



## wwPDB EM Validation Summary Report ⓘ

Jul 9, 2025 – 03:32 am BST

PDB ID : 9HCD / pdb\_00009hcd  
EMDB ID : EMD-52045  
Title : Mouse mitoribosome large subunit assembly intermediate (with uL16m) bound to MRM3-dimer, DDX28 and the MALSU-L0R8F8-mt-ACP complex, state A2 (SAMC knock-out)  
Authors : Singh, V.; Rorbach, J.; Freyer, C.; Amunts, A.; Wredenber, A.  
Deposited on : 2024-11-08  
Resolution : 4.63 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

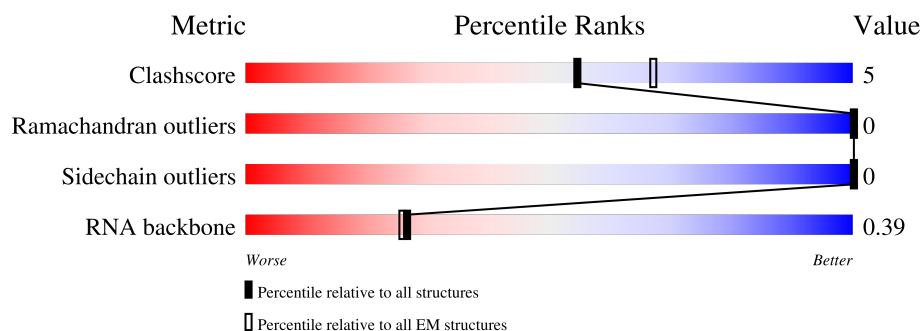
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.63 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1584	
2	B	68	
3	D	246	
4	E	348	
5	F	294	
6	H	268	
7	I	262	

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Mol	Chain	Length	Quality of chain
8	J	192	
9	K	178	
10	L	145	
11	M	295	
12	N	251	
13	O	176	
14	P	180	
15	Q	292	
16	R	149	
17	S	209	
18	T	206	
19	U	146	
20	V	216	
21	X	294	
22	Y	252	
23	Z	160	
24	0	187	
25	5	423	
26	6	380	
27	7	336	
28	8	206	
29	9	135	
30	a	142	
31	b	159	
32	c	308	

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Mol	Chain	Length	Quality of chain
33	d	306	
34	e	283	
35	f	211	
36	g	166	
37	h	159	
38	i	128	
39	j	121	
40	k	118	
41	l	135	
42	o	102	
43	p	206	
44	q	222	
45	r	196	
46	s	442	
47	u	228	
48	v	70	
49	w	156	
50	x	418	
50	y	418	
51	z	540	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	FES	r	201	-	-	X	-

## 2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 177802 atoms, of which 83096 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 (1584-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1129	Total	C	H	N	O	P	0	0
			36135	10793	12123	4354	7736	1129		

- Molecule 2 is a RNA chain called tRNA-Phe (68-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	61	Total	C	H	N	O	P	0	0
			1960	585	657	240	417	61		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	172	Total	C	H	N	O	S	0	0
			2708	835	1373	253	240	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	264	Total	C	H	N	O	S	0	0
			4219	1367	2097	361	388	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	214	Total	C	H	N	O	S	0	0
			3483	1113	1755	305	304	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	H	95	Total	C	H	N	O		0	0
			1593	492	814	150	137			

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	154	Total	C	H	N	O	S	0	0
			2575	810	1330	222	207	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	142	Total	C	H	N	O	S	0	0
			2220	690	1145	191	191	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	171	Total	C	H	N	O	S	0	0
			2794	894	1398	253	243	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	115	Total	C	H	N	O	S	0	0
			1837	560	944	174	155	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	M	249	Total	C	H	N	O	S	0	0
			4090	1285	2080	365	355	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	N	195	Total	C	H	N	O	S	0	0
			3209	1035	1608	285	271	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	O	144	Total	C	H	N	O	S	0	0
			2398	751	1215	220	207	5		

- Molecule 14 is a protein called Large ribosomal subunit protein uL18m.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	P	141	Total	C	H	N	O	S	0	0
			2302	725	1148	221	203	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	Q	217	Total	C	H	N	O	S	0	0
			3612	1150	1822	309	322	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	R	131	Total	C	H	N	O	S	0	0
			2214	685	1137	214	175	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
17	S	159	Total	C	H	N	O	S	0	0
			2673	840	1372	233	226	2		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22m.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	T	166	Total	C	H	N	O	S	0	0
			2771	871	1402	256	234	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	U	125	Total	C	H	N	O	S	0	0
			2072	664	1038	193	174	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
20	V	198	Total	C	H	N	O	S	0	0
			3250	1026	1622	302	294	6		

- Molecule 21 is a protein called Large ribosomal subunit protein bL28m, Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	X	242	Total	C	H	N	O	S	0	0
			4072	1304	2051	358	355	4		

- Molecule 22 is a protein called Large ribosomal subunit protein uL29m.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	Y	176	Total	C	H	N	O	S	0	0
			3076	973	1553	290	255	5		

- Molecule 23 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Z	115	Total	C	H	N	O	S	0	0
			1913	598	979	171	162	3		

- Molecule 24 is a protein called Large ribosomal subunit protein bL32m.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	0	108	Total	C	H	N	O	S	0	0
			1789	546	908	174	155	6		

- Molecule 25 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	5	387	Total	C	H	N	O	S	0	0
			6355	2045	3187	554	560	9		

- Molecule 26 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	6	287	Total	C	H	N	O	S	0	0
			4793	1573	2342	447	425	6		

- Molecule 27 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	7	292	Total	C	H	N	O	S	0	0
			4757	1517	2378	409	438	15		

- Molecule 28 is a protein called Large ribosomal subunit protein mL40.



Mol	Chain	Residues	Atoms						AltConf	Trace
28	8	59	Total	C	H	N	O	S	0	0
			977	306	484	87	98	2		

- Molecule 29 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	9	96	Total	C	H	N	O	S	0	0
			1550	510	772	123	144	1		

- Molecule 30 is a protein called Large ribosomal subunit protein mL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	a	103	Total	C	H	N	O	S	0	0
			1703	542	843	156	159	3		

- Molecule 31 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	b	148	Total	C	H	N	O	S	0	0
			2376	731	1195	234	214	2		

- Molecule 32 is a protein called Large ribosomal subunit protein mL44.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	c	279	Total	C	H	N	O	S	0	0
			4502	1440	2256	389	409	8		

- Molecule 33 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	d	204	Total	C	H	N	O	S	0	0
			3359	1085	1671	299	293	11		

- Molecule 34 is a protein called Large ribosomal subunit protein mL46.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	e	177	Total	C	H	N	O	S	0	0
			2911	922	1474	258	252	5		

- Molecule 35 is a protein called Large ribosomal subunit protein mL48.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	f	89	Total	C	H	N	O	S	0	0
			1418	452	704	120	138	4		

- Molecule 36 is a protein called Large ribosomal subunit protein mL49.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	g	132	Total	C	H	N	O	S	0	0
			2184	709	1094	187	192	2		

- Molecule 37 is a protein called Large ribosomal subunit protein mL50.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	h	110	Total	C	H	N	O	S	0	0
			1740	552	868	156	160	4		

- Molecule 38 is a protein called Large ribosomal subunit protein mL51.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	i	92	Total	C	H	N	O	S	0	0
			1601	514	811	152	122	2		

- Molecule 39 is a protein called Large ribosomal subunit protein mL52.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	j	85	Total	C	H	N	O	S	0	0
			1376	426	692	135	121	2		

- Molecule 40 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	k	80	Total	C	H	N	O	S	0	0
			1268	393	639	114	117	5		

- Molecule 41 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	l	76	Total	C	H	N	O	S	0	0
			1266	403	631	114	116	2		

- Molecule 42 is a protein called Large ribosomal subunit protein mL63.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	o	78	Total	C	H	N	O	S	0	0
			1263	402	623	118	116	4		

- Molecule 43 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	p	132	Total	C	H	N	O	S	0	0
			2201	682	1112	205	198	4		

- Molecule 44 is a protein called Large ribosomal subunit protein mL64.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	q	97	Total	C	H	N	O	S	0	0
			1584	501	785	155	142	1		

- Molecule 45 is a protein called Large ribosomal subunit protein mL66.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	r	156	Total	C	H	N	O	S	0	0
			2586	806	1319	241	209	11		

- Molecule 46 is a protein called Large ribosomal subunit protein mL65.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	s	377	Total	C	H	N	O	S	0	0
			6100	1938	3055	555	540	12		

- Molecule 47 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	u	125	Total	C	H	N	O	S	0	0
			2041	659	1012	170	191	9		

- Molecule 48 is a protein called Predicted gene, 55359.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	v	69	Total	C	H	N	O	S	0	0
			1189	374	603	112	99	1		

- Molecule 49 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	w	79	Total	C	H	N	O	S	0	0
			1277	410	640	95	127	5		

- Molecule 50 is a protein called rRNA methyltransferase 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	x	295	Total	C	H	N	O	S	0	0
			4661	1478	2356	399	420	8		
50	y	293	Total	C	H	N	O	S	0	0
			4631	1469	2340	397	417	8		

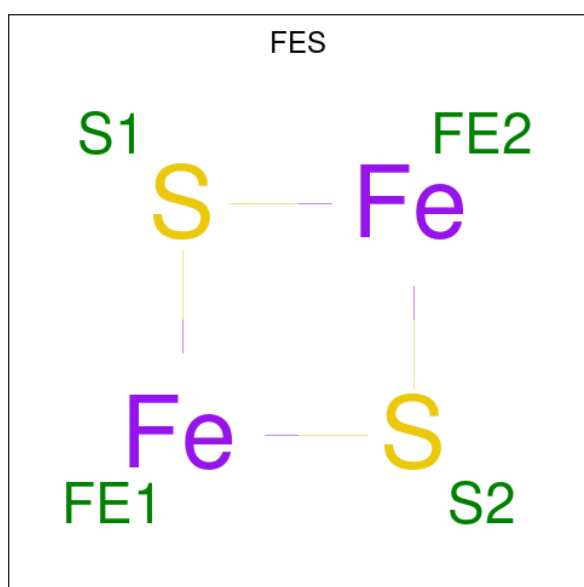
- Molecule 51 is a protein called Probable ATP-dependent RNA helicase DDX28.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	z	454	Total	C	H	N	O	S	0	0
			7163	2237	3639	636	642	9		

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	0	1	Total	Zn	0
			1	1	

- Molecule 53 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).

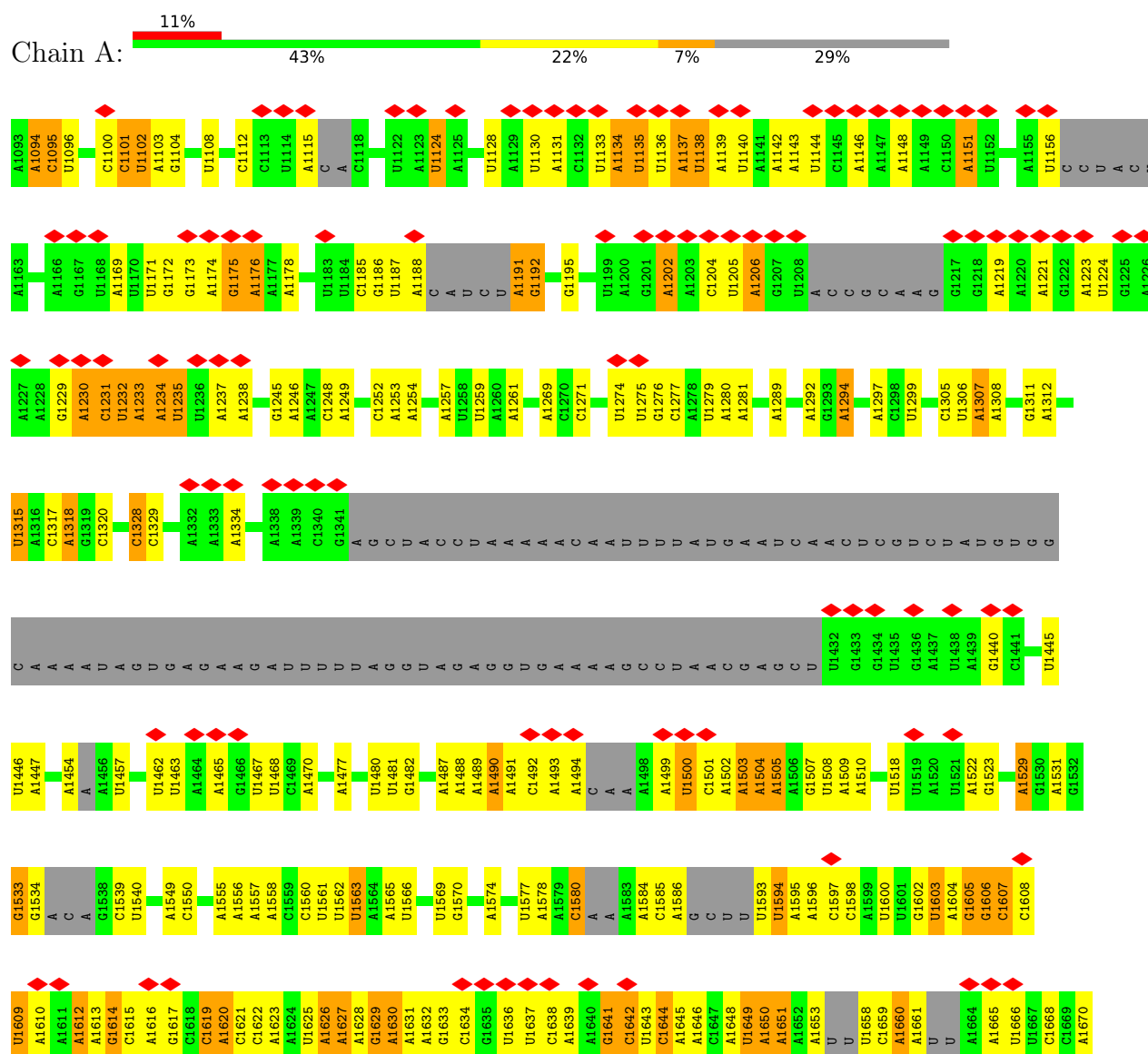


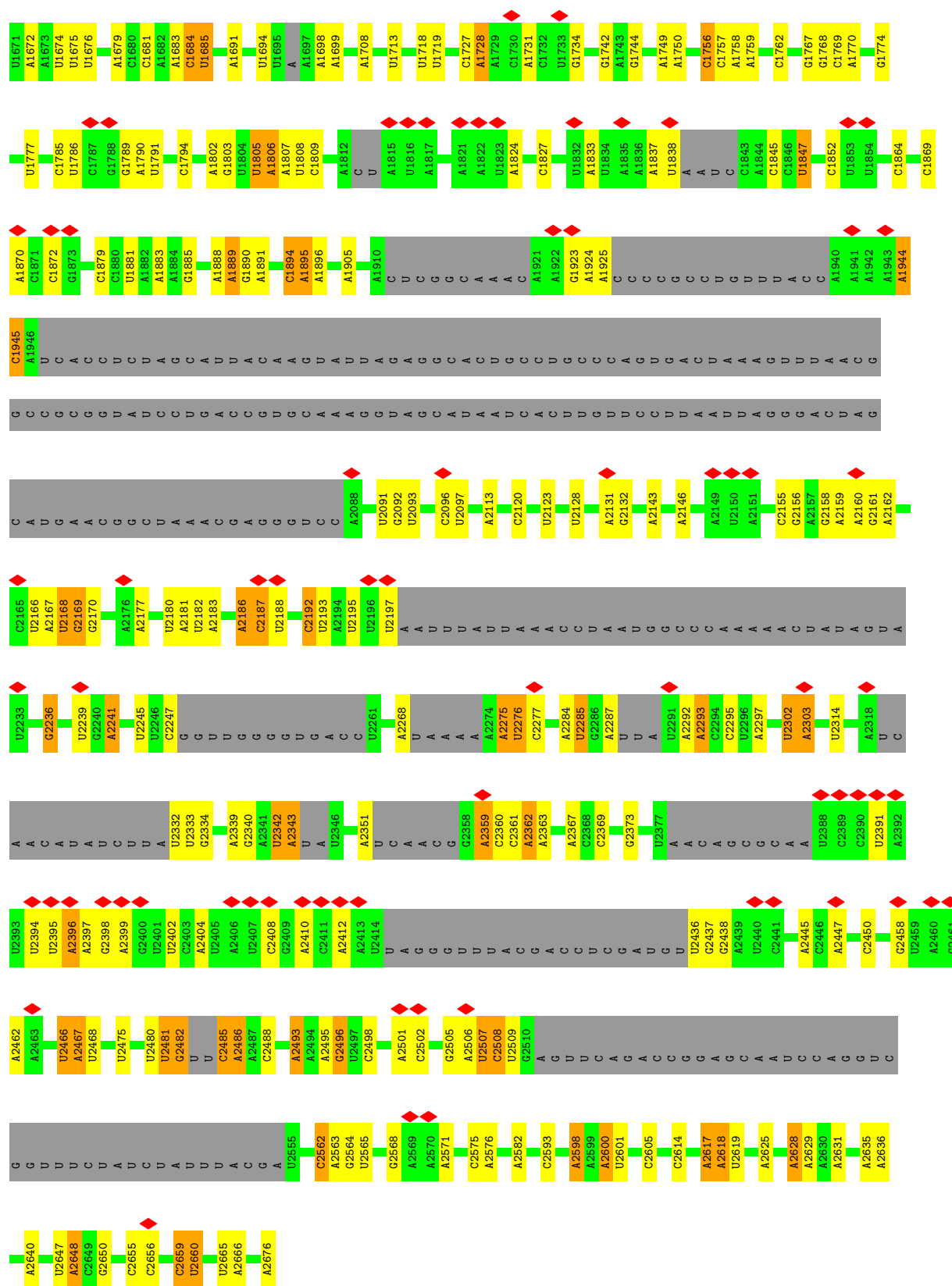
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
53	r	1	4	2	2	0

### 3 Residue-property plots

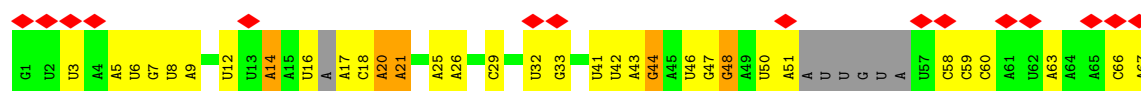
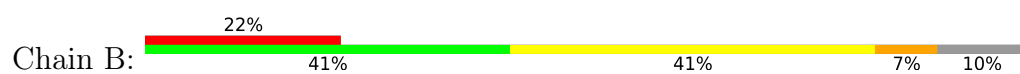
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA (1584-MER)

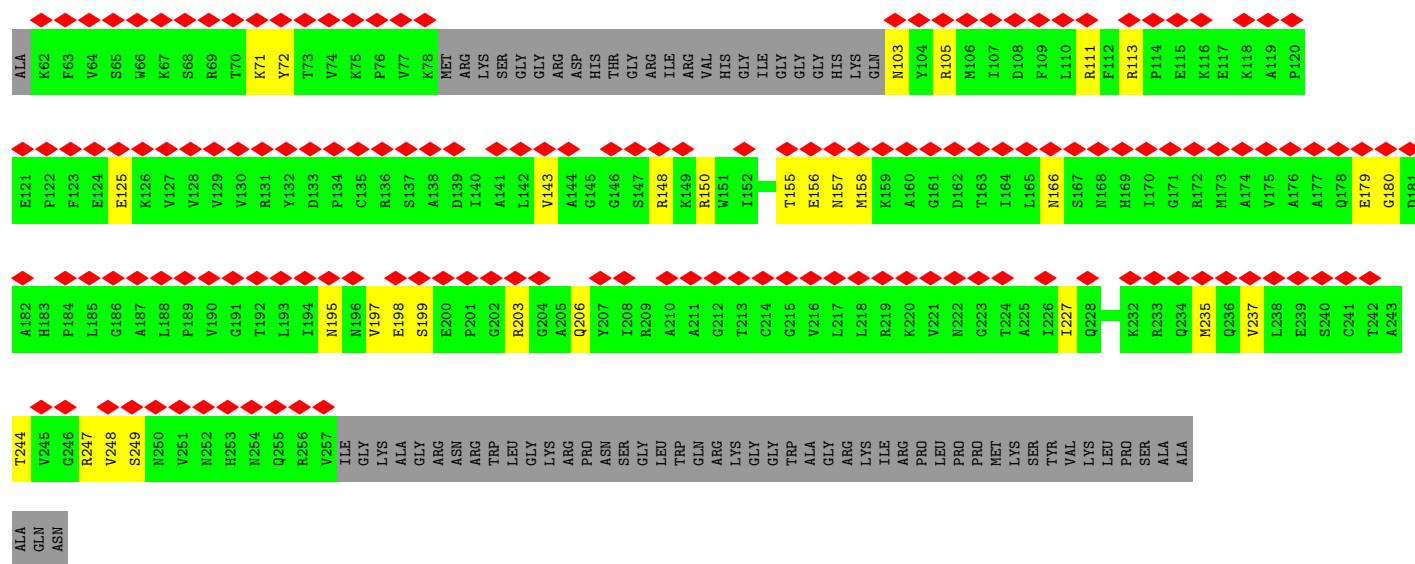




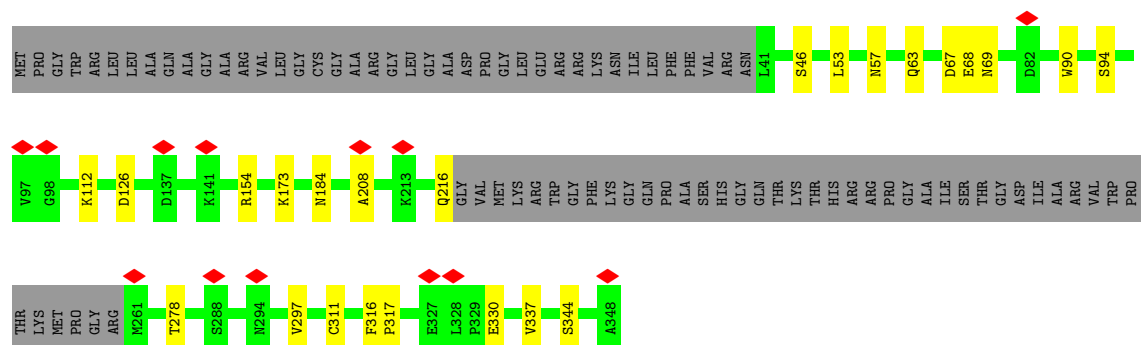
- Molecule 2: tRNA-Phe (68-MER)



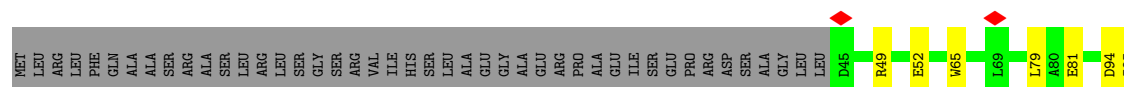
• Molecule 3: Large ribosomal subunit protein uL2m



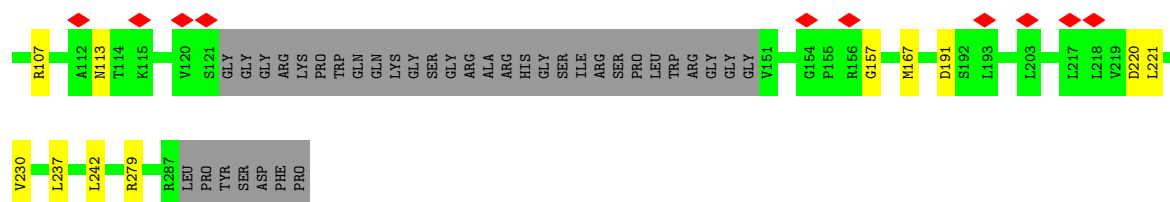
• Molecule 4: Large ribosomal subunit protein uL3m



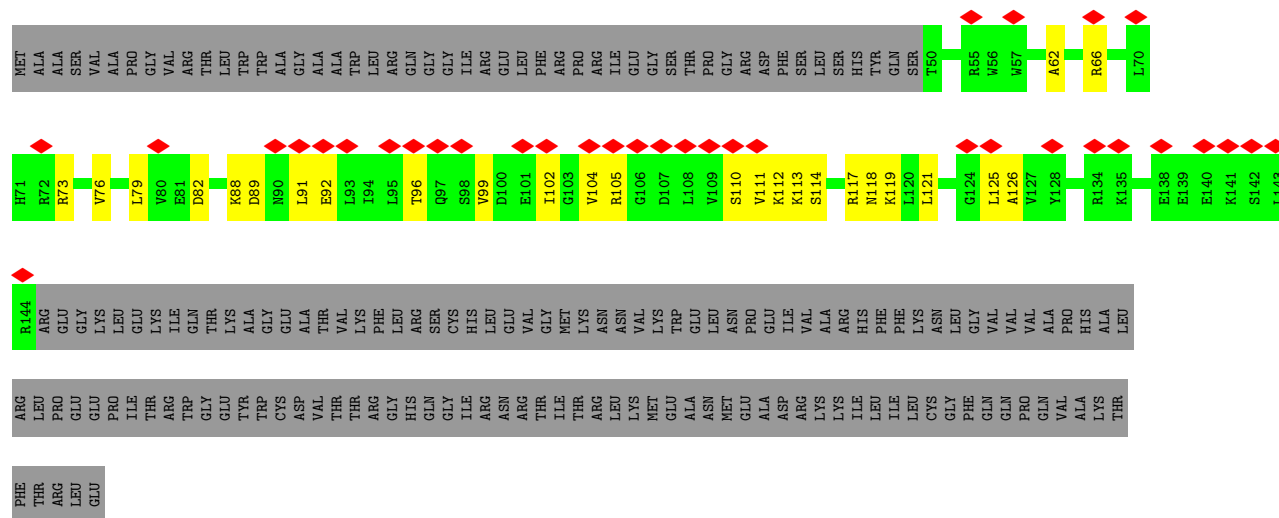
• Molecule 5: Large ribosomal subunit protein uL4m



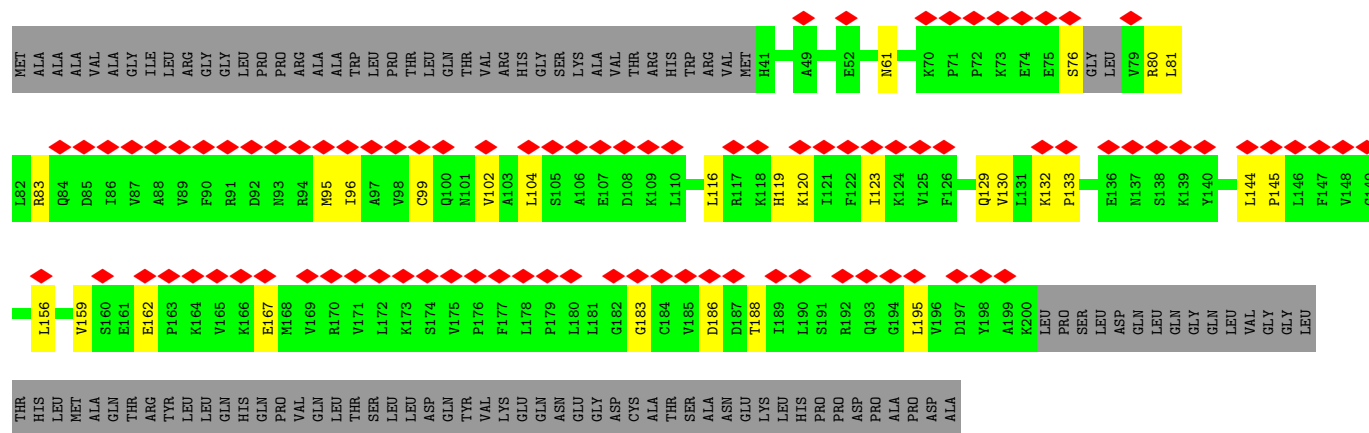




• Molecule 6: Large ribosomal subunit protein bL9m

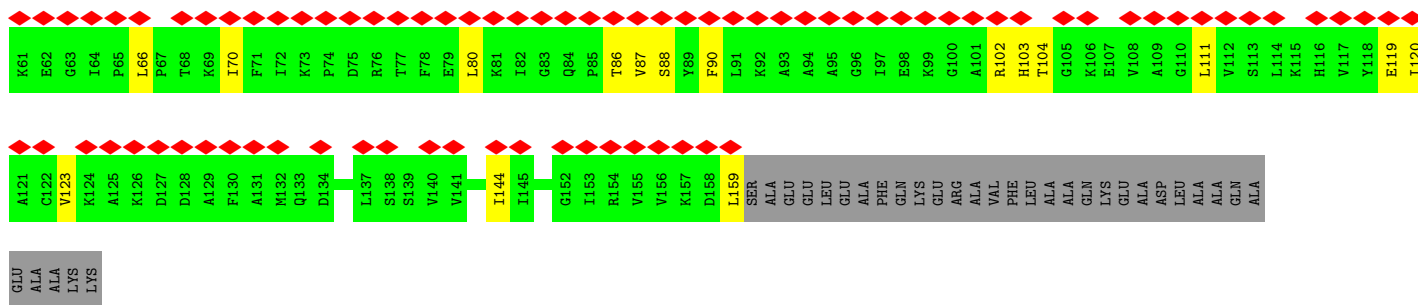


• Molecule 7: Large ribosomal subunit protein uL10m

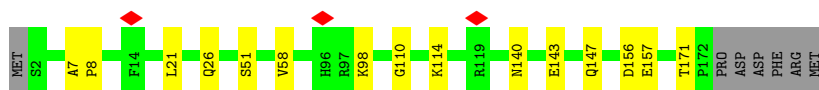
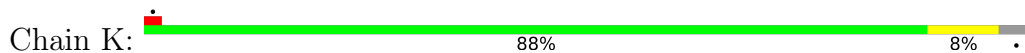


• Molecule 8: Large ribosomal subunit protein uL11m

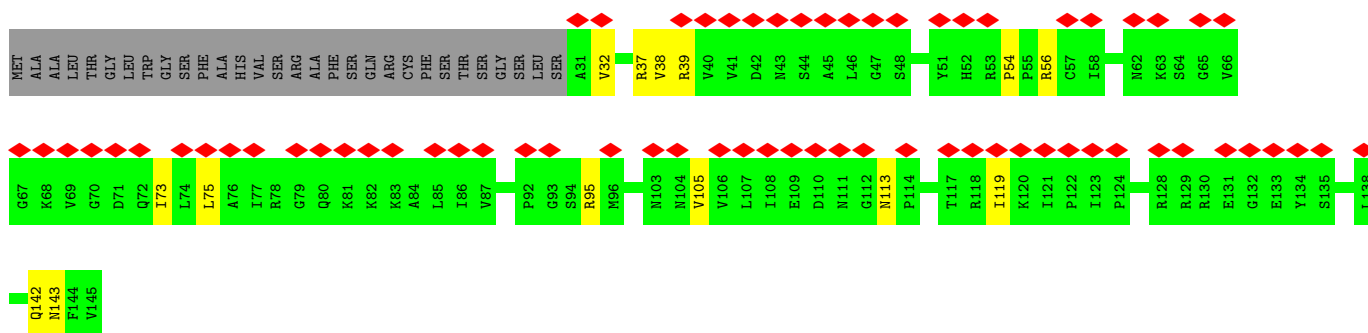




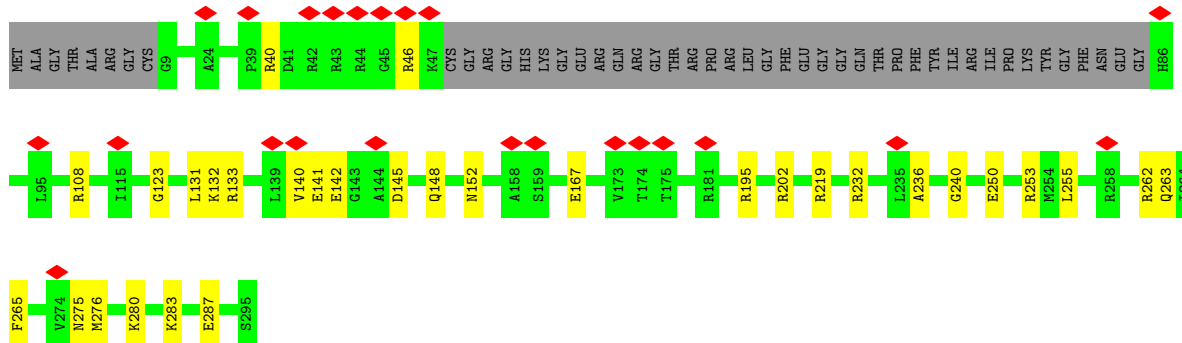
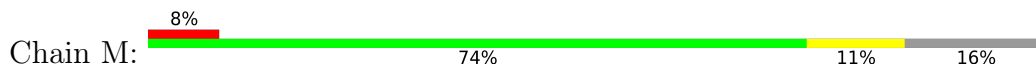
- Molecule 9: Large ribosomal subunit protein uL13m



- Molecule 10: Large ribosomal subunit protein uL14m

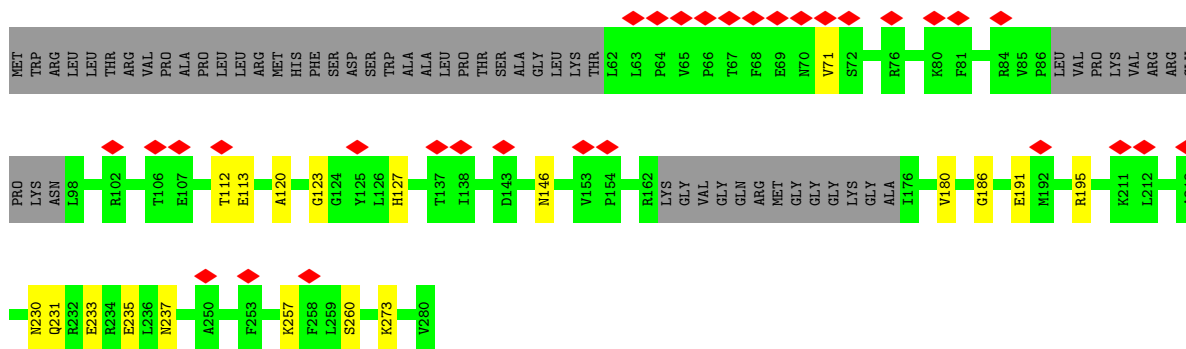


- Molecule 11: Large ribosomal subunit protein uL15m

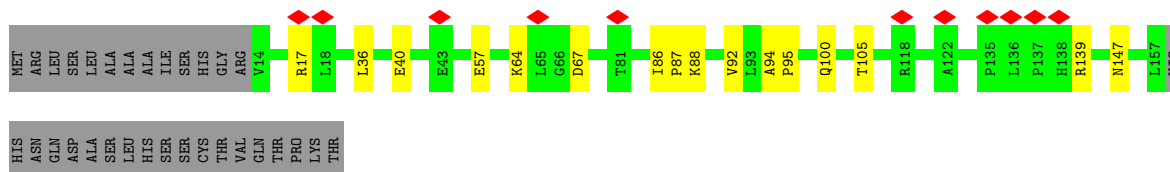


- Molecule 12: Large ribosomal subunit protein uL16m

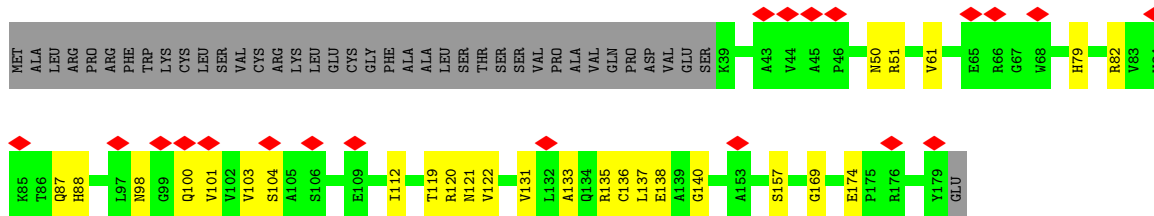




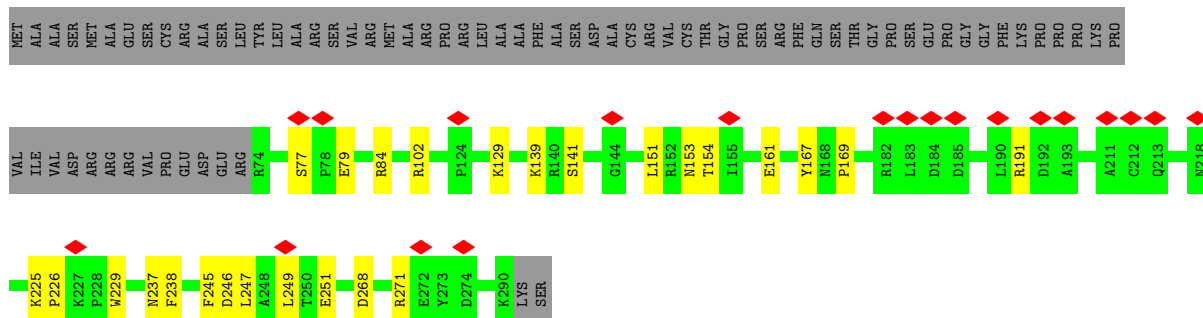
- Molecule 13: Large ribosomal subunit protein bL17m



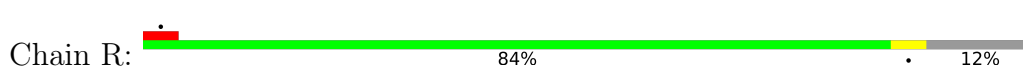
- Molecule 14: Large ribosomal subunit protein uL18m

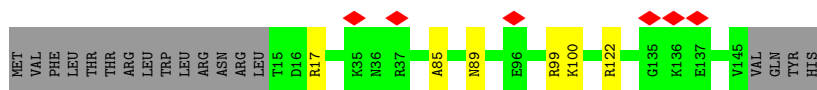


- Molecule 15: Large ribosomal subunit protein bL19m

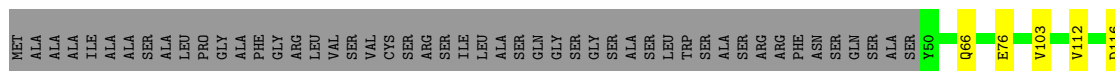


- Molecule 16: Large ribosomal subunit protein bL20m

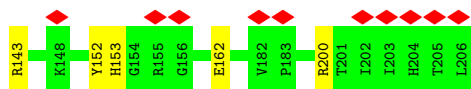
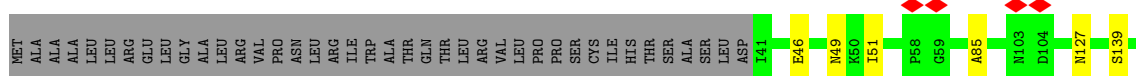
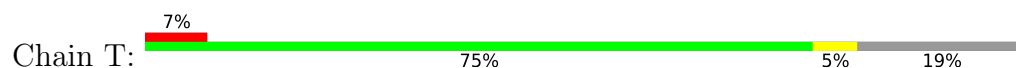




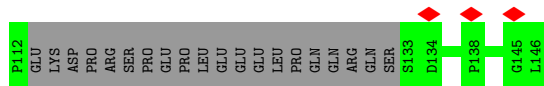
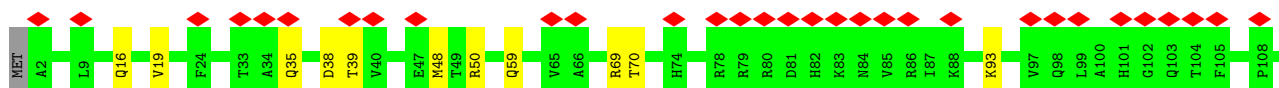
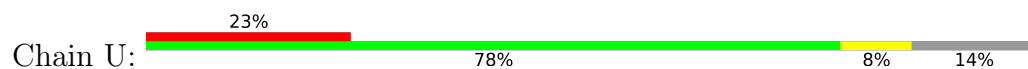
- Molecule 17: Large ribosomal subunit protein bL21m



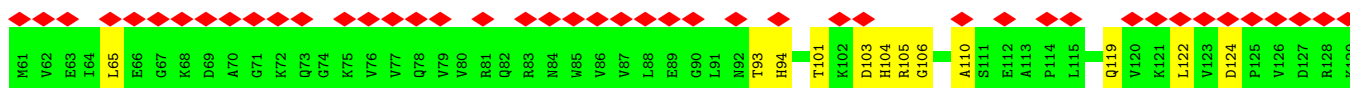
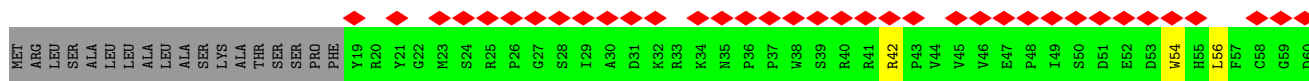
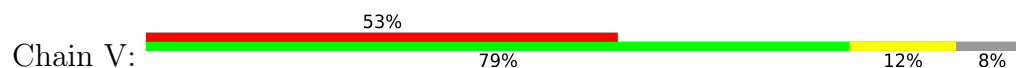
- Molecule 18: Large ribosomal subunit protein uL22m

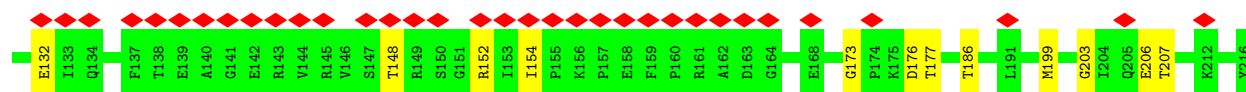


- Molecule 19: Large ribosomal subunit protein uL23m

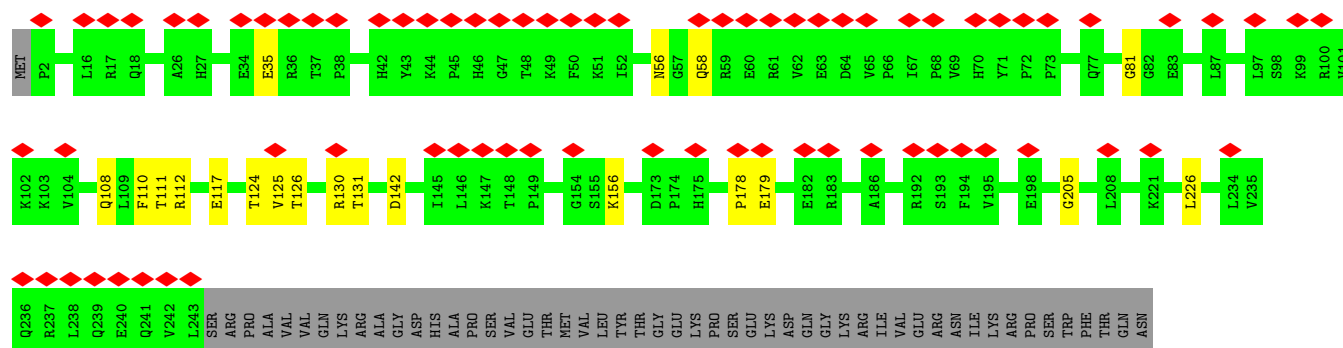
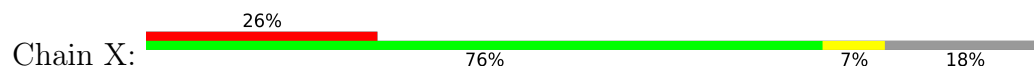


- Molecule 20: Large ribosomal subunit protein uL24m

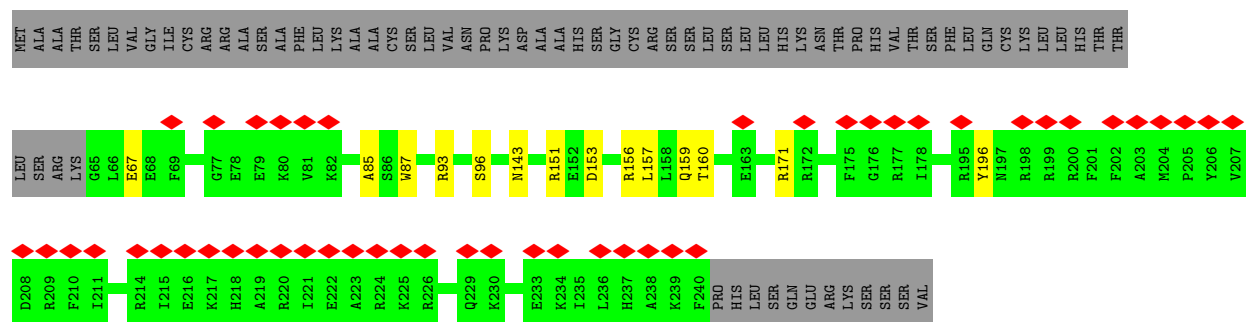




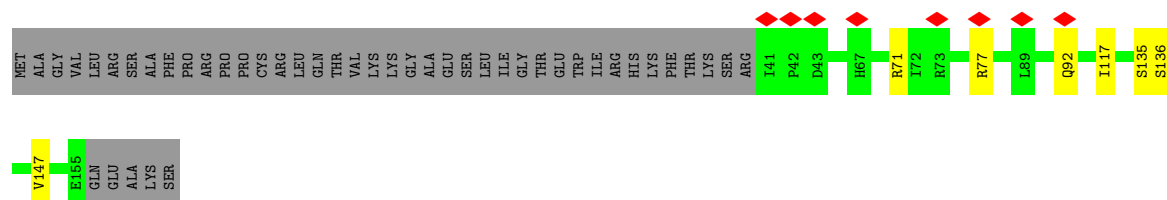
- Molecule 21: Large ribosomal subunit protein bL28m, Large ribosomal subunit protein bL32m



- Molecule 22: Large ribosomal subunit protein uL29m



- Molecule 23: Large ribosomal subunit protein uL30m

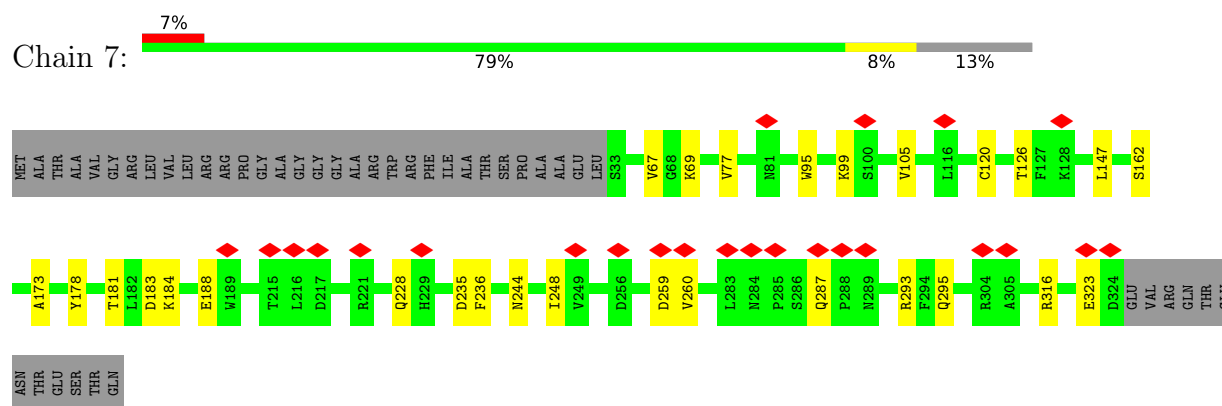


- Molecule 24: Large ribosomal subunit protein bL32m

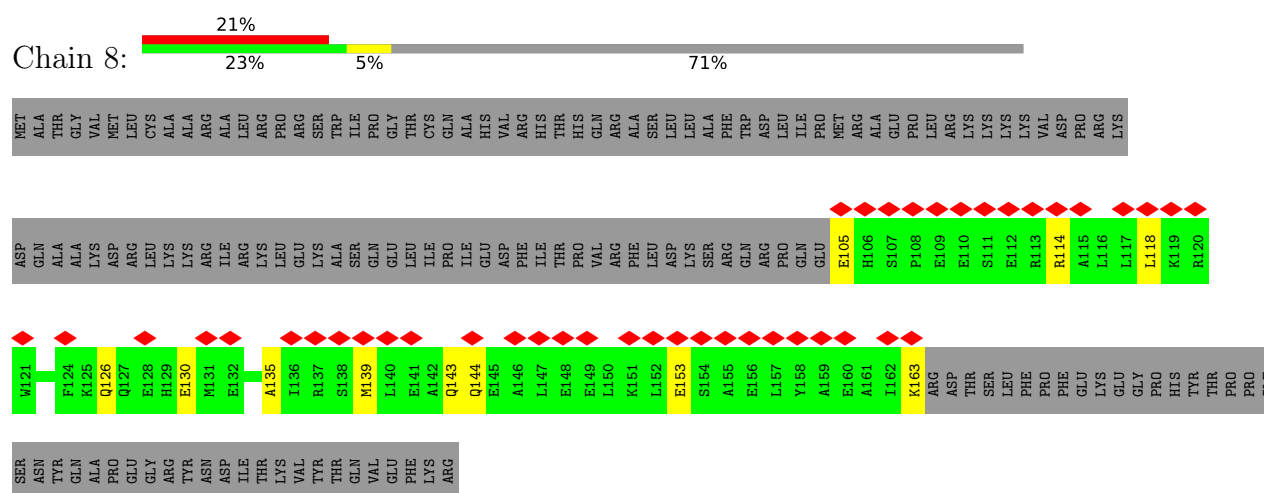




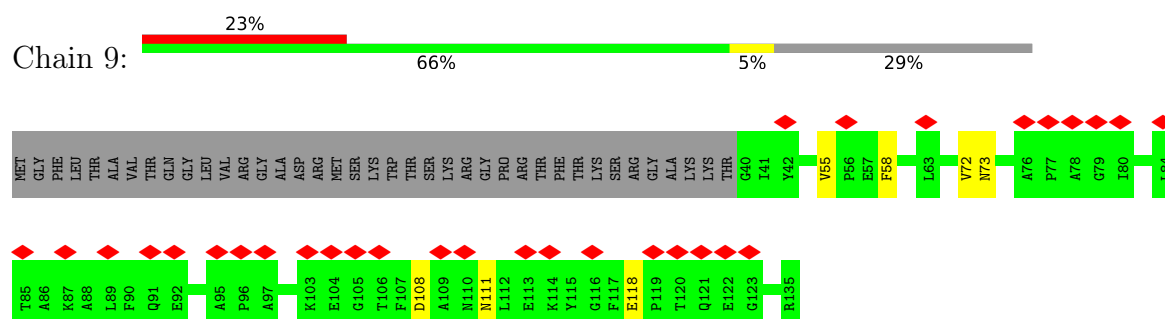
- Molecule 27: Large ribosomal subunit protein mL39



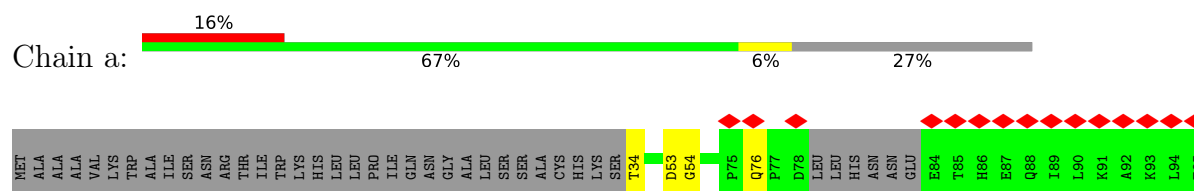
- Molecule 28: Large ribosomal subunit protein mL40

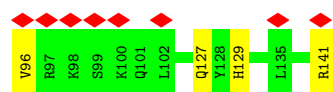


- Molecule 29: Large ribosomal subunit protein mL41

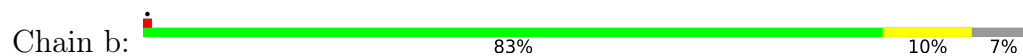


- Molecule 30: Large ribosomal subunit protein mL42

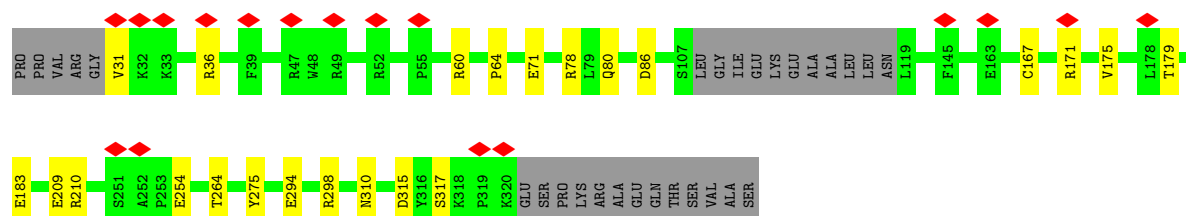
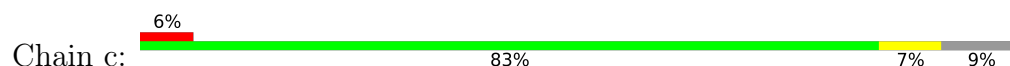




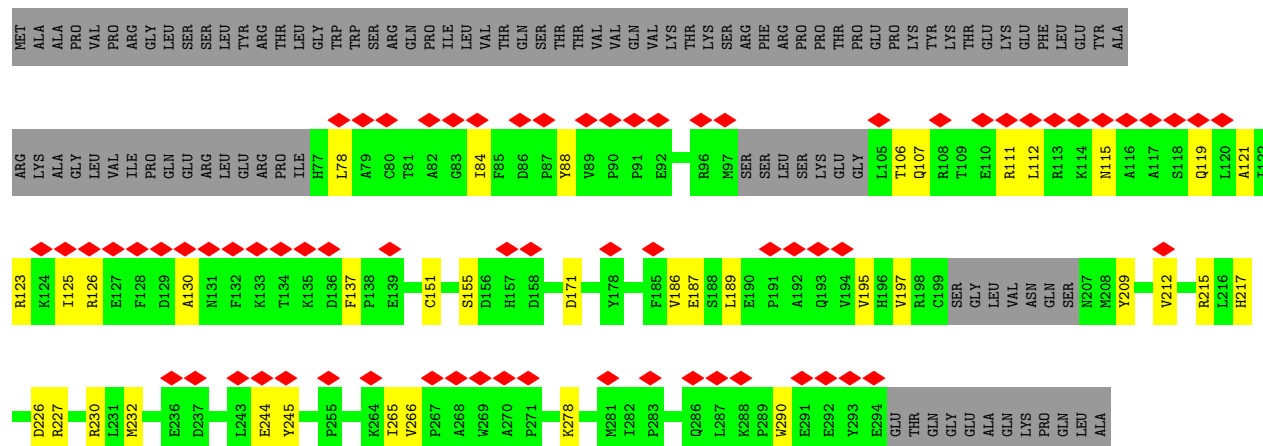
- Molecule 31: Large ribosomal subunit protein mL43



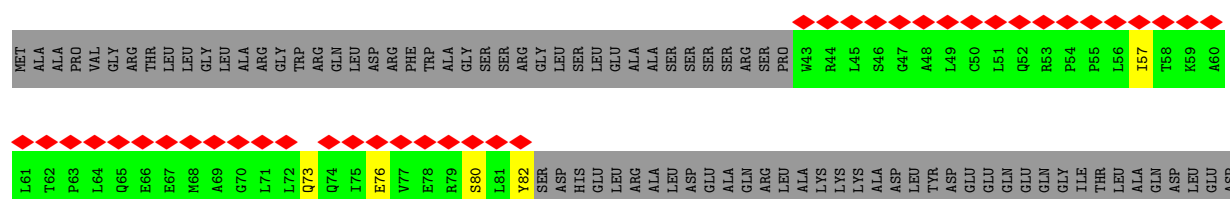
- Molecule 32: Large ribosomal subunit protein mL44



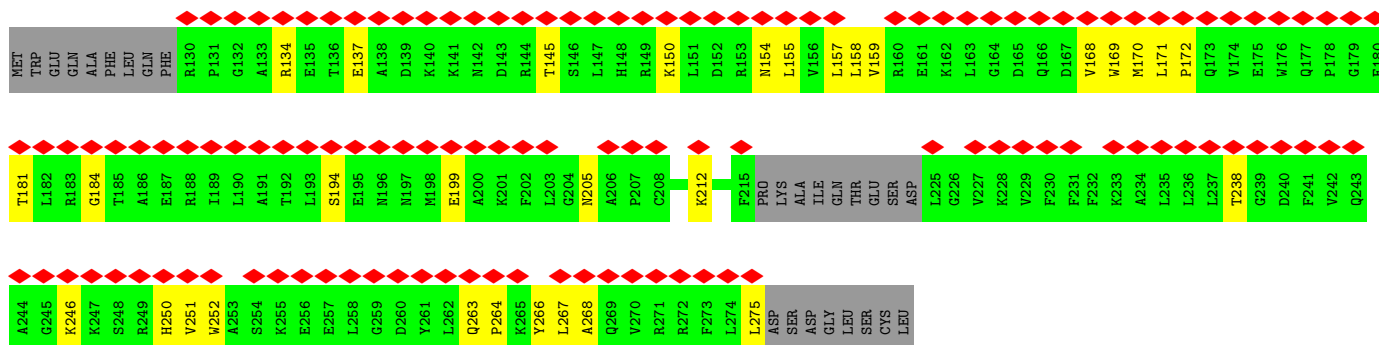
- Molecule 33: Large ribosomal subunit protein mL45



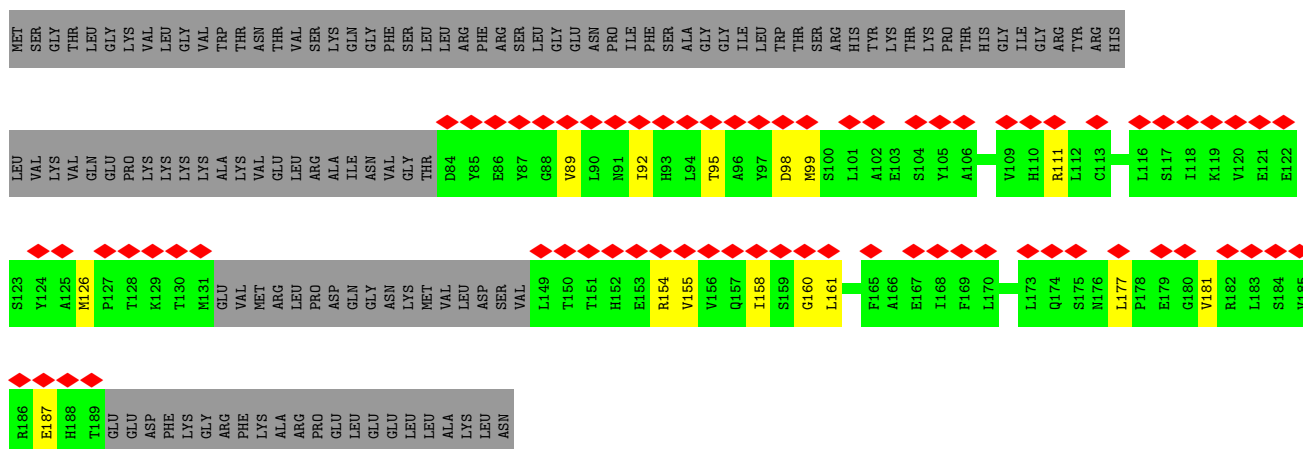
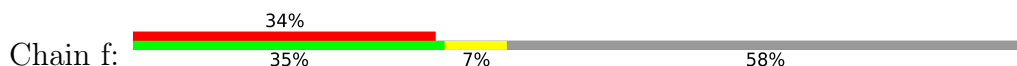
- Molecule 34: Large ribosomal subunit protein mL46



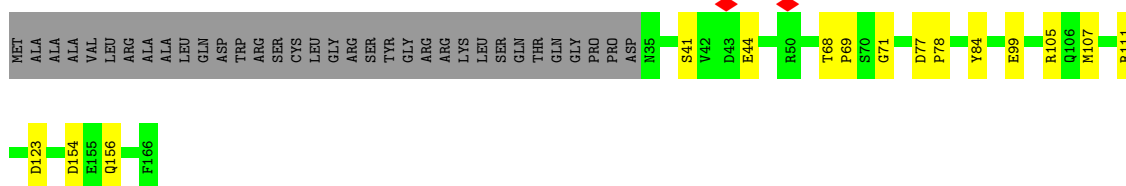




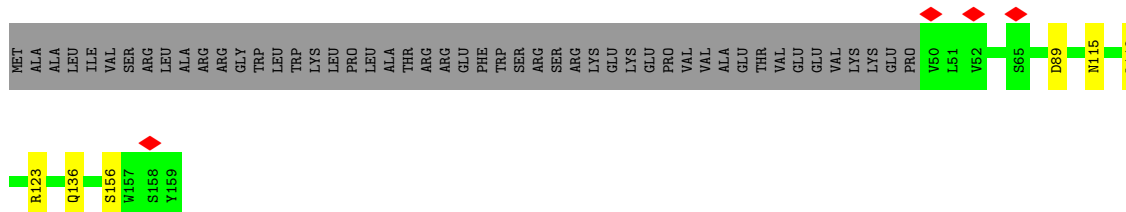
• Molecule 35: Large ribosomal subunit protein mL48



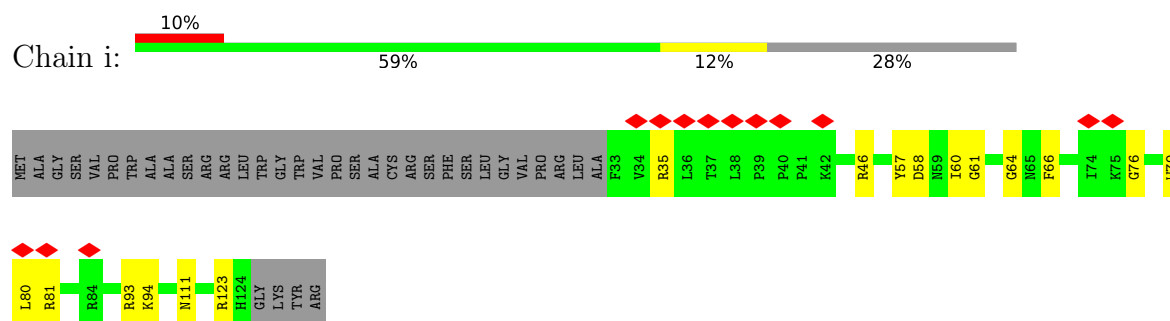
• Molecule 36: Large ribosomal subunit protein mL49



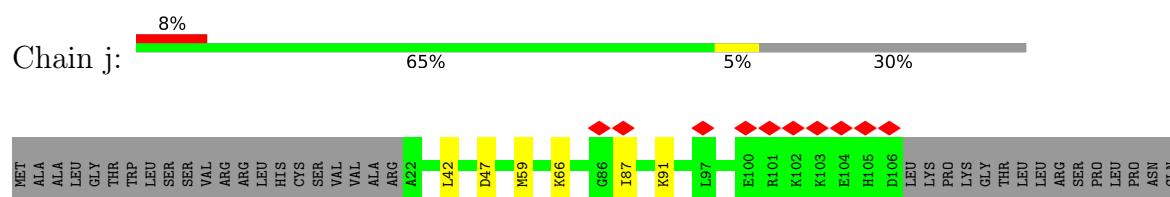
• Molecule 37: Large ribosomal subunit protein mL50



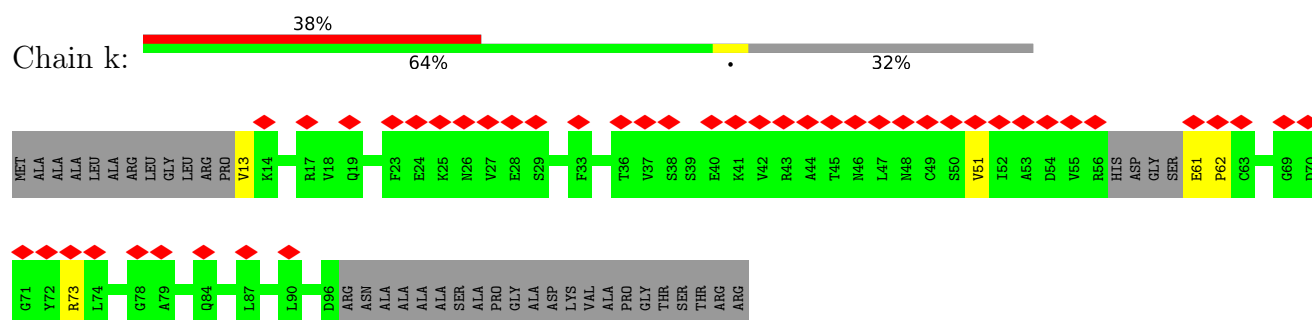
- Molecule 38: Large ribosomal subunit protein mL51



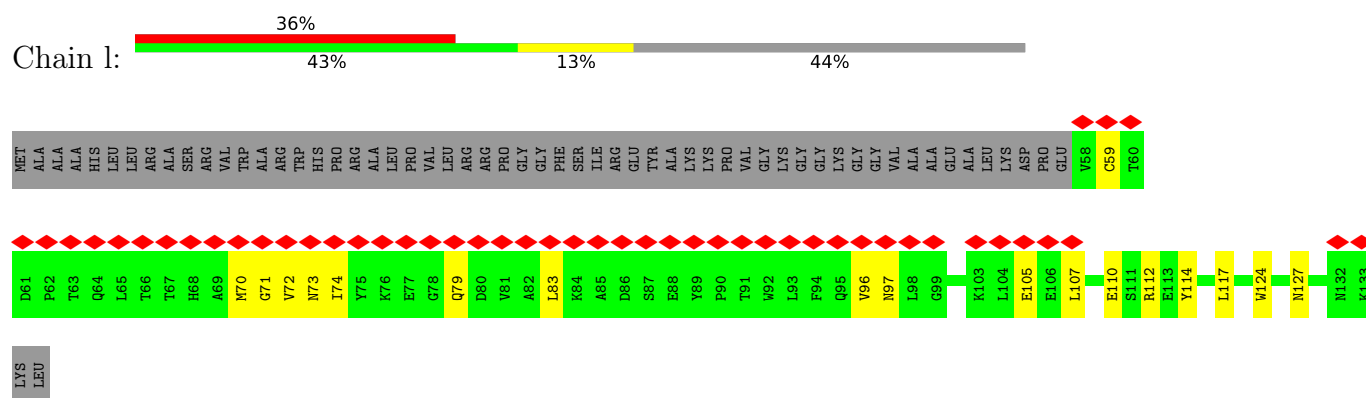
- Molecule 39: Large ribosomal subunit protein mL52



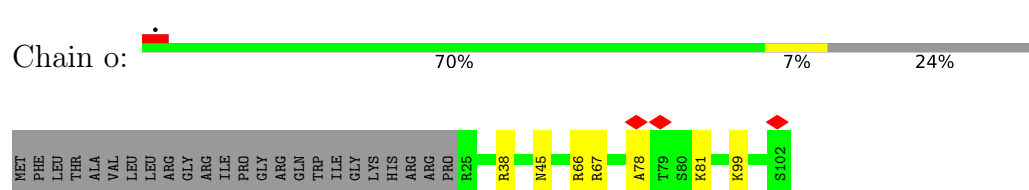
- Molecule 40: Large ribosomal subunit protein mL53



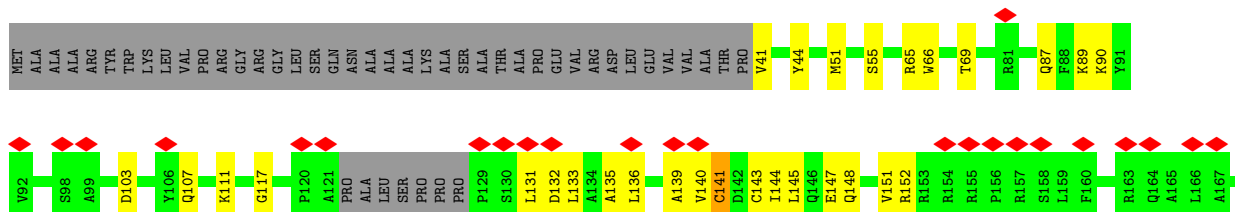
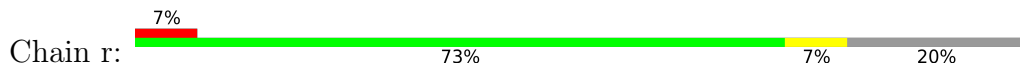
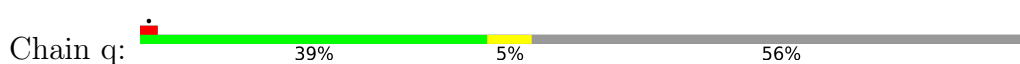
- Molecule 41: Large ribosomal subunit protein mL54

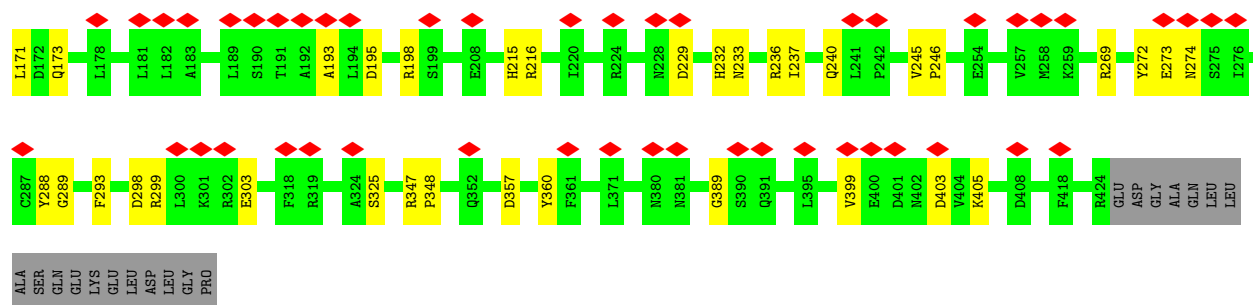


- Molecule 42: Large ribosomal subunit protein mL63

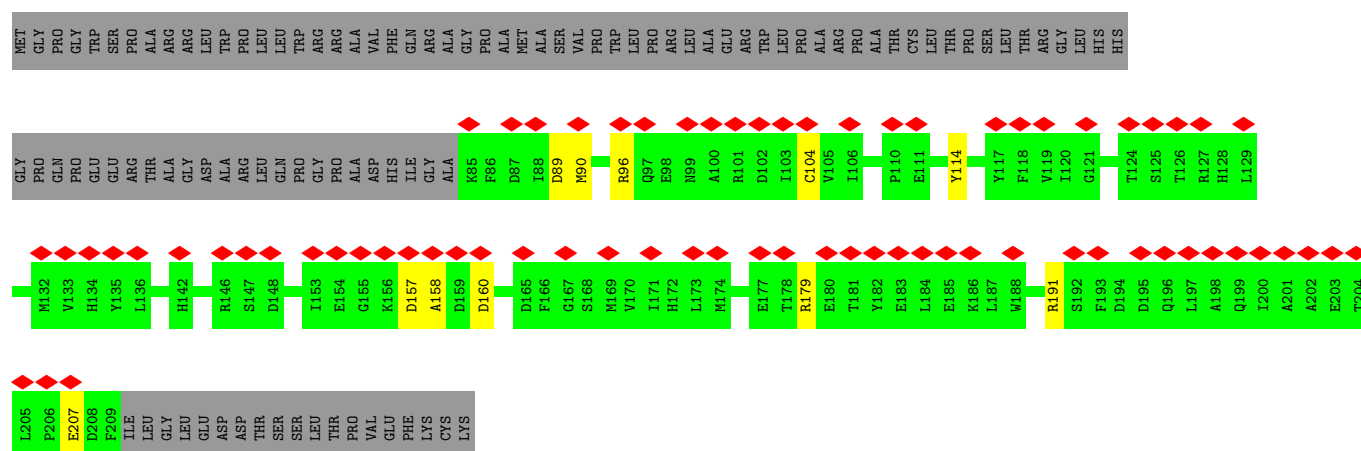


- Chain p: 

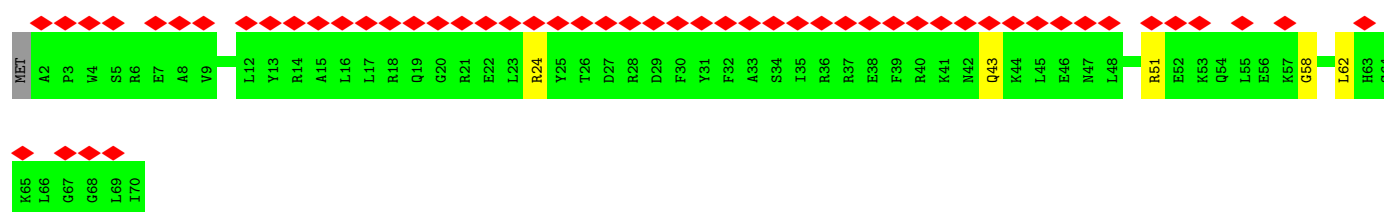
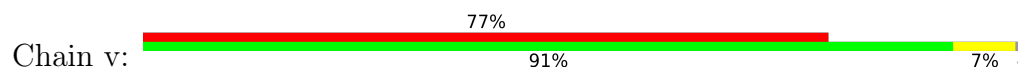




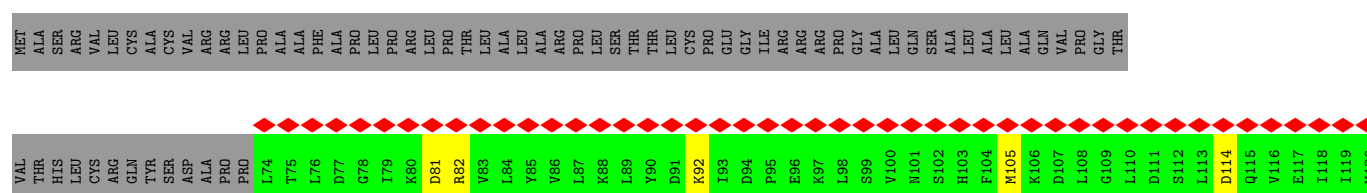
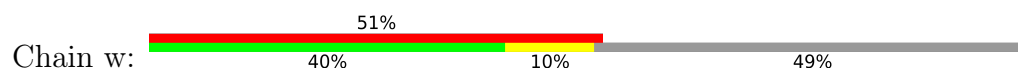
- Molecule 47: Mitochondrial assembly of ribosomal large subunit protein 1

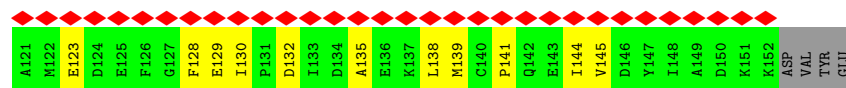


- Molecule 48: Predicted gene, 55359

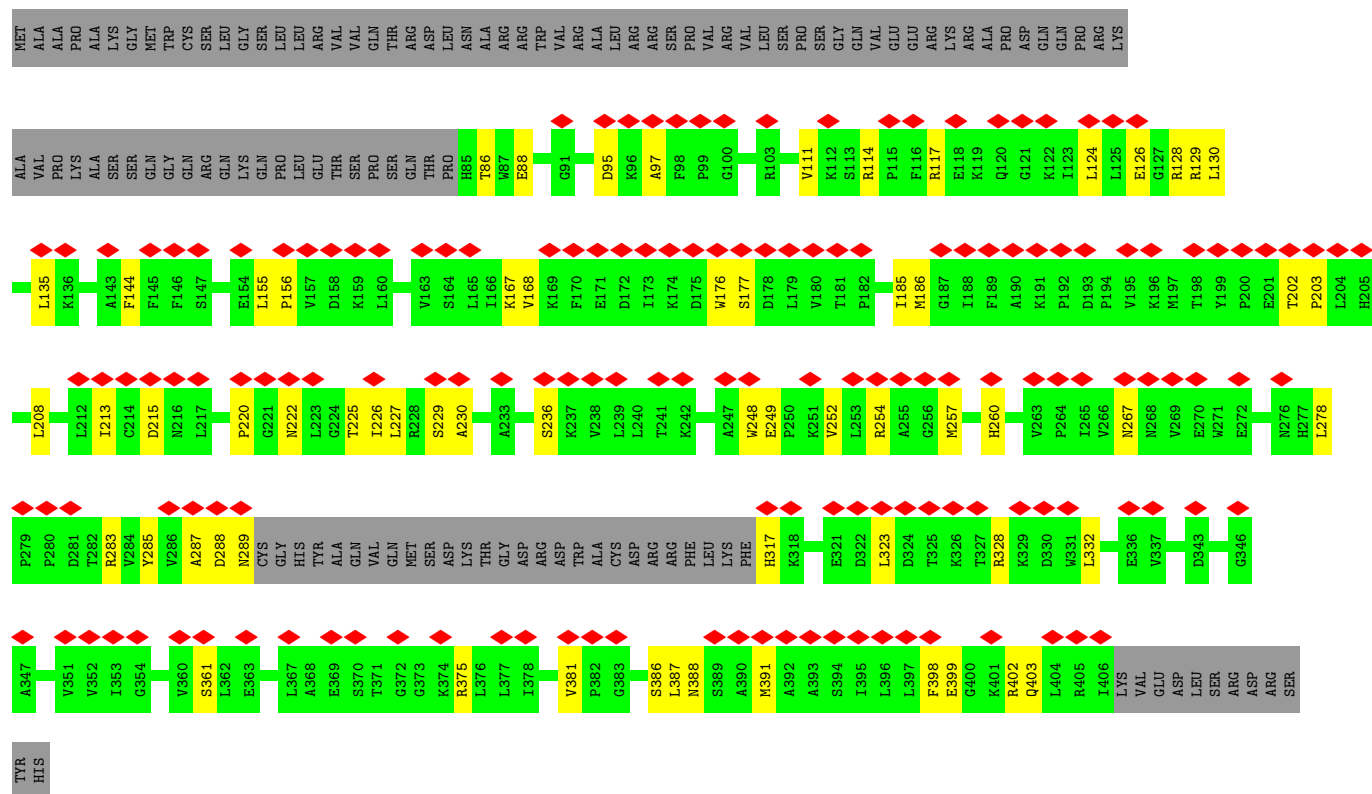
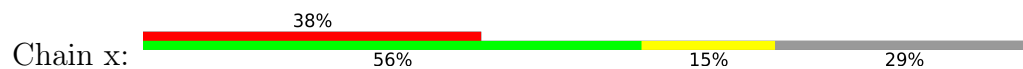


- Molecule 49: Acyl carrier protein, mitochondrial

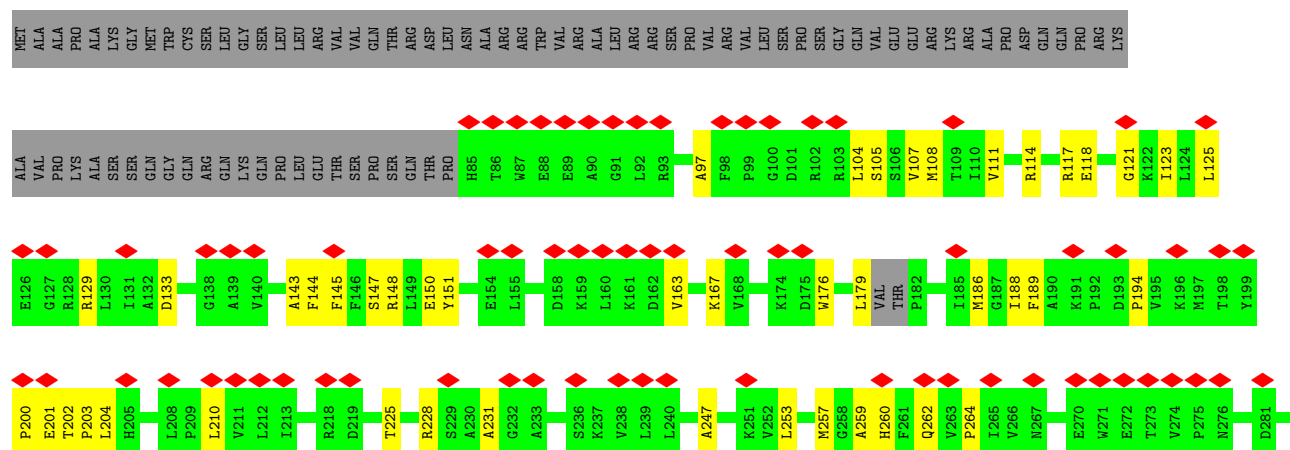


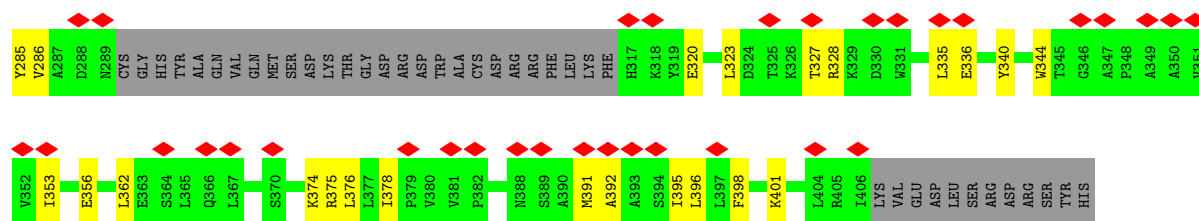


• Molecule 50: rRNA methyltransferase 3, mitochondrial

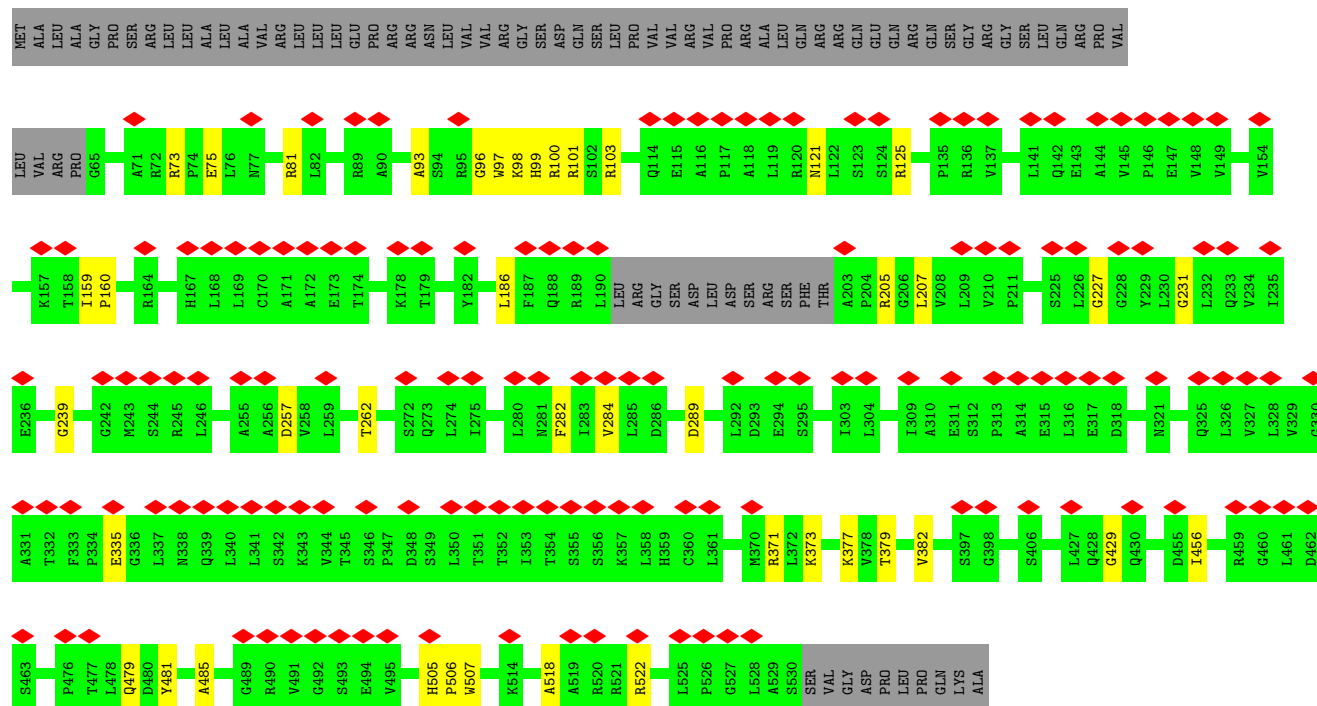
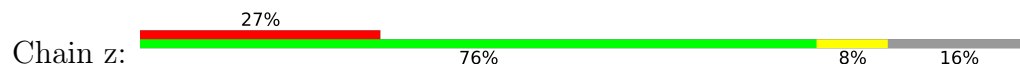


• Molecule 50: rRNA methyltransferase 3, mitochondrial





• Molecule 51: Probable ATP-dependent RNA helicase DDX28



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8965	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.573	Depositor
Minimum map value	-0.200	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	457.2936, 457.2936, 457.2936	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84684, 0.84684, 0.84684	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.07	0/26872	0.18	0/41762
2	B	0.09	0/1459	0.21	0/2266
3	D	0.07	0/1357	0.23	0/1831
4	E	0.06	0/2186	0.19	0/2972
5	F	0.07	0/1772	0.20	0/2415
6	H	0.08	0/793	0.23	0/1066
7	I	0.09	0/1273	0.23	0/1722
8	J	0.08	0/1093	0.23	0/1472
9	K	0.07	0/1436	0.20	0/1948
10	L	0.08	0/908	0.23	0/1224
11	M	0.08	0/2054	0.23	0/2776
12	N	0.07	0/1646	0.20	0/2220
13	O	0.07	0/1206	0.20	0/1626
14	P	0.07	0/1181	0.20	0/1600
15	Q	0.07	0/1832	0.21	0/2471
16	R	0.06	0/1096	0.17	0/1469
17	S	0.08	0/1328	0.23	0/1798
18	T	0.07	0/1402	0.19	0/1885
19	U	0.07	0/1062	0.20	0/1441
20	V	0.07	0/1669	0.20	0/2259
21	X	0.07	0/2075	0.20	0/2806
22	Y	0.06	0/1561	0.17	0/2093
23	Z	0.07	0/959	0.21	0/1298
24	0	0.07	0/896	0.20	0/1200
25	5	0.07	0/3256	0.21	0/4432
26	6	0.08	0/2530	0.21	0/3431
27	7	0.07	0/2436	0.22	0/3300
28	8	0.07	0/499	0.17	0/666
29	9	0.09	0/800	0.23	0/1082
30	a	0.07	0/884	0.20	0/1197
31	b	0.07	0/1203	0.21	0/1625
32	c	0.07	0/2297	0.19	0/3106



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	d	0.08	0/1736	0.21	0/2353
34	e	0.08	0/1465	0.22	0/1971
35	f	0.08	0/726	0.20	0/983
36	g	0.08	0/1126	0.23	0/1533
37	h	0.07	0/894	0.20	0/1216
38	i	0.06	0/813	0.20	0/1092
39	j	0.06	0/698	0.18	0/937
40	k	0.07	0/636	0.19	0/857
41	l	0.07	0/651	0.20	0/882
42	o	0.06	0/655	0.17	0/880
43	p	0.07	0/1104	0.22	0/1476
44	q	0.07	0/825	0.20	0/1126
45	r	0.07	0/1301	0.22	0/1756
46	s	0.09	0/3118	0.24	0/4232
47	u	0.07	0/1053	0.20	0/1425
48	v	0.07	0/596	0.20	0/795
49	w	0.10	0/646	0.27	0/869
50	x	0.10	0/2357	0.26	0/3198
50	y	0.09	0/2342	0.25	0/3174
51	z	0.07	0/3592	0.21	0/4876
All	All	0.07	0/99355	0.20	0/140090

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
46	s	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	s	141	CYS	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	24012	12123	12152	177	0
2	B	1303	657	658	14	0
3	D	1335	1373	1373	21	0
4	E	2122	2097	2097	18	0
5	F	1728	1755	1754	14	0
6	H	779	814	814	16	0
7	I	1245	1330	1330	22	0
8	J	1075	1145	1145	22	0
9	K	1396	1398	1398	10	0
10	L	893	944	944	10	0
11	M	2010	2080	2080	25	0
12	N	1601	1608	1608	12	0
13	O	1183	1215	1215	10	0
14	P	1154	1148	1148	21	0
15	Q	1790	1822	1822	19	0
16	R	1077	1137	1137	5	0
17	S	1301	1372	1372	15	0
18	T	1369	1402	1402	11	0
19	U	1034	1038	1038	8	0
20	V	1628	1622	1622	18	0
21	X	2021	2051	2051	14	0
22	Y	1523	1553	1553	10	0
23	Z	934	979	979	7	0
24	0	881	908	908	12	0
25	5	3168	3187	3187	15	0
26	6	2451	2342	2342	39	0
27	7	2379	2378	2378	19	0
28	8	493	484	484	10	0
29	9	778	772	772	6	0
30	a	860	843	843	7	0
31	b	1181	1195	1195	13	0
32	c	2246	2256	2256	17	0
33	d	1688	1671	1670	32	0
34	e	1437	1474	1474	26	0
35	f	714	704	704	12	0
36	g	1090	1094	1094	13	0
37	h	872	868	867	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	i	790	811	811	13	0
39	j	684	692	692	6	0
40	k	629	639	639	4	0
41	l	635	631	631	16	0
42	o	640	623	623	6	0
43	p	1089	1112	1112	15	0
44	q	799	785	785	6	0
45	r	1267	1319	1319	12	0
46	s	3045	3055	3055	49	0
47	u	1029	1012	1012	8	0
48	v	586	603	603	4	0
49	w	637	640	640	12	0
50	x	2305	2356	2356	53	0
50	y	2291	2340	2340	58	0
51	z	3524	3639	3639	34	0
52	0	1	0	0	0	0
53	r	4	0	0	2	0
All	All	94706	83096	83123	840	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 840 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:8:139:MET:HE1	34:e:275:LEU:HD23	1.47	0.93
1:A:2168:U:O2'	51:z:99:HIS:O	1.91	0.88
1:A:1597:C:N4	1:A:1644:C:OP1	2.08	0.86
50:x:124:LEU:HD21	50:x:186:MET:HE3	1.58	0.83
1:A:2168:U:OP2	51:z:73:ARG:NH1	2.12	0.83

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	168/246 (68%)	165 (98%)	3 (2%)	0	100	100
4	E	260/348 (75%)	251 (96%)	9 (4%)	0	100	100
5	F	210/294 (71%)	210 (100%)	0	0	100	100
6	H	93/268 (35%)	89 (96%)	4 (4%)	0	100	100
7	I	150/262 (57%)	146 (97%)	4 (3%)	0	100	100
8	J	140/192 (73%)	138 (99%)	2 (1%)	0	100	100
9	K	169/178 (95%)	168 (99%)	1 (1%)	0	100	100
10	L	113/145 (78%)	110 (97%)	3 (3%)	0	100	100
11	M	245/295 (83%)	242 (99%)	3 (1%)	0	100	100
12	N	189/251 (75%)	186 (98%)	3 (2%)	0	100	100
13	O	142/176 (81%)	140 (99%)	2 (1%)	0	100	100
14	P	139/180 (77%)	138 (99%)	1 (1%)	0	100	100
15	Q	215/292 (74%)	211 (98%)	4 (2%)	0	100	100
16	R	129/149 (87%)	129 (100%)	0	0	100	100
17	S	157/209 (75%)	154 (98%)	3 (2%)	0	100	100
18	T	164/206 (80%)	164 (100%)	0	0	100	100
19	U	121/146 (83%)	121 (100%)	0	0	100	100
20	V	196/216 (91%)	196 (100%)	0	0	100	100
21	X	240/294 (82%)	239 (100%)	1 (0%)	0	100	100
22	Y	174/252 (69%)	174 (100%)	0	0	100	100
23	Z	113/160 (71%)	112 (99%)	1 (1%)	0	100	100
24	0	106/187 (57%)	106 (100%)	0	0	100	100
25	5	383/423 (90%)	378 (99%)	5 (1%)	0	100	100
26	6	279/380 (73%)	274 (98%)	5 (2%)	0	100	100
27	7	290/336 (86%)	287 (99%)	3 (1%)	0	100	100
28	8	57/206 (28%)	57 (100%)	0	0	100	100
29	9	94/135 (70%)	94 (100%)	0	0	100	100
30	a	99/142 (70%)	96 (97%)	3 (3%)	0	100	100
31	b	146/159 (92%)	140 (96%)	6 (4%)	0	100	100
32	c	275/308 (89%)	275 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	d	198/306 (65%)	196 (99%)	2 (1%)	0	100	100
34	e	171/283 (60%)	159 (93%)	12 (7%)	0	100	100
35	f	85/211 (40%)	81 (95%)	4 (5%)	0	100	100
36	g	130/166 (78%)	129 (99%)	1 (1%)	0	100	100
37	h	108/159 (68%)	104 (96%)	4 (4%)	0	100	100
38	i	90/128 (70%)	90 (100%)	0	0	100	100
39	j	83/121 (69%)	82 (99%)	1 (1%)	0	100	100
40	k	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
41	l	74/135 (55%)	74 (100%)	0	0	100	100
42	o	76/102 (74%)	75 (99%)	1 (1%)	0	100	100
43	p	124/206 (60%)	122 (98%)	2 (2%)	0	100	100
44	q	95/222 (43%)	95 (100%)	0	0	100	100
45	r	152/196 (78%)	146 (96%)	6 (4%)	0	100	100
46	s	373/442 (84%)	359 (96%)	14 (4%)	0	100	100
47	u	123/228 (54%)	121 (98%)	2 (2%)	0	100	100
48	v	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
49	w	77/156 (49%)	76 (99%)	1 (1%)	0	100	100
50	x	291/418 (70%)	282 (97%)	9 (3%)	0	100	100
50	y	287/418 (69%)	279 (97%)	8 (3%)	0	100	100
51	z	450/540 (83%)	444 (99%)	6 (1%)	0	100	100
All	All	8386/11660 (72%)	8245 (98%)	141 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	143/197 (73%)	143 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	237/298 (80%)	237 (100%)	0	100	100
5	F	190/250 (76%)	190 (100%)	0	100	100
6	H	86/231 (37%)	86 (100%)	0	100	100
7	I	143/230 (62%)	143 (100%)	0	100	100
8	J	116/152 (76%)	116 (100%)	0	100	100
9	K	151/158 (96%)	151 (100%)	0	100	100
10	L	99/122 (81%)	99 (100%)	0	100	100
11	M	219/252 (87%)	219 (100%)	0	100	100
12	N	172/216 (80%)	172 (100%)	0	100	100
13	O	125/152 (82%)	125 (100%)	0	100	100
14	P	123/157 (78%)	123 (100%)	0	100	100
15	Q	197/258 (76%)	197 (100%)	0	100	100
16	R	110/128 (86%)	110 (100%)	0	100	100
17	S	145/180 (81%)	145 (100%)	0	100	100
18	T	147/180 (82%)	147 (100%)	0	100	100
19	U	112/133 (84%)	112 (100%)	0	100	100
20	V	176/190 (93%)	176 (100%)	0	100	100
21	X	219/265 (83%)	219 (100%)	0	100	100
22	Y	162/228 (71%)	162 (100%)	0	100	100
23	Z	108/146 (74%)	108 (100%)	0	100	100
24	0	97/170 (57%)	97 (100%)	0	100	100
25	5	349/372 (94%)	349 (100%)	0	100	100
26	6	254/335 (76%)	254 (100%)	0	100	100
27	7	269/301 (89%)	269 (100%)	0	100	100
28	8	51/182 (28%)	51 (100%)	0	100	100
29	9	83/114 (73%)	83 (100%)	0	100	100
30	a	97/129 (75%)	97 (100%)	0	100	100
31	b	130/138 (94%)	130 (100%)	0	100	100
32	c	243/266 (91%)	243 (100%)	0	100	100
33	d	182/272 (67%)	182 (100%)	0	100	100
34	e	152/238 (64%)	152 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	f	80/185 (43%)	80 (100%)	0	100	100
36	g	122/148 (82%)	122 (100%)	0	100	100
37	h	100/143 (70%)	100 (100%)	0	100	100
38	i	84/111 (76%)	84 (100%)	0	100	100
39	j	68/99 (69%)	68 (100%)	0	100	100
40	k	72/95 (76%)	72 (100%)	0	100	100
41	l	70/112 (62%)	70 (100%)	0	100	100
42	o	65/85 (76%)	65 (100%)	0	100	100
43	p	118/177 (67%)	118 (100%)	0	100	100
44	q	84/187 (45%)	84 (100%)	0	100	100
45	r	141/168 (84%)	141 (100%)	0	100	100
46	s	329/378 (87%)	329 (100%)	0	100	100
47	u	115/197 (58%)	115 (100%)	0	100	100
48	v	60/61 (98%)	60 (100%)	0	100	100
49	w	73/135 (54%)	73 (100%)	0	100	100
50	x	251/358 (70%)	251 (100%)	0	100	100
50	y	249/358 (70%)	249 (100%)	0	100	100
51	z	390/464 (84%)	390 (100%)	0	100	100
All	All	7558/10101 (75%)	7558 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
45	r	79	HIS
50	y	206	HIS
46	s	233	ASN
46	s	402	ASN
51	z	104	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1101/1584 (69%)	352 (31%)	25 (2%)
2	B	59/68 (86%)	24 (40%)	1 (1%)
All	All	1160/1652 (70%)	376 (32%)	26 (2%)

5 of 376 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1094	A
1	A	1095	C
1	A	1100	C
1	A	1101	C
1	A	1102	U

5 of 26 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1894	C
1	A	2275	A
1	A	2659	C
1	A	2182	U
1	A	2302	U

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
53	FES	r	201	7,45	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
53	FES	r	201	7,45	-	-	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	r	201	FES	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

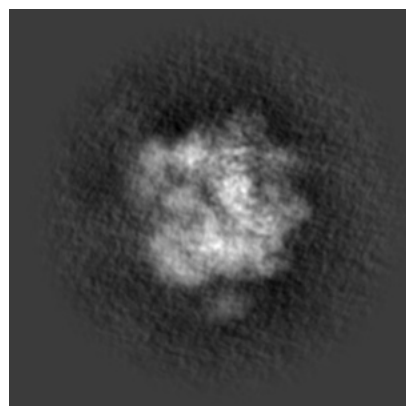
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52045. These allow visual inspection of the internal detail of the map and identification of artifacts.

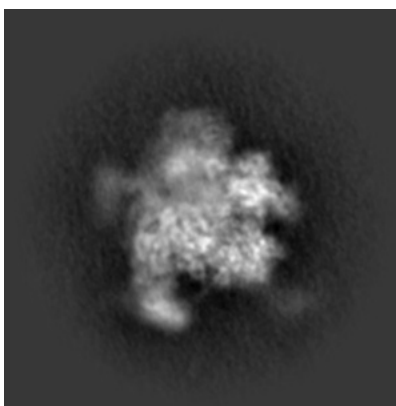
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

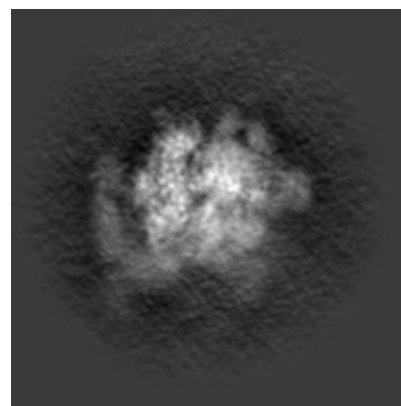
#### 6.1.1 Primary map



X

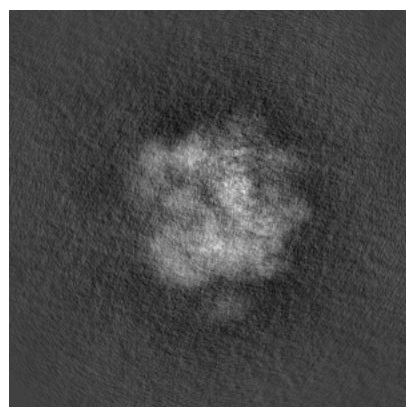


Y

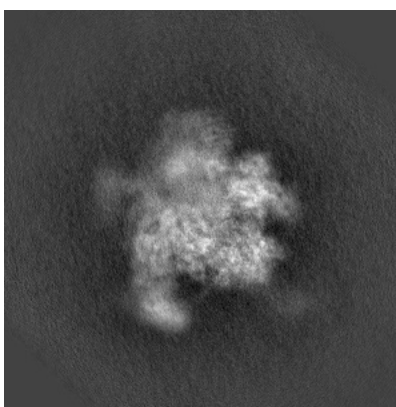


Z

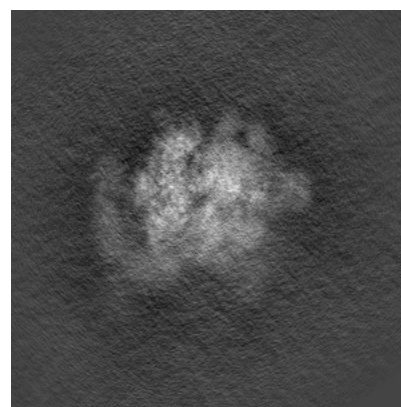
#### 6.1.2 Raw map



X



Y

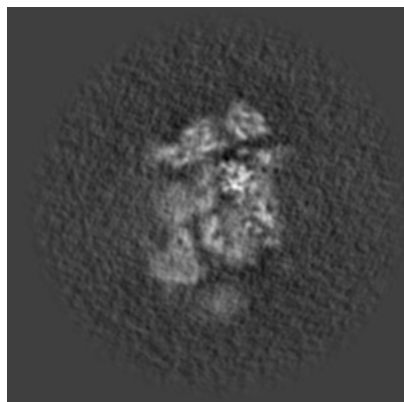


Z

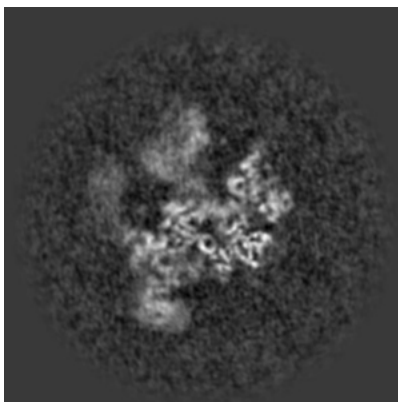
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

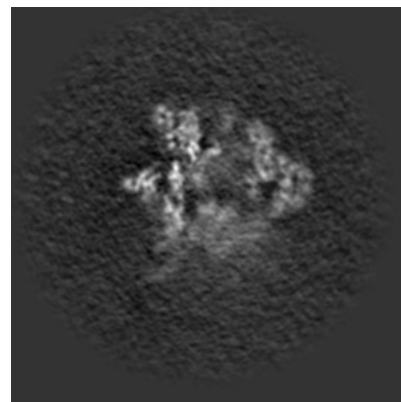
### 6.2.1 Primary map



X Index: 270

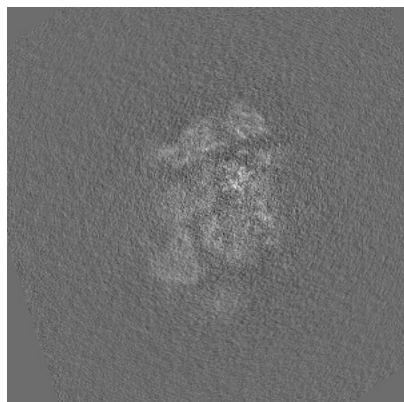


Y Index: 270

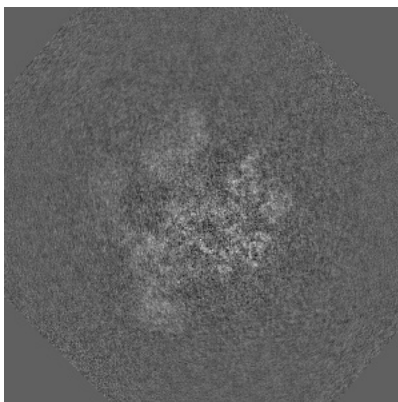


Z Index: 270

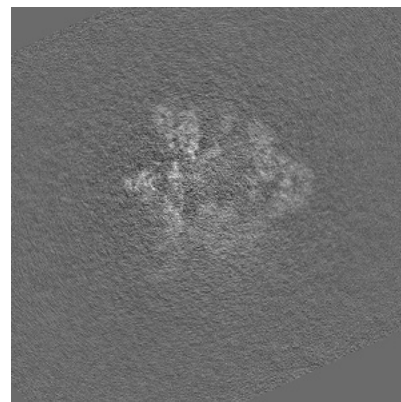
### 6.2.2 Raw map



X Index: 270



Y Index: 270

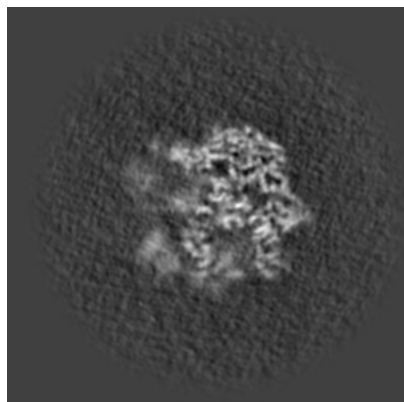


Z Index: 270

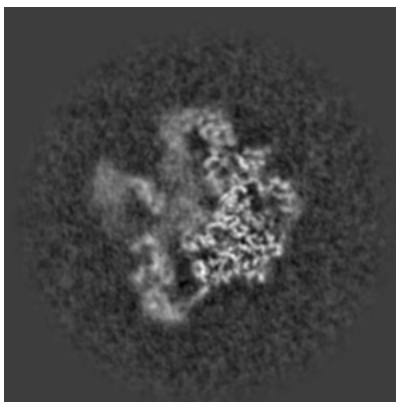
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

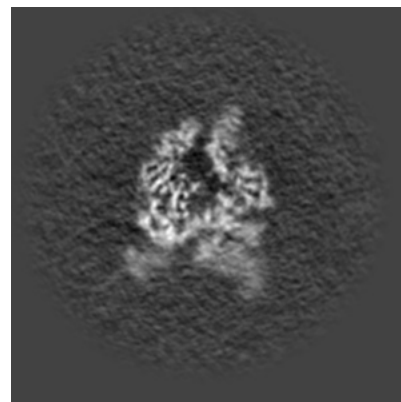
### 6.3.1 Primary map



X Index: 219

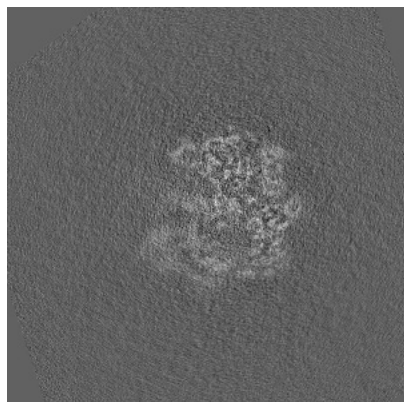


Y Index: 300

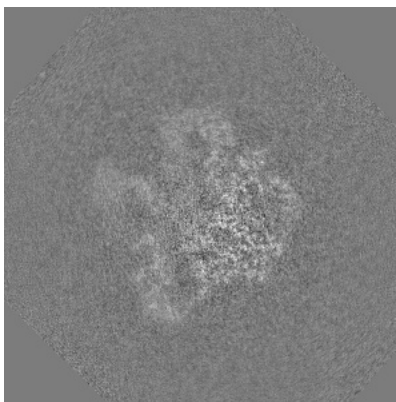


Z Index: 339

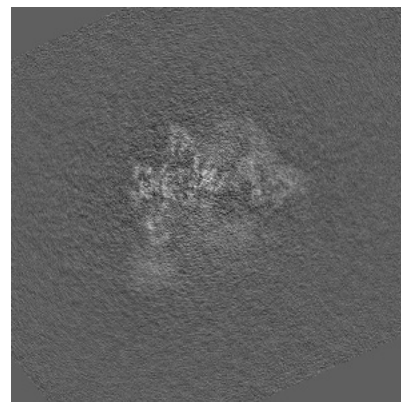
### 6.3.2 Raw map



X Index: 229



Y Index: 300



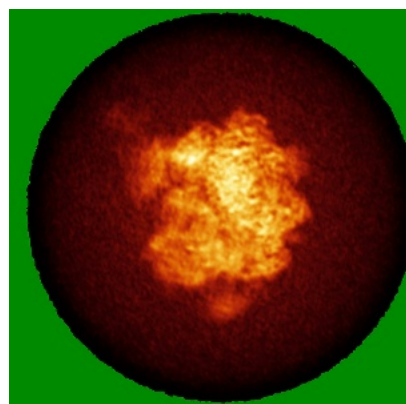
Z Index: 295

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

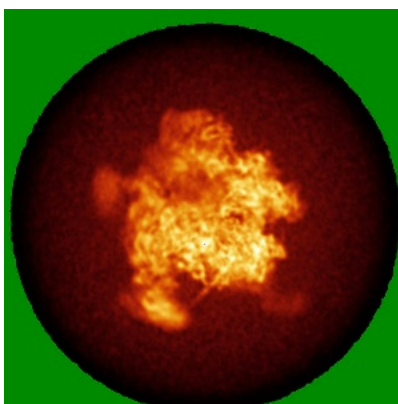


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

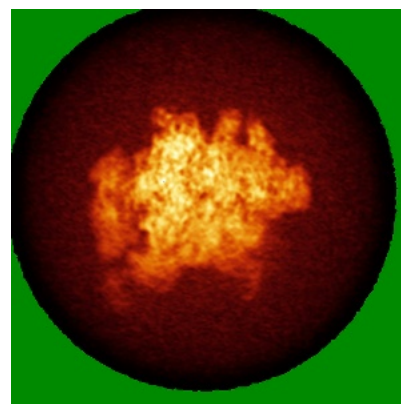
### 6.4.1 Primary map



X

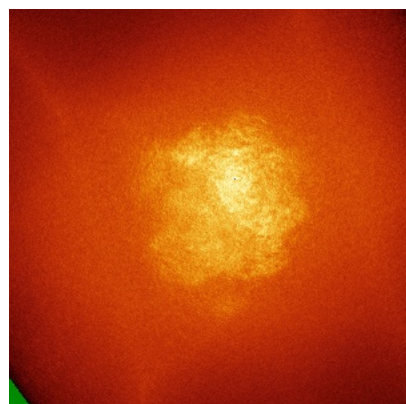


Y

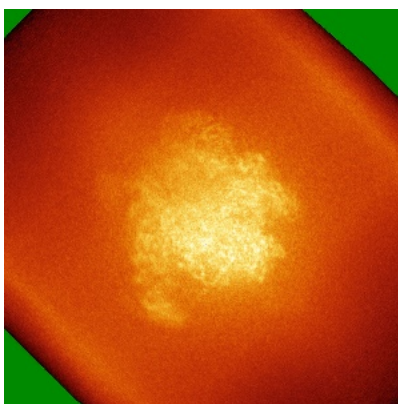


Z

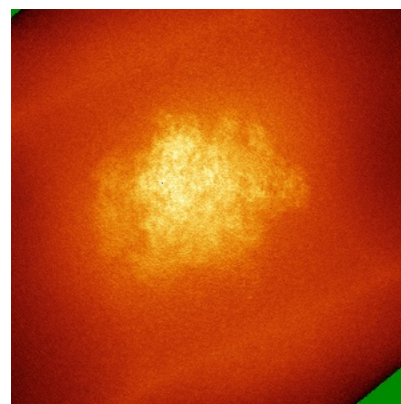
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

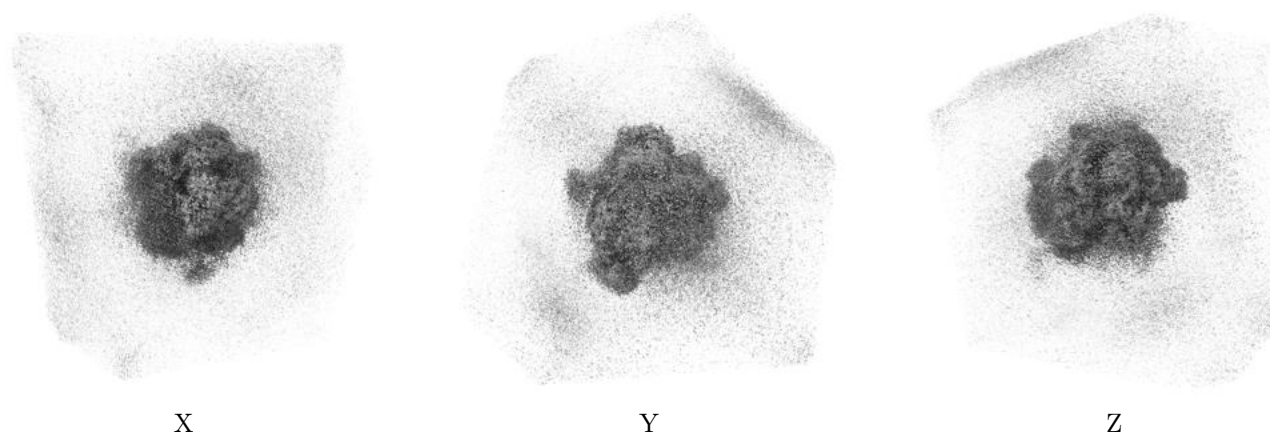
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

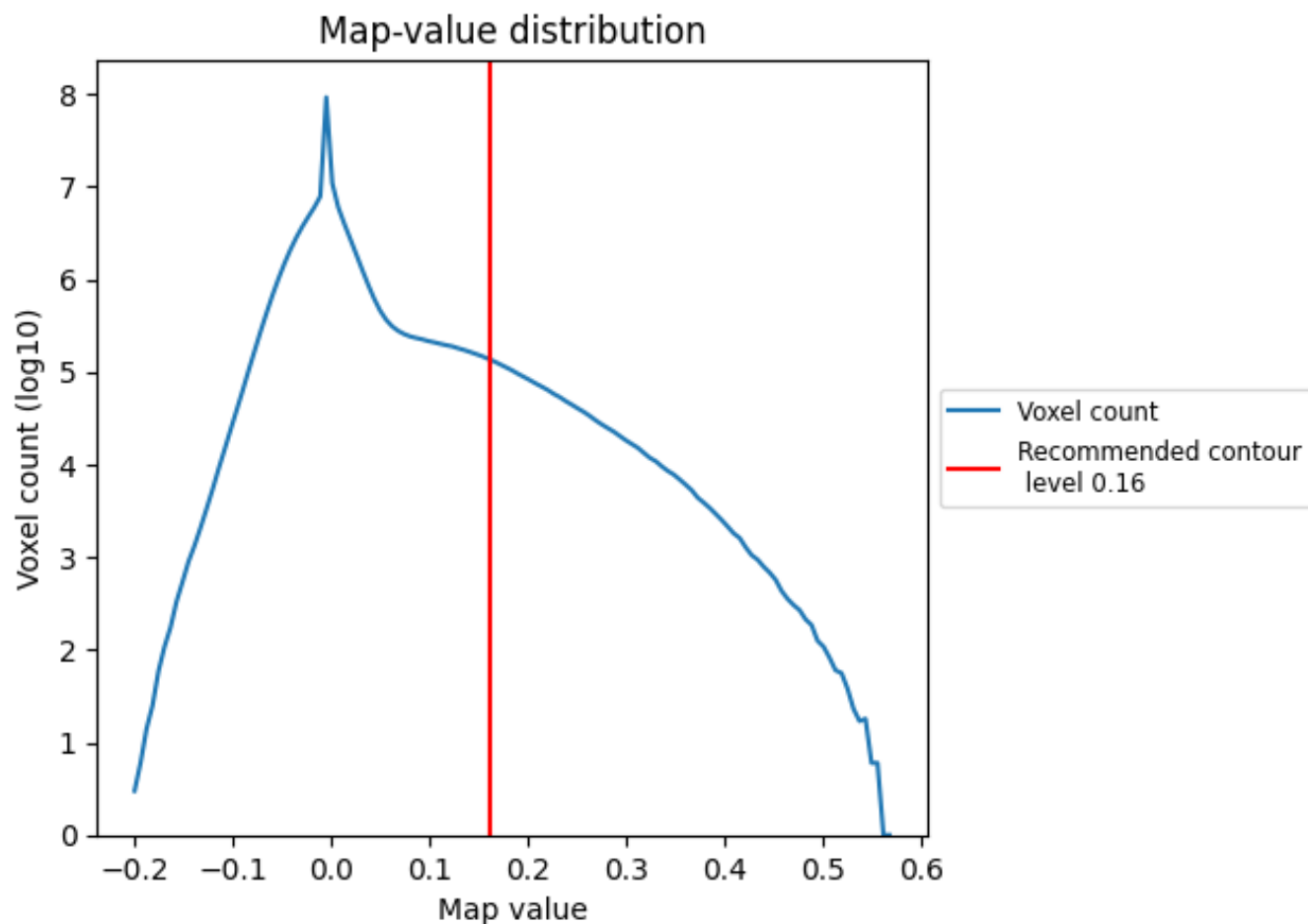
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

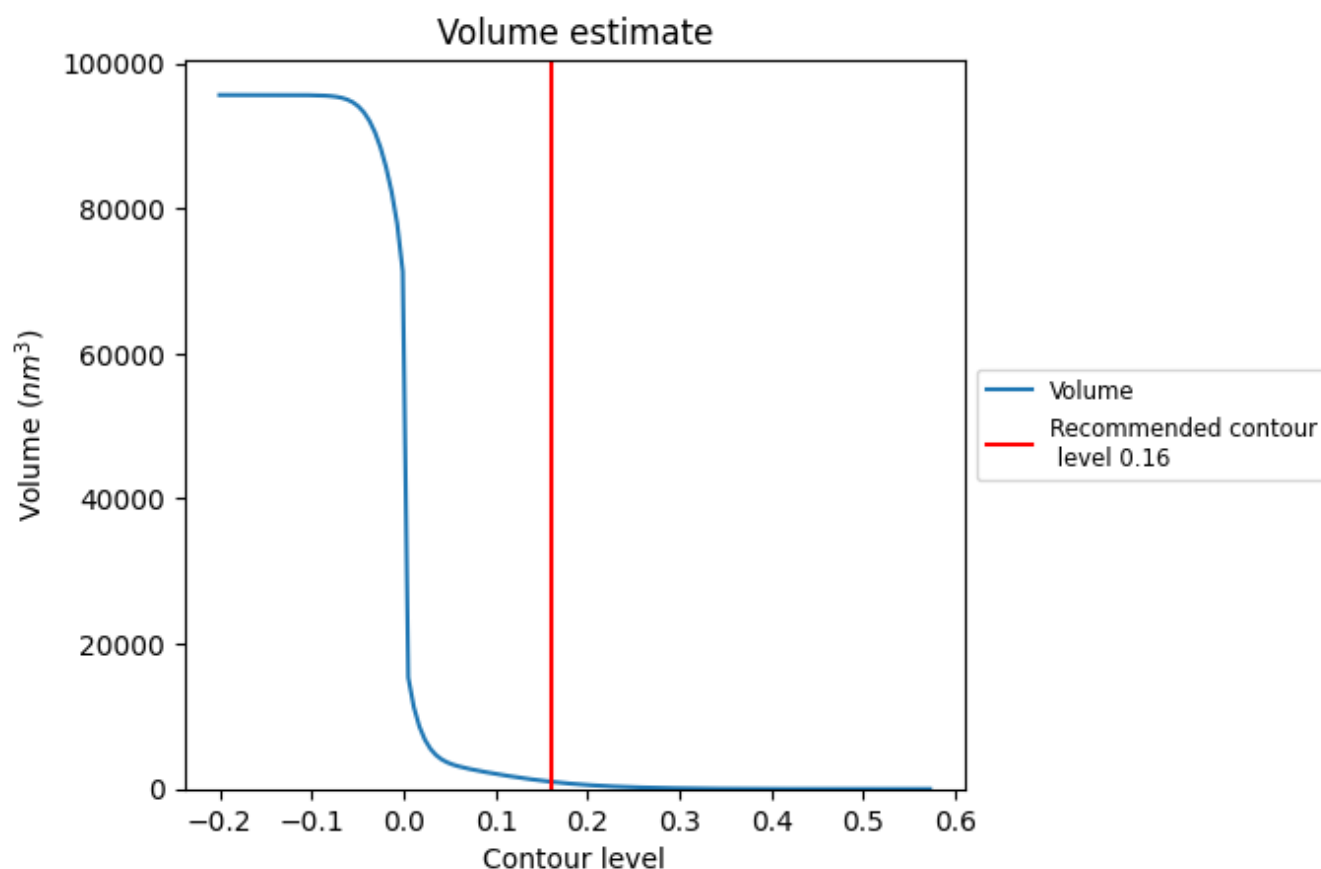
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

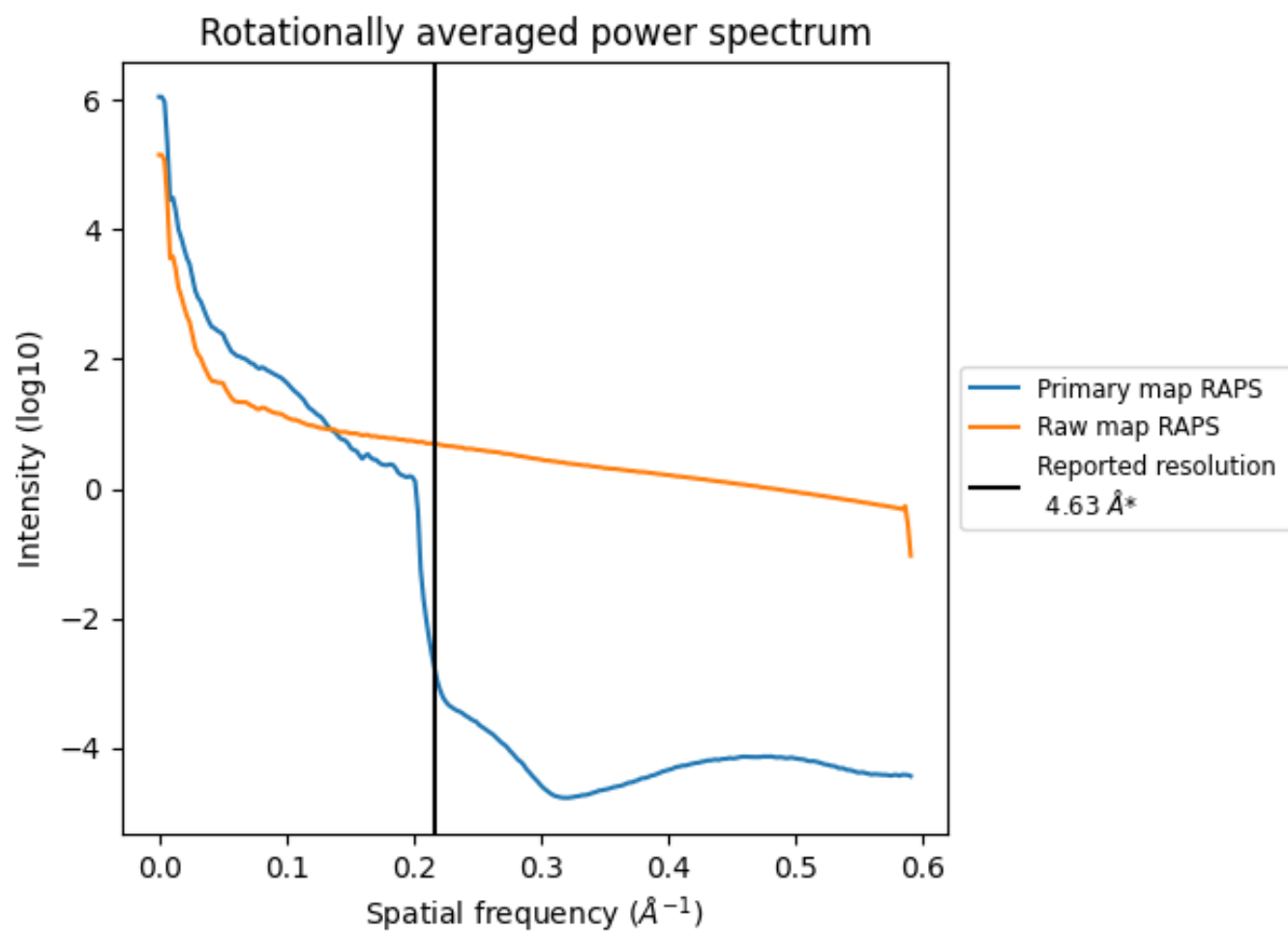


The volume at the recommended contour level is 1002 nm<sup>3</sup>; this corresponds to an approximate mass of 905 kDa.

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 ⓘ

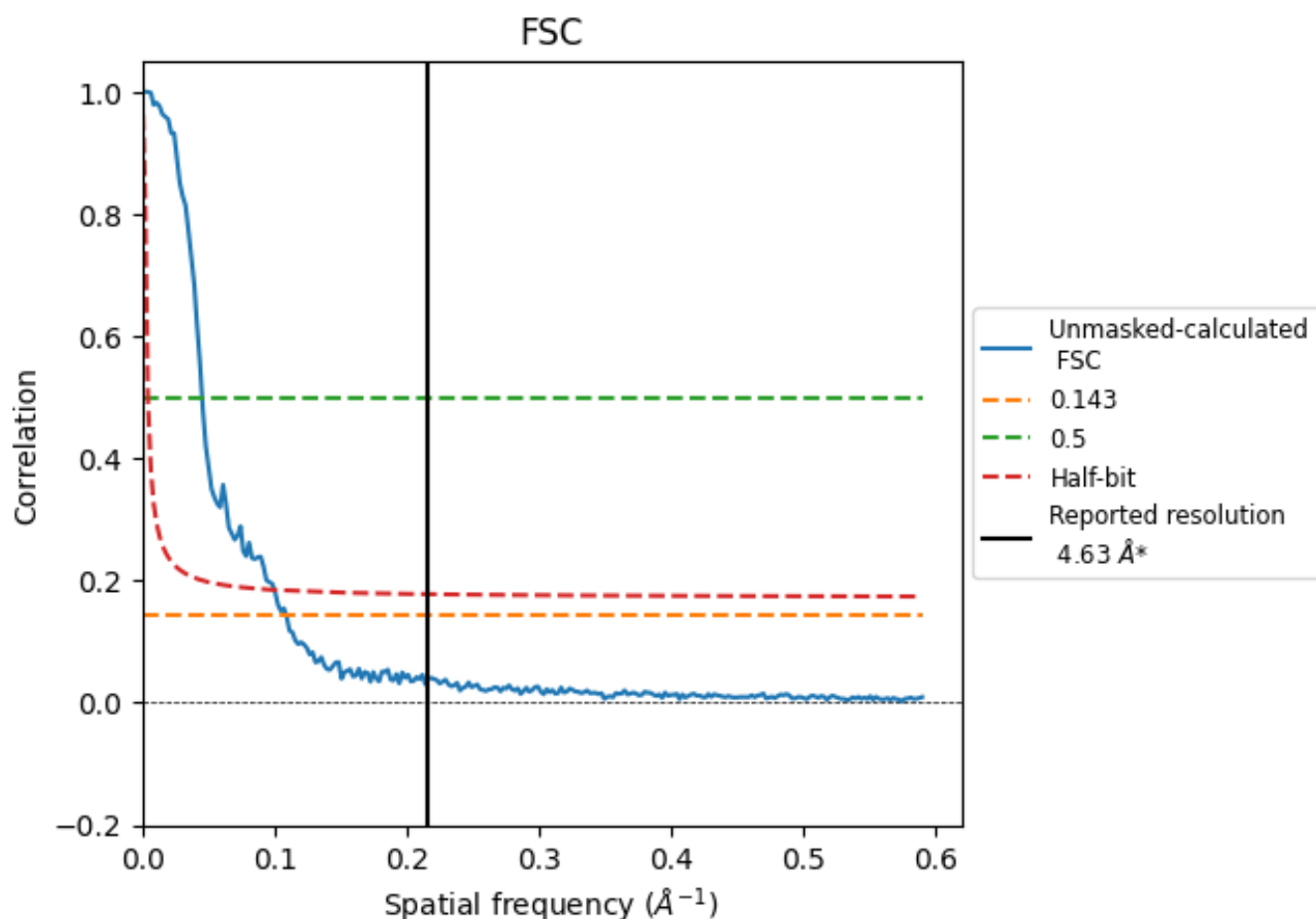


\*Reported resolution corresponds to spatial frequency of 0.216  $\text{\AA}^{-1}$

## 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 0.216 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

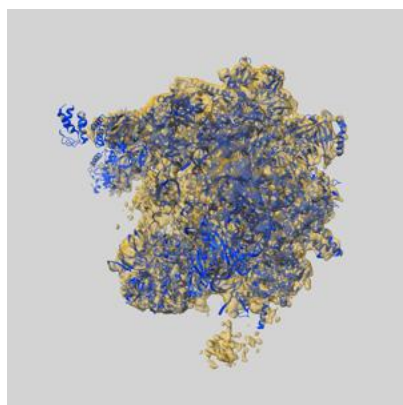
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.63	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.17	22.08	10.00

\*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 9.17 differs from the reported value 4.63 by more than 10 %

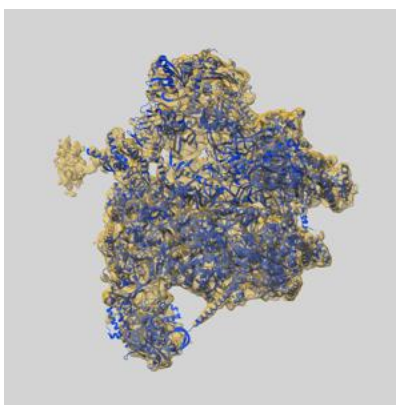
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52045 and PDB model 9HCD. Per-residue inclusion information can be found in section [3](#) on page [14](#).

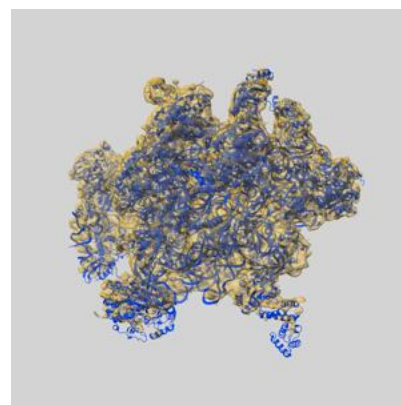
### 9.1 Map-model overlay [i](#)



X



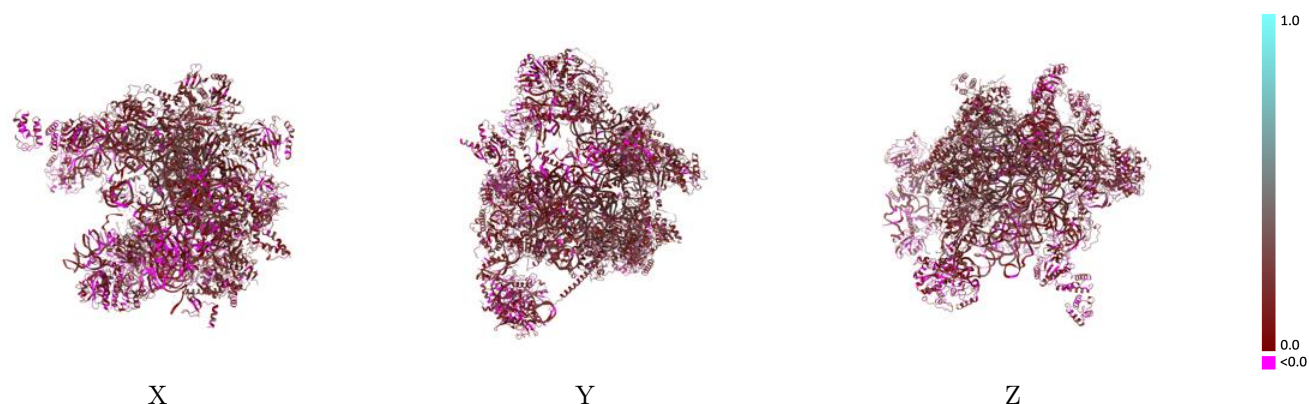
Y



Z

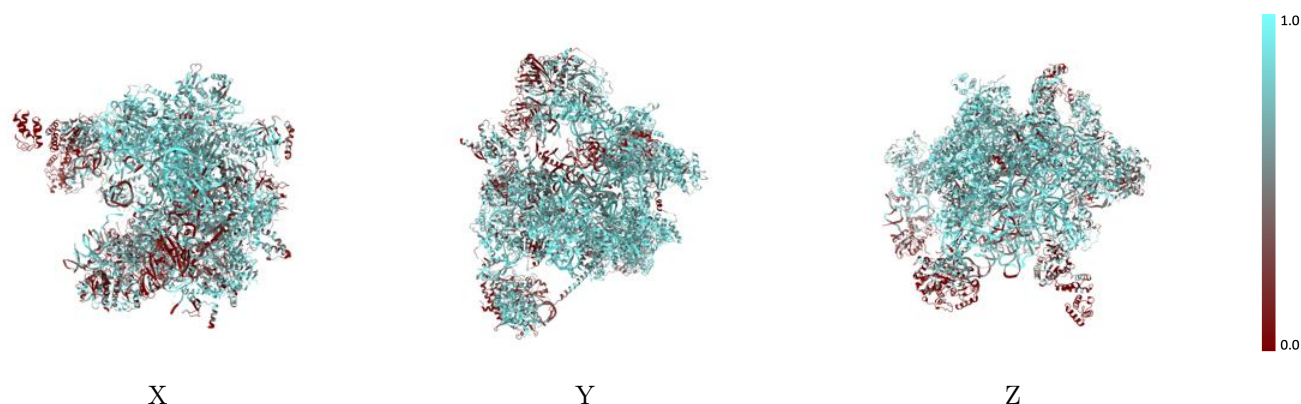
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



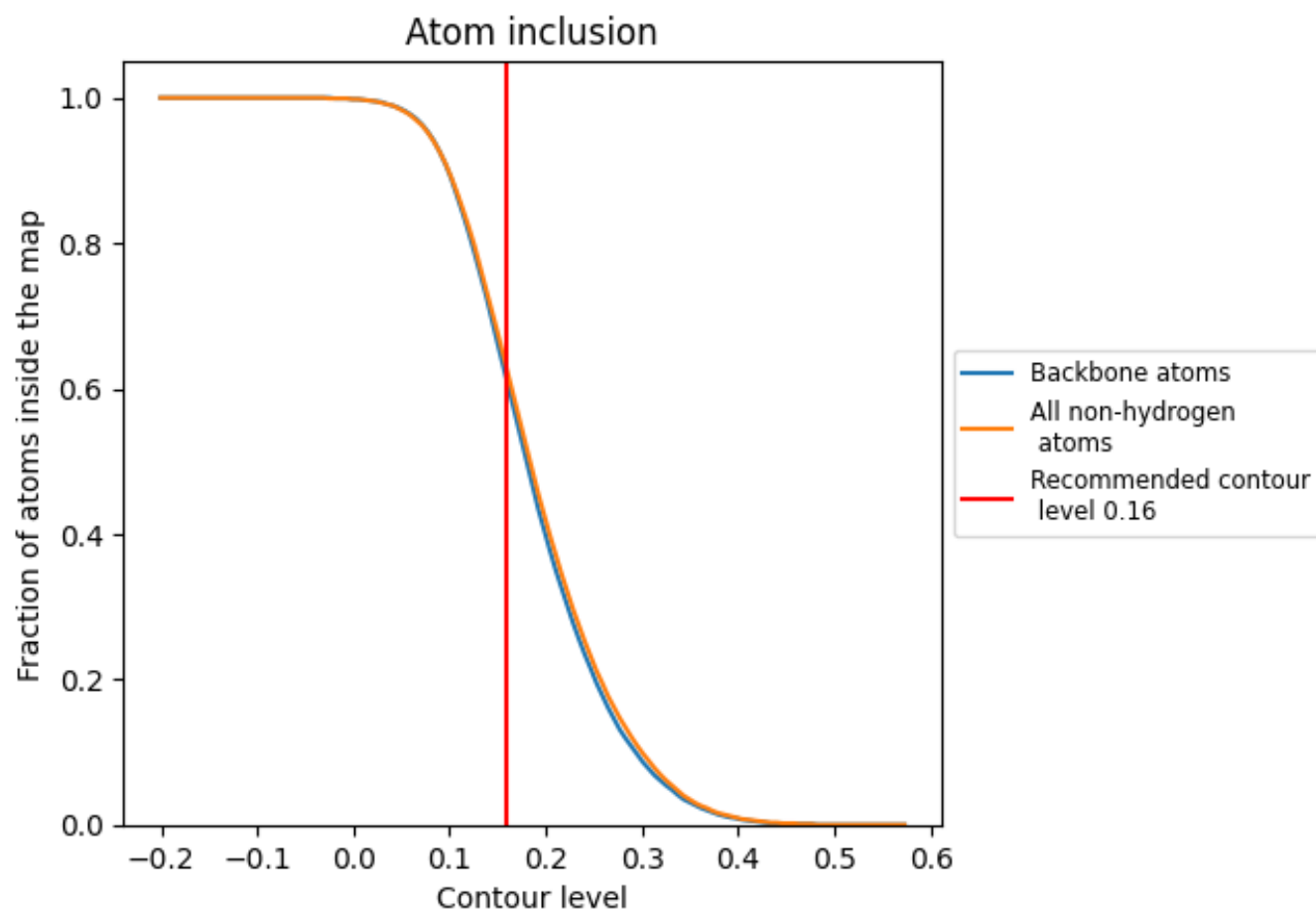
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 62% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6240	 0.1560
0	 0.7580	 0.2100
5	 0.3560	 0.1140
6	 0.6310	 0.1010
7	 0.7450	 0.1850
8	 0.2660	 0.0880
9	 0.6250	 0.1200
A	 0.7530	 0.1710
B	 0.6680	 0.1140
D	 0.1280	 0.0200
E	 0.7890	 0.1780
F	 0.7480	 0.1900
H	 0.5630	 0.0970
I	 0.3460	 0.0990
J	 0.1300	 0.0670
K	 0.7920	 0.2410
L	 0.3520	 0.1170
M	 0.7140	 0.1830
N	 0.6810	 0.1650
O	 0.7520	 0.1930
P	 0.7490	 0.1230
Q	 0.7180	 0.1720
R	 0.7140	 0.2100
S	 0.7460	 0.2360
T	 0.7140	 0.1870
U	 0.5960	 0.1570
V	 0.3590	 0.1220
X	 0.5530	 0.1420
Y	 0.6060	 0.1340
Z	 0.7040	 0.2330
a	 0.6050	 0.2280
b	 0.7800	 0.2350
c	 0.7390	 0.1980
d	 0.5700	 0.1520
e	 0.0900	 0.0480



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Chain	Atom inclusion	Q-score
f	 0.2120	 0.0620
g	 0.8290	 0.2250
h	 0.7690	 0.2130
i	 0.6580	 0.1910
j	 0.6810	 0.2170
k	 0.3570	 0.1320
l	 0.3310	 0.0970
o	 0.7500	 0.2130
p	 0.5840	 0.1540
q	 0.7680	 0.2210
r	 0.7890	 0.2000
s	 0.6440	 0.1650
u	 0.3540	 0.0930
v	 0.1990	 0.0910
w	 0.0110	 0.0990
x	 0.4060	 0.0730
y	 0.5560	 0.1100
z	 0.5250	 0.1560