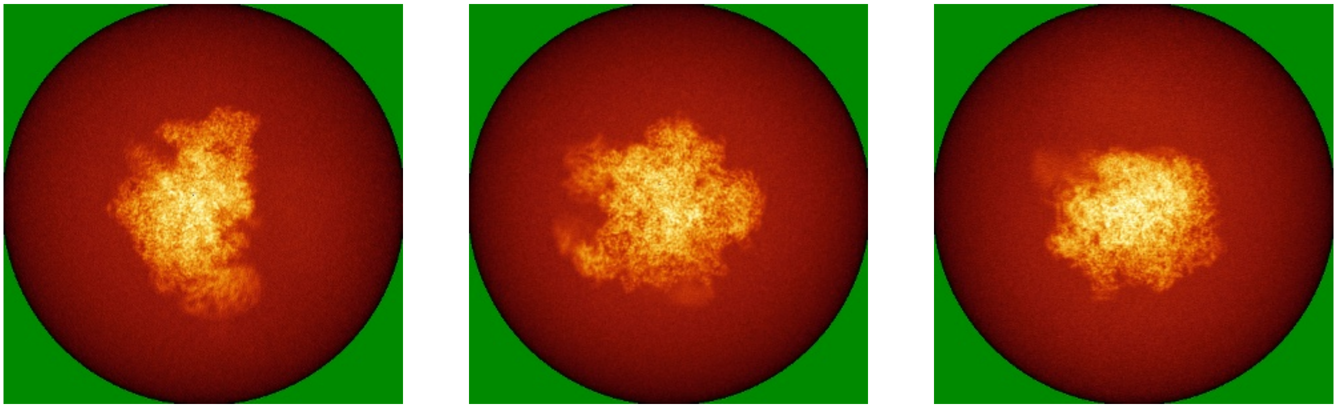
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X Y Z

6.4.2 Raw map

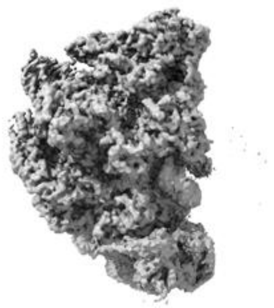


X Y Z

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

6.5.1 Primary map



X

Y

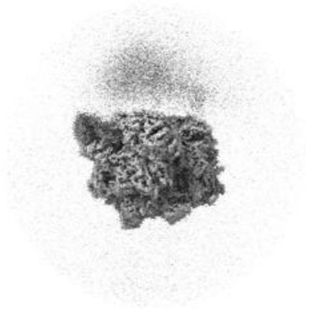
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X

Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

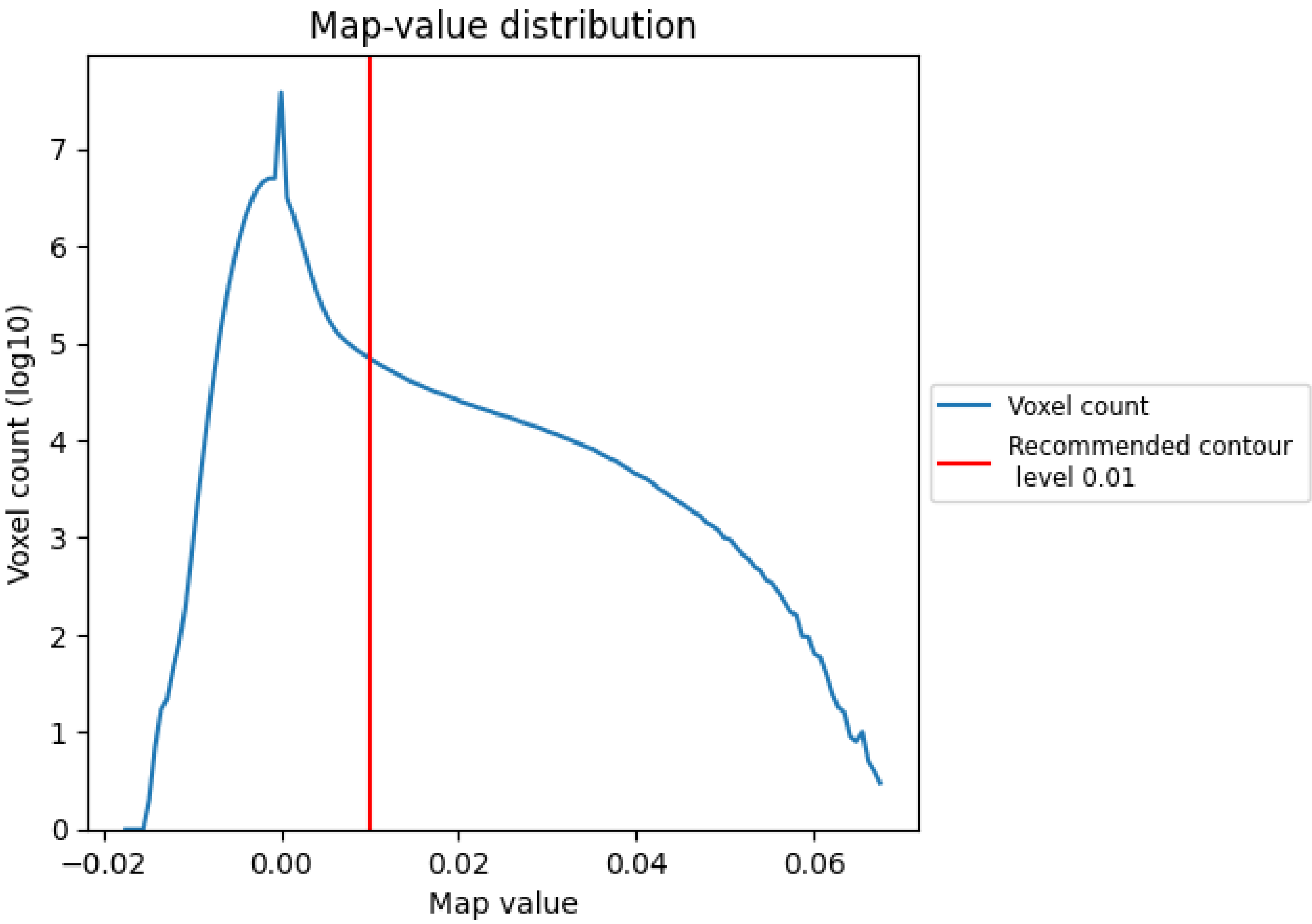
6.6 Mask visualisation

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

7 Map analysis ⓘ

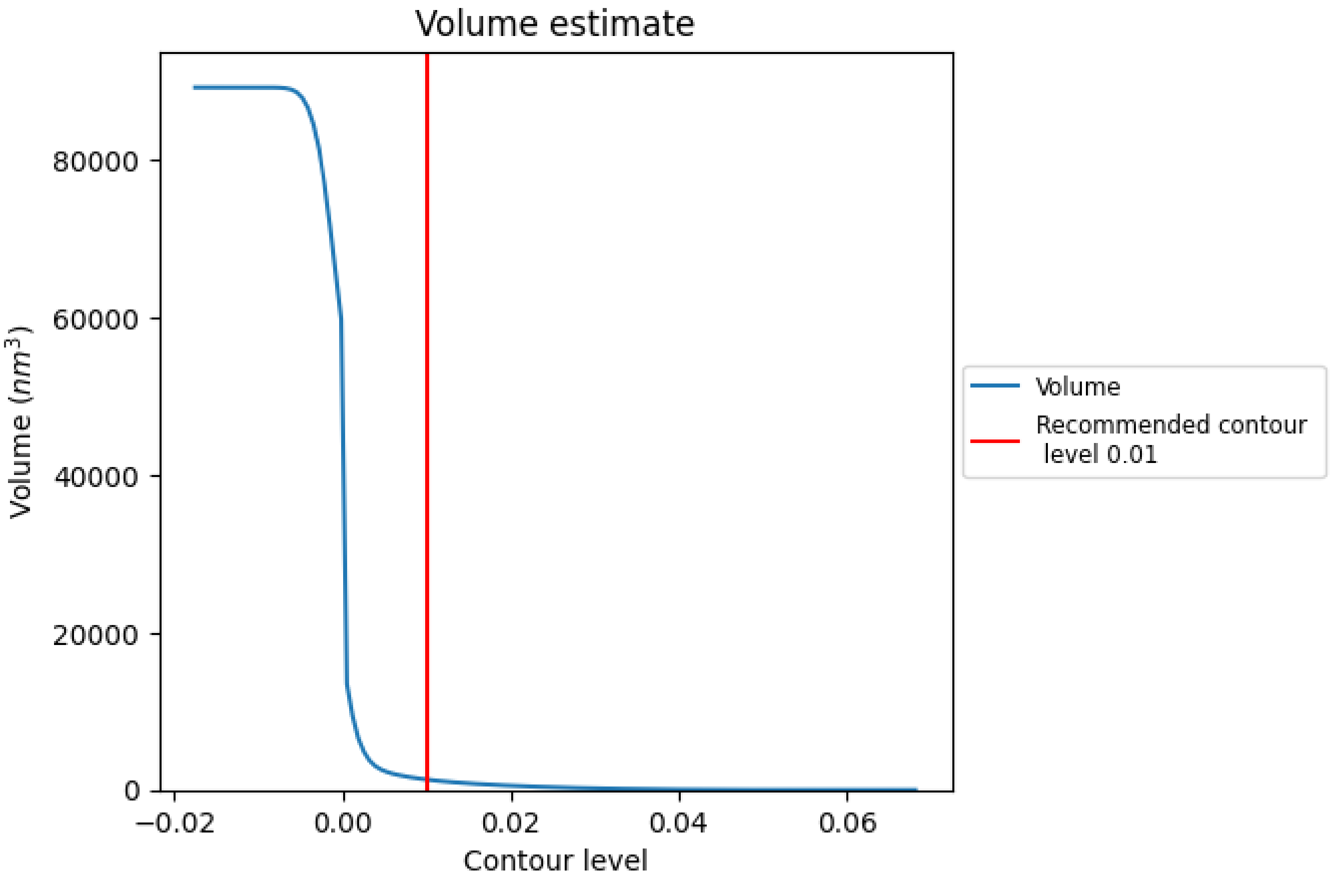
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

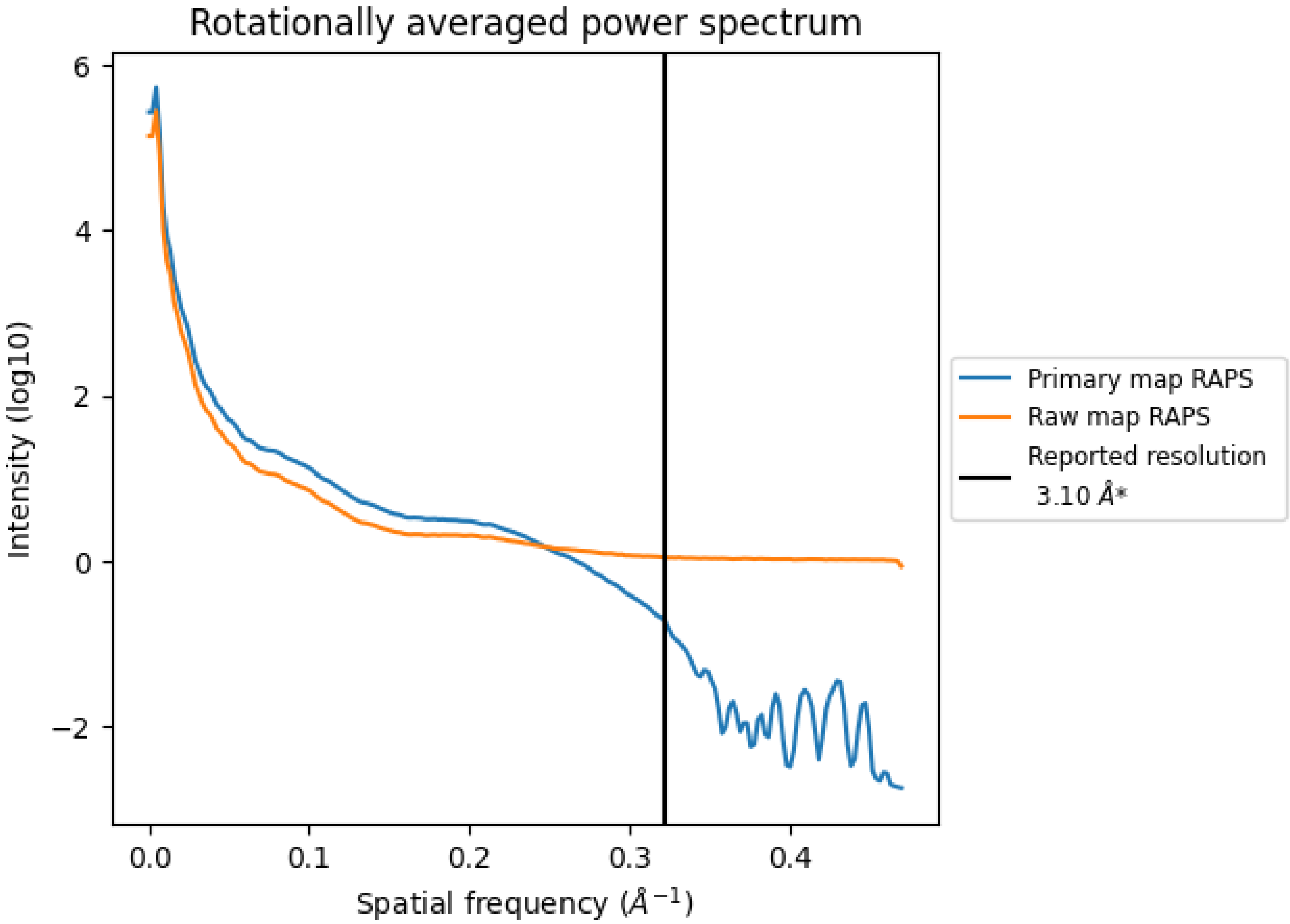
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1320 nm^3; this corresponds to an approximate mass of 1193 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 ⓘ

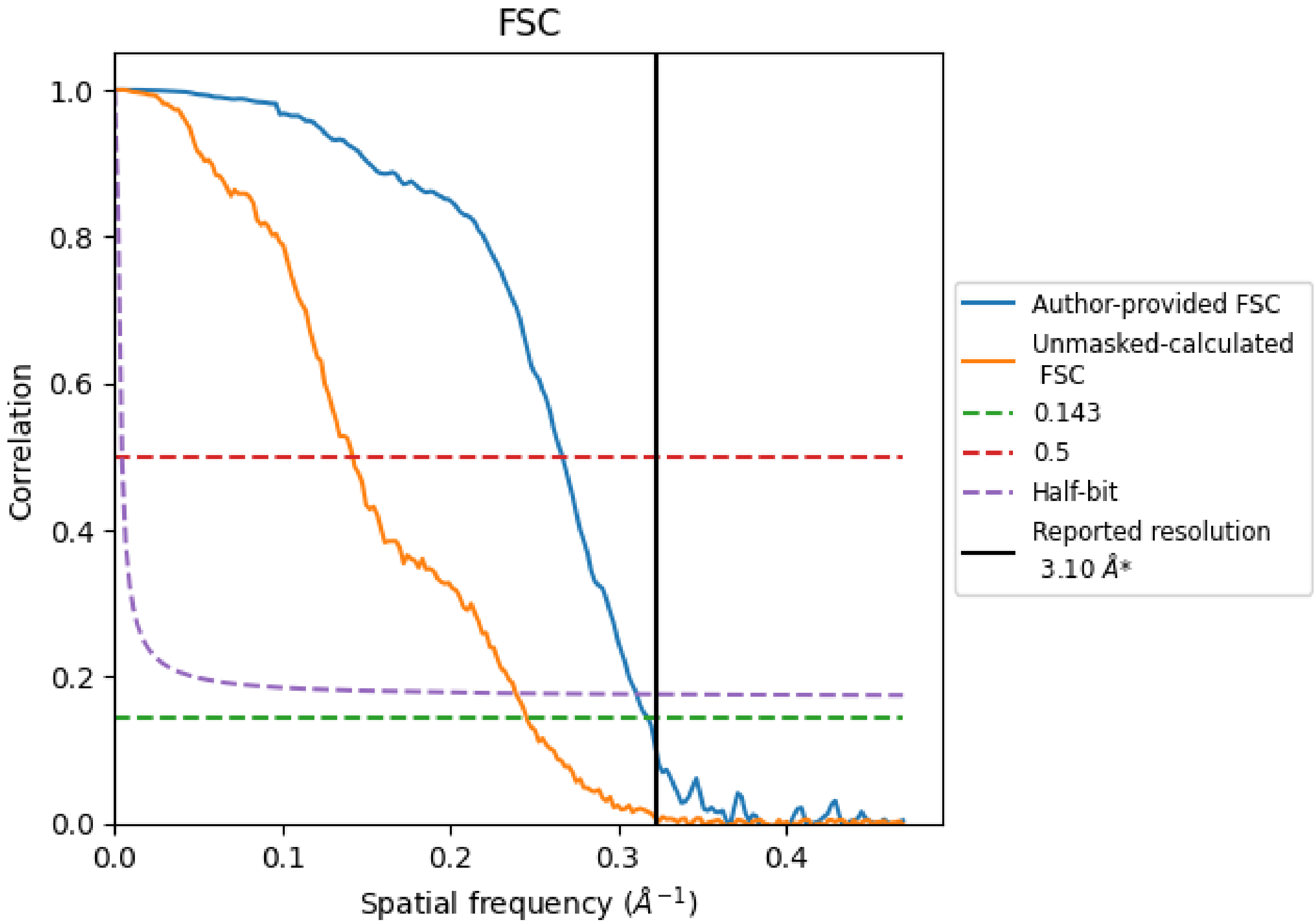


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8.2 Resolution estimates ⓘ

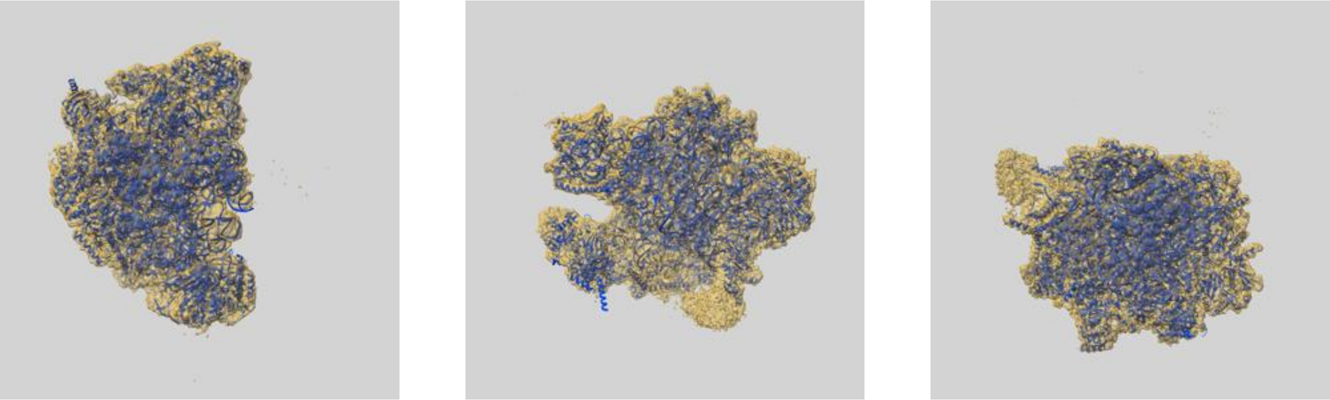
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.14	3.75	3.21
Unmasked-calculated*	4.07	7.05	4.18

*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 4.07 differs from the reported value 3.1 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-38635 and PDB model 8XT3. Per-residue inclusion information can be found in section 3 on page 14.

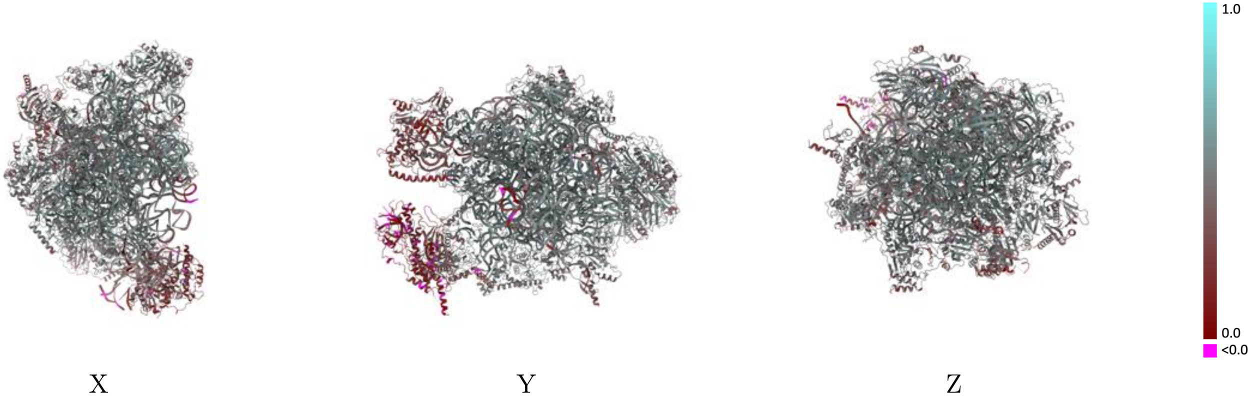
9.1 Map-model overlay (i)



X Y Z

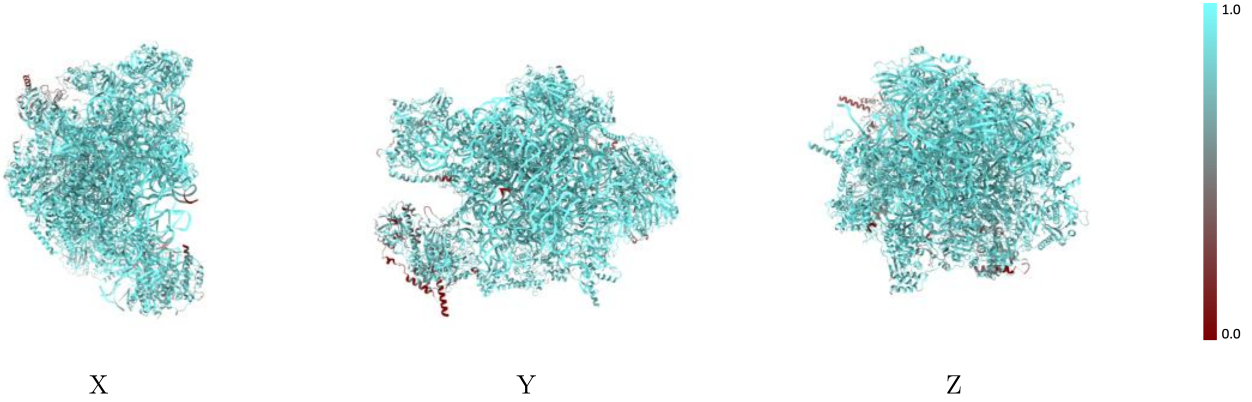
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



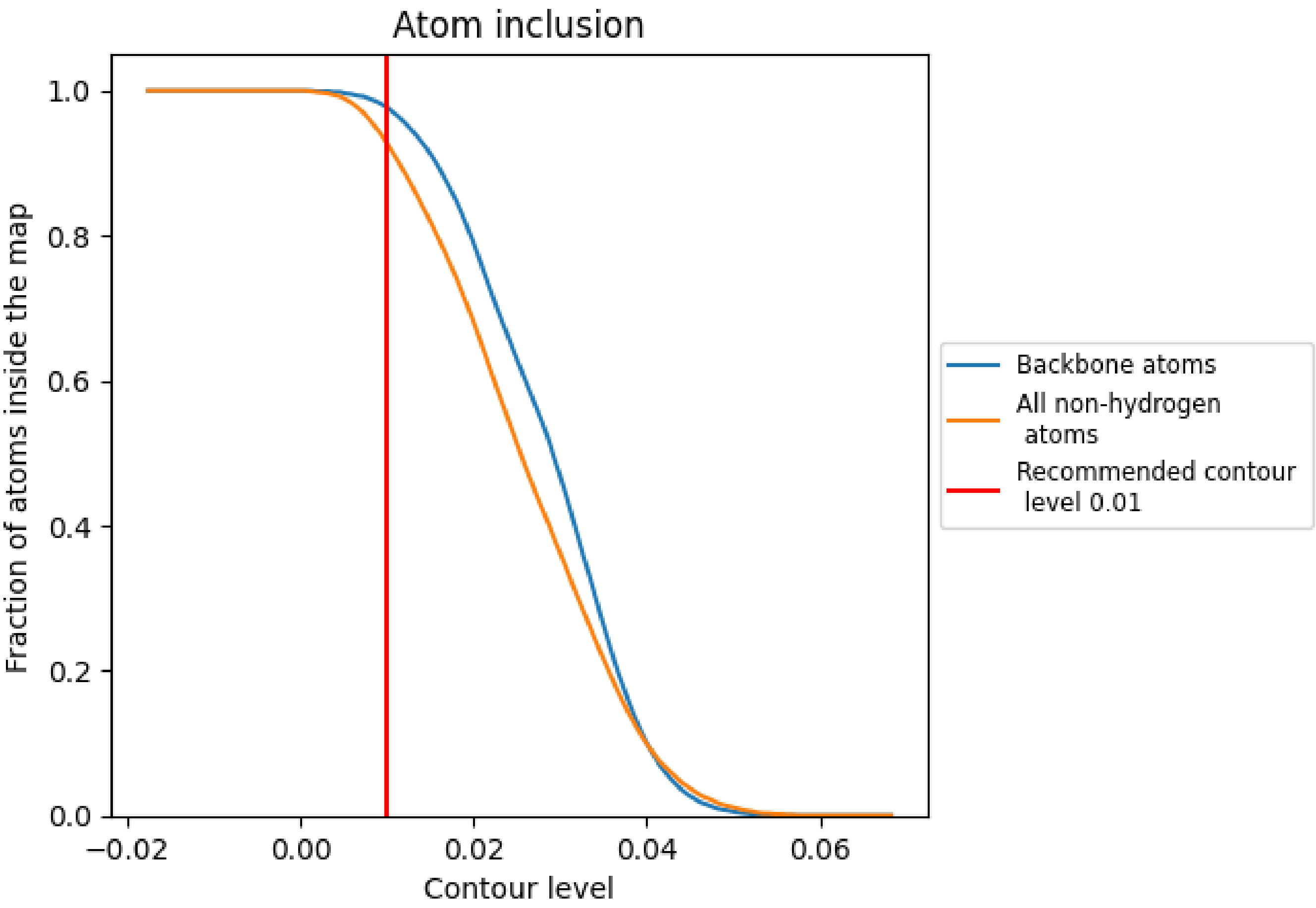
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9270	0.4670
L1	0.9910	0.5010
L2	0.9400	0.2700
L3	0.9000	0.3830
L4	0.7920	0.3100
L5	0.6770	0.1810
L6	0.9660	0.5210
L7	0.8980	0.4400
L8	0.8570	0.4210
LB	0.9510	0.5170
LC	0.9610	0.5080
LD	0.9580	0.5200
LI	0.9250	0.4440
LJ	0.8680	0.3660
LK	0.7680	0.2450
LM	0.9680	0.5130
LN	0.9450	0.4990
LO	0.9450	0.5090
LP	0.9490	0.5000
LQ	0.9600	0.5040
LR	0.9390	0.4520
LS	0.9180	0.4830
LT	0.9600	0.5140
LU	0.9440	0.5130
LV	0.9420	0.5160
LW	0.8930	0.4820
LX	0.7550	0.4280
La	0.9860	0.5350
Lb	0.9030	0.4780
Ld	0.9430	0.5170
Lf	0.9340	0.4980
Lg	0.9500	0.4880
Lh	0.9830	0.5380
Li	0.9800	0.5410
Lj	0.9820	0.5350

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Chain	Atom inclusion	Q-score
Lk	0.9230	0.4830
Ll	0.9070	0.4050
Lm	0.8920	0.4280
Ln	0.5910	0.1870
Lo	0.8840	0.4740
Lp	0.9130	0.4750
Lq	0.9620	0.5190
Lr	0.9170	0.4750
Ls	0.6910	0.3970
Lt	0.5210	0.1400
Lu	0.9360	0.4910
Lv	0.6810	0.2410
Lw	0.9560	0.4950
Lx	0.8340	0.4250
Ly	0.9760	0.5250
Lz	0.9220	0.4730
SR	0.9730	0.5060
Sf	0.9460	0.5000