



wwPDB EM Validation Summary Report ⓘ

Jun 8, 2022 – 07:46 pm BST

PDB ID : 7PKT
EMDB ID : EMD-13480
Title : Large subunit of the Chlamydomonas reinhardtii mitoribosome
Authors : Waltz, F.; Soufari, H.; Hashem, Y.
Deposited on : 2021-08-26
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

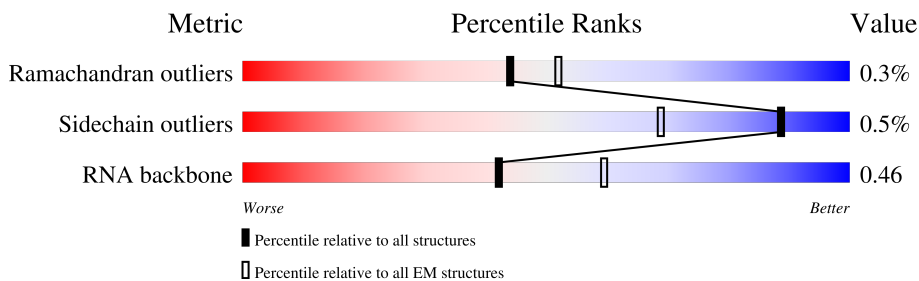
EMDB validation analysis : 0.0.1.dev8
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

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 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	a	383	
2	b	417	
3	c	427	
4	d	216	
5	f	304	
6	i	277	
7	j	120	
8	k	337	

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Mol	Chain	Length	Quality of chain
9	l	270	49% 50% 50%
10	m	183	19% 95%
11	n	312	22% 54% 45%
12	o	115	96%
13	p	370	7% 53% 45%
14	q	377	5% 43% 57%
15	r	226	11% 69% 30%
16	s	309	18% 67% 32%
17	t	366	35% 52% 48%
18	u	173	10% 76% 23%
19	v	153	57% 78% 22%
20	w	127	14% 93% 6%
21	x	214	78% 22%
22	y	123	8% 58% 42%
23	z	59	22% 88% 10%
24	A	280	18% 82%
25	B	151	15% 83% 15%
26	e	207	79% 79% 21%
27	D	172	54% 54% 45%
28	E	112	11% 71% 29%
29	F	141	91% 9%
30	G	259	76% 76% 23%
31	I	132	12% 72% 27%
32	J	134	42% 85% 15%
33	K	249	20% 77% 22%

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Mol	Chain	Length	Quality of chain
34	L	206	6% 67% 33%
35	C	36	100% 100%
36	M	876	26% 49% 51%
37	N	455	43% 61% 38%
38	O	688	56% 84% 15%
39	P	530	16% 82% 17%
40	Q	820	39% 60% 39%
41	R	653	40% 57% 42%
42	S	334	34% 72% 27%
43	X	31	26% 100%
44	Y	172	85% 87% 13%
45	Z	49	43% 100%
46	1	162	22% 67% 28% 5%
47	2	86	6% 71% 27%
48	0	75	49% 49% 45% 5%
49	3	184	82% 15%
50	4	118	8% 75% 24%
51	5	149	79% 52% 42% 5%
52	6	136	70% 25% 5%
53	7	578	41% 67% 29%
54	8	413	55% 59% 34% 7%

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 103129 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal_L2_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	263	Total	C	N	O	S	0	0
			1993	1238	398	354	3		

- Molecule 2 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	304	Total	C	N	O	S	0	0
			2325	1481	430	403	11		

- Molecule 3 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	318	Total	C	N	O	S	0	0
			2497	1571	491	431	4		

- Molecule 4 is a protein called uL5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	184	Total	C	N	O	S	0	0
			1382	885	242	249	6		

- Molecule 5 is a protein called 50S ribosomal protein L9, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	f	60	Total	C	N	O	S	0	0
			464	289	92	81	2		

- Molecule 6 is a protein called Mitochondrial ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	i	152	Total	C	N	O	S	0	0
			1234	788	230	213	3		

- Molecule 7 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	j	120	941	604	173	161	3	0	0

- Molecule 8 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	k	210	1620	1018	311	286	5	0	0

- Molecule 9 is a protein called Ribosomal_L16 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	l	136	1079	689	209	176	5	0	0

- Molecule 10 is a protein called Mitochondrial ribosomal protein L17,bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	m	177	1459	911	297	248	3	0	0

- Molecule 11 is a protein called Mitochondrial ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	n	173	1406	897	262	240	7	0	0

- Molecule 12 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	o	110	890	561	180	145	4	0	0

- Molecule 13 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	p	204	1606	1022	301	281	2	0	0

- Molecule 14 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	q	161	Total	C	N	O	S	0	0
			1270	795	246	221	8		

- Molecule 15 is a protein called Mitochondrial ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	158	Total	C	N	O	S	0	0
			1335	847	256	227	5		

- Molecule 16 is a protein called KOW domain-containing protein,uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	s	210	Total	C	N	O	S	0	0
			1565	983	284	294	4		

- Molecule 17 is a protein called Ribosomal_TL5_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	t	192	Total	C	N	O	S	0	0
			1489	942	282	257	8		

- Molecule 18 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	u	133	Total	C	N	O	S	0	0
			1007	633	194	177	3		

- Molecule 19 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	v	120	Total	C	N	O	S	0	0
			997	627	196	171	3		

- Molecule 20 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	w	120	Total	C	N	O	S	0	0
			974	611	185	173	5		

- Molecule 21 is a protein called Ribosomal_L30 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	x	167	Total	C	N	O	S	0	0
			1397	882	279	232	4		

- Molecule 22 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	y	71	Total	C	N	O	S	0	0
			542	335	105	97	5		

- Molecule 23 is a protein called Mitochondrial ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	z	53	Total	C	N	O	S	0	0
			439	290	77	71	1		

- Molecule 24 is a protein called bL34m.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	A	50	Total	C	N	O	0	0
			427	259	100	68		

- Molecule 25 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B	128	Total	C	N	O	S	0	0
			1058	664	218	175	1		

- Molecule 26 is a protein called Plastid ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	e	164	Total	C	N	O	S	0	0
			1238	785	223	226	4		

- Molecule 27 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	D	94	Total	C	N	O	S	0	0
			740	467	135	134	4		

- Molecule 28 is a protein called mL41.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	E	79	Total	C	N	O	0	0
			636	409	119	108		

- Molecule 29 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F	129	Total	C	N	O	S	0	0
			1036	650	199	182	5		

- Molecule 30 is a protein called Mitochondrial ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	G	199	Total	C	N	O	S	0	0
			1482	924	268	286	4		

- Molecule 31 is a protein called mL63/57/60.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	I	97	Total	C	N	O	S	0	0
			780	490	152	133	5		

- Molecule 32 is a protein called mL59/64.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	J	114	Total	C	N	O	S	0	0
			842	529	156	154	3		

- Molecule 33 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	K	195	Total	C	N	O	S	0	0
			1571	987	305	276	3		

- Molecule 34 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L	137	Total	C	N	O	S	0	0
			1167	735	234	195	3		

- Molecule 35 is a protein called bL36m.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	C	36	Total	C	N	O	0	0
			180	108	36	36		

- Molecule 36 is a protein called mL113.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	M	430	Total	C	N	O	S	0	0
			3152	1965	617	561	9		

- Molecule 37 is a protein called mL114.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	283	Total	C	N	O	S	0	0
			2116	1337	397	377	5		

- Molecule 38 is a protein called mL115.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O	584	Total	C	N	O	S	0	0
			4260	2671	792	778	19		

- Molecule 39 is a protein called mL116.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	P	438	Total	C	N	O	S	0	0
			3151	1979	602	564	6		

- Molecule 40 is a protein called mL117.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Q	498	Total	C	N	O	S	0	0
			3073	1893	581	587	12		

- Molecule 41 is a protein called mL118.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	R	376	Total	C	N	O	S	0	0
			2594	1616	511	461	6		

- Molecule 42 is a protein called mL119.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	S	244	1967	1211	376	362	18	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	257	THR	GLY	conflict	UNP A0A2K3D424

- Molecule 43 is a protein called Unk1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	X	31	155	93	31	31	0	0

- Molecule 44 is a protein called PPR*.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	Y	149	745	447	149	149	0	0

- Molecule 45 is a protein called Unk2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	Z	49	245	147	49	49	0	0

- Molecule 46 is a RNA chain called L1 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
46	1	162	3440	1541	607	1130	162	0	0

- Molecule 47 is a RNA chain called L2a rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
47	2	86	1821	816	311	608	86	0	0

- Molecule 48 is a RNA chain called L3a rRNA (5S).

Mol	Chain	Residues	Atoms					AltConf	Trace
48	0	75	Total	C	N	O	P	0	0
			1592	713	280	524	75		

- Molecule 49 is a RNA chain called L3b rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3	184	Total	C	N	O	P	0	0
			3933	1757	709	1283	184		

- Molecule 50 is a RNA chain called L4 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	4	118	Total	C	N	O	P	0	0
			2538	1135	478	807	118		

- Molecule 51 is a RNA chain called L5 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	5	149	Total	C	N	O	P	0	0
			3156	1412	545	1050	149		

- Molecule 52 is a RNA chain called L6 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	6	136	Total	C	N	O	P	0	0
			2913	1306	542	929	136		

- Molecule 53 is a RNA chain called L7 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	7	578	Total	C	N	O	P	0	0
			12344	5521	2237	4008	578		

- Molecule 54 is a RNA chain called L8 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	8	413	Total	C	N	O	P	0	0
			8792	3931	1558	2890	413		

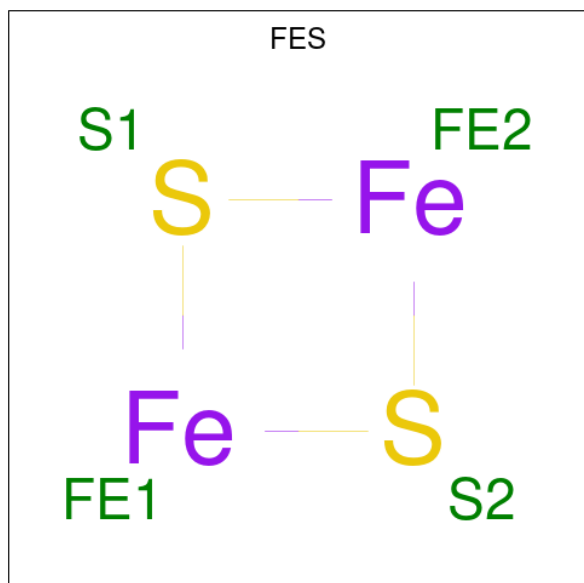
- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
55	y	1	Total Zn 1 1	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
56	Q	1	Total Mg 1 1	0
56	1	6	Total Mg 6 6	0
56	2	7	Total Mg 7 7	0
56	0	1	Total Mg 1 1	0
56	3	12	Total Mg 12 12	0
56	4	8	Total Mg 8 8	0
56	5	3	Total Mg 3 3	0
56	6	6	Total Mg 6 6	0
56	7	18	Total Mg 18 18	0
56	8	7	Total Mg 7 7	0

- Molecule 57 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

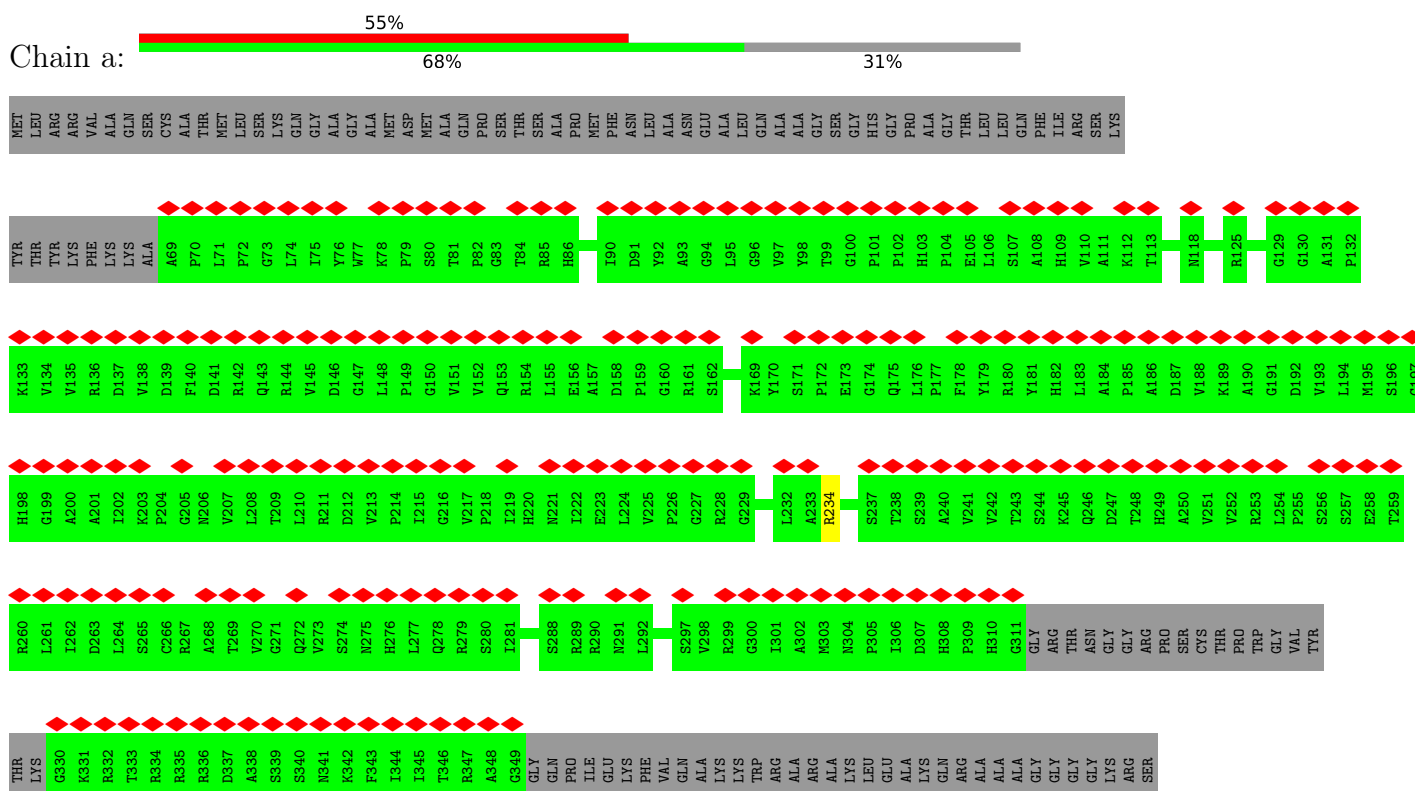


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
57	S	1	4	2	2	0

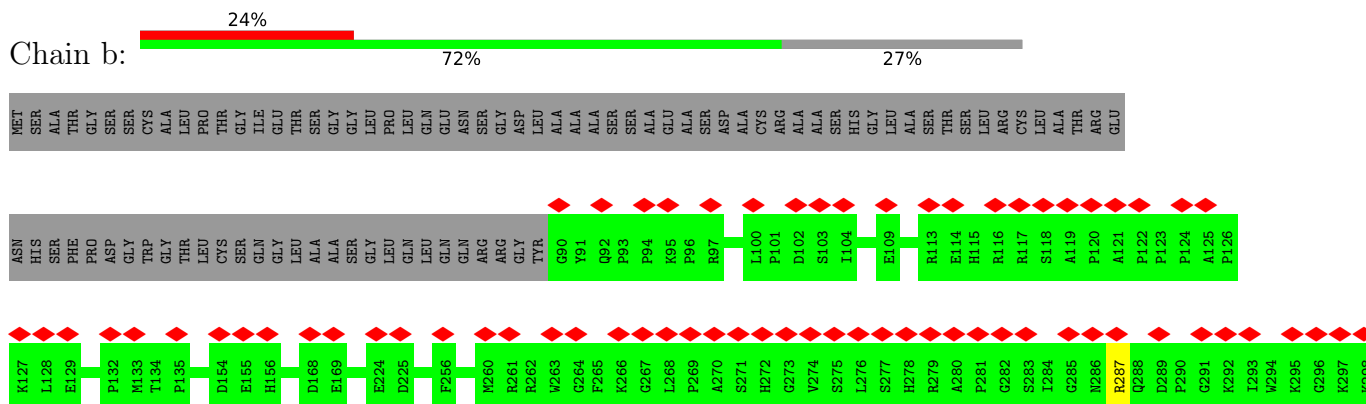
3 Residue-property plots

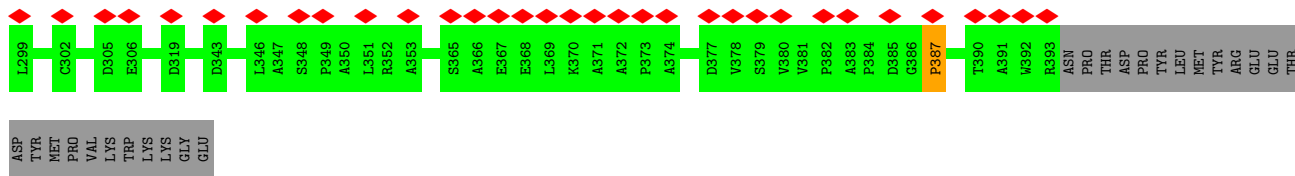
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ribosomal_L2_C domain-containing protein

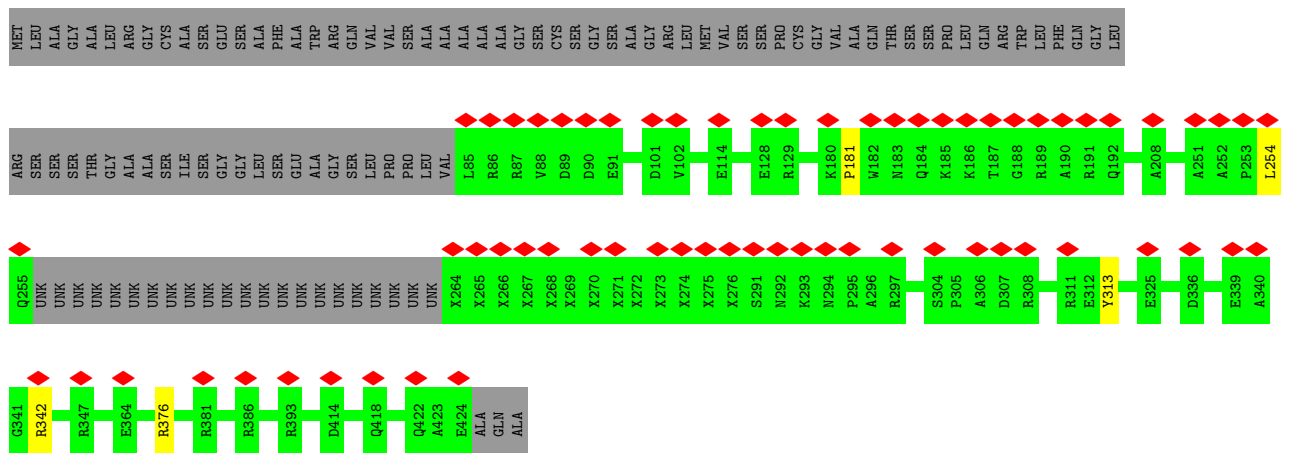
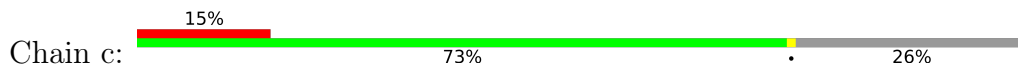


• Molecule 2: uL3m

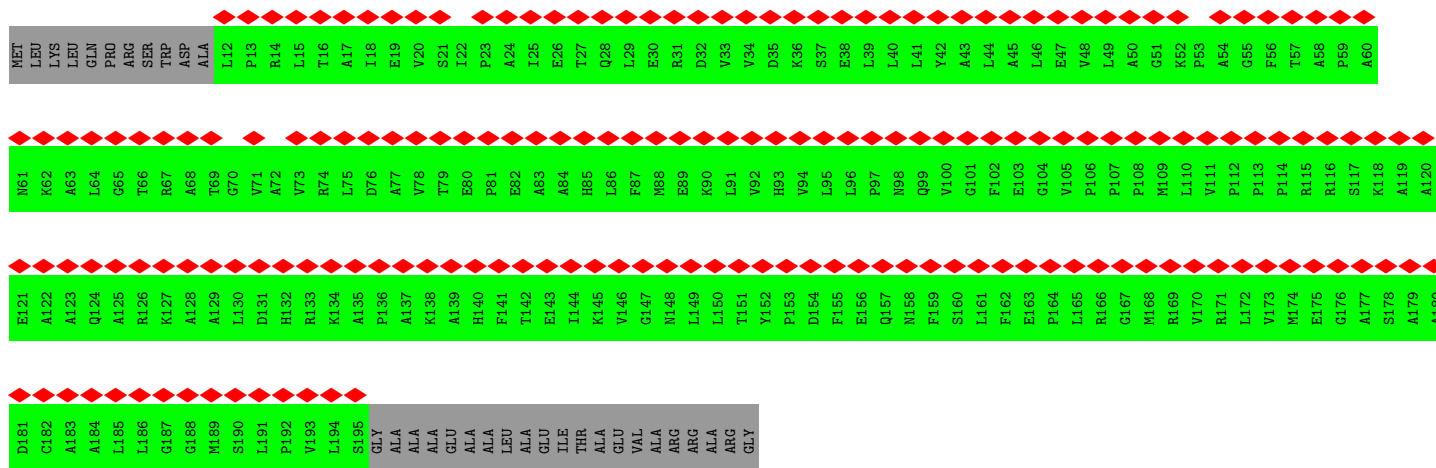
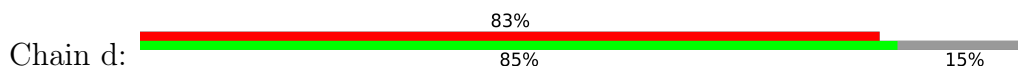




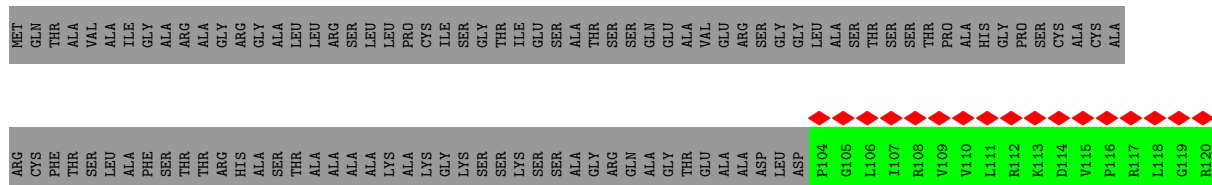
• Molecule 3: uL4m

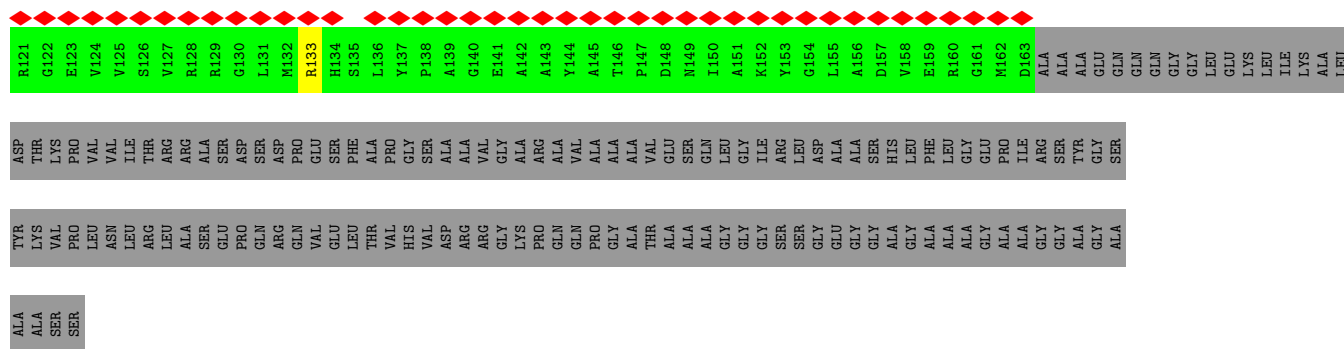


• Molecule 4: uL5m

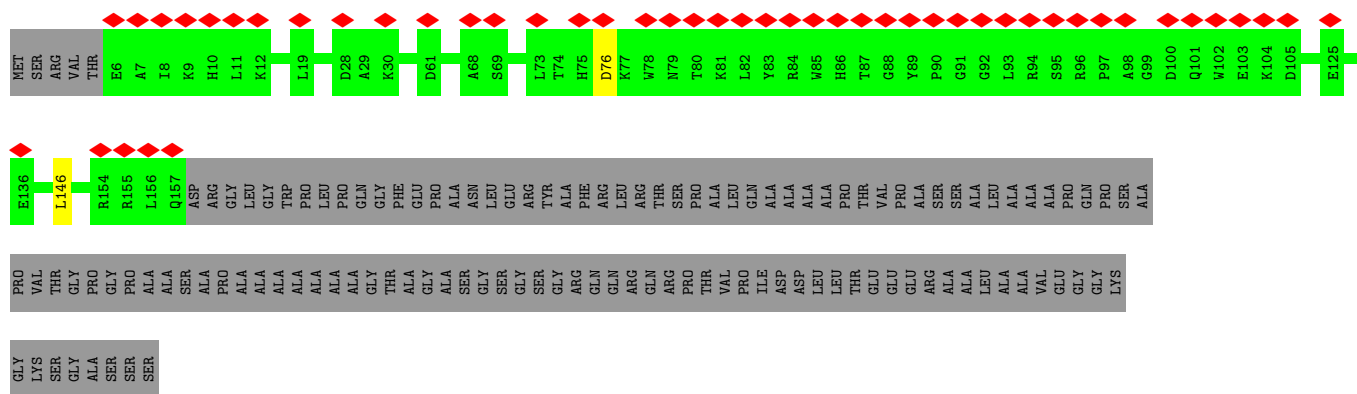


• Molecule 5: 50S ribosomal protein L9, chloroplactic

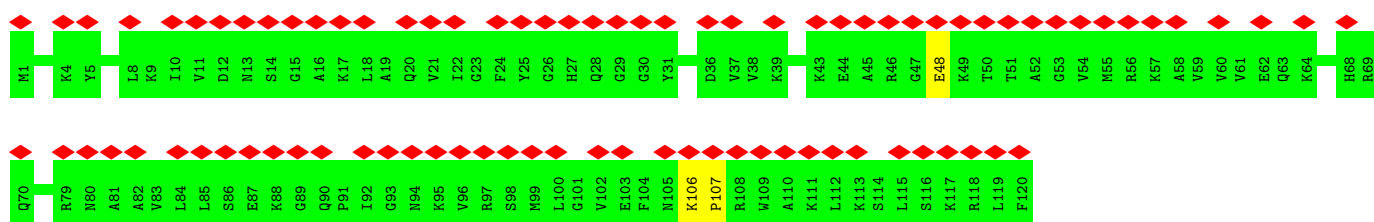




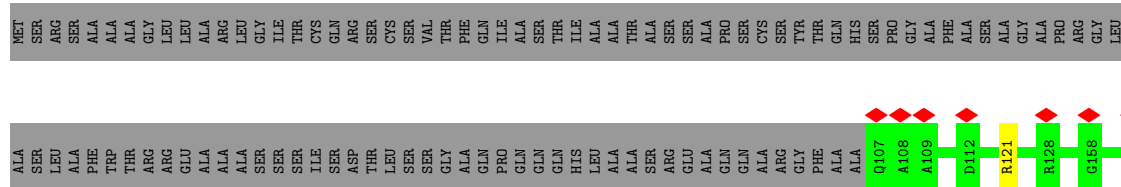
• Molecule 6: Mitochondrial ribosomal protein L13

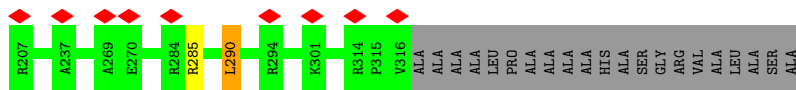


• Molecule 7: uL14m

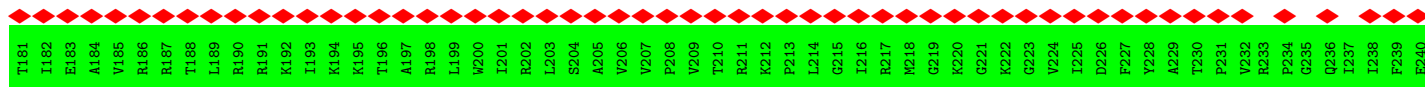
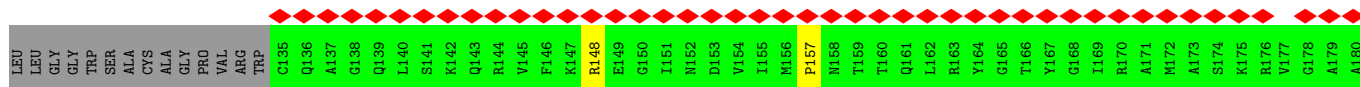
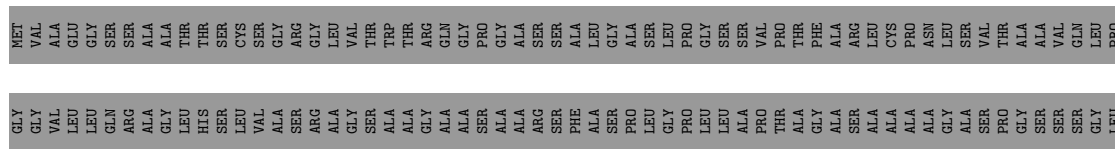


• Molecule 8: Ribosomal_L18e/L15P domain-containing protein

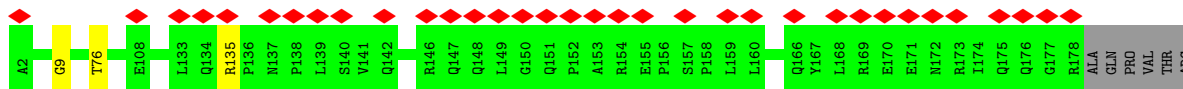




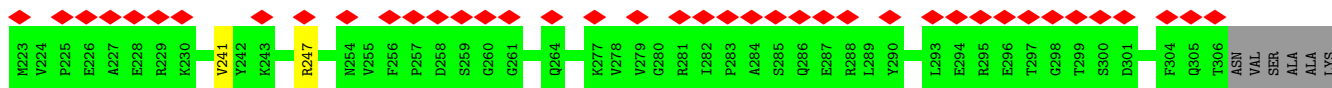
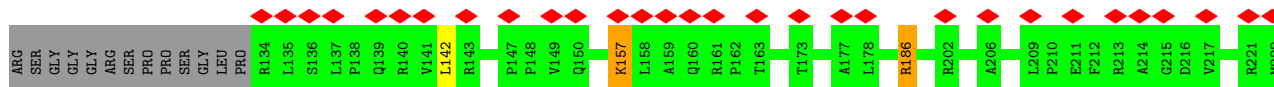
• Molecule 9: Ribosomal_L16 domain-containing protein



• Molecule 10: Mitochondrial ribosomal protein L17,bL17m

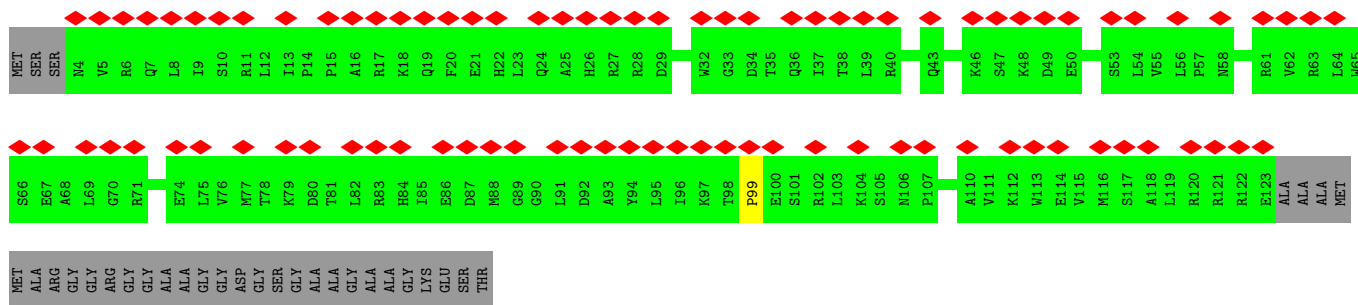


• Molecule 11: Mitochondrial ribosomal protein L19

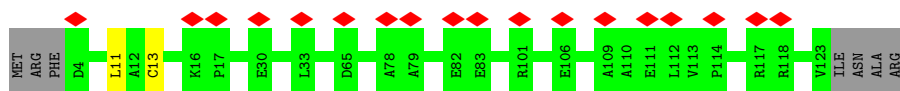


• Molecule 12: 50S ribosomal protein L20

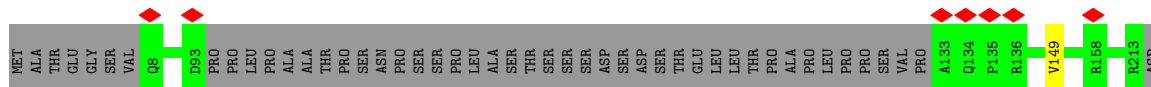
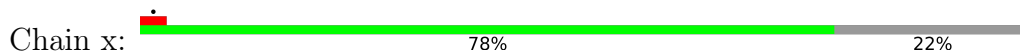




- Molecule 20: uL29m



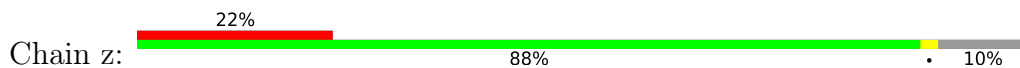
- Molecule 21: Ribosomal_L30 domain-containing protein



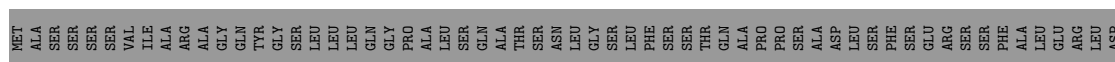
- Molecule 22: bL32m

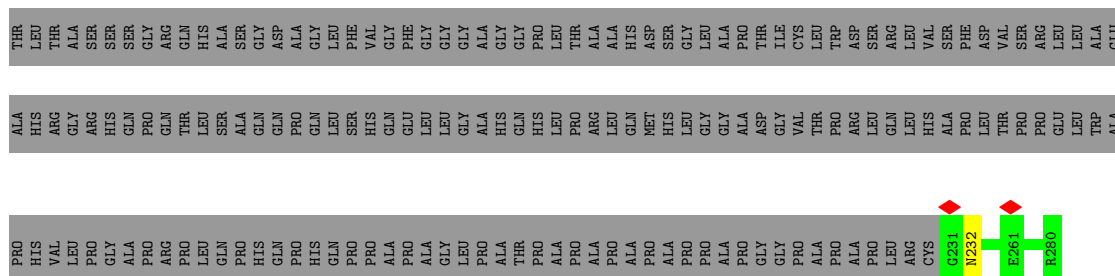


- Molecule 23: Mitochondrial ribosomal protein L33

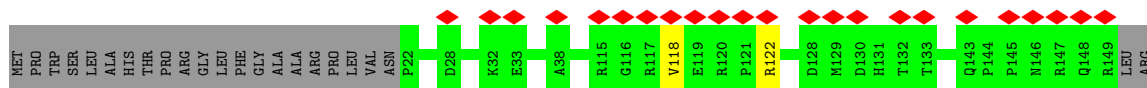
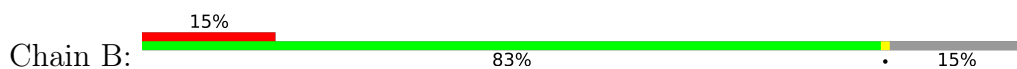


- Molecule 24: bL34m

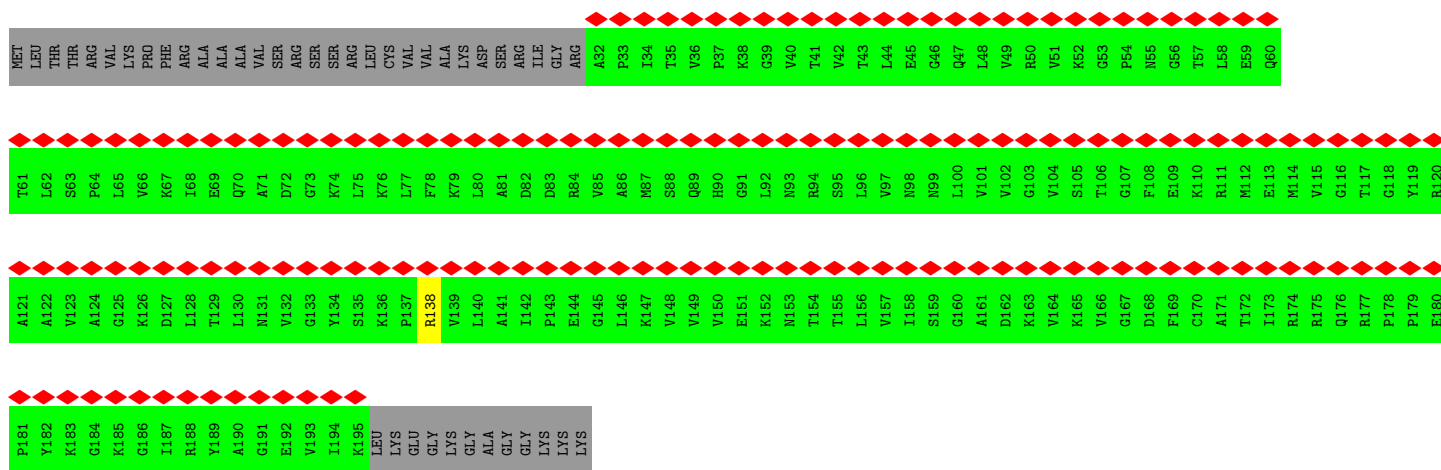
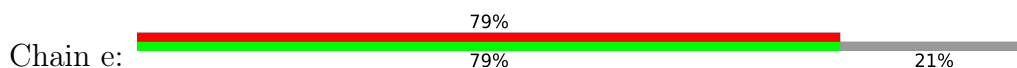




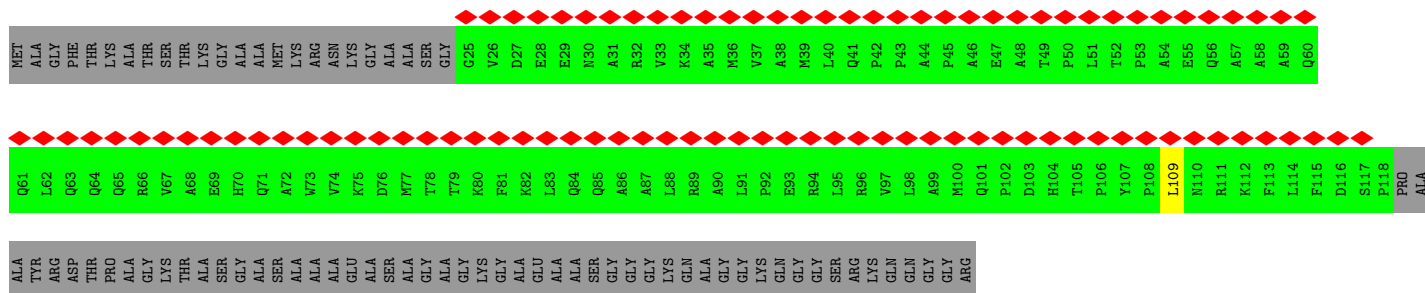
• Molecule 25: bL35m



• Molecule 26: Plastid ribosomal protein L6

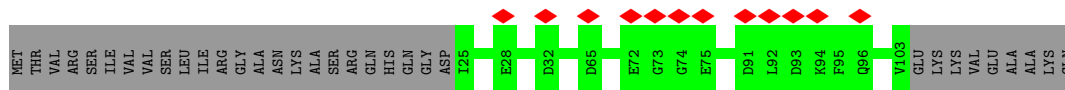


• Molecule 27: mL40

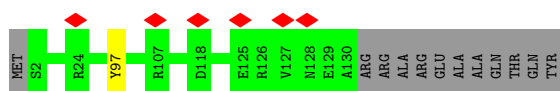
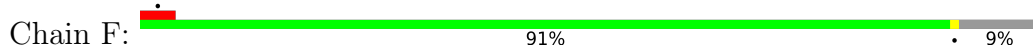


• Molecule 28: mL41

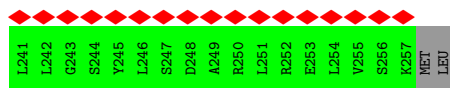
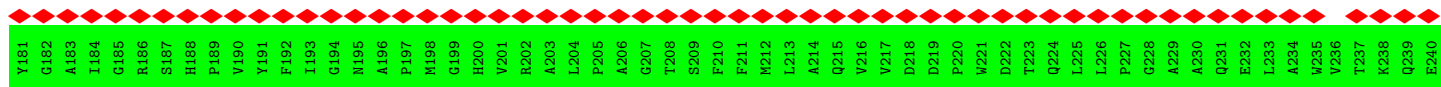
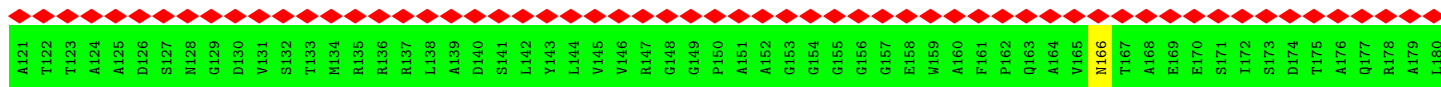
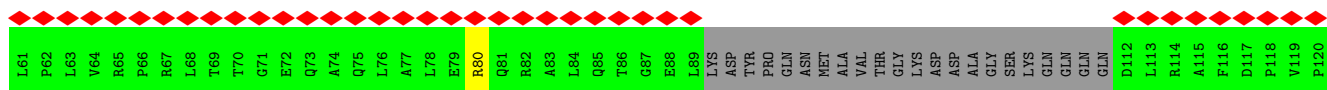
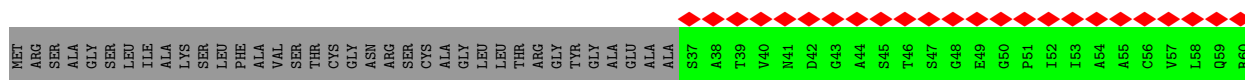




• Molecule 29: mL43



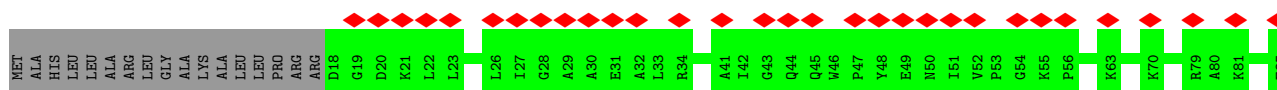
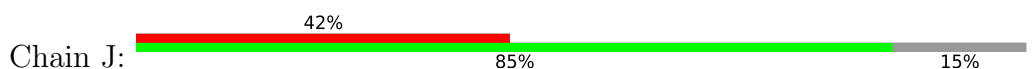
• Molecule 30: Mitochondrial ribosomal protein L17

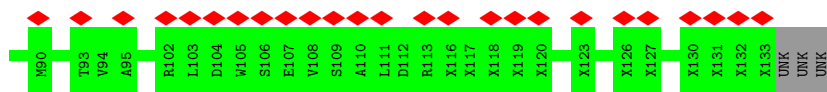


• Molecule 31: mL63/57/60

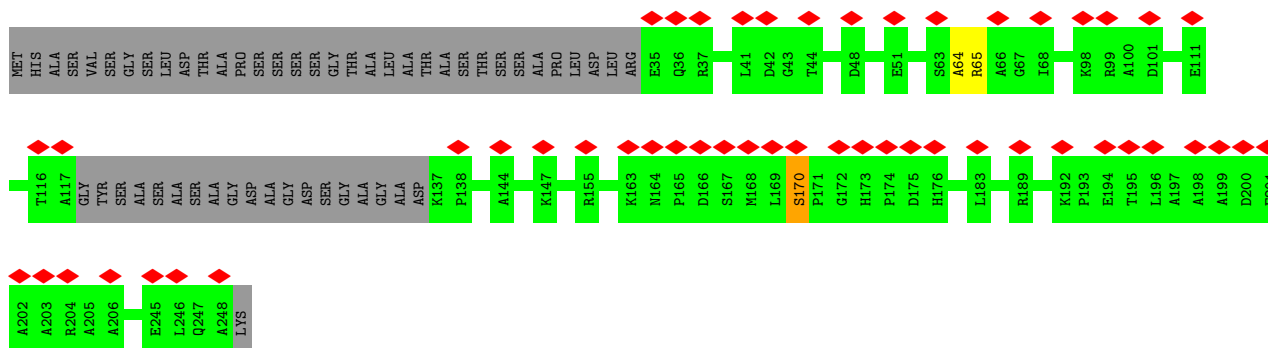
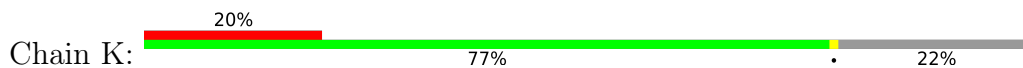


• Molecule 32: mL59/64

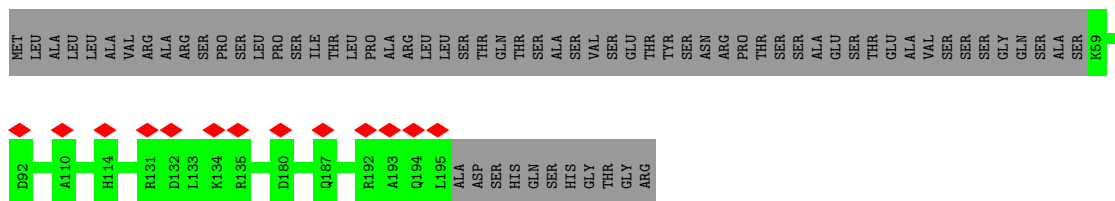




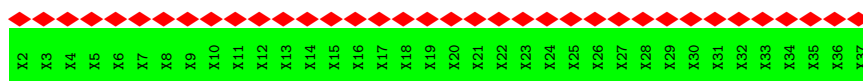
• Molecule 33: mL80



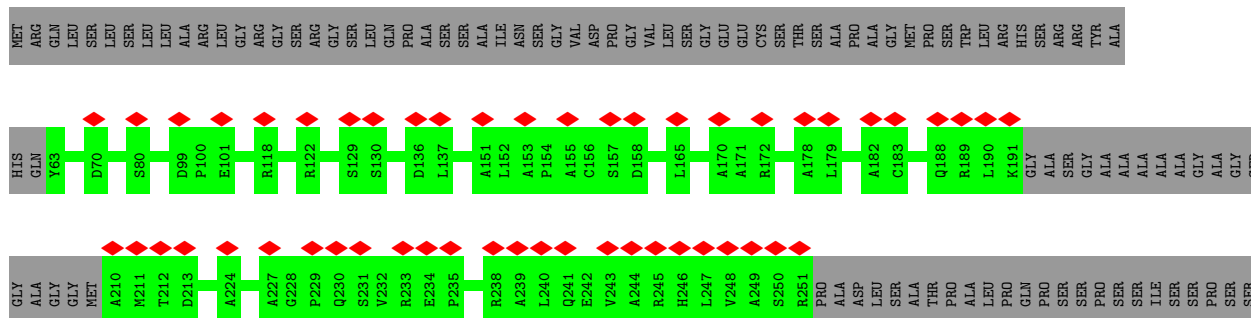
• Molecule 34: mL87

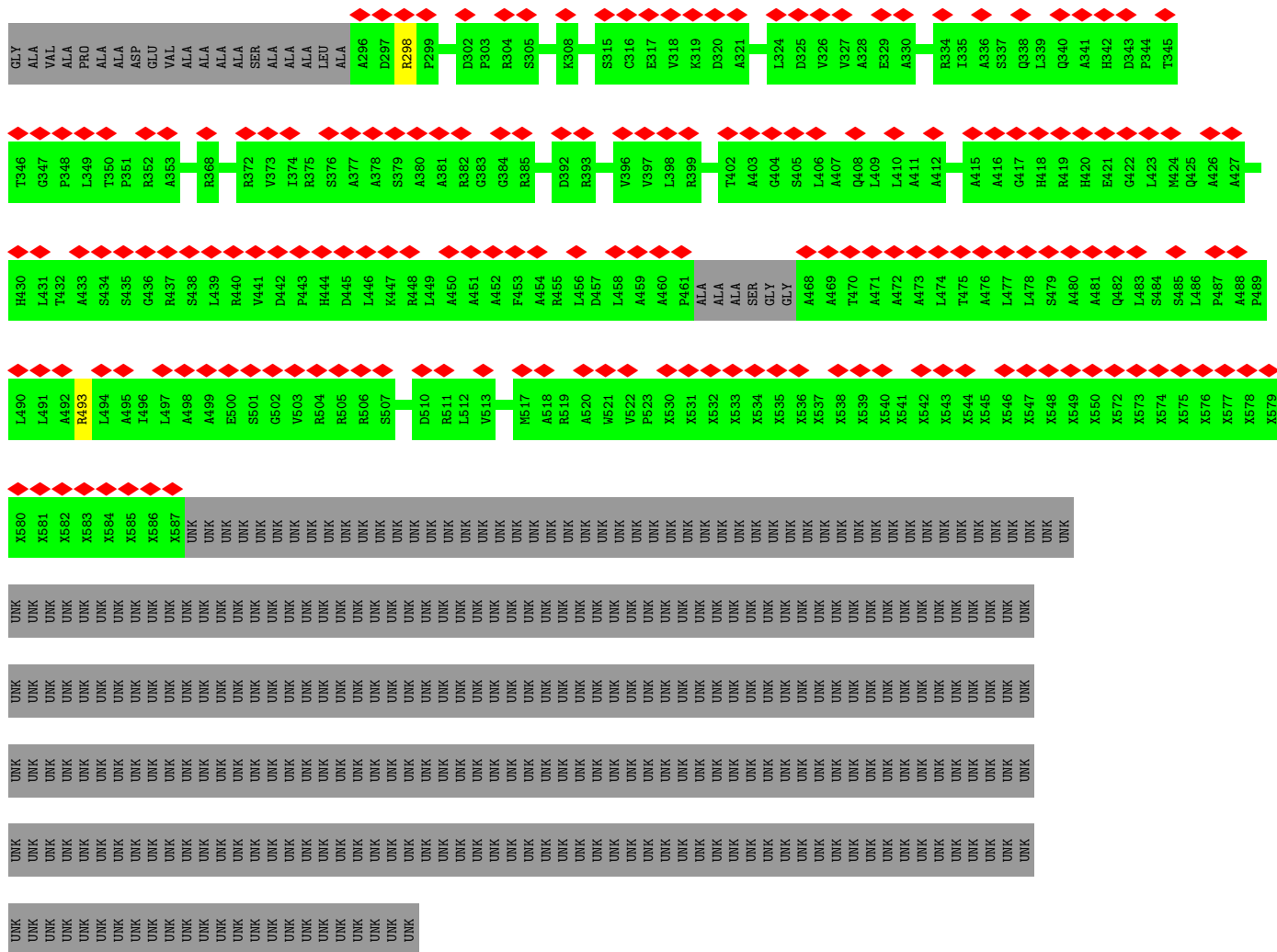


• Molecule 35: bL36m

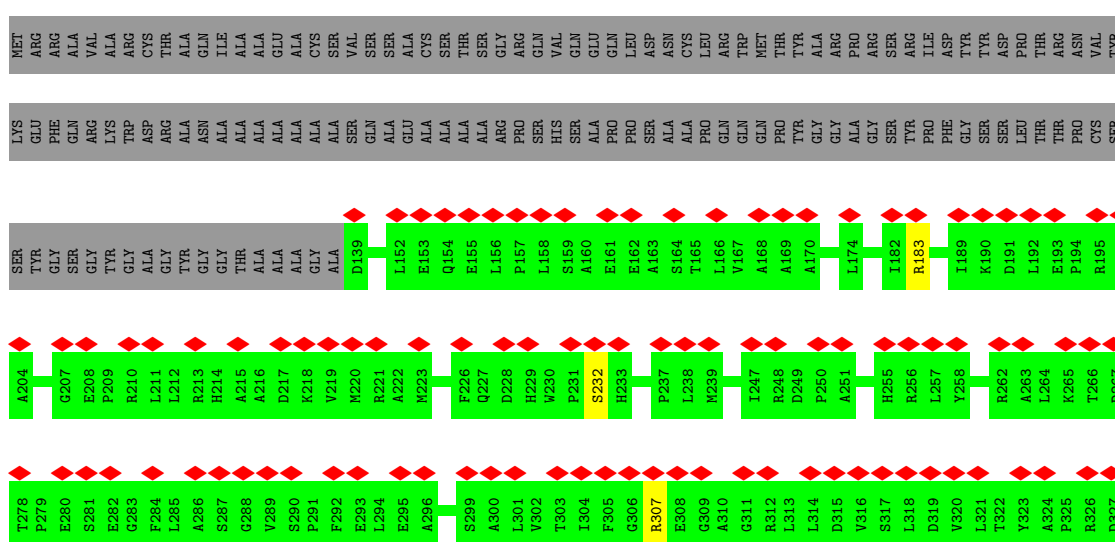
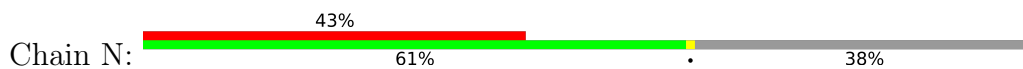


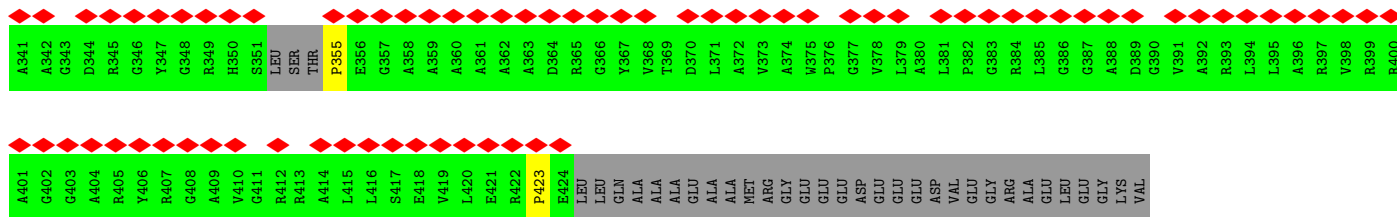
• Molecule 36: mL113



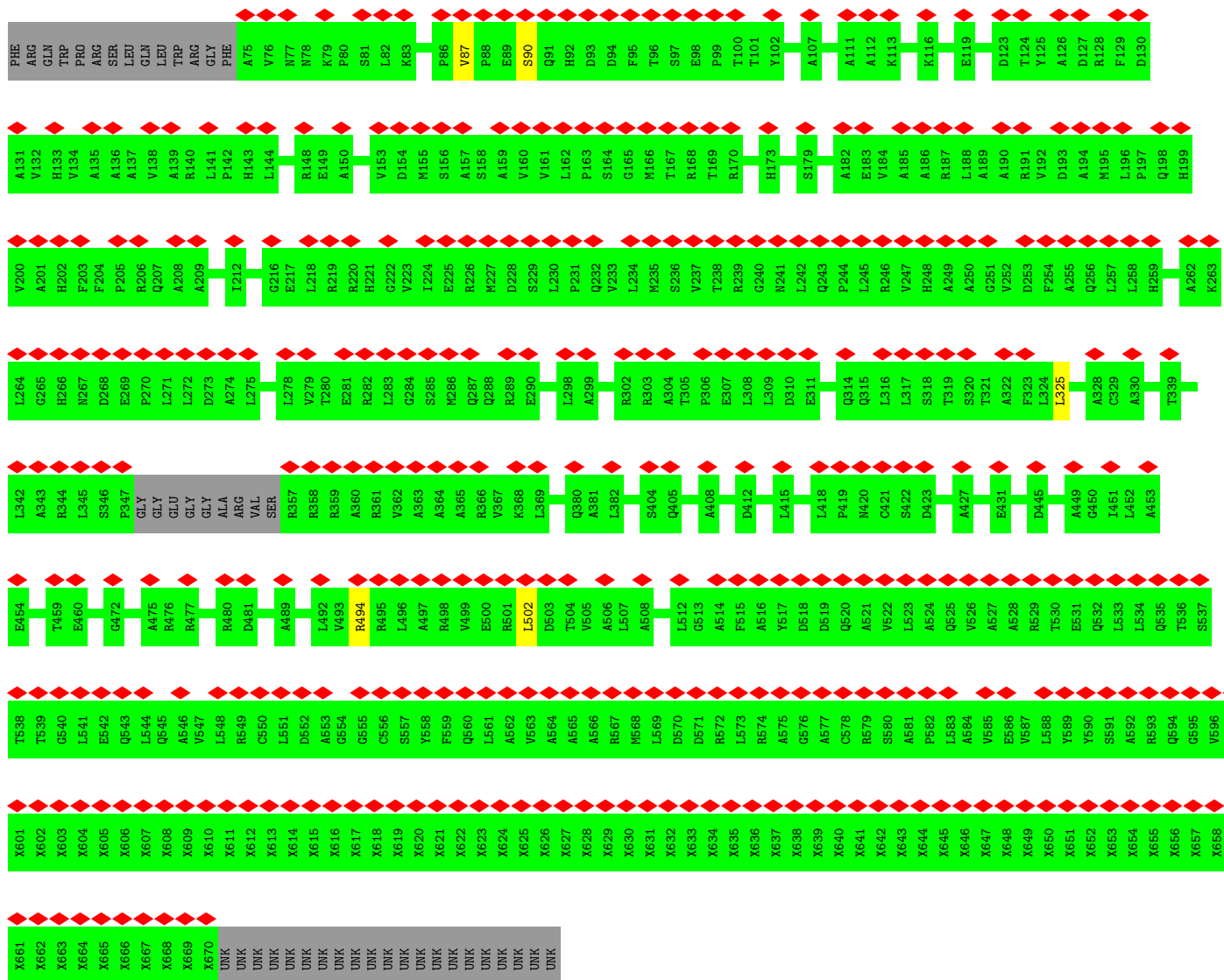
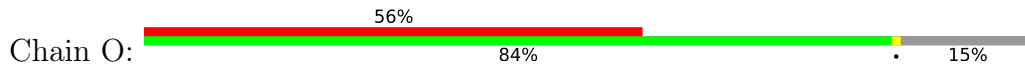


● Molecule 37: mL114

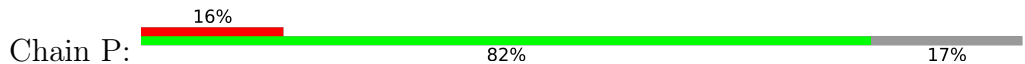


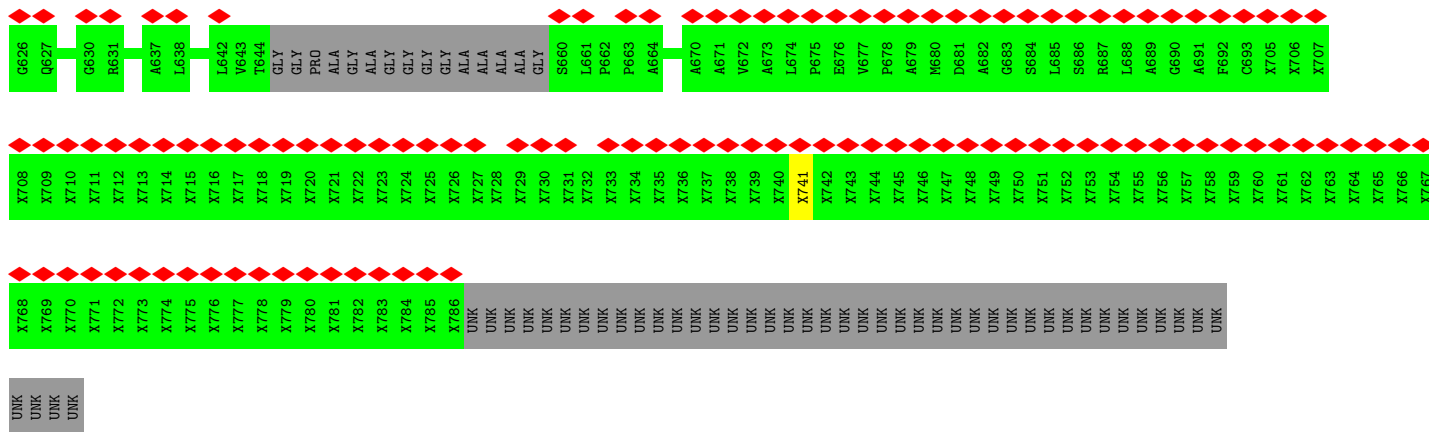


• Molecule 38: mL115

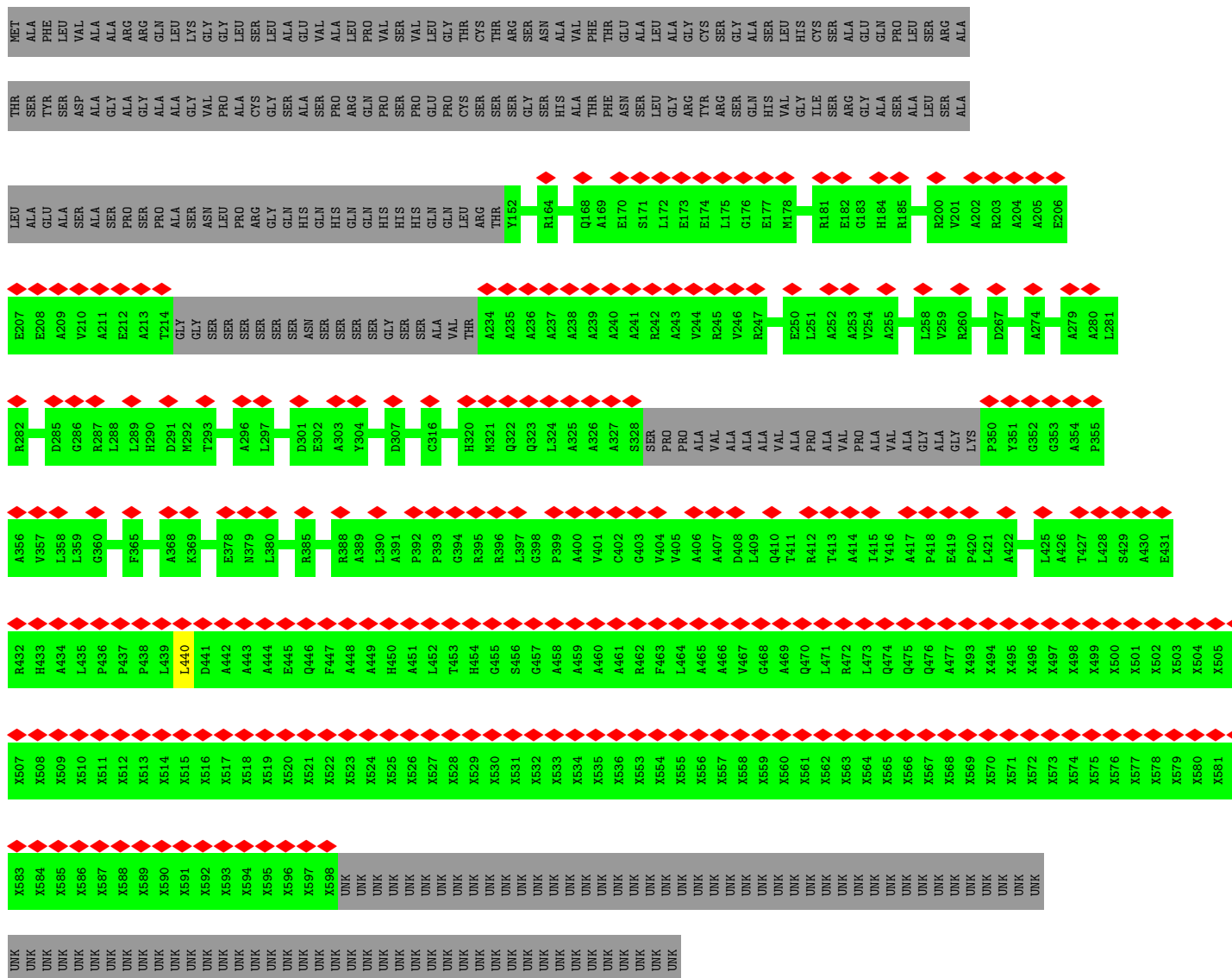
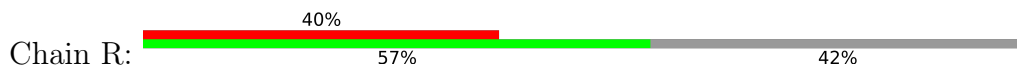


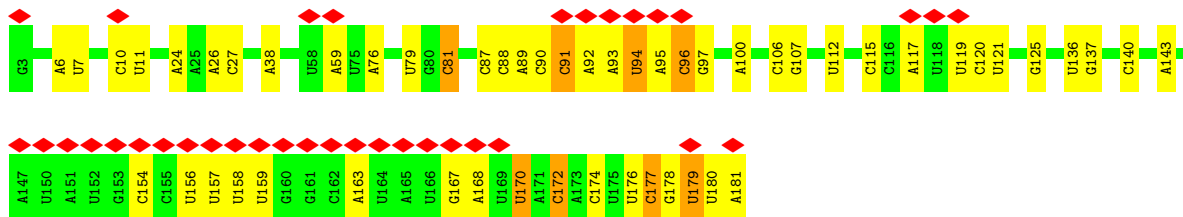
• Molecule 39: mL116



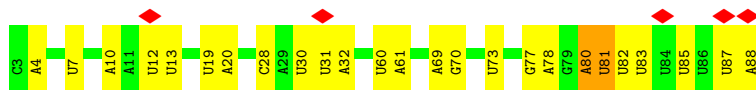


• Molecule 41: mL118





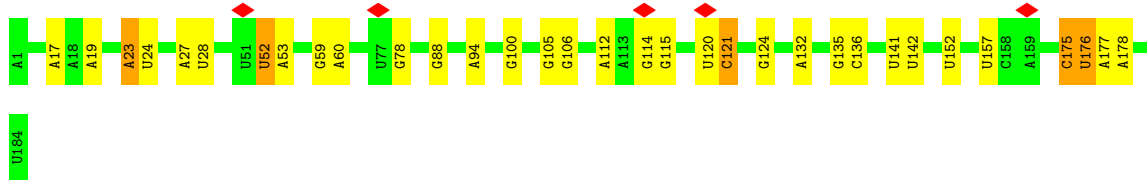
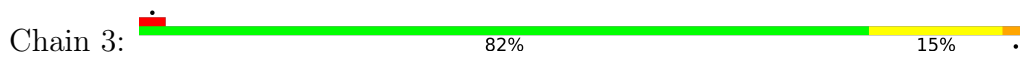
• Molecule 47: L2a rRNA



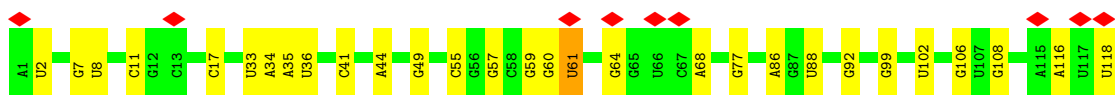
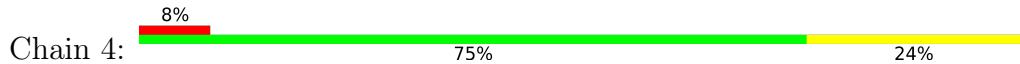
• Molecule 48: L3a rRNA (5S)



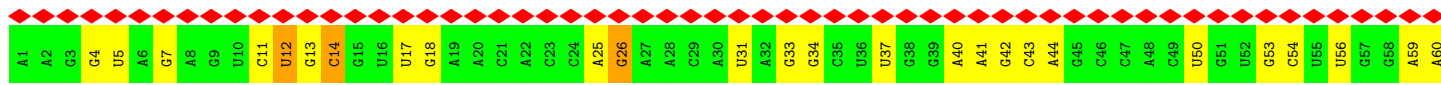
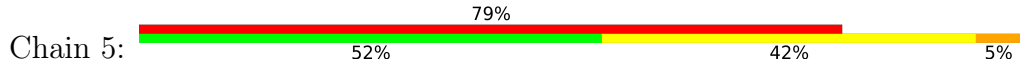
• Molecule 49: L3b rRNA



• Molecule 50: L4 rRNA

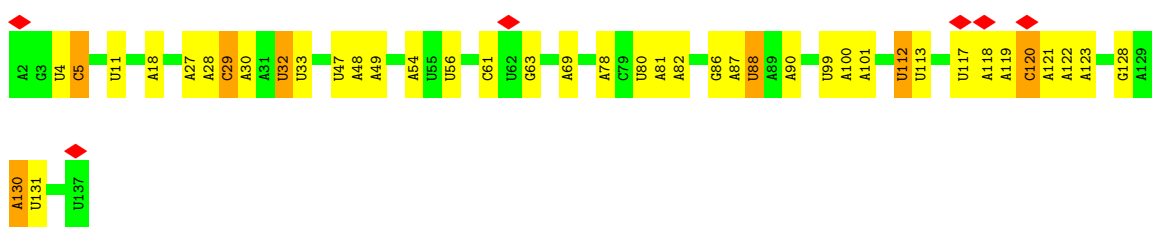


• Molecule 51: L5 rRNA

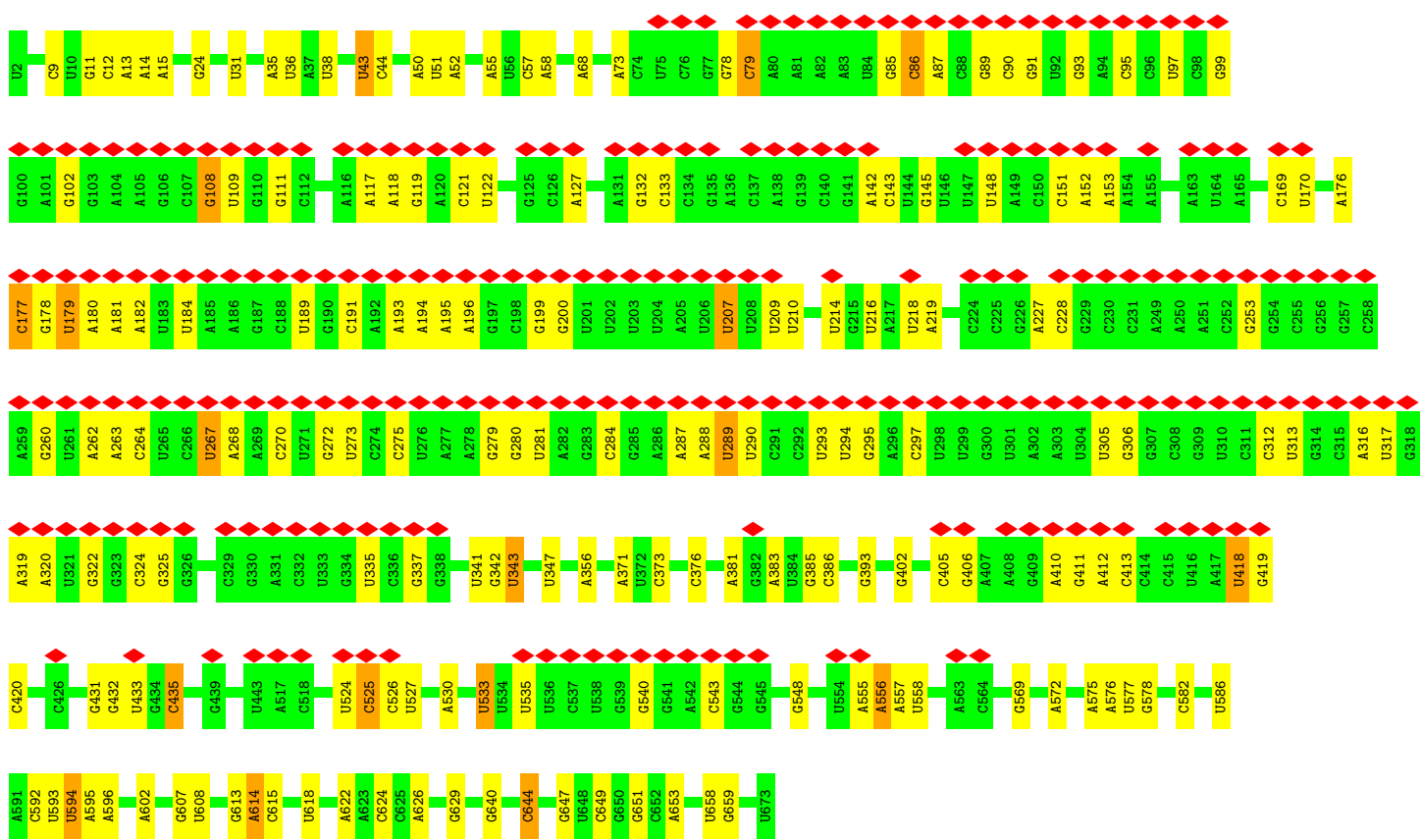
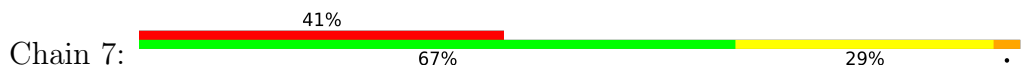




• Molecule 52: L6 rRNA

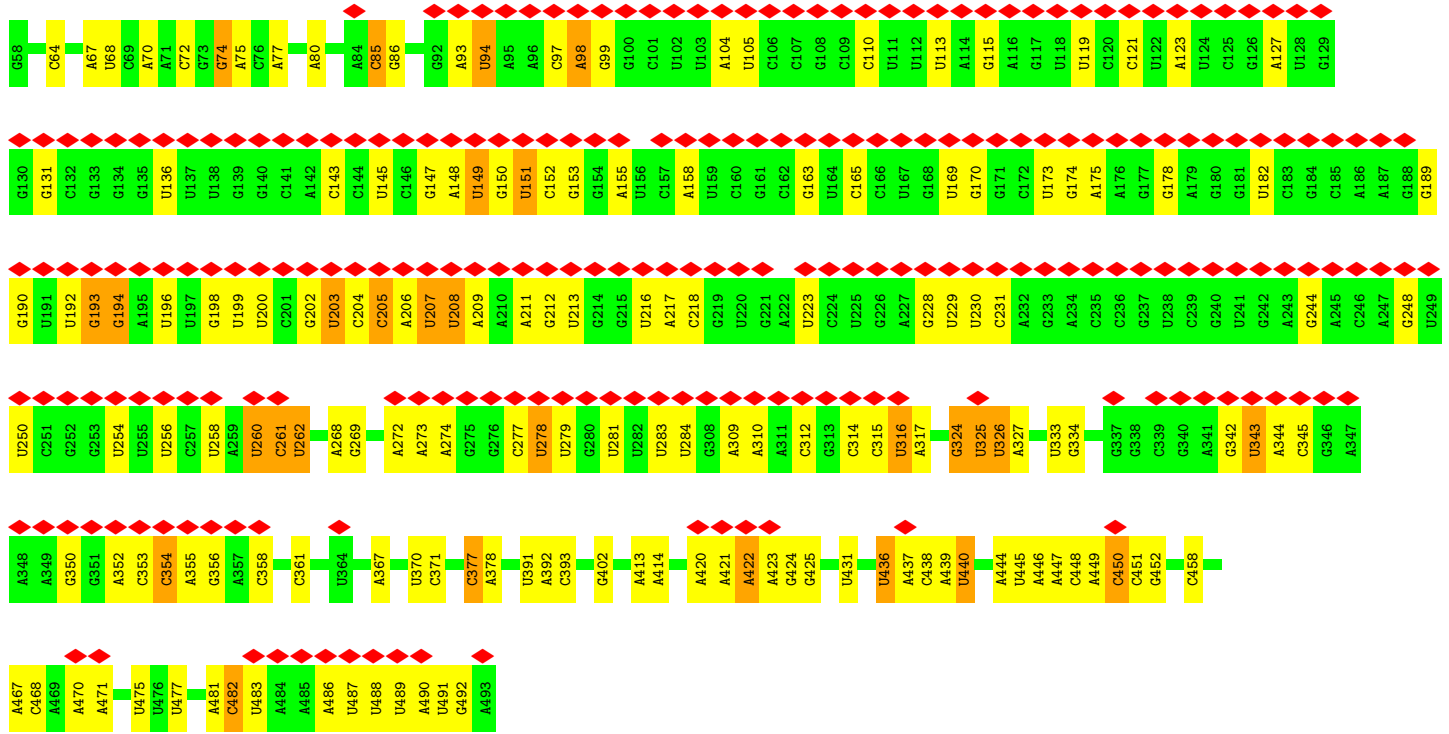


• Molecule 53: L7 rRNA



• Molecule 54: L8 rRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101291	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.092	Depositor
Minimum map value	-0.045	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	432.0, 432.0, 432.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9, 0.9, 0.9	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.61	0/2039	0.73	1/2766 (0.0%)
2	b	0.59	0/2397	0.75	1/3264 (0.0%)
3	c	0.60	0/2492	0.76	1/3374 (0.0%)
4	d	0.64	0/1410	0.78	0/1918
5	f	0.63	0/471	0.82	0/633
6	i	0.32	0/1266	0.65	2/1711 (0.1%)
7	j	0.63	0/959	0.77	1/1284 (0.1%)
8	k	0.58	0/1655	0.76	0/2237
9	l	0.60	0/1098	0.71	0/1474
10	m	0.60	0/1488	0.79	1/2009 (0.0%)
11	n	0.60	0/1440	0.87	4/1954 (0.2%)
12	o	0.36	0/905	0.64	0/1211
13	p	0.58	0/1640	0.83	2/2231 (0.1%)
14	q	0.38	0/1300	0.67	0/1754
15	r	0.36	0/1370	0.69	1/1854 (0.1%)
16	s	0.61	0/1442	0.76	0/1958
17	t	0.63	0/1517	0.79	0/2057
18	u	0.59	0/994	0.75	1/1342 (0.1%)
19	v	0.30	0/1017	0.68	0/1372
20	w	0.58	0/992	0.71	0/1339
21	x	0.39	1/1434 (0.1%)	0.65	0/1933
22	y	0.63	0/555	0.81	0/748
23	z	0.35	0/449	0.78	0/600
24	A	0.34	0/433	0.73	0/575
25	B	0.57	0/1094	0.74	0/1481
26	e	0.64	0/1254	0.75	0/1692
27	D	0.29	0/757	0.69	1/1030 (0.1%)
28	E	0.57	0/650	0.71	0/877
29	F	0.36	0/1058	0.68	0/1428
30	G	0.60	0/1509	0.68	0/2054
31	I	0.33	0/795	0.73	2/1069 (0.2%)
32	J	0.60	0/769	0.78	0/1039

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	K	0.58	0/1615	0.72	0/2192
34	L	0.35	0/1205	0.63	0/1630
36	M	0.58	0/3027	0.70	0/4123
37	N	0.64	1/2163 (0.0%)	0.77	2/2937 (0.1%)
38	O	0.31	0/3974	0.71	2/5407 (0.0%)
39	P	0.31	0/3195	0.73	3/4362 (0.1%)
40	Q	3.55	6/1969 (0.3%)	0.74	2/2668 (0.1%)
41	R	0.31	0/2184	0.72	1/2967 (0.0%)
42	S	0.35	0/1947	0.74	1/2603 (0.0%)
46	1	0.59	0/3844	1.29	61/5979 (1.0%)
47	2	0.60	0/2034	0.99	4/3164 (0.1%)
48	0	0.44	0/1779	1.28	18/2768 (0.7%)
49	3	0.58	0/4401	1.10	17/6859 (0.2%)
50	4	0.64	0/2846	1.16	24/4437 (0.5%)
51	5	0.44	0/3522	1.24	36/5477 (0.7%)
52	6	0.66	0/3266	1.16	29/5088 (0.6%)
53	7	0.45	0/13815	1.12	110/21523 (0.5%)
54	8	0.43	0/9830	1.21	117/15312 (0.8%)
All	All	0.70	8/105265 (0.0%)	0.96	445/151764 (0.3%)

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
8	k	0	1
13	p	0	1
19	v	0	1
23	z	0	1
29	F	0	1
33	K	0	2
38	O	0	2
40	Q	0	2
42	S	0	1
All	All	0	12

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	Q	556	ARG	CZ-NH2	151.26	3.29	1.33
40	Q	608	HIS	CG-CD2	22.03	1.73	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	Q	608	HIS	CG-ND1	20.18	1.83	1.38
40	Q	608	HIS	CD2-NE2	18.87	1.81	1.42
40	Q	608	HIS	CE1-NE2	15.09	1.67	1.32

The worst 5 of 445 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	8	450	C	N1-C2-O2	13.02	126.71	118.90
40	Q	556	ARG	NE-CZ-NH1	-12.68	113.96	120.30
54	8	450	C	C2-N1-C1'	12.01	132.01	118.80
54	8	325	U	C2-N1-C1'	11.43	131.42	117.70
49	3	175	C	N1-C2-O2	11.37	125.72	118.90

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	F	97	TYR	Peptide
8	k	290	LEU	Mainchain
13	p	265	ARG	Mainchain
19	v	99	PRO	Peptide
23	z	19	ALA	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
1	a	259/383 (68%)	251 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	302/417 (72%)	284 (94%)	16 (5%)	2 (1%)	22	60
3	c	301/427 (70%)	288 (96%)	11 (4%)	2 (1%)	22	60
4	d	182/216 (84%)	168 (92%)	14 (8%)	0	100	100
5	f	58/304 (19%)	54 (93%)	4 (7%)	0	100	100
6	i	150/277 (54%)	139 (93%)	11 (7%)	0	100	100
7	j	118/120 (98%)	109 (92%)	8 (7%)	1 (1%)	19	57
8	k	208/337 (62%)	198 (95%)	8 (4%)	2 (1%)	15	53
9	l	134/270 (50%)	127 (95%)	6 (4%)	1 (1%)	22	60
10	m	175/183 (96%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	n	171/312 (55%)	163 (95%)	6 (4%)	2 (1%)	13	48
12	o	108/115 (94%)	107 (99%)	1 (1%)	0	100	100
13	p	200/370 (54%)	187 (94%)	11 (6%)	2 (1%)	15	53
14	q	159/377 (42%)	150 (94%)	9 (6%)	0	100	100
15	r	154/226 (68%)	142 (92%)	11 (7%)	1 (1%)	25	64
16	s	177/309 (57%)	159 (90%)	16 (9%)	2 (1%)	14	50
17	t	186/366 (51%)	172 (92%)	14 (8%)	0	100	100
18	u	124/173 (72%)	121 (98%)	2 (2%)	1 (1%)	19	57
19	v	118/153 (77%)	107 (91%)	11 (9%)	0	100	100
20	w	118/127 (93%)	110 (93%)	8 (7%)	0	100	100
21	x	163/214 (76%)	157 (96%)	6 (4%)	0	100	100
22	y	69/123 (56%)	63 (91%)	6 (9%)	0	100	100
23	z	51/59 (86%)	48 (94%)	3 (6%)	0	100	100
24	A	48/280 (17%)	46 (96%)	2 (4%)	0	100	100
25	B	126/151 (83%)	116 (92%)	9 (7%)	1 (1%)	19	57
26	e	162/207 (78%)	150 (93%)	12 (7%)	0	100	100
27	D	92/172 (54%)	80 (87%)	12 (13%)	0	100	100
28	E	77/112 (69%)	74 (96%)	3 (4%)	0	100	100
29	F	127/141 (90%)	116 (91%)	11 (9%)	0	100	100
30	G	195/259 (75%)	184 (94%)	11 (6%)	0	100	100
31	I	95/132 (72%)	93 (98%)	2 (2%)	0	100	100
32	J	94/134 (70%)	84 (89%)	10 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	K	191/249 (77%)	184 (96%)	6 (3%)	1 (0%)	29	68
34	L	135/206 (66%)	126 (93%)	9 (7%)	0	100	100
36	M	385/876 (44%)	368 (96%)	17 (4%)	0	100	100
37	N	279/455 (61%)	262 (94%)	16 (6%)	1 (0%)	34	72
38	O	509/688 (74%)	459 (90%)	50 (10%)	0	100	100
39	P	430/530 (81%)	400 (93%)	30 (7%)	0	100	100
40	Q	260/820 (32%)	237 (91%)	23 (9%)	0	100	100
41	R	280/653 (43%)	264 (94%)	16 (6%)	0	100	100
42	S	230/334 (69%)	210 (91%)	20 (9%)	0	100	100
All	All	7400/12257 (60%)	6926 (94%)	454 (6%)	20 (0%)	44	76

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	p	221	ALA
13	p	266	PRO
2	b	287	ARG
3	c	181	PRO
10	m	9	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	209/295 (71%)	209 (100%)	0	100	100
2	b	244/331 (74%)	244 (100%)	0	100	100
3	c	254/313 (81%)	252 (99%)	2 (1%)	81	93
4	d	144/164 (88%)	144 (100%)	0	100	100
5	f	47/209 (22%)	46 (98%)	1 (2%)	53	82
6	i	133/214 (62%)	133 (100%)	0	100	100
7	j	99/99 (100%)	98 (99%)	1 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	k	165/247 (67%)	164 (99%)	1 (1%)	86	95
9	l	112/197 (57%)	111 (99%)	1 (1%)	78	92
10	m	152/157 (97%)	151 (99%)	1 (1%)	84	94
11	n	153/245 (62%)	151 (99%)	2 (1%)	69	89
12	o	93/96 (97%)	93 (100%)	0	100	100
13	p	172/303 (57%)	168 (98%)	4 (2%)	50	80
14	q	128/269 (48%)	128 (100%)	0	100	100
15	r	143/184 (78%)	143 (100%)	0	100	100
16	s	156/157 (99%)	155 (99%)	1 (1%)	86	95
17	t	161/287 (56%)	160 (99%)	1 (1%)	86	95
18	u	100/122 (82%)	100 (100%)	0	100	100
19	v	109/122 (89%)	109 (100%)	0	100	100
20	w	106/112 (95%)	104 (98%)	2 (2%)	57	84
21	x	148/189 (78%)	148 (100%)	0	100	100
22	y	56/104 (54%)	56 (100%)	0	100	100
23	z	49/54 (91%)	49 (100%)	0	100	100
24	A	45/219 (20%)	44 (98%)	1 (2%)	52	81
25	B	108/126 (86%)	107 (99%)	1 (1%)	78	92
26	e	135/168 (80%)	134 (99%)	1 (1%)	84	94
27	D	77/116 (66%)	77 (100%)	0	100	100
28	E	66/93 (71%)	66 (100%)	0	100	100
29	F	112/121 (93%)	112 (100%)	0	100	100
30	G	151/195 (77%)	149 (99%)	2 (1%)	69	89
31	I	82/105 (78%)	82 (100%)	0	100	100
32	J	75/87 (86%)	75 (100%)	0	100	100
33	K	158/193 (82%)	157 (99%)	1 (1%)	86	95
34	L	115/172 (67%)	115 (100%)	0	100	100
36	M	287/369 (78%)	285 (99%)	2 (1%)	84	94
37	N	201/335 (60%)	199 (99%)	2 (1%)	76	91
38	O	403/466 (86%)	402 (100%)	1 (0%)	93	98
39	P	301/353 (85%)	301 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	Q	191/313 (61%)	191 (100%)	0	100	100
41	R	199/336 (59%)	199 (100%)	0	100	100
42	S	206/254 (81%)	206 (100%)	0	100	100
All	All	6045/8491 (71%)	6017 (100%)	28 (0%)	89	96

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	t	120	ARG
38	O	494	ARG
24	A	232	ASN
36	M	493	ARG
20	w	13	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
20	w	94	GLN
26	e	93	ASN
38	O	315	GLN
33	K	173	HIS
38	O	256	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	1	159/162 (98%)	43 (27%)	1 (0%)
47	2	85/86 (98%)	24 (28%)	2 (2%)
48	0	74/75 (98%)	31 (41%)	0
49	3	183/184 (99%)	32 (17%)	1 (0%)
50	4	117/118 (99%)	22 (18%)	0
51	5	146/149 (97%)	62 (42%)	1 (0%)
52	6	135/136 (99%)	35 (25%)	3 (2%)
53	7	574/578 (99%)	158 (27%)	5 (0%)
54	8	411/413 (99%)	153 (37%)	9 (2%)
All	All	1884/1901 (99%)	560 (29%)	22 (1%)

5 of 560 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	1	6	A
46	1	7	U
46	1	10	C
46	1	24	A
46	1	26	A

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	8	212	G
54	8	316	U
54	8	309	A
54	8	324	G
52	6	120	C

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 71 ligands modelled in this entry, 70 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	$\# Z > 2$
57	FES	S	401	42	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	FES	S	401	42	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
40	Q	6
53	7	3
44	Y	3
46	1	2
41	R	2
51	5	2
36	M	2
3	c	1
54	8	1
38	O	1
42	S	1
16	s	1
32	J	1

The worst 5 of 26 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	59:A	O3'	75:U	P	56.66
1	R	536:UNK	C	553:UNK	N	27.93
1	c	276:UNK	C	291:SER	N	25.05

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	111:U	O3'	117:A	P	21.41
1	R	477:ALA	C	493:UNK	N	21.21

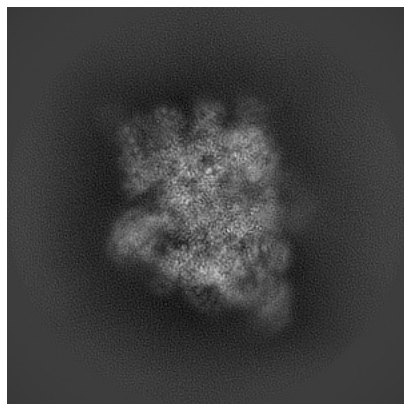
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13480. These allow visual inspection of the internal detail of the map and identification of artifacts.

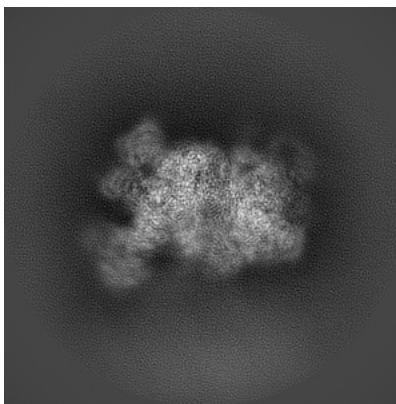
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

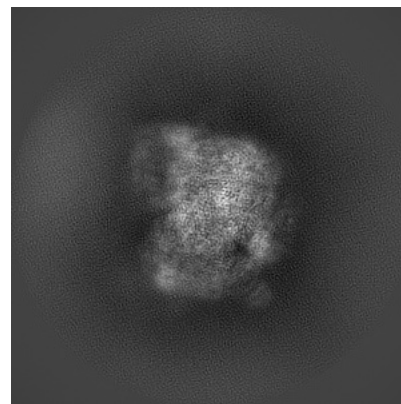
6.1.1 Primary map



X

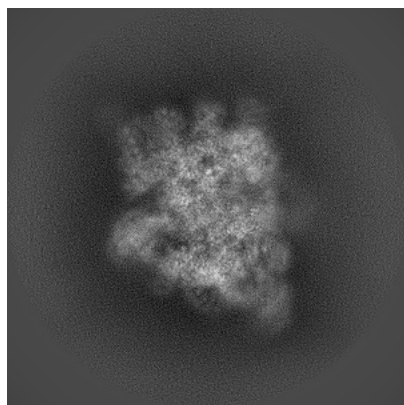


Y

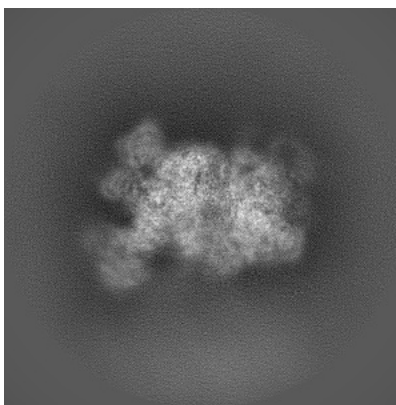


Z

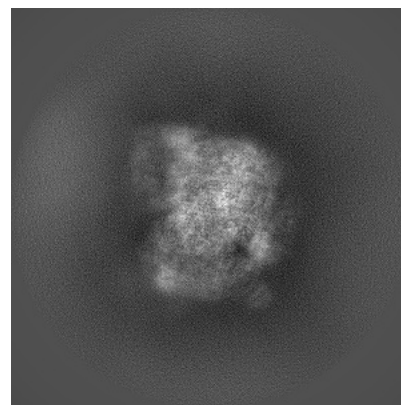
6.1.2 Raw map



X



Y

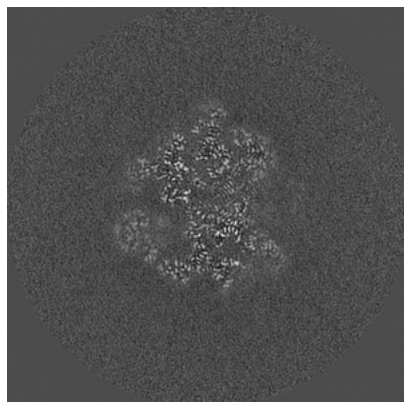


Z

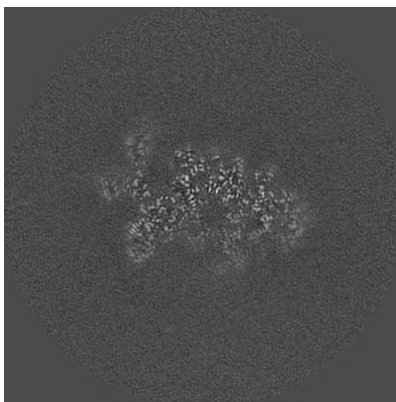
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

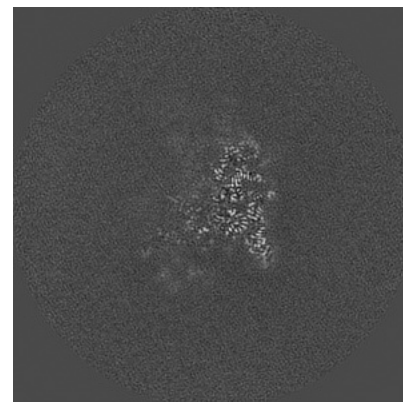
6.2.1 Primary map



X Index: 240

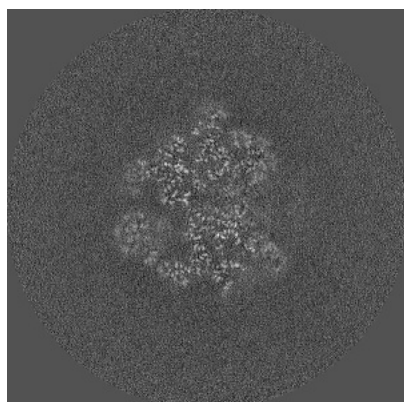


Y Index: 240

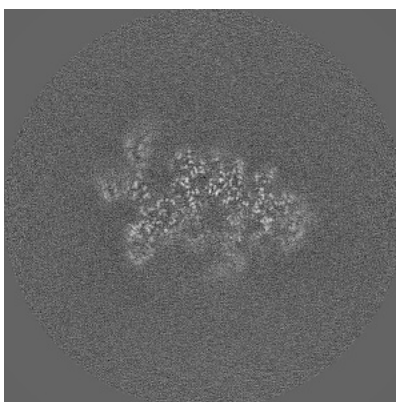


Z Index: 240

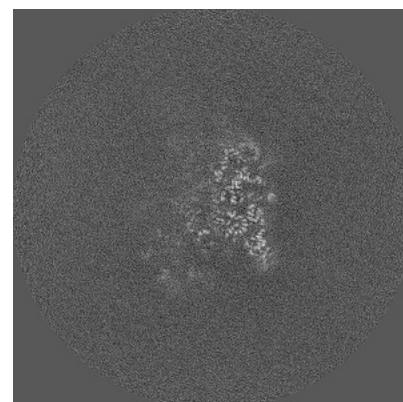
6.2.2 Raw map



X Index: 240



Y Index: 240

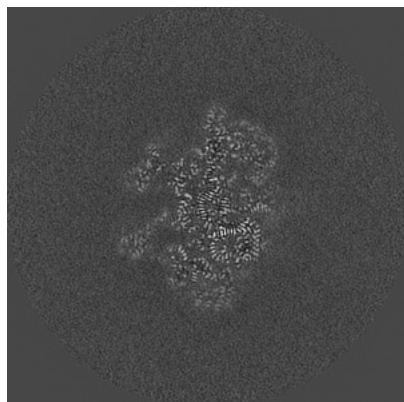


Z Index: 240

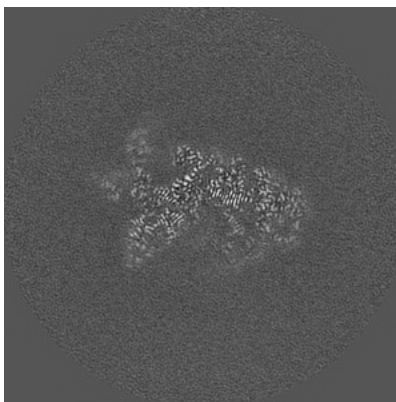
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

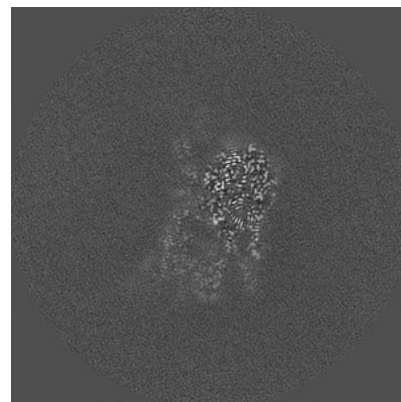
6.3.1 Primary map



X Index: 256

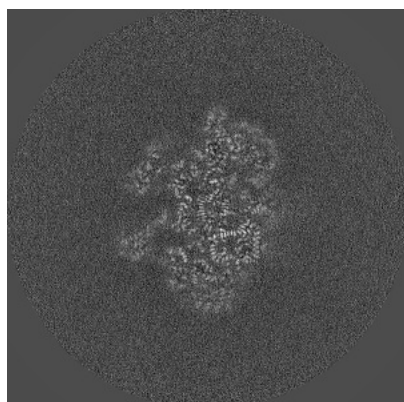


Y Index: 245

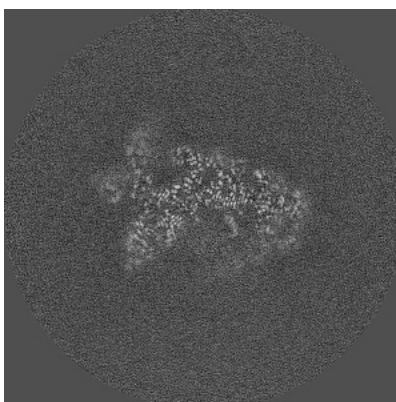


Z Index: 217

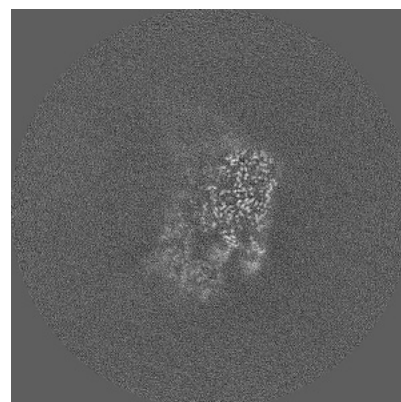
6.3.2 Raw map



X Index: 256



Y Index: 246



Z Index: 225

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

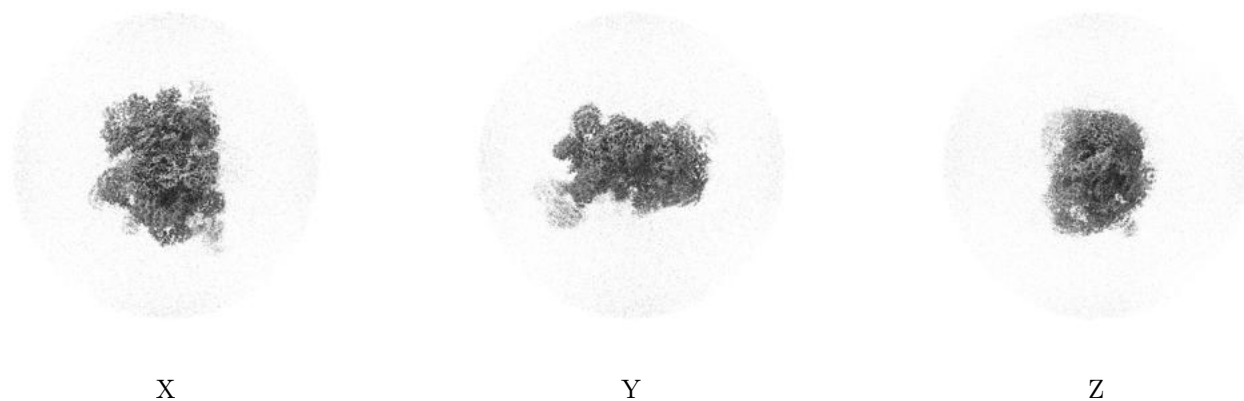
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

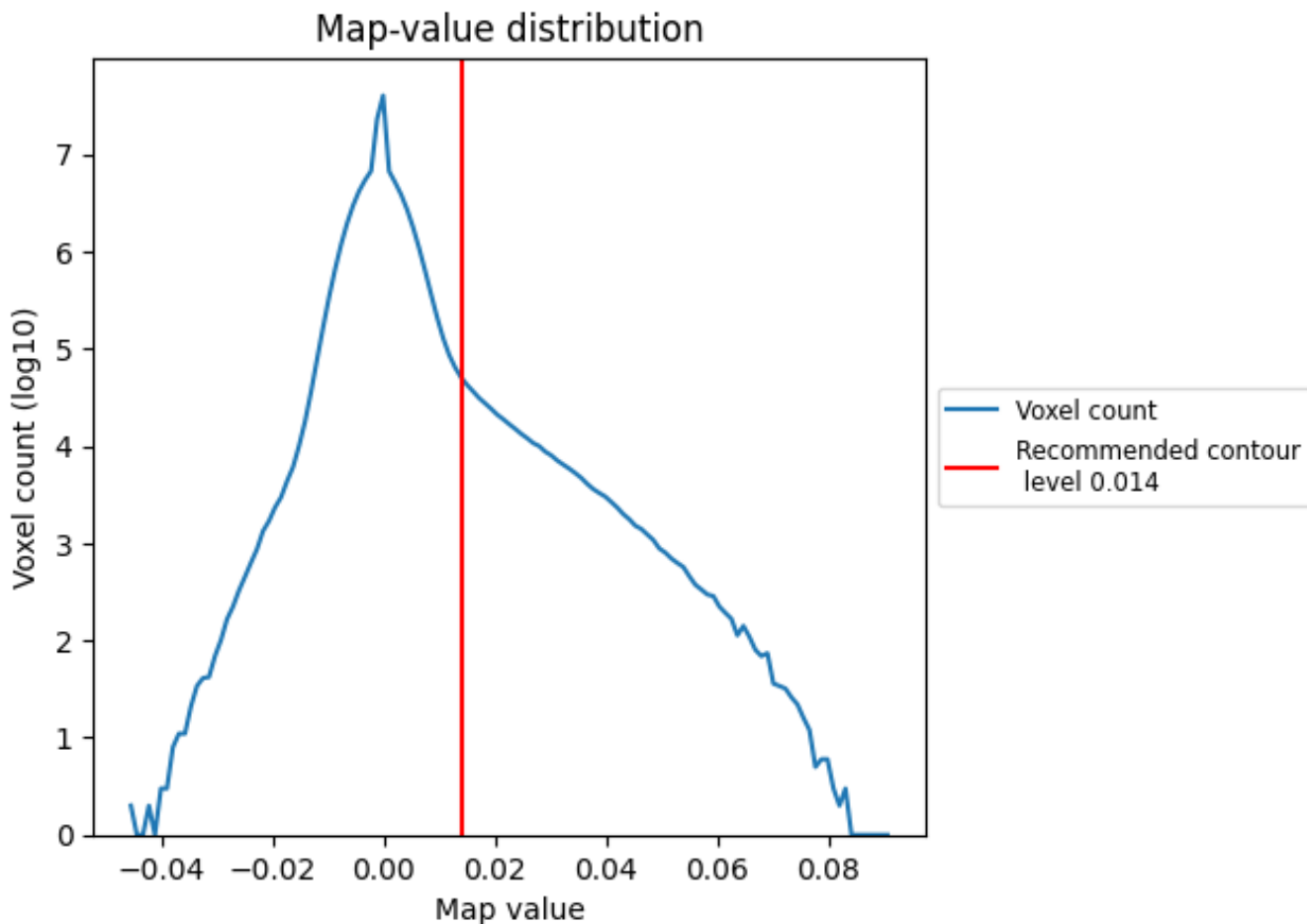
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

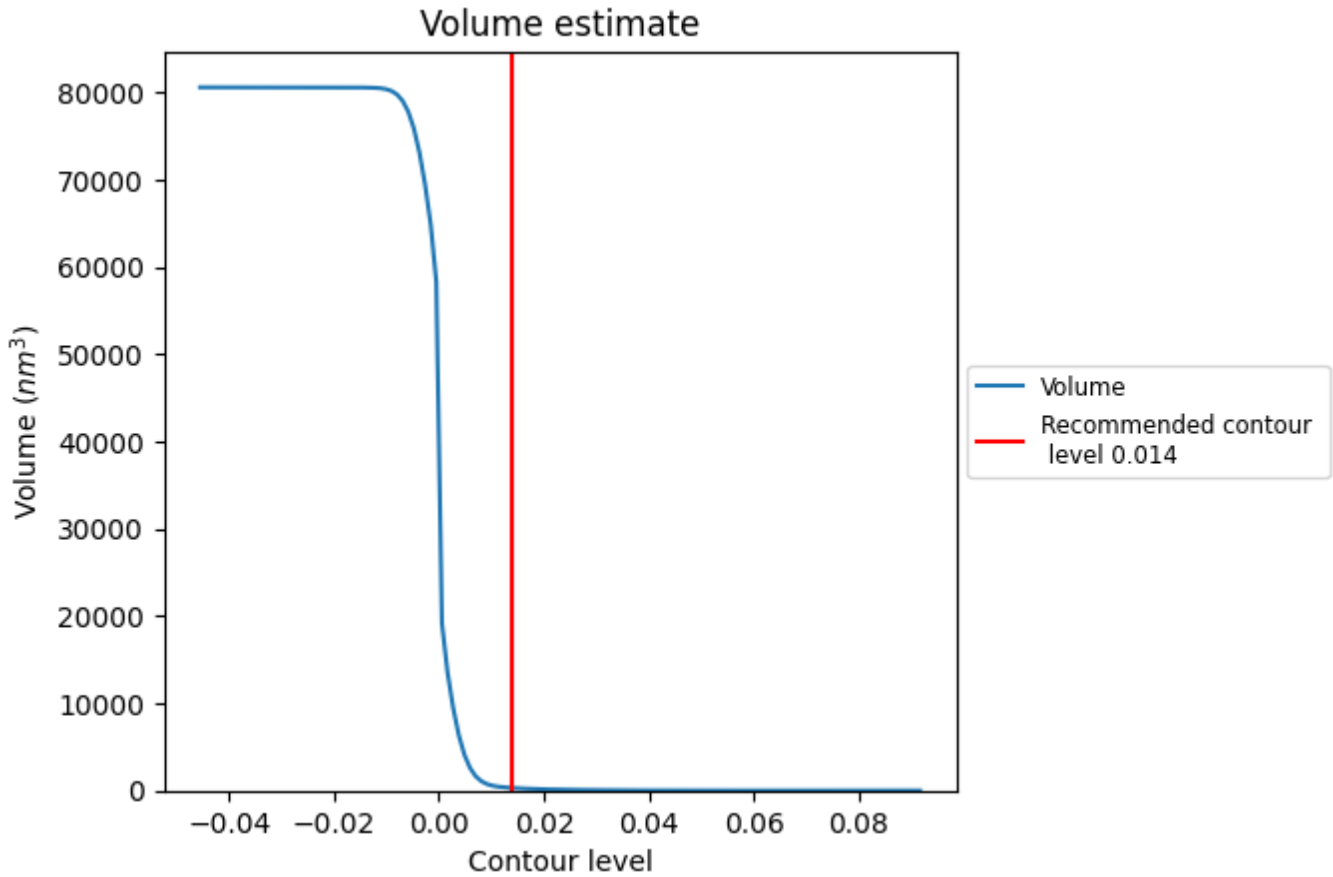
This section contains the results of statistical analysis of the map.

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.

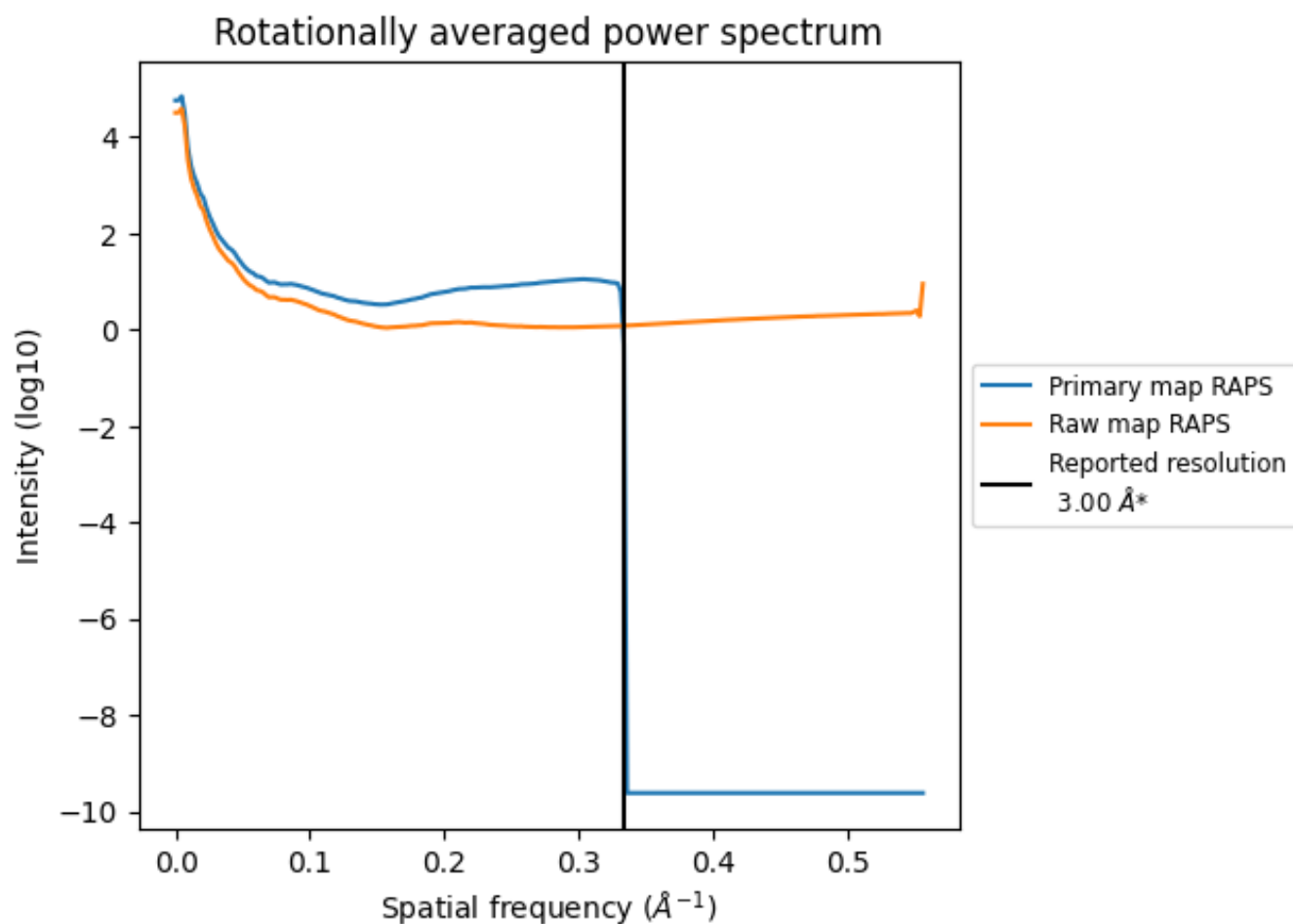
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 297 nm³; this corresponds to an approximate mass of 268 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

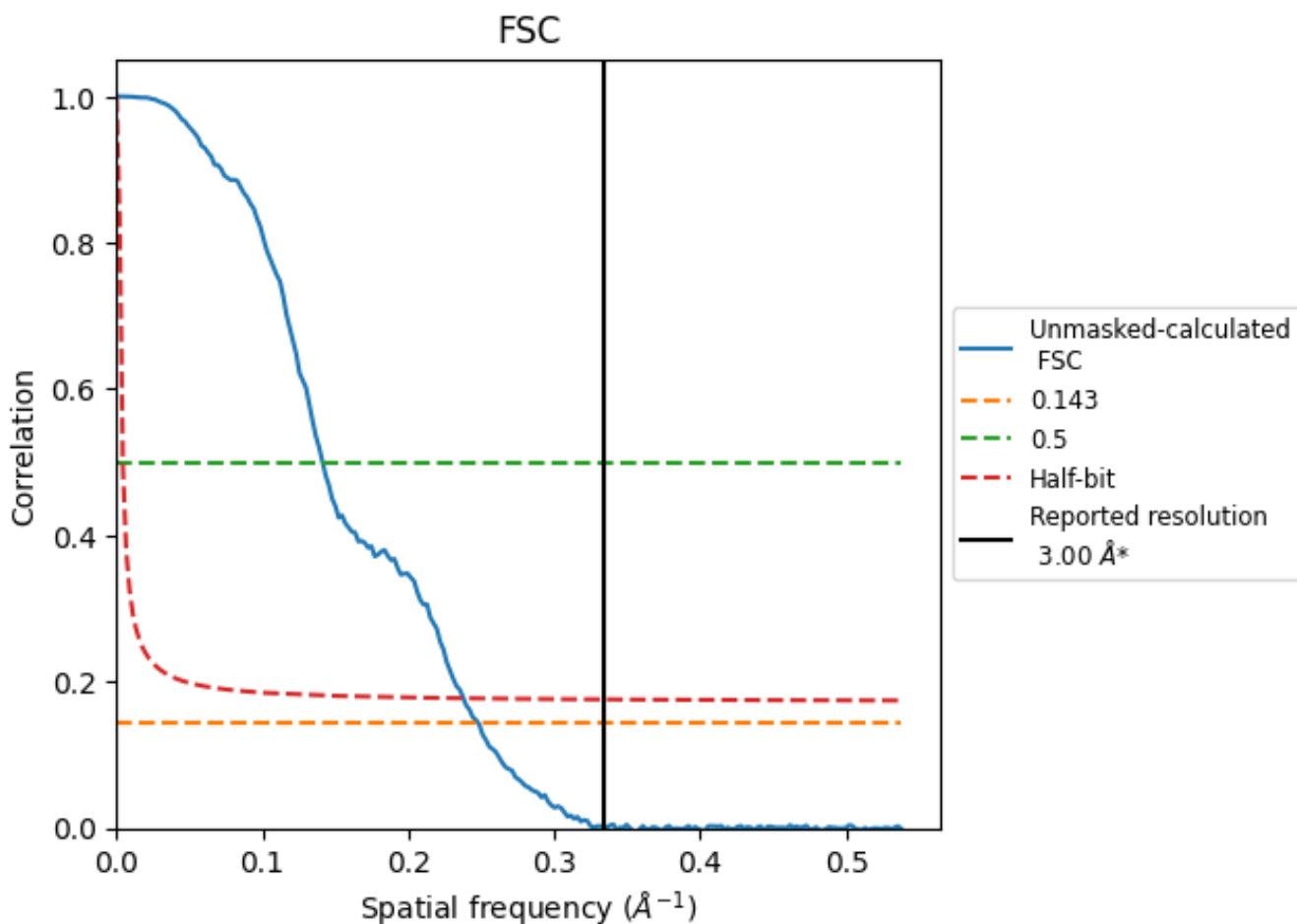


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333\AA^{-1}

8.2 Resolution estimates [i](#)

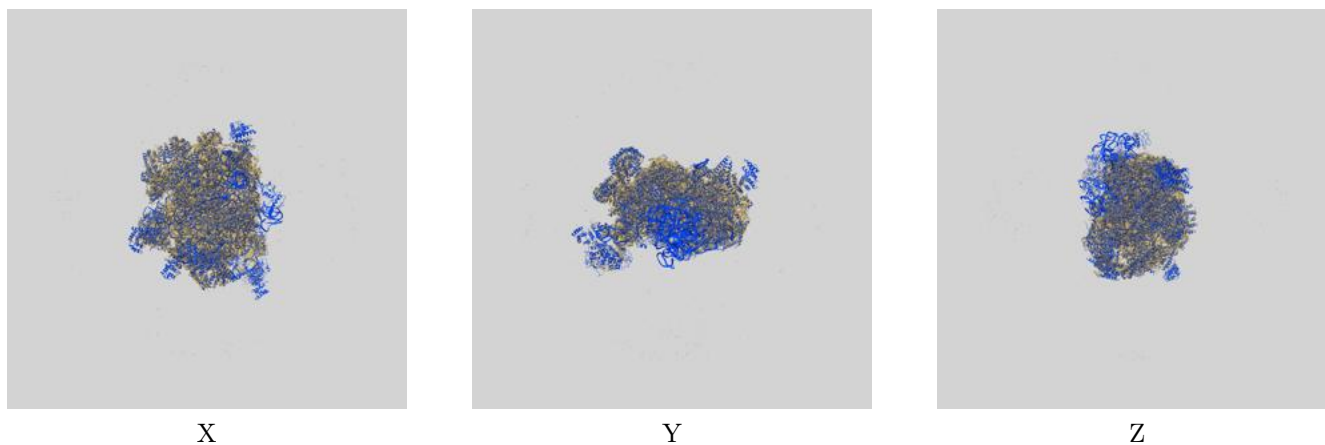
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	7.08	4.21

*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 4.03 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

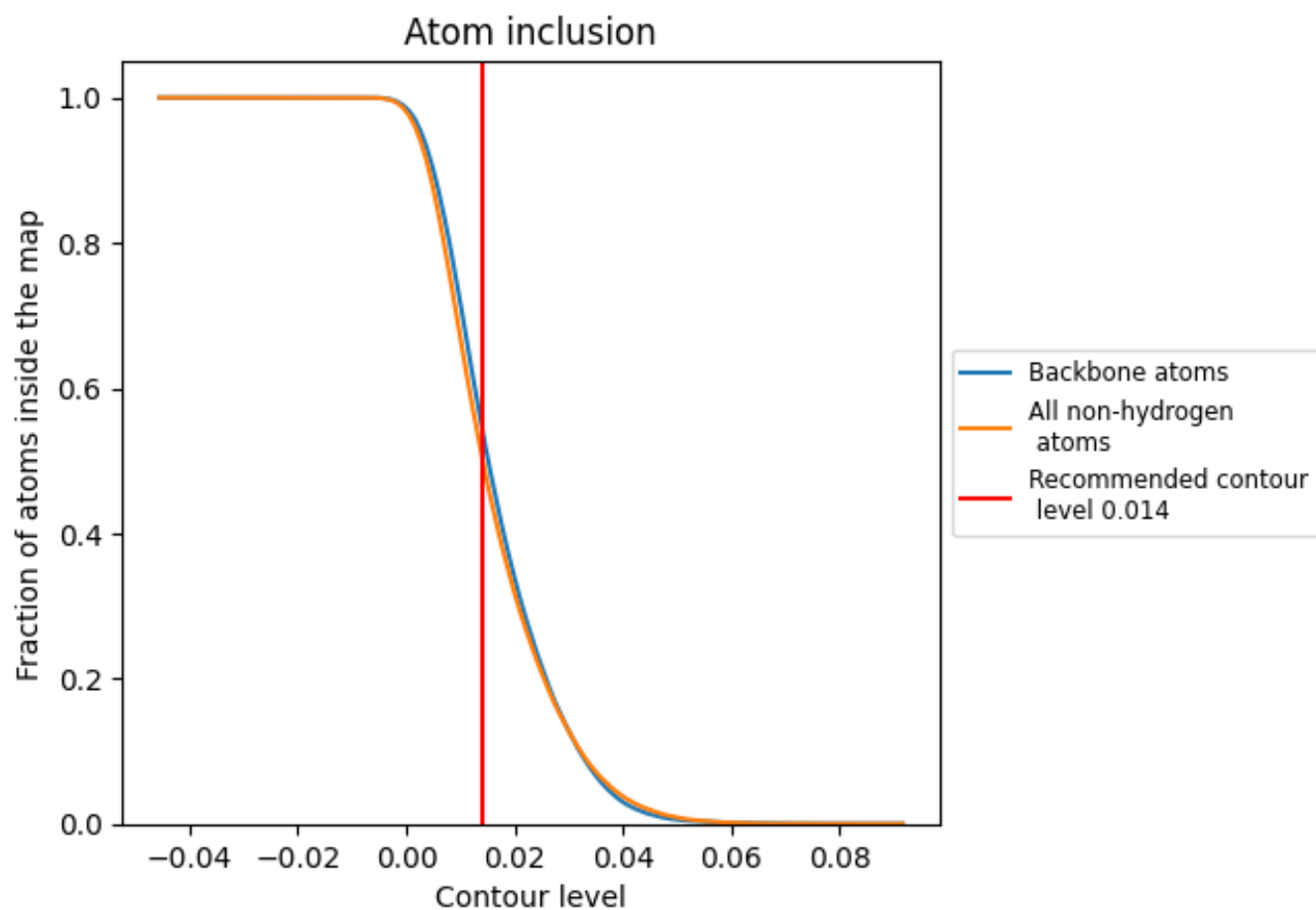
This section contains information regarding the fit between EMDB map EMD-13480 and PDB model 7PKT. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.014 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 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.