



Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 07:02 am GMT

PDB ID : 7NSI
EMDB ID : EMD-12568
Title : 55S mammalian mitochondrial ribosome with mtRRF (pre) and tRNA(P/E)
Authors : Kummer, E.; Schubert, K.; Ban, N.
Deposited on : 2021-03-07
Resolution : 4.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

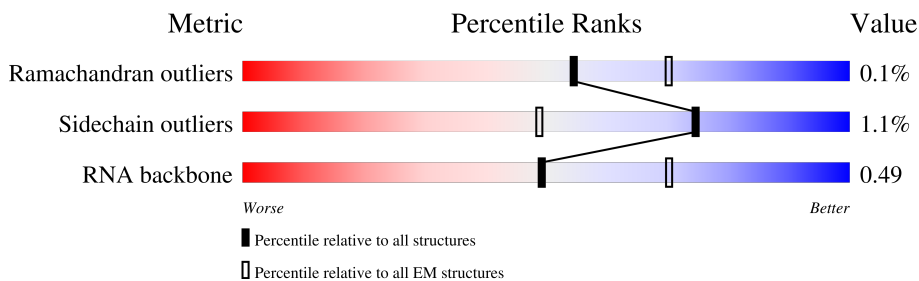
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 4.60 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	B0	148	
2	B1	256	
3	B2	252	
4	B3	161	
5	B4	126	
6	B5	188	
7	B6	65	
8	BB	73	

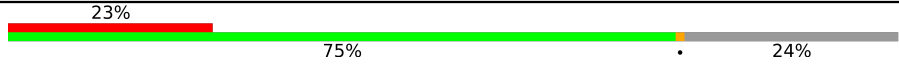
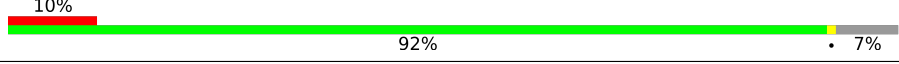
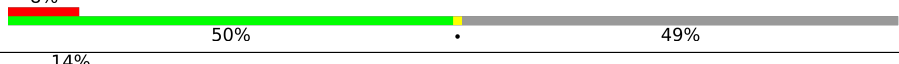


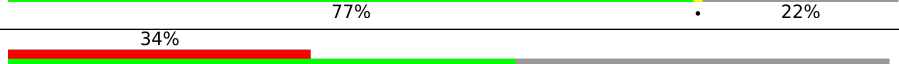
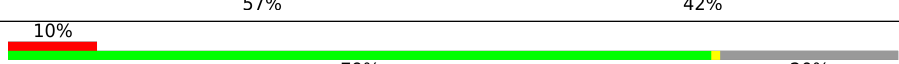
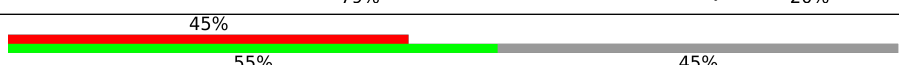
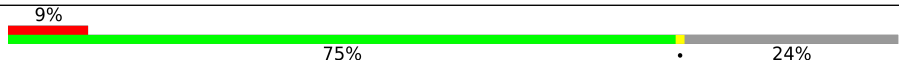

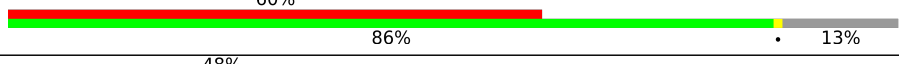
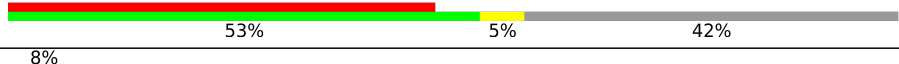
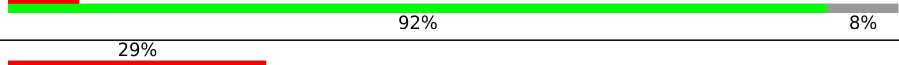

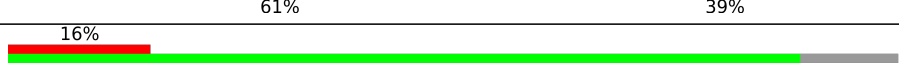
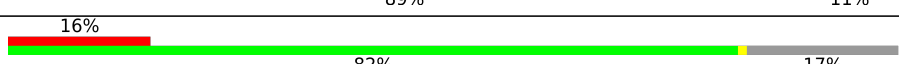


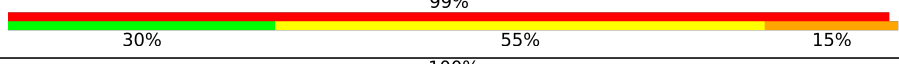
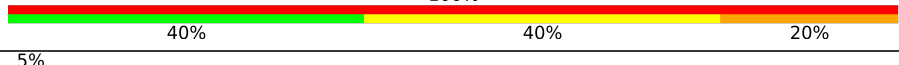





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	B7	95	5% 48% 52%
10	BD	306	11% 78% 22%
11	BE	399	7% 76% 23%
12	BF	294	12% 84% 15%
13	BG	257	64% 72% 25%
14	BI	268	13% 36% 63%
15	BJ	262	60% 81% 19%
16	BK	192	84% 91% 8%
17	BN	178	8% 99%
18	BO	145	8% 79% 21%
19	BP	296	15% 97%
20	BQ	251	14% 88% 12%
21	BR	169	12% 90% 9%
22	BS	180	8% 79% 21%
23	BT	292	13% 77% 21%
24	BU	149	14% 94% 6%
25	BV	209	7% 73% 26%
26	BW	210	13% 79% 21%
27	BX	150	30% 99%
28	BY	216	64% 94% 5%
29	Ba	423	14% 92% 7%
30	Bb	380	12% 92% 7%
31	Bc	334	12% 88% 12%
32	Bd	206	36% 65% 33%
33	Be	135	38% 90% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	Bf	142	
35	Bg	159	
36	B8	188	
37	Bh	332	
38	Bi	306	
39	Bj	279	
40	Bk	269	
41	Bl	166	
42	Bm	198	
43	Bn	128	
44	Bo	124	
45	Bp	112	
46	Bq	138	
47	Bt	102	
48	Bu	205	
49	Bv	222	
50	Bw	433	
51	Bx	196	
52	AA	962	
53	B9	100	
54	AV	71	
55	AX	5	
56	BA	1571	
57	AB	289	
58	AC	167	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	AE	430	45% 78% 20%
60	AF	276	29% 43% 56%
61	AG	242	69% 86% 14%
62	AI	397	57% 82% 17%
63	AJ	200	64% 70% 30%
64	AK	196	46% 70% 30%
65	AL	139	25% 78% 22%
66	AN	128	57% 77% 21%
67	AO	239	42% 73% 27%
68	AP	135	44% 87% 13%
69	AQ	130	30% 86% 14%
70	AR	143	33% 66% 32%
71	AU	87	43% 98% ..
72	AZ	18	83% 100%
73	Aa	382	45% 75% 24%
74	Ab	190	37% 71% 29%
75	Ac	173	34% 97% ..
76	Ad	205	36% 84% 14%
77	Ae	455	66% 82% 15%
78	Af	188	27% 52% 47%
79	Ag	410	68% 85% 14%
80	Ah	387	26% 31% 69%
81	Ai	106	75% 92% 7%
82	Aj	218	72% 97%
83	Ak	325	71% 84% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
84	Am	118	
85	An	199	
86	Ao	690	
87	Ap	258	
88	CL	198	
88	DL	198	
88	EL	198	
88	FL	198	
88	GL	198	
88	HL	198	

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 174700 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 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B0	110	857	553	156	145	3	0	0

- Molecule 2 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B1	244	2036	1315	363	353	5	0	0

- Molecule 3 is a protein called Mitochondrial ribosomal protein L47.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B2	179	1548	992	290	260	6	0	0

- Molecule 4 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B3	118	968	622	178	165	3	0	0

- Molecule 5 is a protein called Mitochondrial ribosomal protein L55.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B4	62	474	296	94	81	3	0	0

- Molecule 6 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B5	110	902	553	181	162	6	0	0

- Molecule 7 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B6	52	425	274	78	71	2	0	0

- Molecule 8 is a RNA chain called CP tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	BB	67	1427	640	261	459	67	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	72	C	A	conflict	GB 45826169
BB	73	A	C	conflict	GB 45826169

- Molecule 9 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B7	46	387	239	89	58	1	0	0

- Molecule 10 is a protein called Ribosomal_L2_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	BD	240	1860	1160	371	319	10	0	0

- Molecule 11 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	BE	307	2420	1554	426	430	10	0	0

- Molecule 12 is a protein called Mitochondrial ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	BF	250	2011	1294	367	344	6	0	0

- Molecule 13 is a protein called Ribosome-recycling factor, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	BG	193	1501	930	269	294	8	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	6	MET	-	initiating methionine	UNP Q96E11
BG	7	HIS	-	expression tag	UNP Q96E11
BG	8	HIS	-	expression tag	UNP Q96E11
BG	9	HIS	-	expression tag	UNP Q96E11
BG	10	HIS	-	expression tag	UNP Q96E11
BG	11	HIS	-	expression tag	UNP Q96E11
BG	12	HIS	-	expression tag	UNP Q96E11
BG	13	GLU	-	expression tag	UNP Q96E11
BG	14	ASN	-	expression tag	UNP Q96E11
BG	15	LEU	-	expression tag	UNP Q96E11
BG	16	TYR	-	expression tag	UNP Q96E11
BG	17	PHE	-	expression tag	UNP Q96E11
BG	18	GLN	-	expression tag	UNP Q96E11
BG	19	SER	-	expression tag	UNP Q96E11
BG	20	GLY	-	expression tag	UNP Q96E11
BG	21	GLY	-	expression tag	UNP Q96E11
BG	22	SER	-	expression tag	UNP Q96E11
BG	23	GLY	-	expression tag	UNP Q96E11
BG	24	SER	-	expression tag	UNP Q96E11
BG	25	GLY	-	expression tag	UNP Q96E11

- Molecule 14 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	BI	98	805	509	155	141		0	0

- Molecule 15 is a protein called 39S ribosomal protein L10, mitochondrial isoform a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	BJ	212	1705	1100	306	290	9	0	0

- Molecule 16 is a protein called 39S ribosomal protein L11, mitochondrial isoform a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BK	176	Total	C	N	O	S	0	0
			1303	830	236	235	2		

- Molecule 17 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BN	177	Total	C	N	O	S	0	0
			1444	926	258	253	7		

- Molecule 18 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BO	115	Total	C	N	O	S	0	0
			896	562	176	154	4		

- Molecule 19 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BP	288	Total	C	N	O	S	0	0
			2312	1473	430	403	6		

- Molecule 20 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BQ	222	Total	C	N	O	S	0	0
			1803	1156	331	306	10		

- Molecule 21 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BR	153	Total	C	N	O	S	0	0
			1240	777	236	222	5		

- Molecule 22 is a protein called 39S ribosomal protein L18, mitochondrial isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BS	143	Total	C	N	O	S	0	0
			1168	733	227	204	4		

- Molecule 23 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	BT	230	1890	1215	325	341	9	0	0

- Molecule 24 is a protein called 39S ribosomal protein L20, mitochondrial isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	BU	140	1159	732	239	185	3	0	0

- Molecule 25 is a protein called 39S ribosomal protein L21, mitochondrial isoform d.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	BV	155	1231	789	219	219	4	0	0

- Molecule 26 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	BW	166	1374	876	258	234	6	0	0

- Molecule 27 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	BX	149	1181	752	227	200	2	0	0

- Molecule 28 is a protein called 39S ribosomal protein L24, mitochondrial isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	BY	206	1678	1056	308	309	5	0	0

- Molecule 29 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Ba	393	3173	2040	556	565	12	0	0

- Molecule 30 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Bb	354	2952	1876	542	525	9	0	0

- Molecule 31 is a protein called TGS domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Bc	295	2408	1541	410	441	16	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bc	328	THR	SER	conflict	UNP A0A4X1UDR3

- Molecule 32 is a protein called Mitochondrial ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Bd	138	1158	729	211	217	1	0	0

- Molecule 33 is a protein called Mitochondrial ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Be	122	972	628	168	173	3	0	0

- Molecule 34 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Bf	108	827	519	154	150	4	0	0

- Molecule 35 is a protein called 39S ribosomal protein L43, mitochondrial isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Bg	148	1167	727	225	212	3	0	0

- Molecule 36 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	B8	95	833	539	163	129	2	0	0

- Molecule 37 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Bh	289	2319	1486	399	426	8	0	0

- Molecule 38 is a protein called Mitochondrial ribosomal protein L45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Bi	260	2138	1370	379	379	10	0	0

- Molecule 39 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Bj	217	1775	1137	311	321	6	0	0

- Molecule 40 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Bk	155	1246	796	214	231	5	0	0

- Molecule 41 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Bl	133	1097	709	192	194	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bl	59	ARG	LYS	conflict	UNP A0A4X1V1G7

- Molecule 42 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bm	109	Total	C	N	O	S	0	0
			893	568	160	162	3		

- Molecule 43 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bn	97	Total	C	N	O	S	0	0
			837	539	166	128	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bo	97	Total	C	N	O	S	0	0
			772	481	148	141	2		

- Molecule 45 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bp	97	Total	C	N	O	S	0	0
			742	459	143	134	6		

- Molecule 46 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bq	80	Total	C	N	O	S	0	0
			672	431	123	116	2		

- Molecule 47 is a protein called Mitochondrial ribosomal protein L57.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Bt	94	Total	C	N	O	S	0	0
			780	485	168	126	1		

- Molecule 48 is a protein called Mitochondrial ribosomal protein L58.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bu	151	Total	C	N	O	S	0	0
			1198	738	233	222	5		

- Molecule 49 is a protein called 39S ribosomal protein L59, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bv	135	Total	C	N	O	S	0	0
			1131	692	223	211	5		

- Molecule 50 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bw	387	Total	C	N	O	S	0	0
			3126	2011	548	555	12		

- Molecule 51 is a protein called Mitochondrial ribosomal protein S18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bx	162	Total	C	N	O	S	0	0
			1325	845	249	224	7		

- Molecule 52 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AA	960	Total	C	N	O	P	0	0
			20411	9162	3708	6581	960		

- Molecule 53 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B9	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 54 is a RNA chain called tRNA (P/E).

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AV	71	Total	C	N	O	P	0	0
			1419	640	147	562	70		

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AX	5	Total	C	N	O	P	0	0
			100	45	10	40	5		

- Molecule 56 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	BA	1544	32844	14750	5972	10578	1544	0	0

- Molecule 57 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	AB	220	1762	1126	326	304	6	0	0

- Molecule 58 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	AC	132	1075	695	195	181	4	0	0

- Molecule 59 is a protein called 28S ribosomal protein S5, mitochondrial isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	AE	343	2732	1707	527	487	11	0	0

- Molecule 60 is a protein called Mitochondrial ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	AF	122	981	620	178	177	6	0	0

- Molecule 61 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	AG	208	1721	1097	314	299	11	0	0

- Molecule 62 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	AI	328	2650	1678	478	481	13	0	0

- Molecule 63 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	AJ	140	1155	746	197	208	4	0	0

- Molecule 64 is a protein called Mitochondrial ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	AK	137	1007	631	193	180	3	0	0

- Molecule 65 is a protein called Mitoribosomal protein us12m, mrps12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	AL	109	840	524	172	138	6	0	0

- Molecule 66 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	AN	101	858	534	174	144	6	0	0

- Molecule 67 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	AO	175	1448	919	272	248	9	0	0

- Molecule 68 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	AP	117	932	588	184	155	5	0	0

- Molecule 69 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	AQ	112	875	568	153	151	3	0	0

- Molecule 70 is a protein called 28S ribosomal protein S18c, mitochondrial isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AR	97	Total	C	N	O	S	0	0
			784	507	132	138	7		

- Molecule 71 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AU	86	Total	C	N	O	S	0	0
			734	453	148	125	8		

- Molecule 72 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	AZ	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 73 is a protein called Mitochondrial ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Aa	292	Total	C	N	O	S	0	0
			2378	1518	409	442	9		

- Molecule 74 is a protein called Mitochondrial ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Ab	135	Total	C	N	O	S	0	0
			1101	709	199	192	1		

- Molecule 75 is a protein called Interferon alpha-inducible protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Ac	169	Total	C	N	O	S	0	0
			1367	876	236	245	10		

- Molecule 76 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Ad	177	Total	C	N	O	S	0	0
			1467	904	288	273	2		

- Molecule 77 is a protein called Mitochondrial ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	Ae	388	3109	1971	535	589	14	0	0

- Molecule 78 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	Af	99	778	494	134	146	4	0	0

- Molecule 79 is a protein called Death associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	Ag	353	2875	1837	515	513	10	0	0

- Molecule 80 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	Ah	120	1015	659	168	185	3	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	133	THR	ALA	conflict	UNP A0A4X1SQW0
Ah	179	ARG	LYS	conflict	UNP A0A4X1SQW0
Ah	180	UNK	ALA	conflict	UNP A0A4X1SQW0

- Molecule 81 is a protein called Mitochondrial ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	Ai	99	824	522	156	143	3	0	0

- Molecule 82 is a protein called Mitochondrial ribosomal protein S34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	Aj	213	1788	1131	338	311	8	0	0

- Molecule 83 is a protein called 28S ribosomal protein S35, mitochondrial isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	Ak	275	2222	1414	380	419	9	0	0

- Molecule 84 is a protein called Coiled-coil-helix-coiled-coil-helix domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	Am	116	930	577	185	160	8	0	0

- Molecule 85 is a protein called Aurora kinase A interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	An	72	639	407	139	92	1	0	0

- Molecule 86 is a protein called Pentatricopeptide repeat domain 3,Pentatricopeptide repeat domain 3,mS39,Pentatricopeptide repeat domain 3,Pentatricopeptide repeat domain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	Ao	572	4527	2899	770	834	24	0	0

- Molecule 87 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
87	Ap	190	1564	991	292	273	8	0	0

- Molecule 88 is a protein called Mitochondrial ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
88	CL	45	317	203	52	62	0	0
88	DL	27	213	137	33	43	0	0
88	EL	28	222	143	35	44	0	0
88	FL	27	213	137	33	43	0	0
88	GL	27	213	137	33	43	0	0
88	HL	26	205	131	32	42	0	0

- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	B3	1	Total 1	Mg 1	0
89	BB	1	Total 1	Mg 1	0
89	BD	3	Total 3	Mg 3	0
89	BE	1	Total 1	Mg 1	0
89	BJ	1	Total 1	Mg 1	0
89	BP	2	Total 2	Mg 2	0
89	BQ	1	Total 1	Mg 1	0
89	Be	1	Total 1	Mg 1	0
89	Bl	1	Total 1	Mg 1	0
89	Bt	1	Total 1	Mg 1	0
89	AA	105	Total 105	Mg 105	0
89	AX	1	Total 1	Mg 1	0
89	BA	204	Total 204	Mg 204	0
89	AB	1	Total 1	Mg 1	0
89	Ag	1	Total 1	Mg 1	0
89	Am	1	Total 1	Mg 1	0
89	An	1	Total 1	Mg 1	0

- Molecule 90 is ZINC ION (three-letter code: ZN) (formula: Zn).

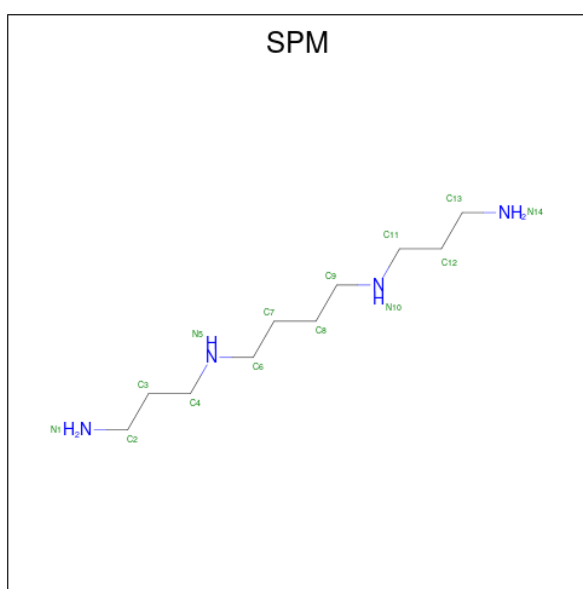
Mol	Chain	Residues	Atoms		AltConf
90	B5	1	Total 1	Zn 1	0
90	Bx	1	Total 1	Zn 1	0

Continued on next page...

Continued from previous page...

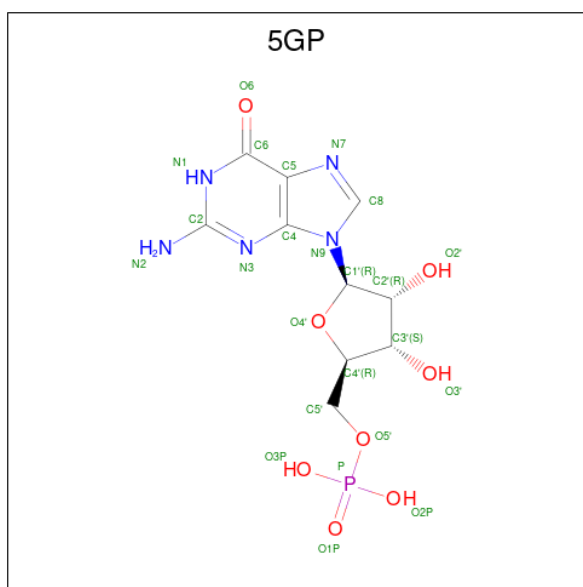
Mol	Chain	Residues	Atoms		AltConf
90	B9	1	Total	Zn	0
			1	1	
90	AR	1	Total	Zn	0
			1	1	
90	Ac	1	Total	Zn	0
			1	1	
90	Ap	1	Total	Zn	0
			1	1	

- Molecule 91 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



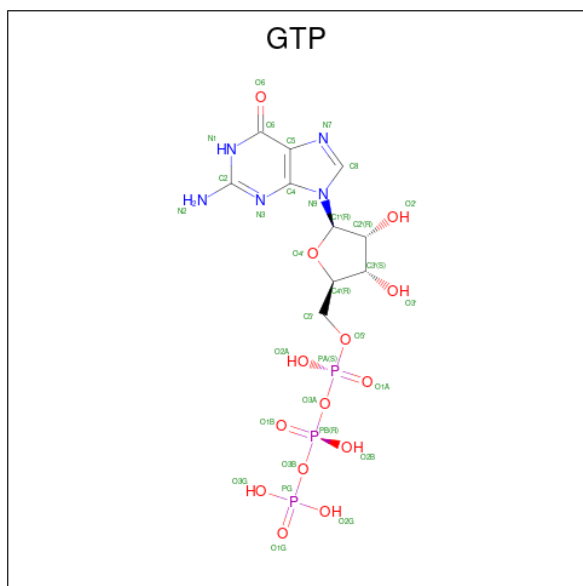
Mol	Chain	Residues	Atoms			AltConf
91	AA	1	Total	C	N	0
			14	10	4	
91	BA	1	Total	C	N	0
			28	20	8	
91	BA	1	Total	C	N	0
			28	20	8	

- Molecule 92 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
92	BA	1	24	10	5	8	1	0

- Molecule 93 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
93	Ag	1	32	10	5	14	3	0

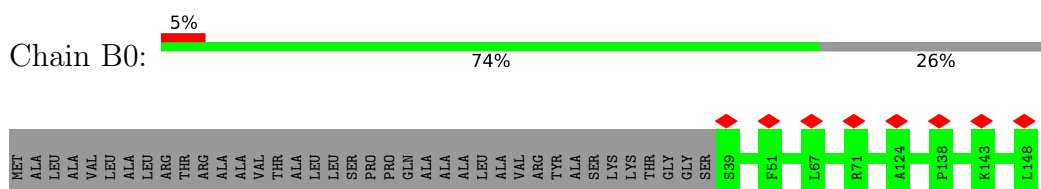
- Molecule 94 is water.

Mol	Chain	Residues	Atoms		AltConf
94	Ag	3	Total 3	O 3	0

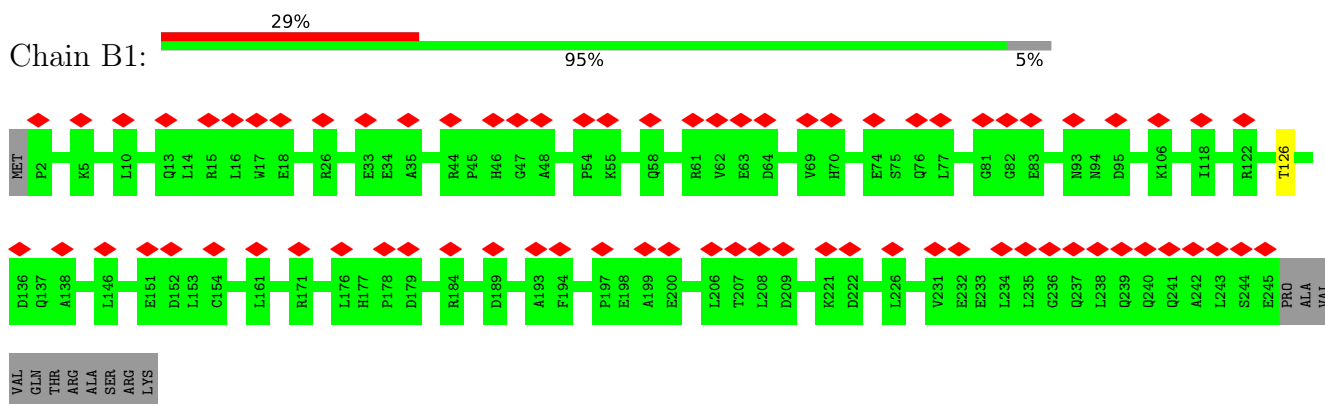
3 Residue-property plots [i](#)

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

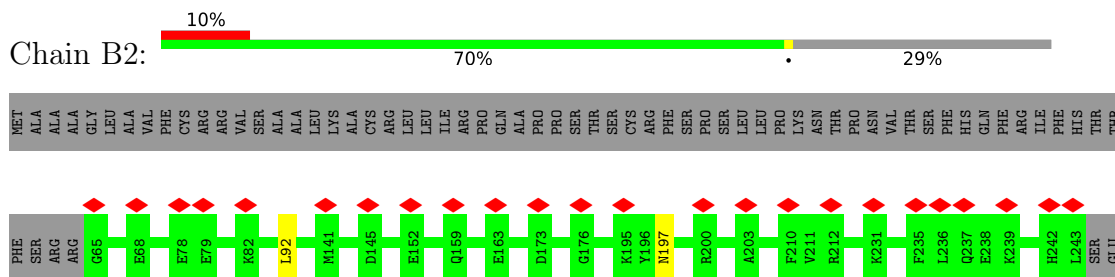
- Molecule 1: 39S ribosomal protein L27, mitochondrial



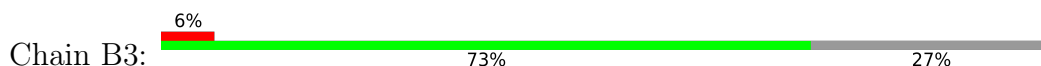
- Molecule 2: 39S ribosomal protein L28, mitochondrial

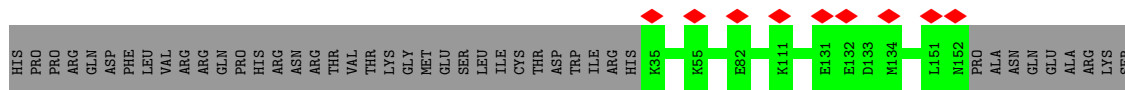


- Molecule 3: Mitochondrial ribosomal protein L47

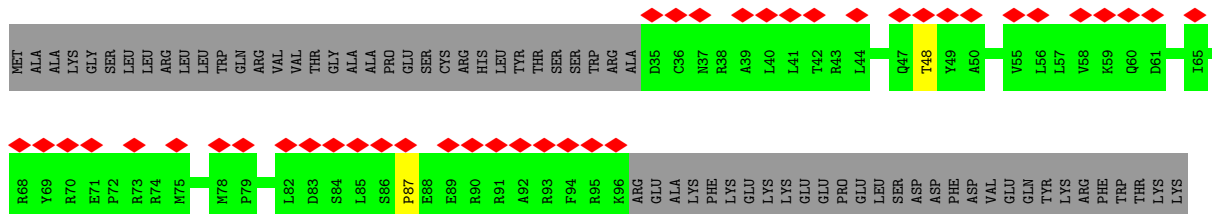


- Molecule 4: 39S ribosomal protein L30, mitochondrial

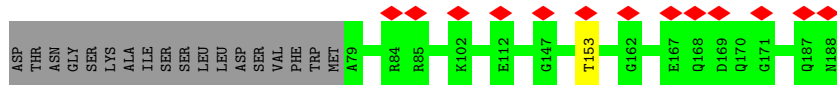




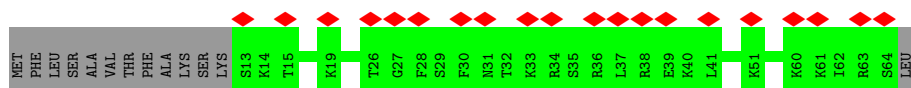
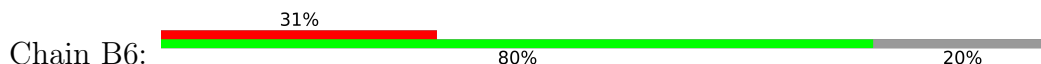
• Molecule 5: Mitochondrial ribosomal protein L55



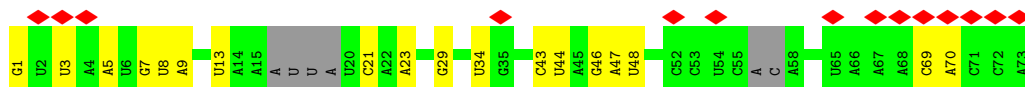
• Molecule 6: bL32m



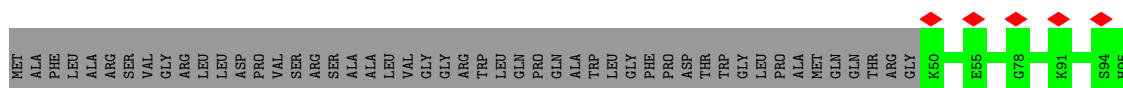
• Molecule 7: 39S ribosomal protein L33, mitochondrial



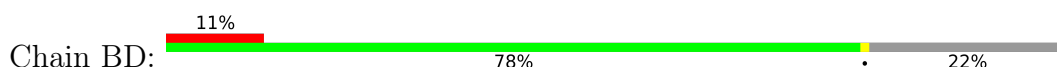
• Molecule 8: CP tRNAPhe

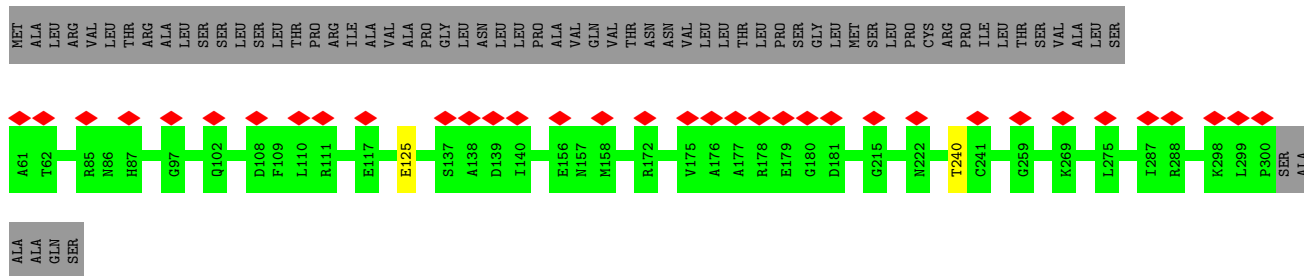


• Molecule 9: 39S ribosomal protein L34, mitochondrial

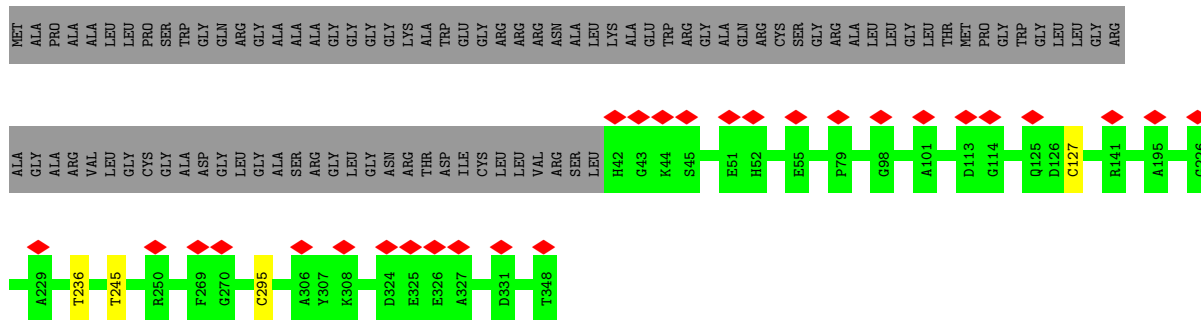
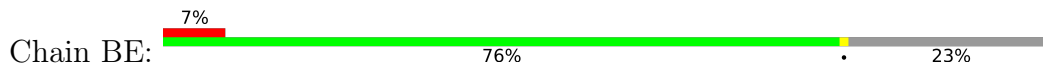


• Molecule 10: Ribosomal_L2_C domain-containing protein

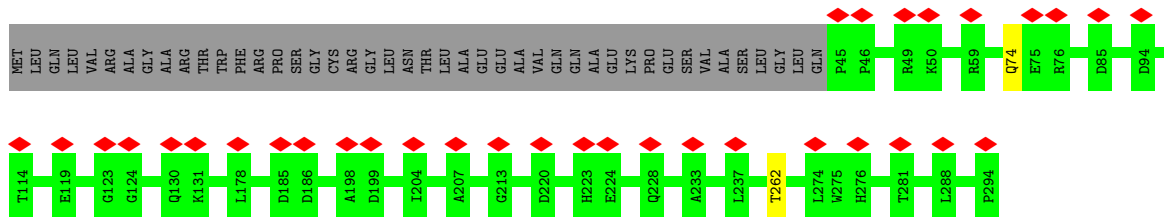
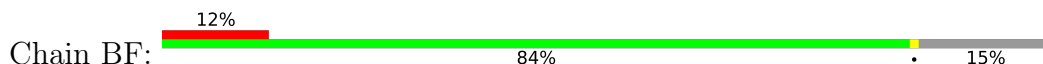




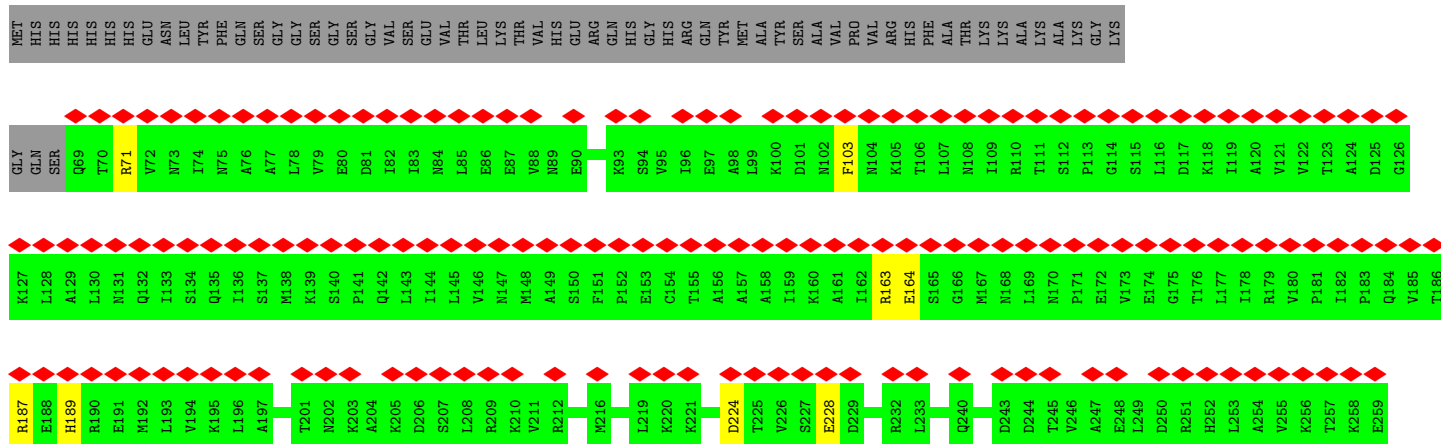
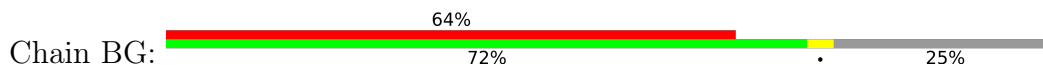
• Molecule 11: ICT1



• Molecule 12: Mitochondrial ribosomal protein L4



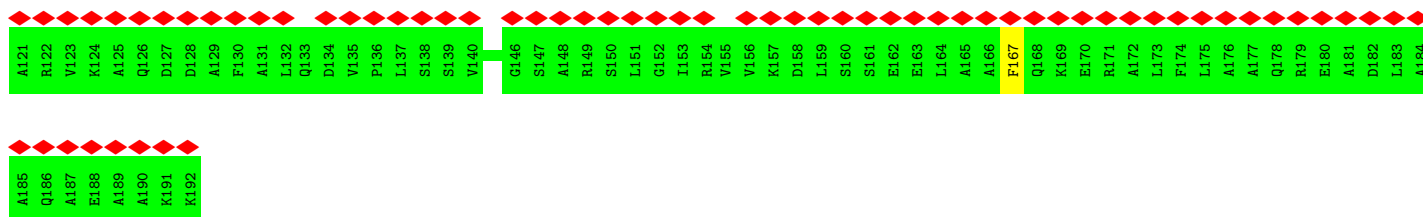
• Molecule 13: Ribosome-recycling factor, mitochondrial



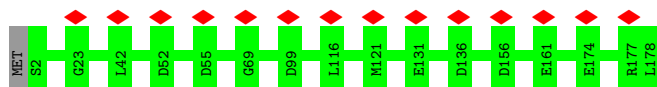


• Molecule 14: 39S ribosomal protein L9, mitochondrial

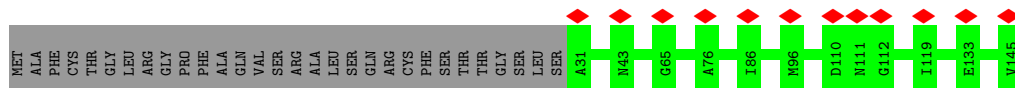
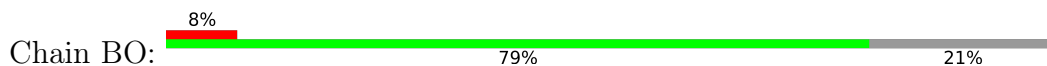




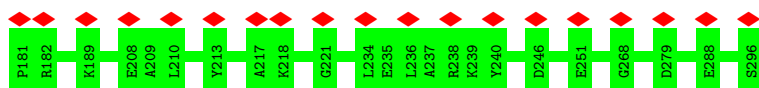
- Molecule 17: 39S ribosomal protein L13, mitochondrial



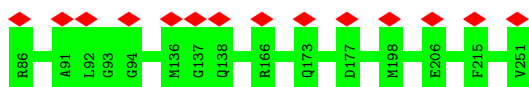
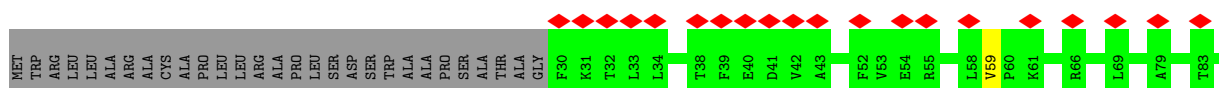
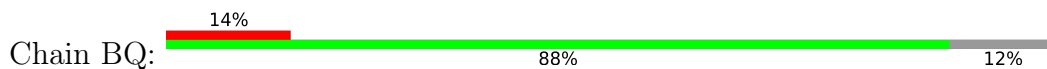
- Molecule 18: uL14m



- Molecule 19: 39S ribosomal protein L15, mitochondrial

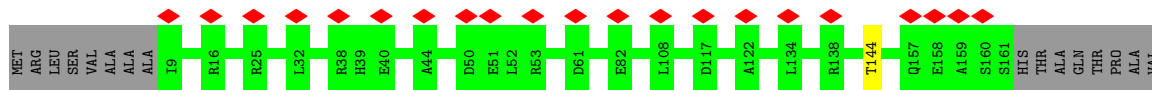


- Molecule 20: 39S ribosomal protein L16, mitochondrial

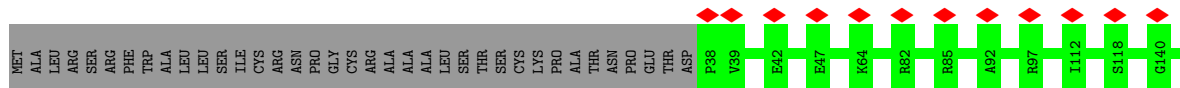
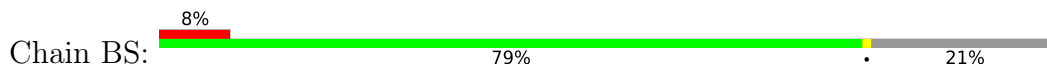


- Molecule 21: 39S ribosomal protein L17, mitochondrial

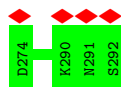
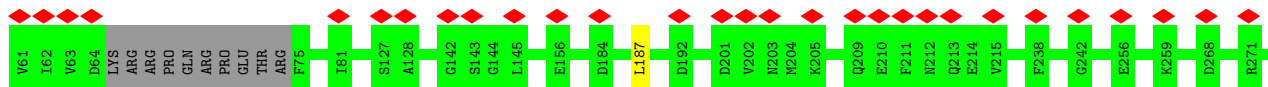
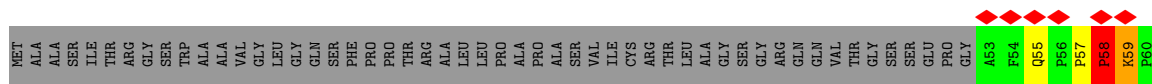
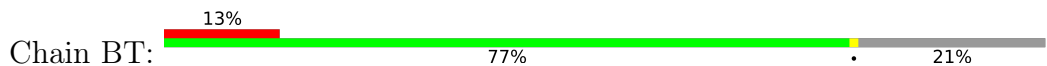




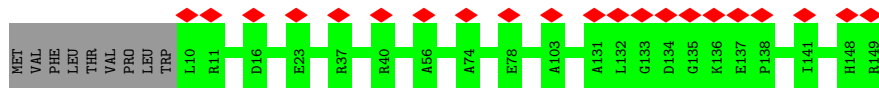
- Molecule 22: 39S ribosomal protein L18, mitochondrial isoform 1



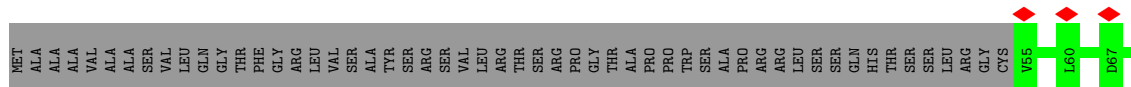
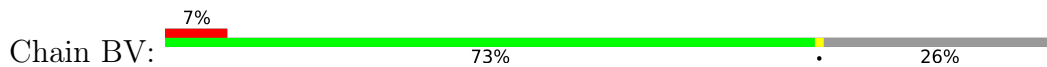
- Molecule 23: 39S ribosomal protein L19, mitochondrial



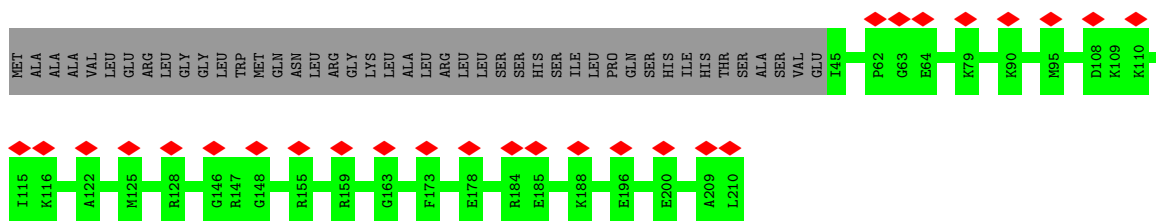
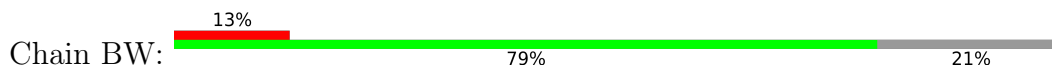
- Molecule 24: 39S ribosomal protein L20, mitochondrial isoform 1



- Molecule 25: 39S ribosomal protein L21, mitochondrial isoform d



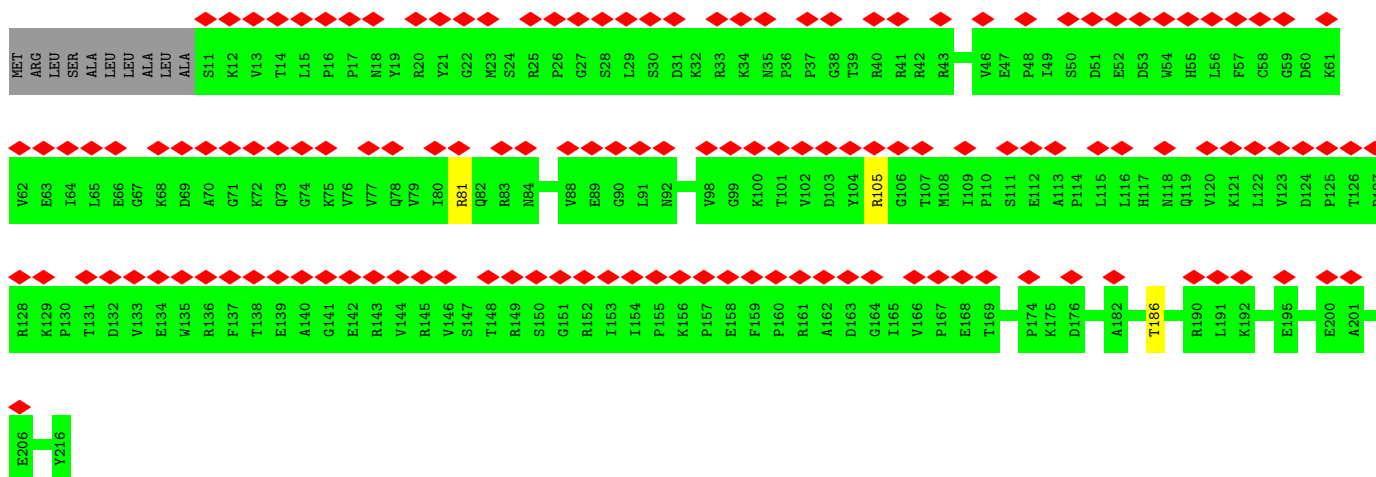
- Molecule 26: 39S ribosomal protein L22, mitochondrial



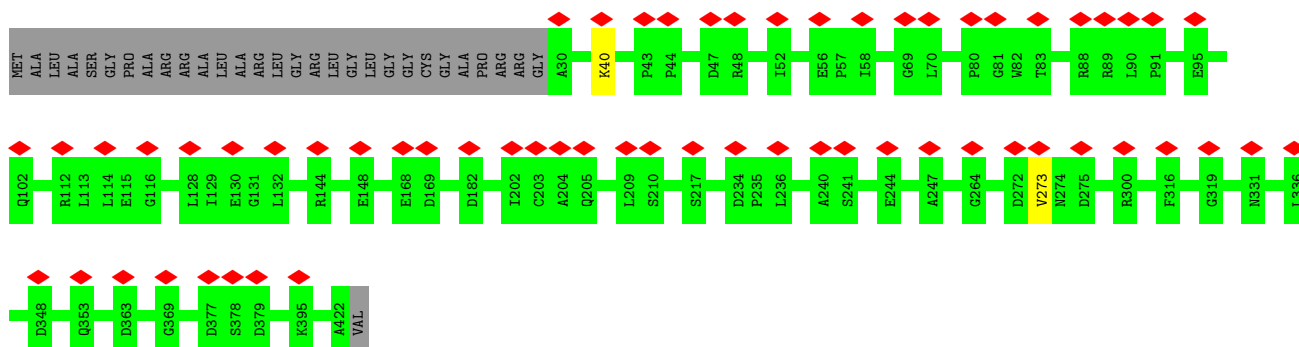
- Molecule 27: 39S ribosomal protein L23, mitochondrial



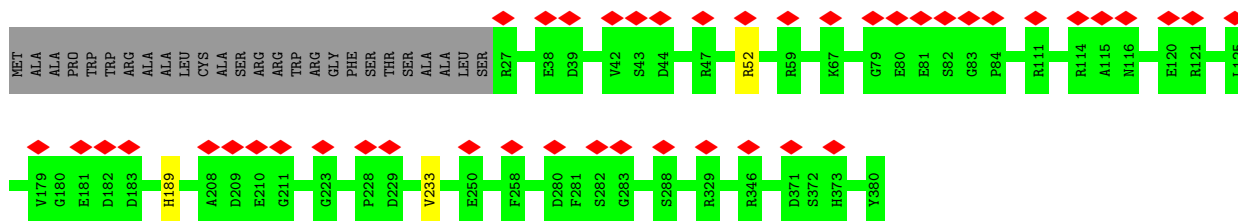
- Molecule 28: 39S ribosomal protein L24, mitochondrial isoform X1



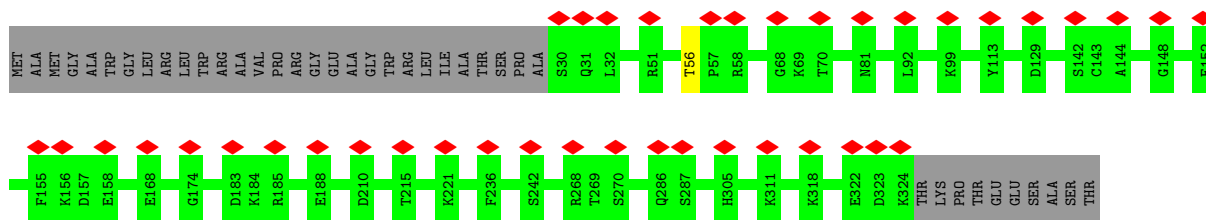
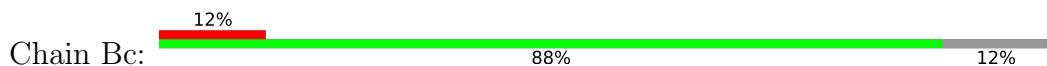
- Molecule 29: 39S ribosomal protein L37, mitochondrial



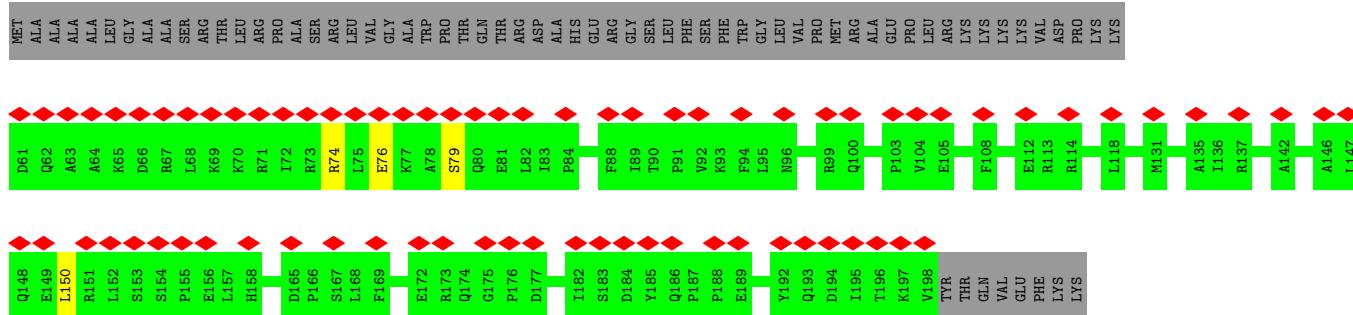
• Molecule 30: 39S ribosomal protein L38, mitochondrial



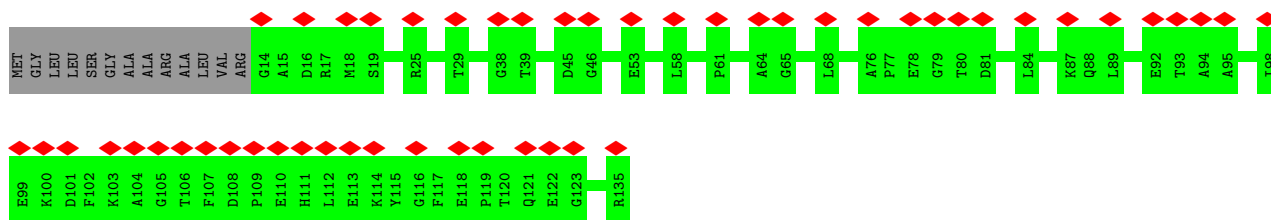
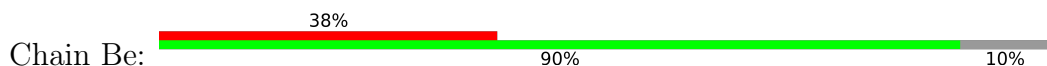
• Molecule 31: TGS domain-containing protein



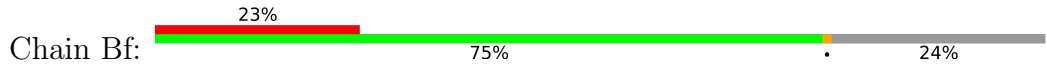
• Molecule 32: Mitochondrial ribosomal protein L40

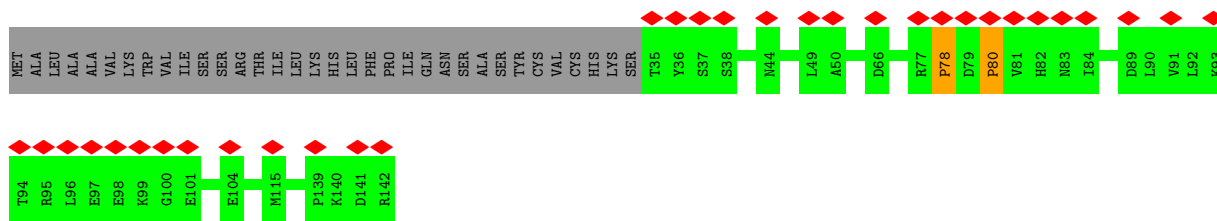


• Molecule 33: Mitochondrial ribosomal protein L41

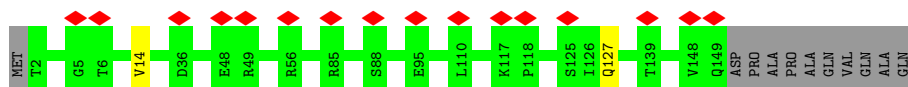
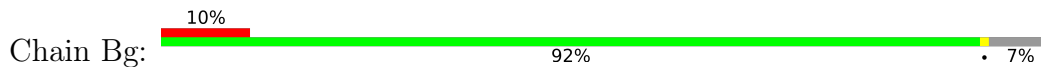


• Molecule 34: mL42

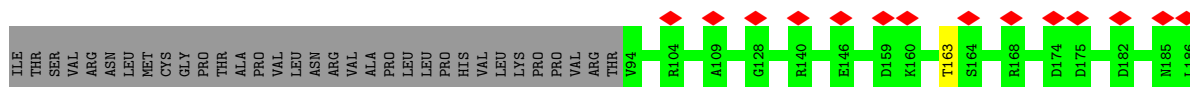
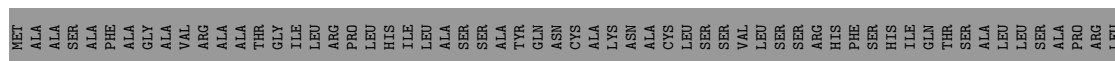




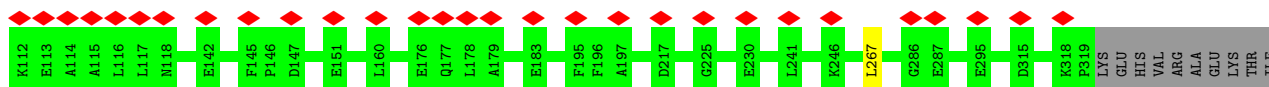
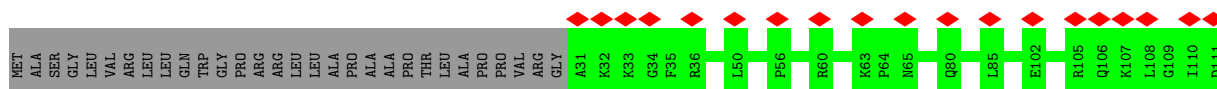
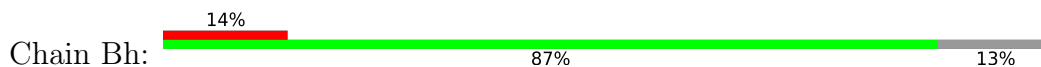
- Molecule 35: 39S ribosomal protein L43, mitochondrial isoform X2



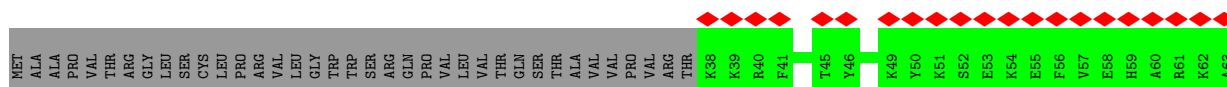
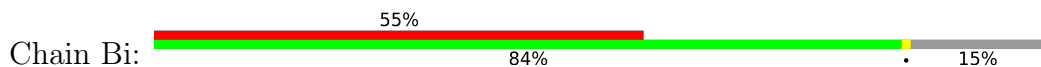
- Molecule 36: 39S ribosomal protein L35, mitochondrial

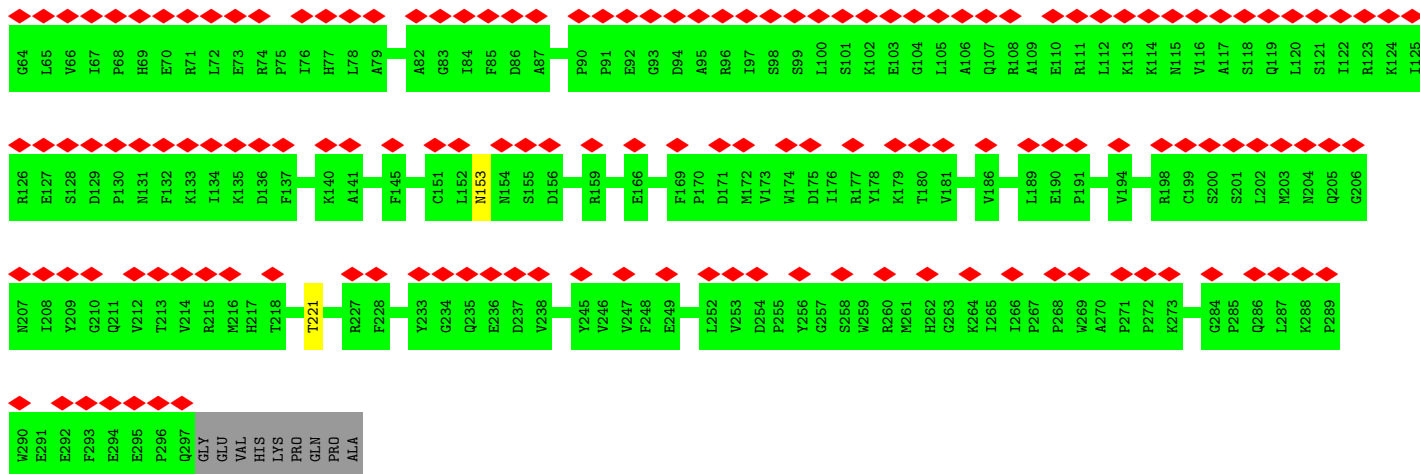


- Molecule 37: 39S ribosomal protein L44, mitochondrial

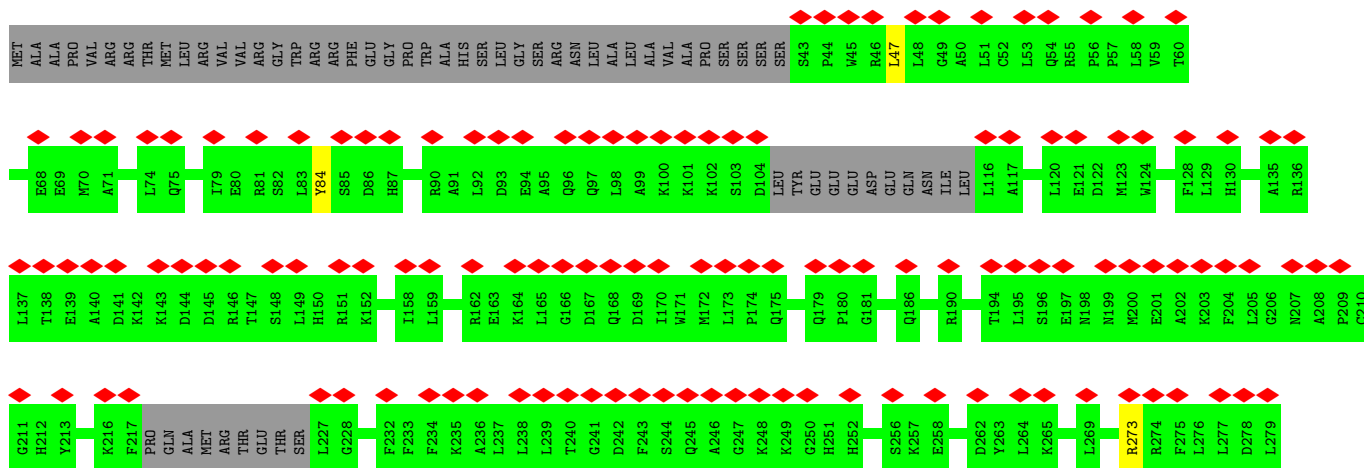
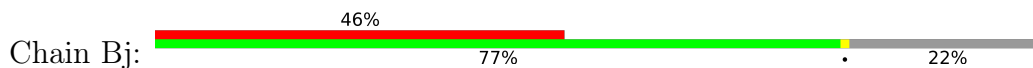


- Molecule 38: Mitochondrial ribosomal protein L45

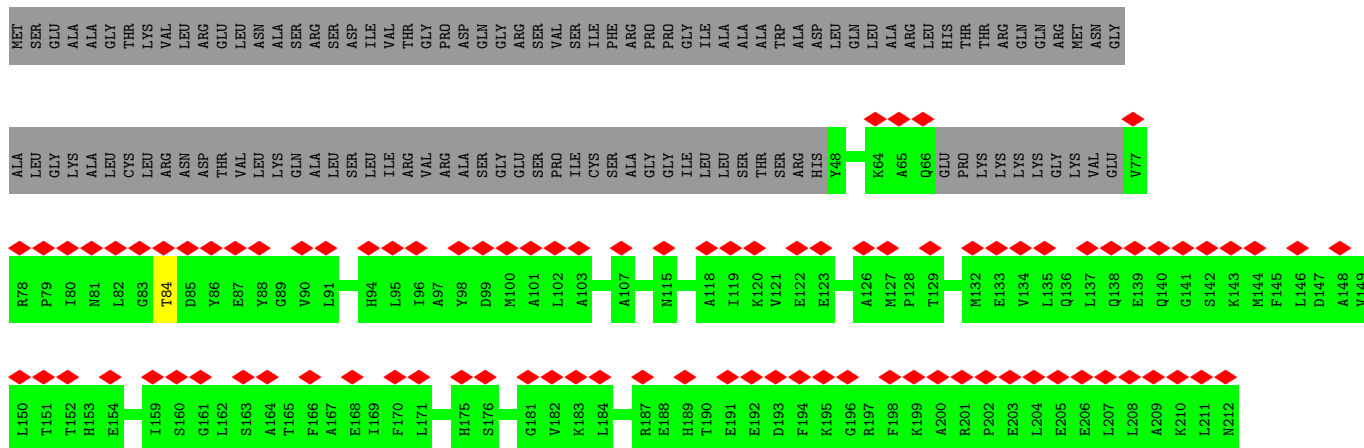




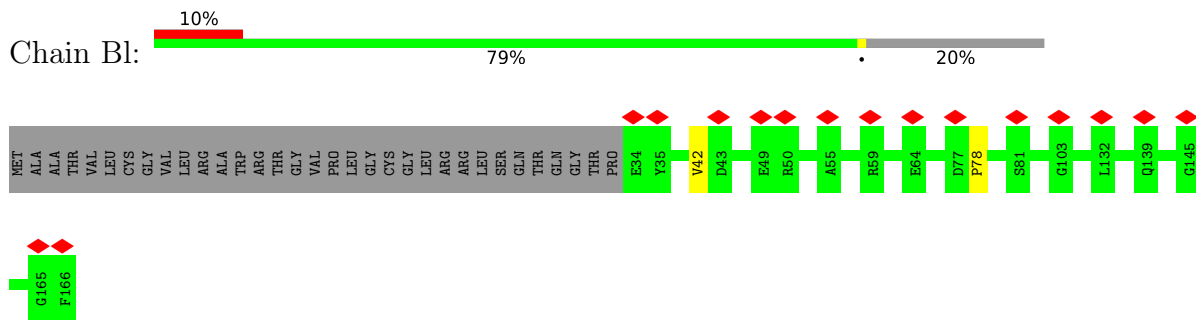
• Molecule 39: 39S ribosomal protein L46, mitochondrial



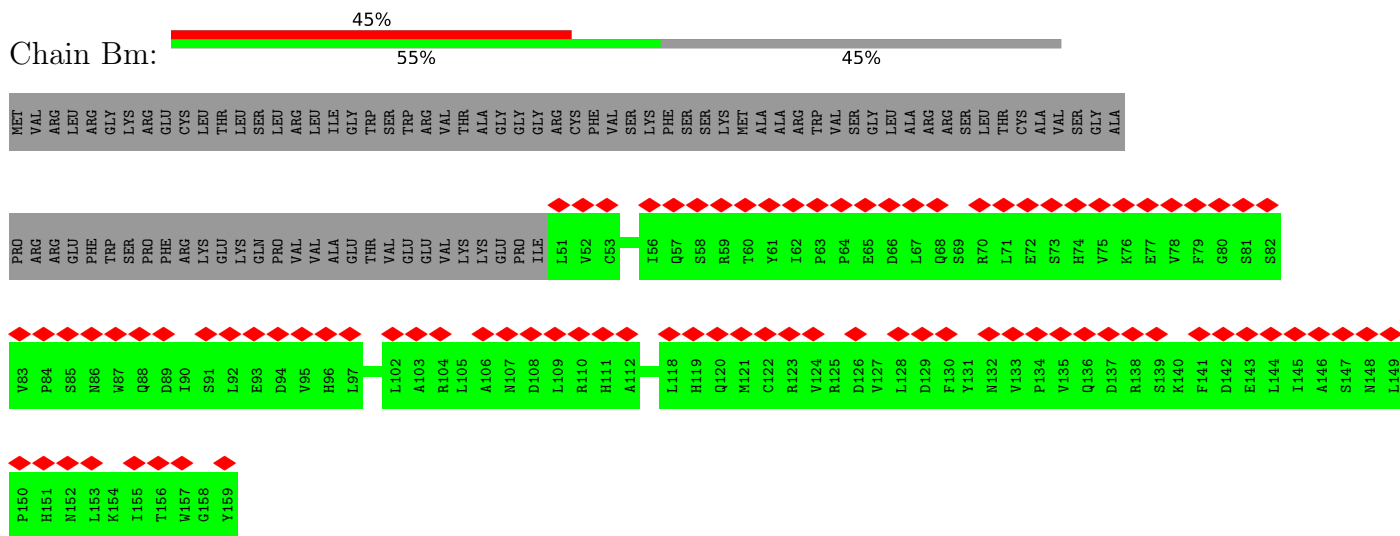
• Molecule 40: 39S ribosomal protein L48, mitochondrial



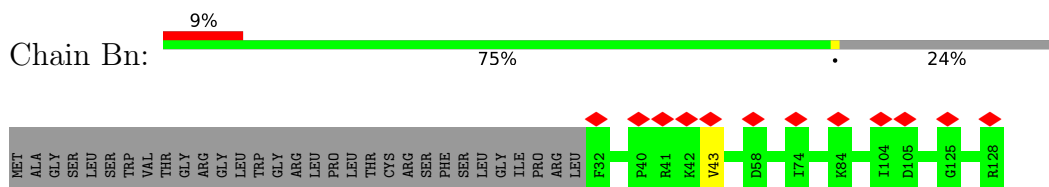
- Molecule 41: 39S ribosomal protein L49, mitochondrial



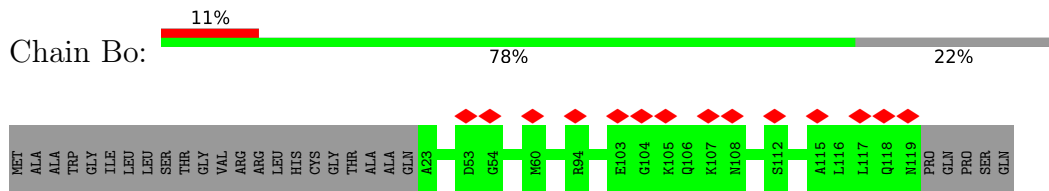
- Molecule 42: 39S ribosomal protein L50, mitochondrial



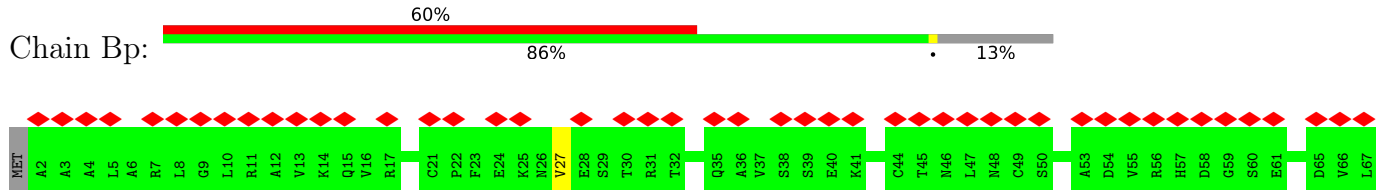
- Molecule 43: 39S ribosomal protein L51, mitochondrial

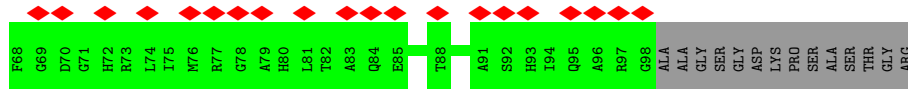


- Molecule 44: 39S ribosomal protein L52, mitochondrial

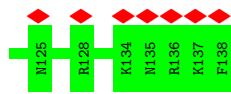
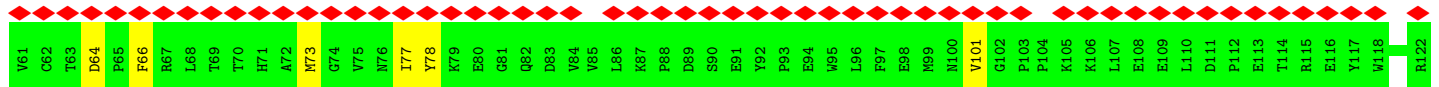
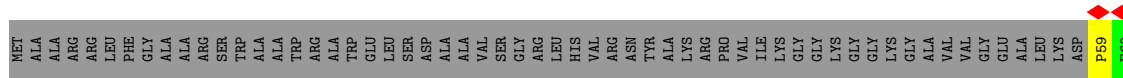


- Molecule 45: mL53

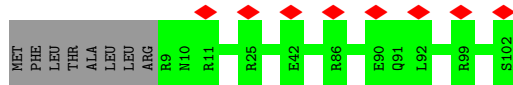
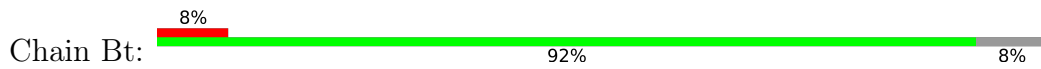




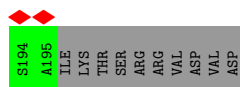
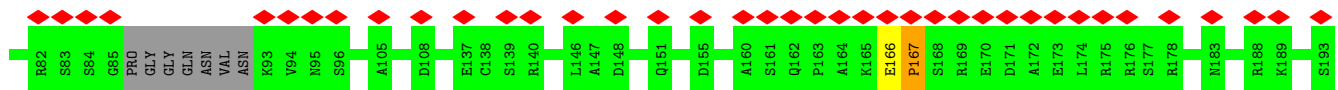
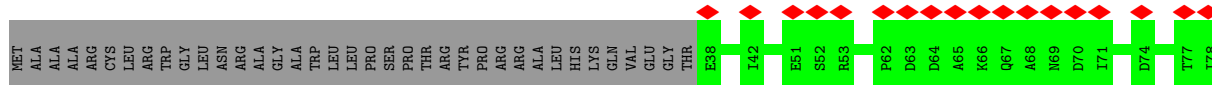
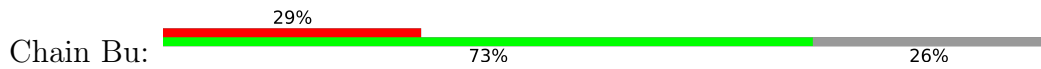
• Molecule 46: 39S ribosomal protein L54, mitochondrial



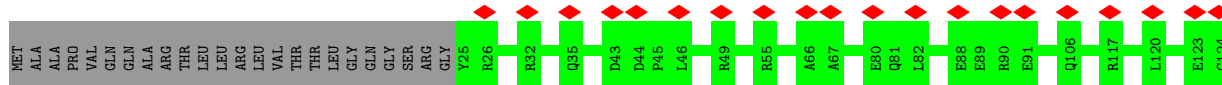
• Molecule 47: Mitochondrial ribosomal protein L57

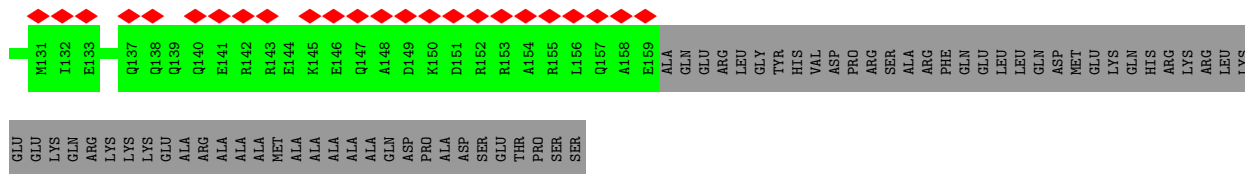


• Molecule 48: Mitochondrial ribosomal protein L58

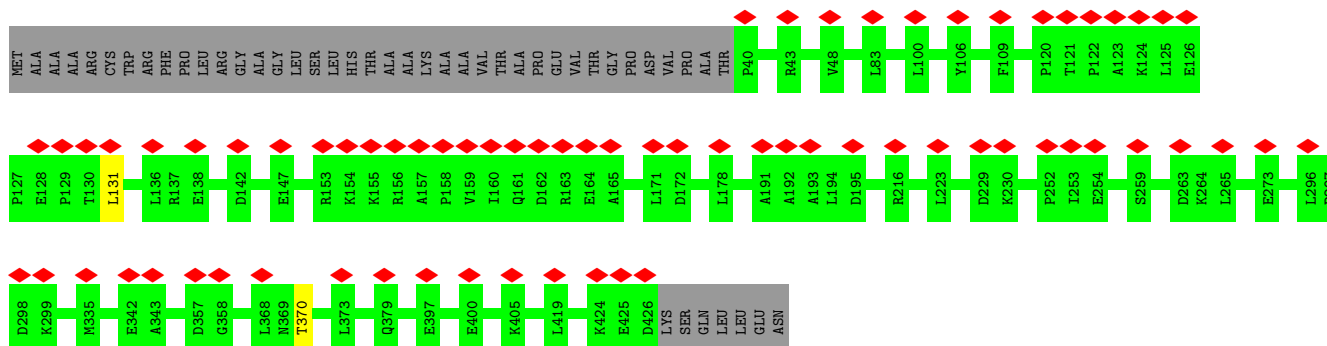
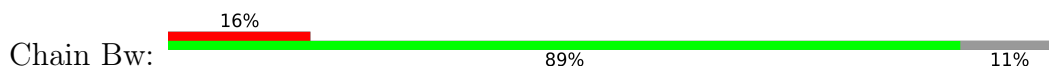


• Molecule 49: 39S ribosomal protein L59, mitochondrial

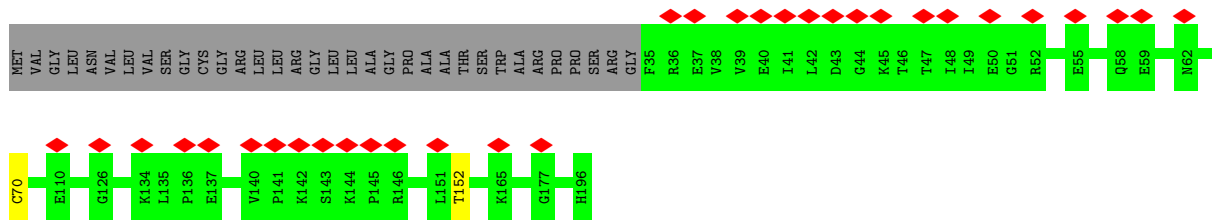
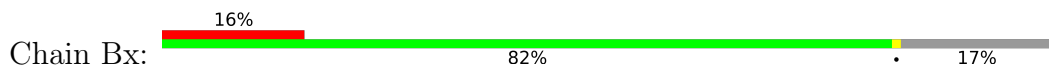




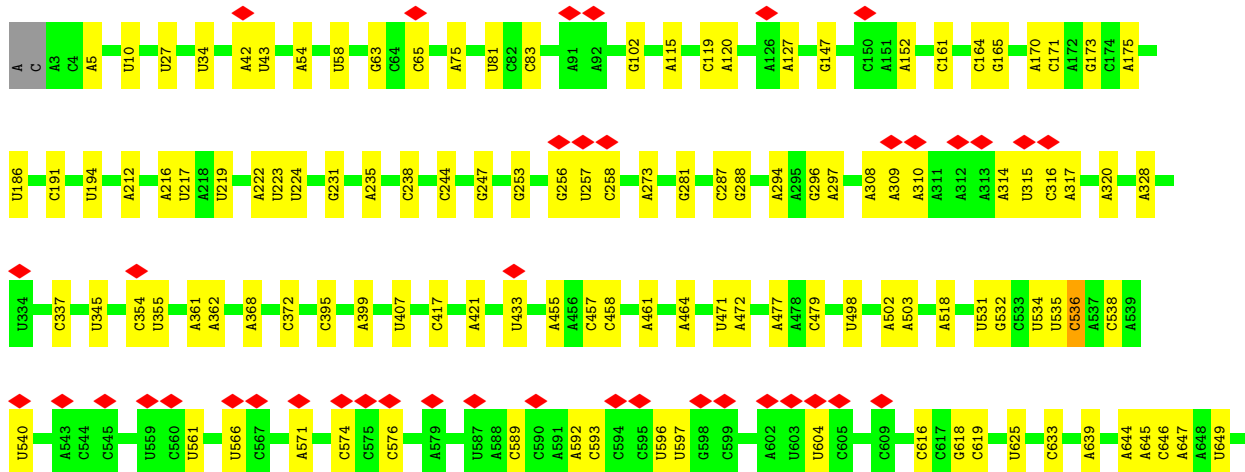
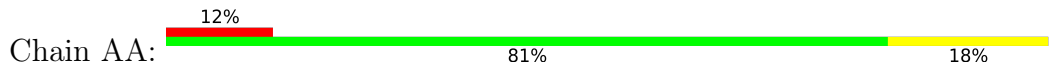
• Molecule 50: 39S ribosomal protein S30, mitochondrial

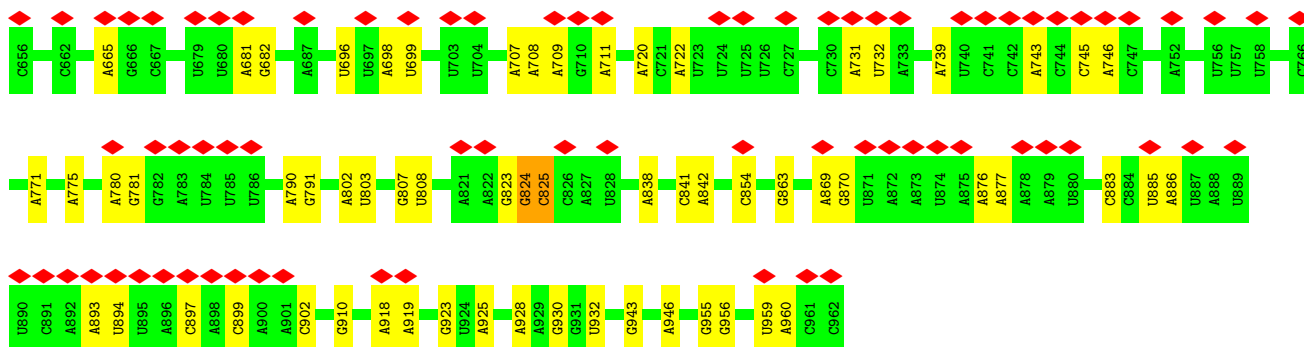


• Molecule 51: Mitochondrial ribosomal protein S18A

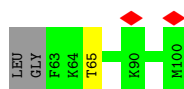
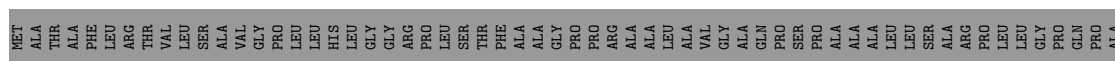


• Molecule 52: 12S rRNA

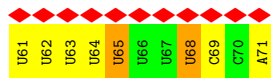
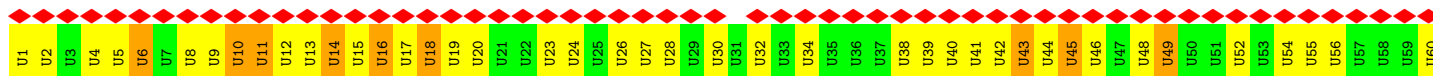




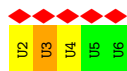
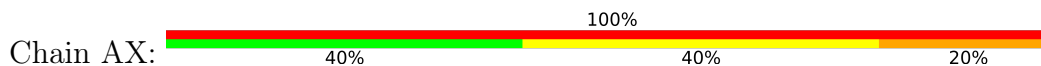
• Molecule 53: Ribosomal protein



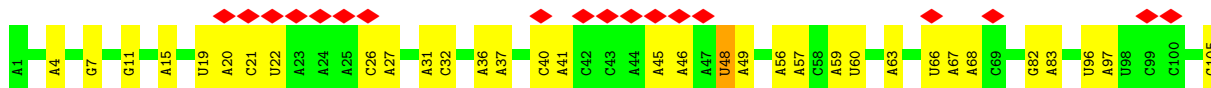
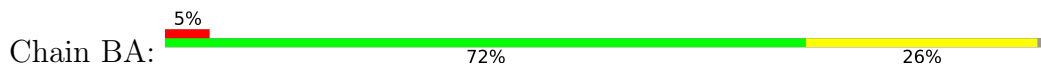
• Molecule 54: tRNA (P/E)

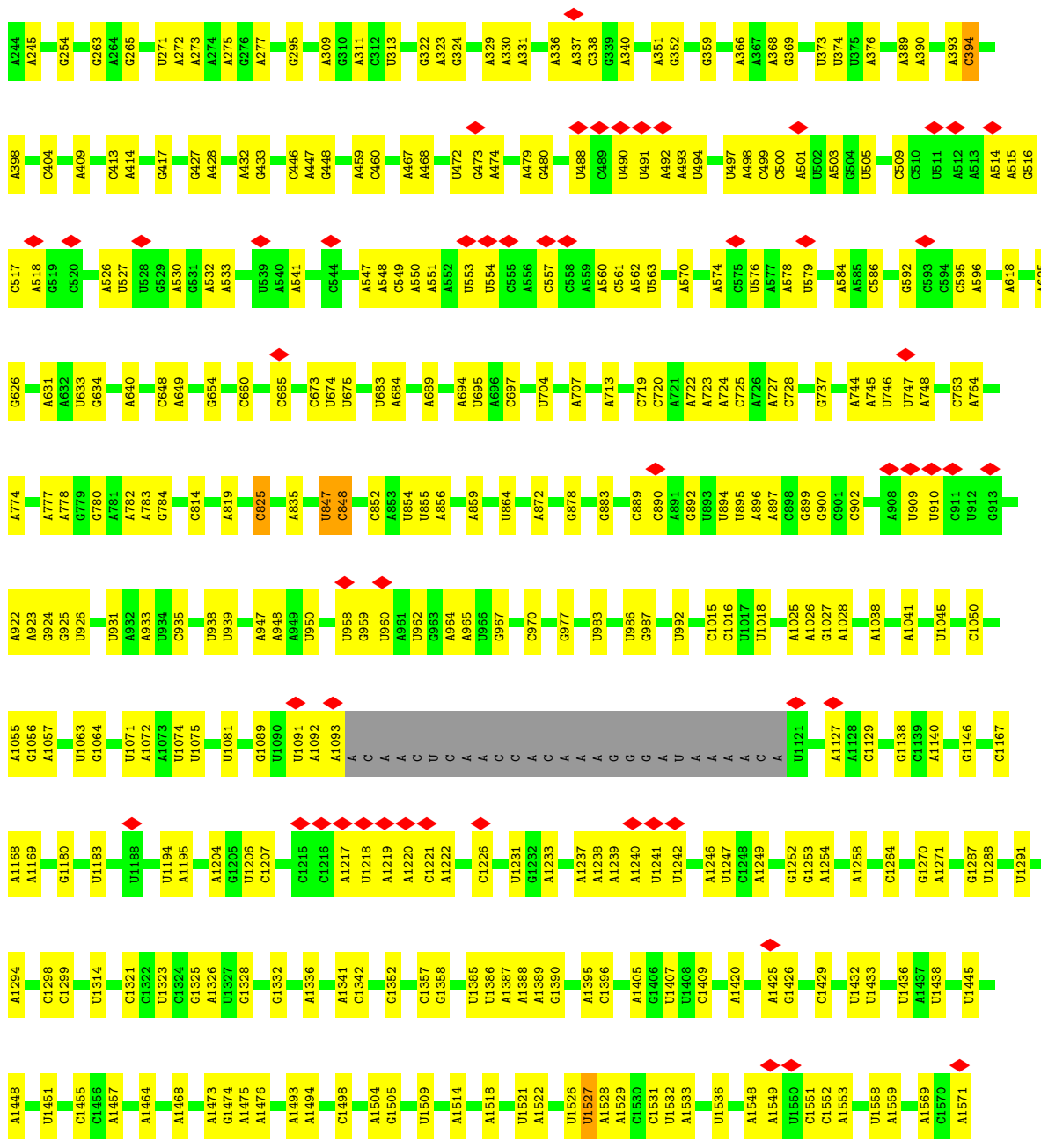


• Molecule 55: mRNA

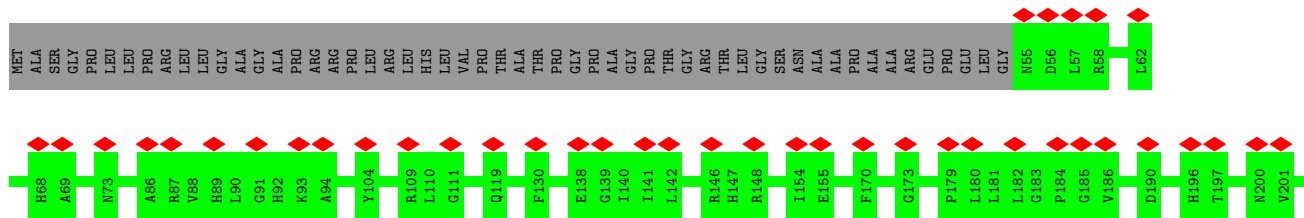
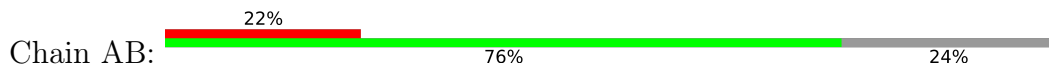


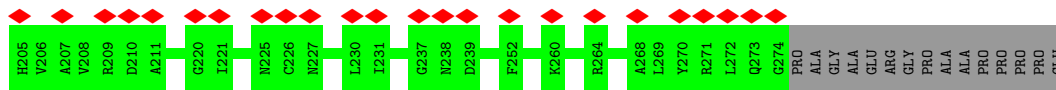
• Molecule 56: 16S rRNA



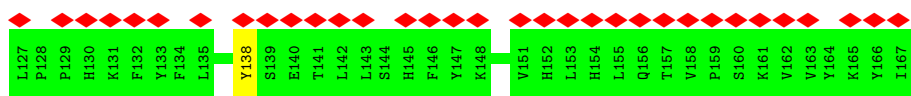
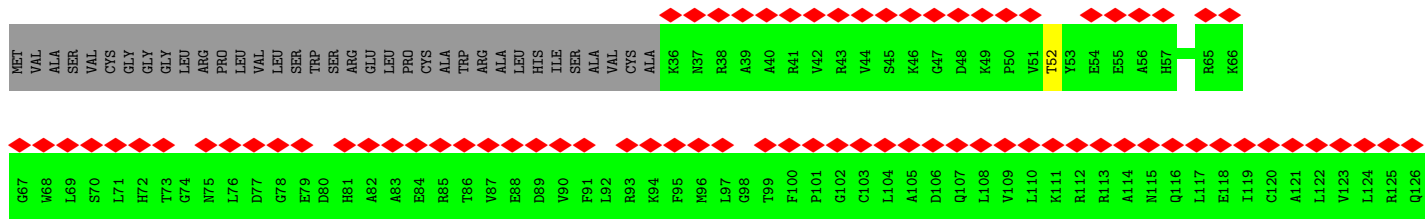
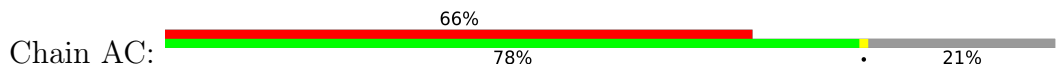


● Molecule 57: 28S ribosomal protein S2, mitochondrial

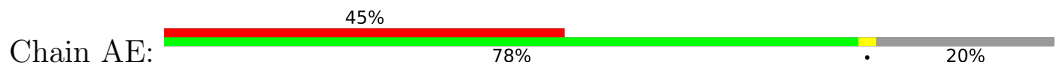




• Molecule 58: 28S ribosomal protein S24, mitochondrial

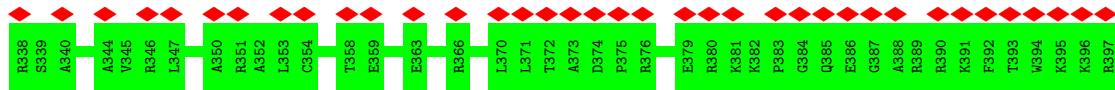
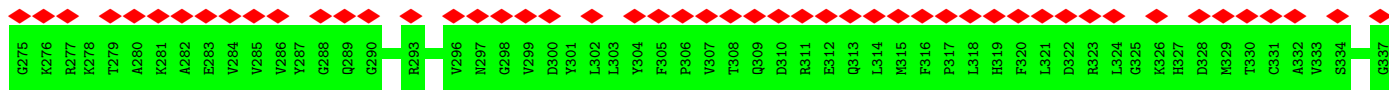


• Molecule 59: 28S ribosomal protein S5, mitochondrial isoform X2

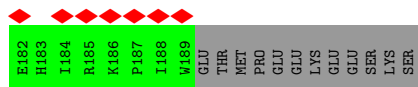
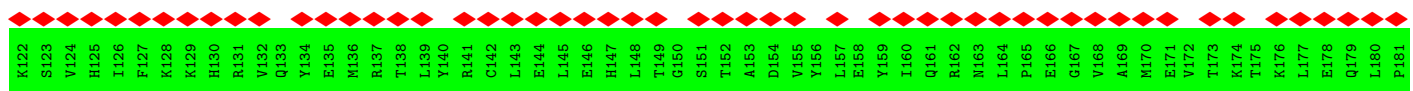
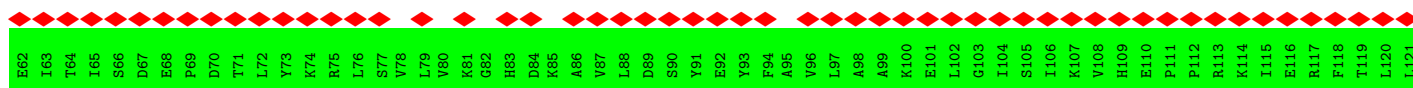
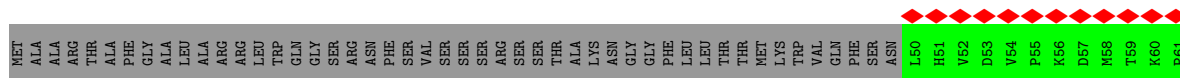


• Molecule 60: Mitochondrial ribosomal protein S6

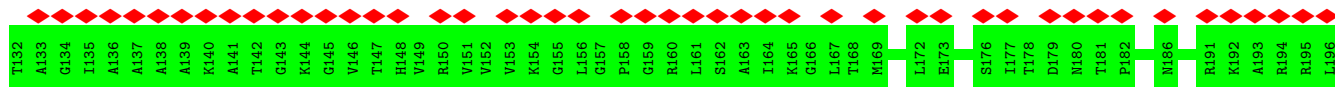
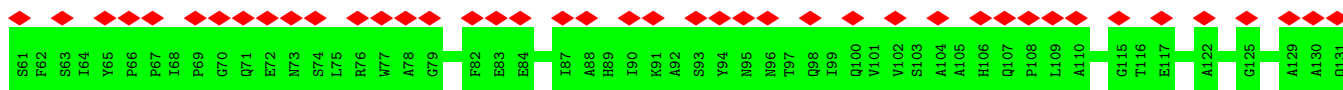
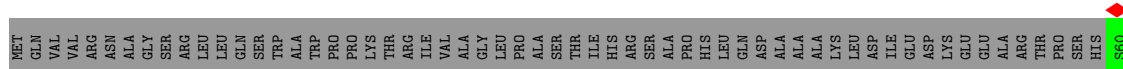
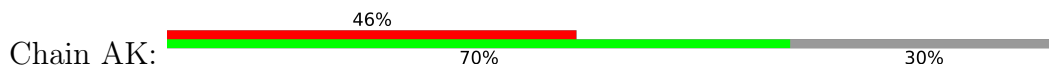




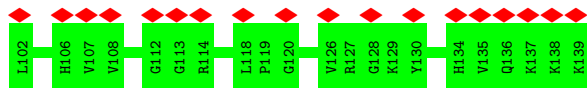
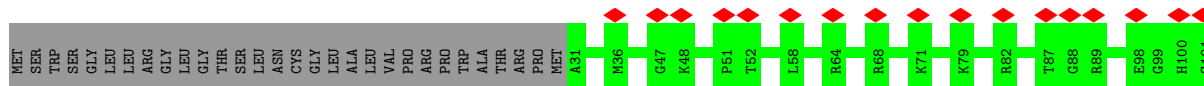
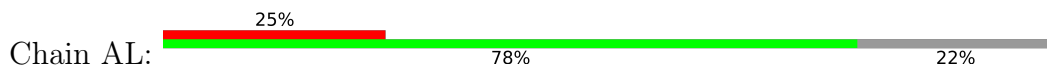
• Molecule 63: 28S ribosomal protein S10, mitochondrial



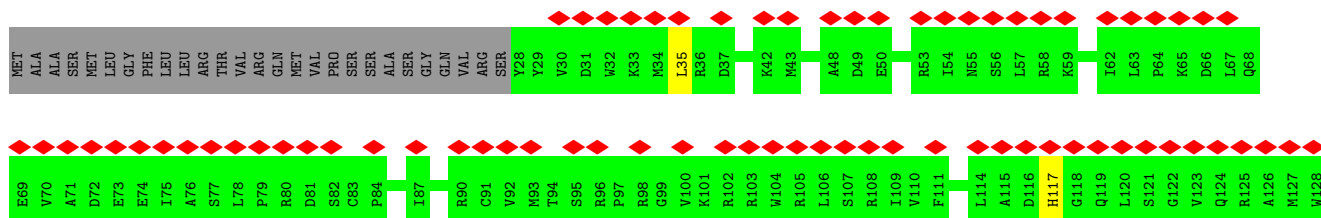
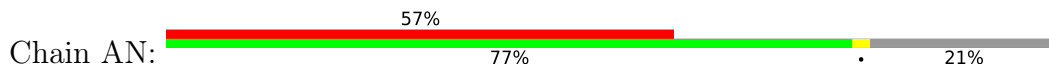
• Molecule 64: Mitochondrial ribosomal protein S11



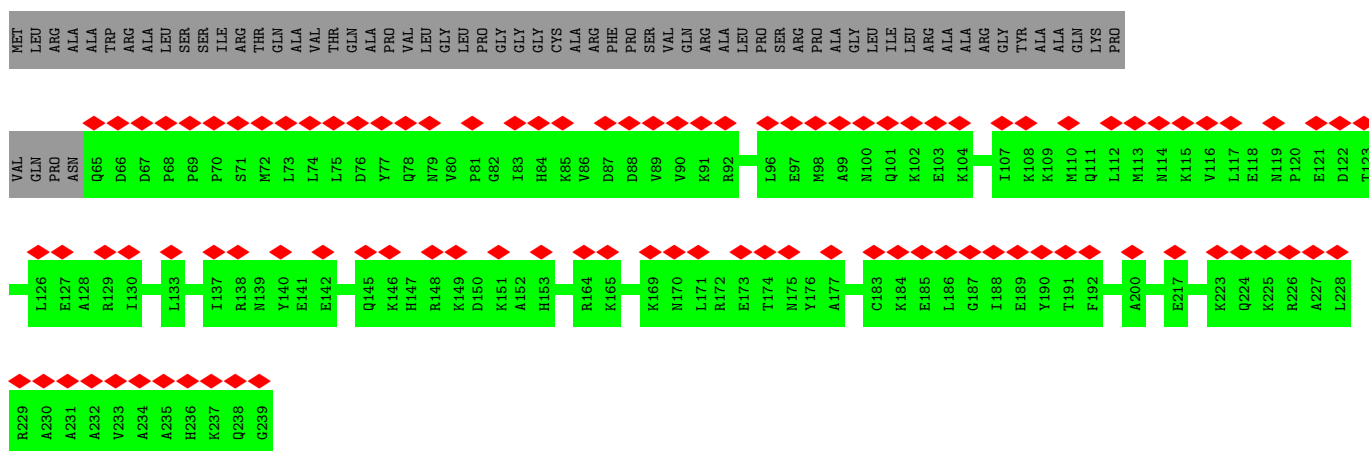
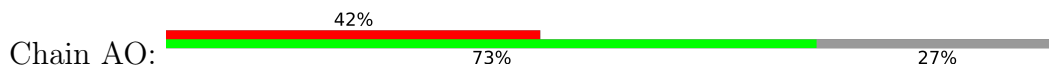
• Molecule 65: Mitoribosomal protein us12m, mrps12



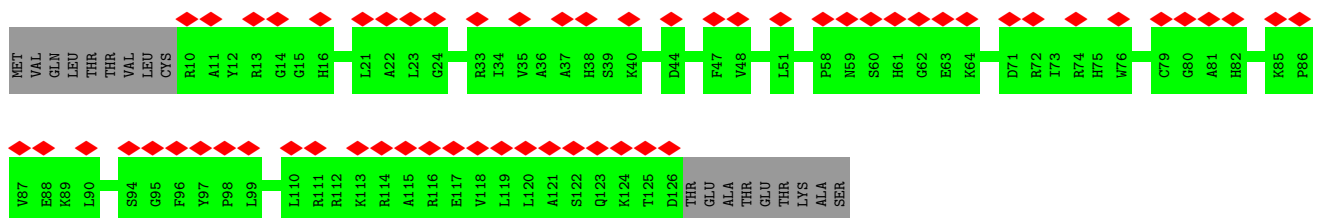
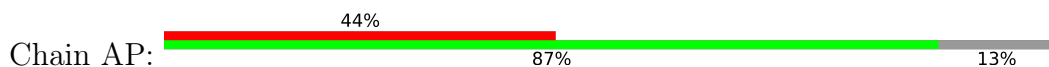
• Molecule 66: 28S ribosomal protein S14, mitochondrial



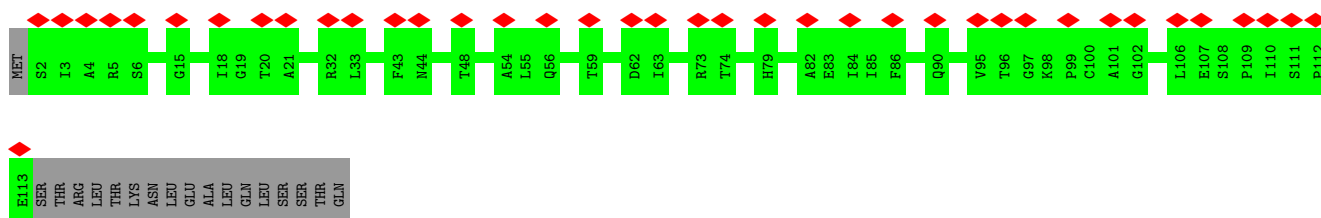
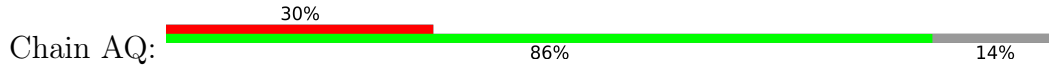
• Molecule 67: 28S ribosomal protein S15, mitochondrial



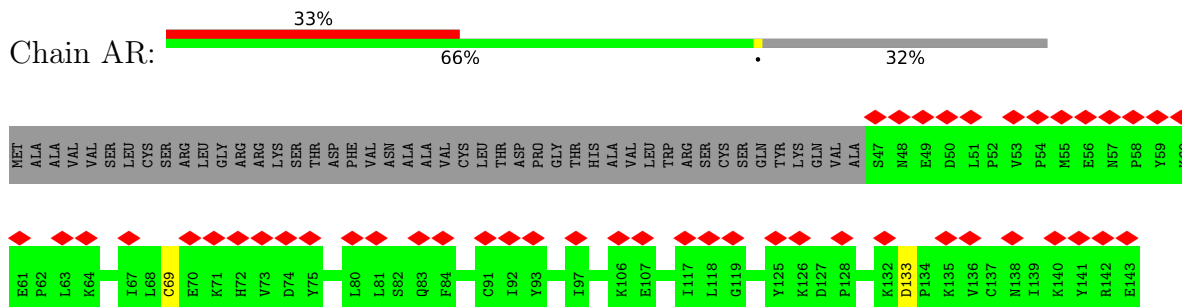
• Molecule 68: 28S ribosomal protein S16, mitochondrial



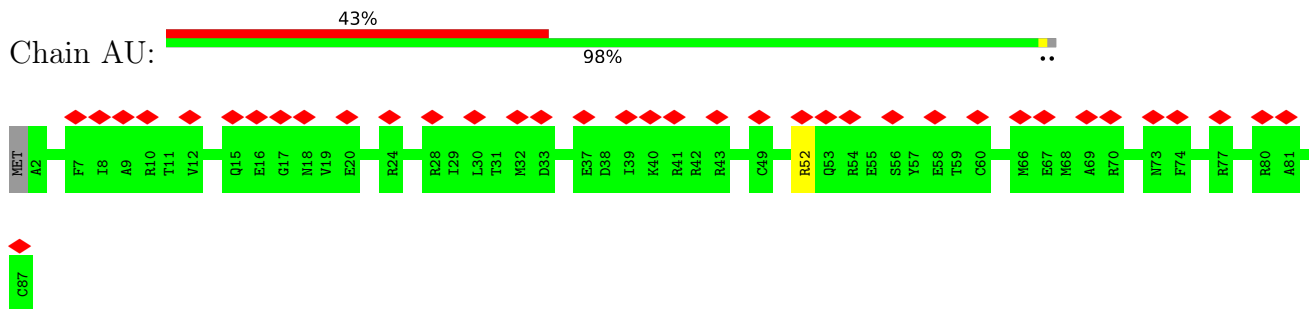
• Molecule 69: uS17m



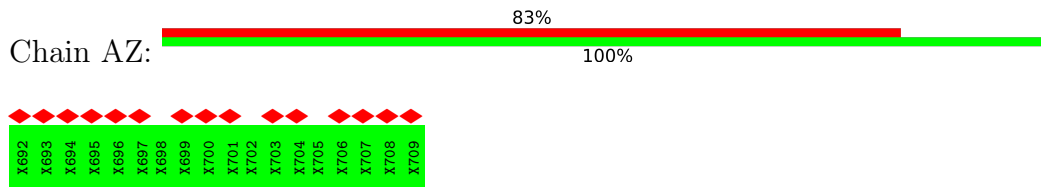
- Molecule 70: 28S ribosomal protein S18c, mitochondrial isoform 1



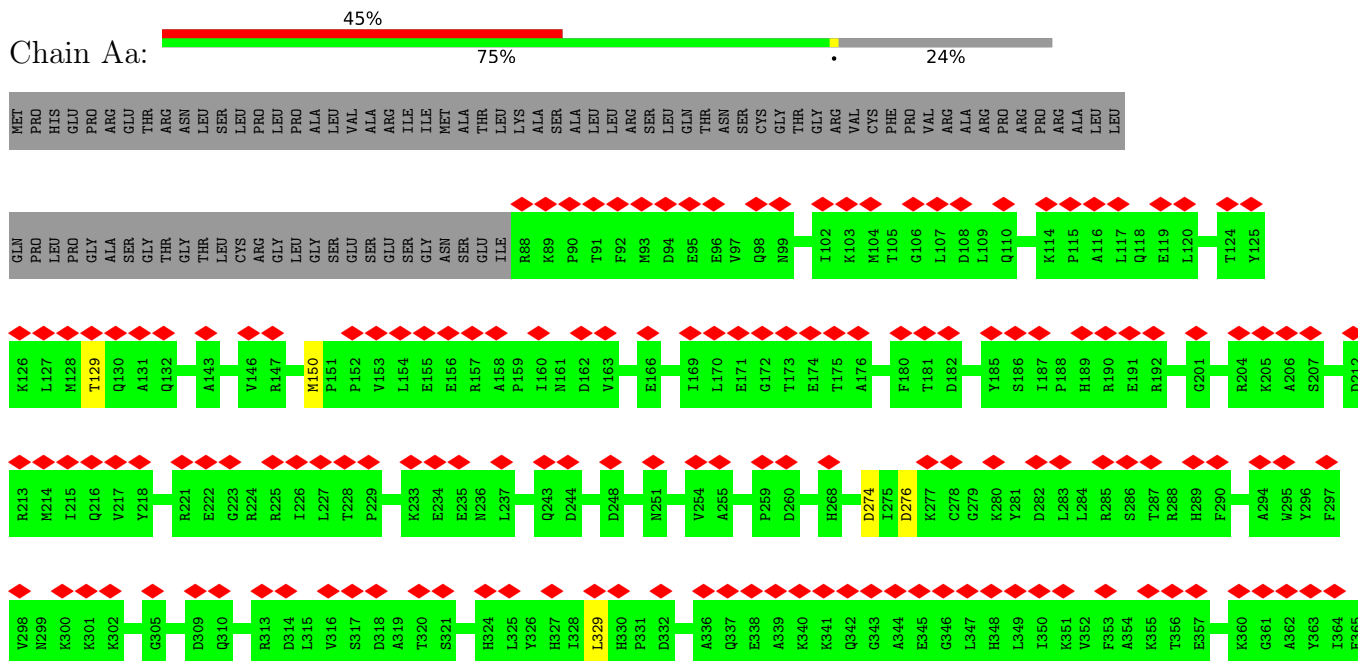
- Molecule 71: 28S ribosomal protein S21, mitochondrial

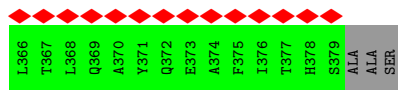


- Molecule 72: unknown

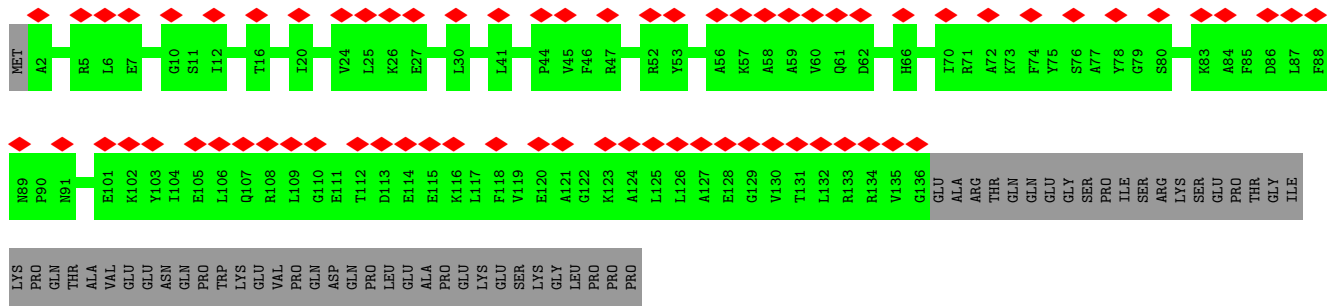
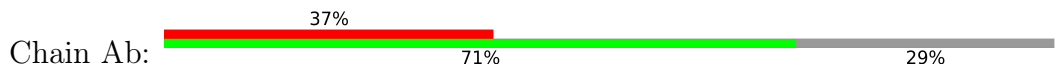


- Molecule 73: Mitochondrial ribosomal protein S22

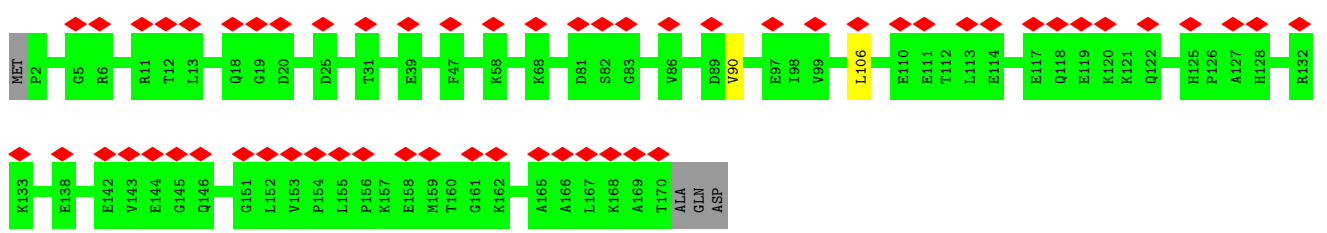




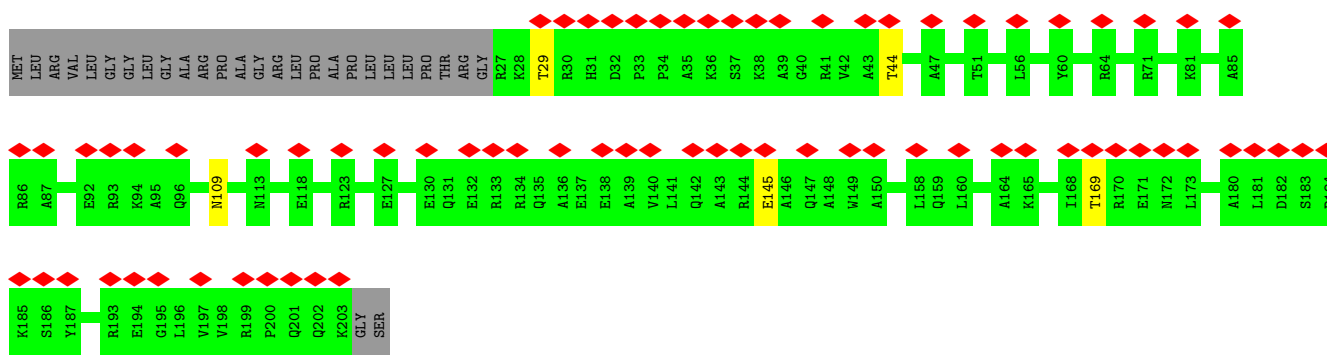
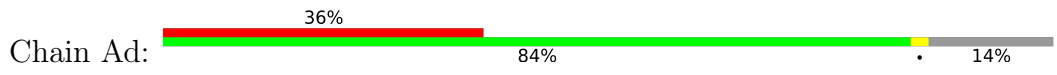
• Molecule 74: Mitochondrial ribosomal protein S23



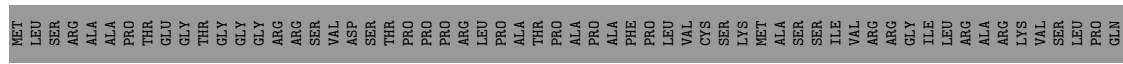
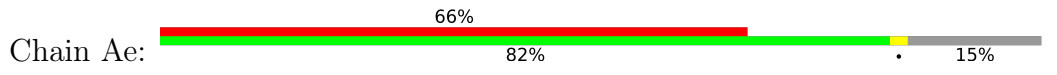
• Molecule 75: Interferon alpha-inducible protein 6

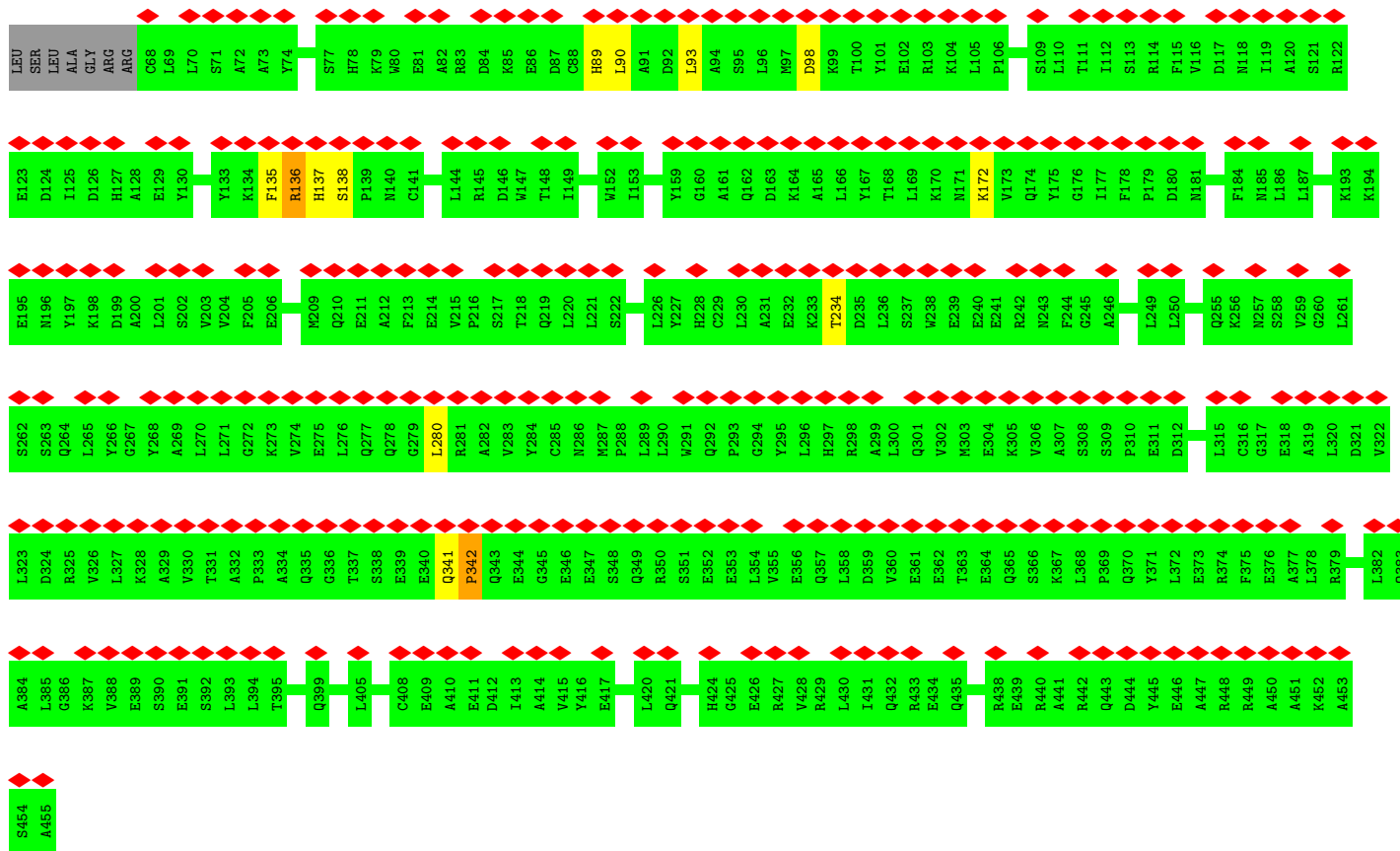


• Molecule 76: 28S ribosomal protein S26, mitochondrial

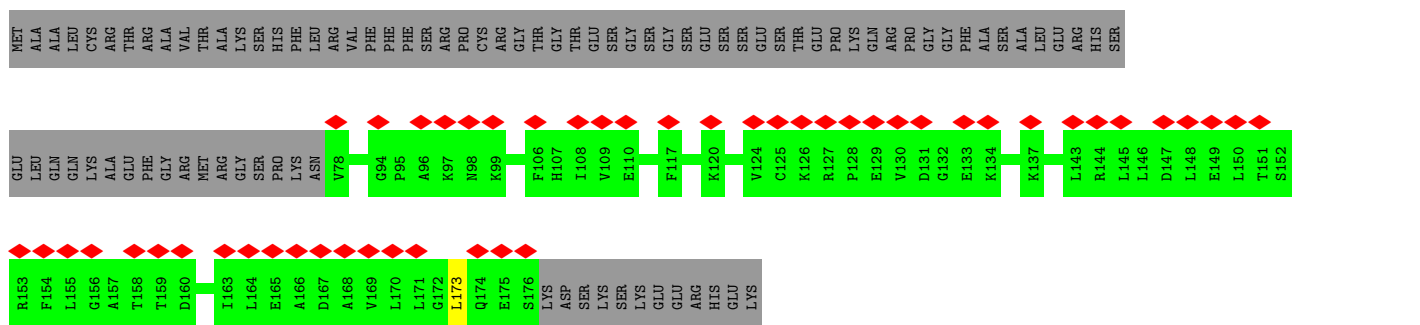


• Molecule 77: Mitochondrial ribosomal protein S27

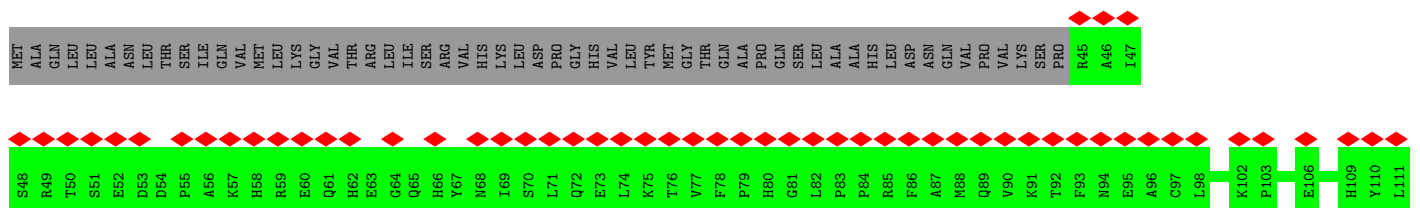
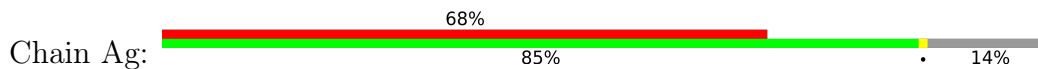




• Molecule 78: 28S ribosomal protein S28, mitochondrial

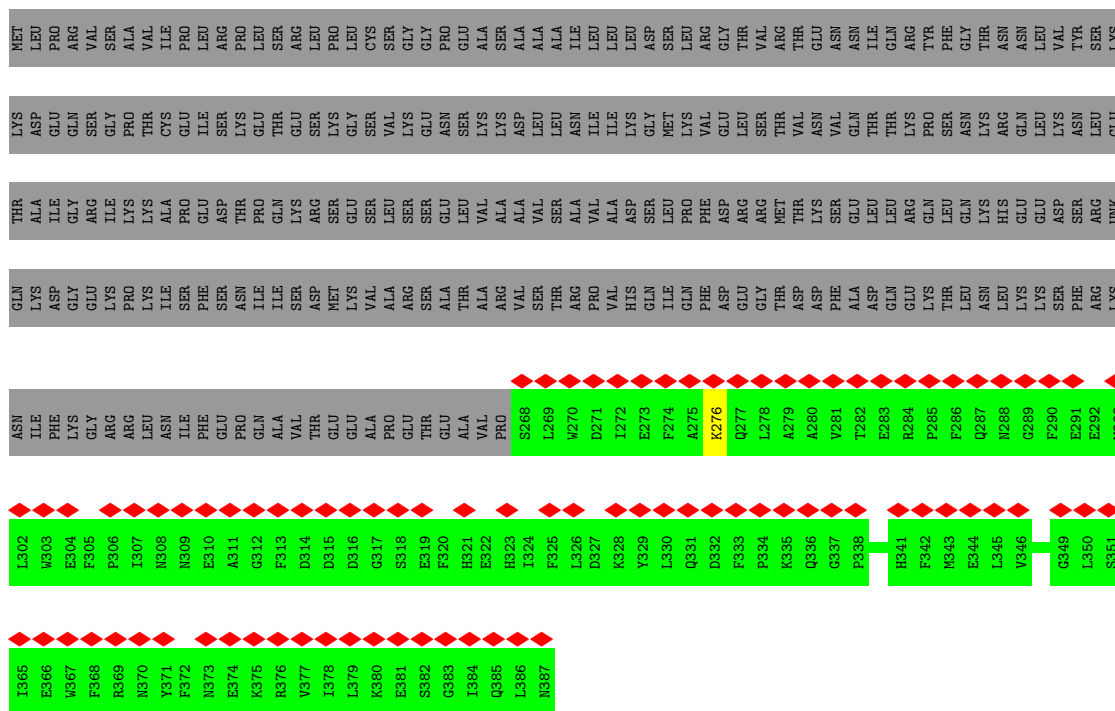


• Molecule 79: Death associated protein 3

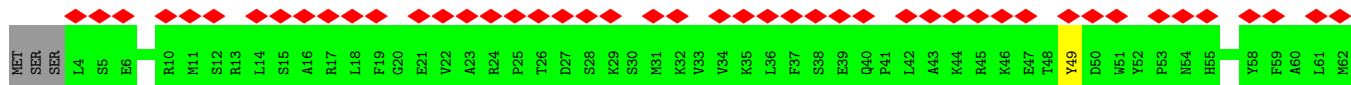
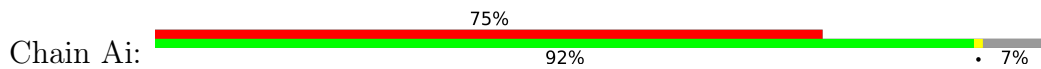


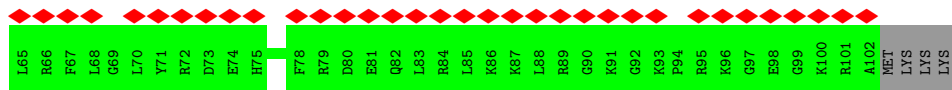


• Molecule 80: 28S ribosomal protein S31, mitochondrial

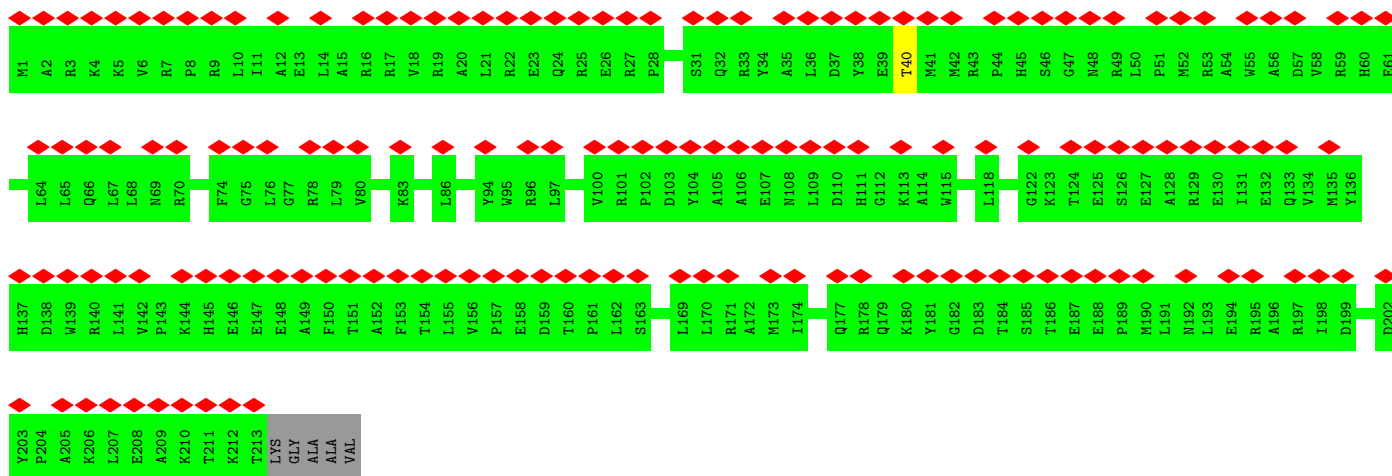
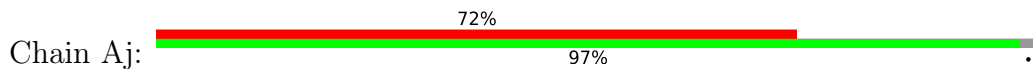


• Molecule 81: Mitochondrial ribosomal protein S33

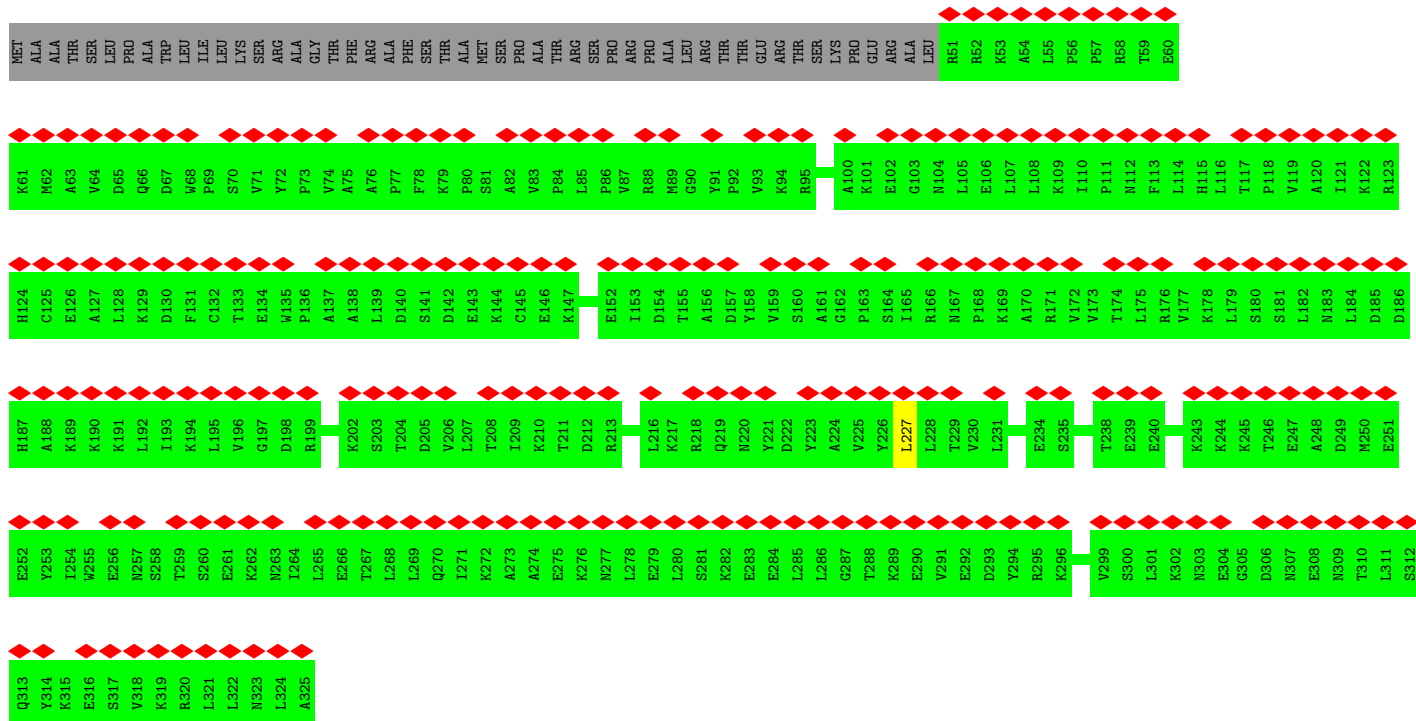
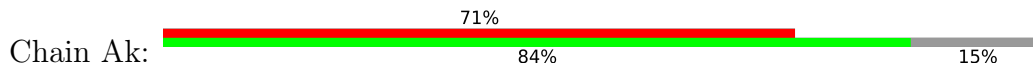




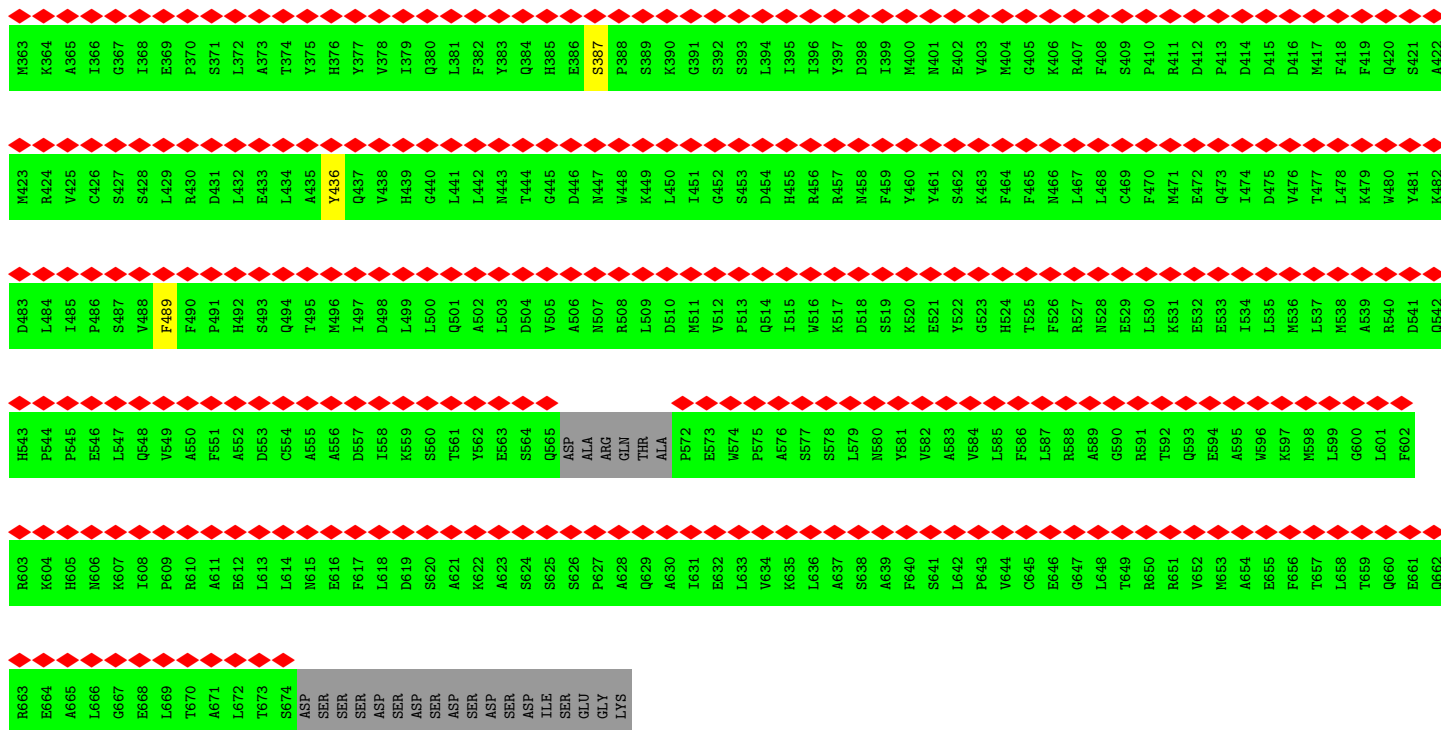
• Molecule 82: Mitochondrial ribosomal protein S34



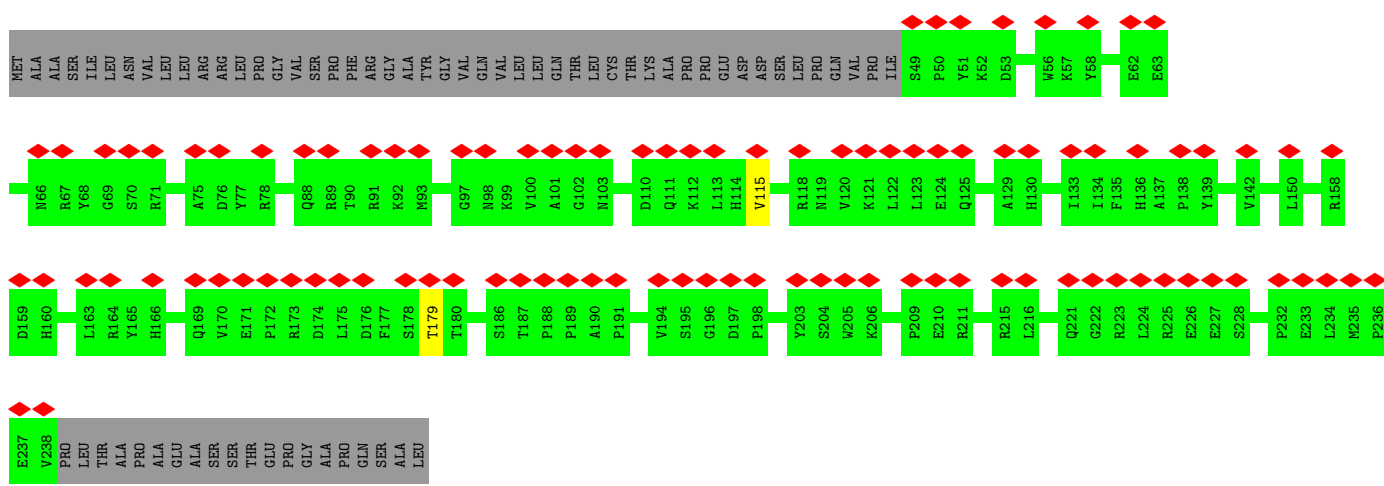
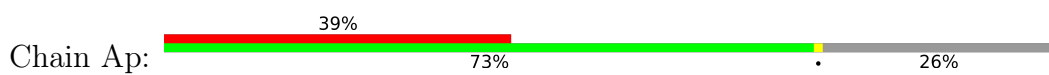
• Molecule 83: 28S ribosomal protein S35, mitochondrial isoform 1



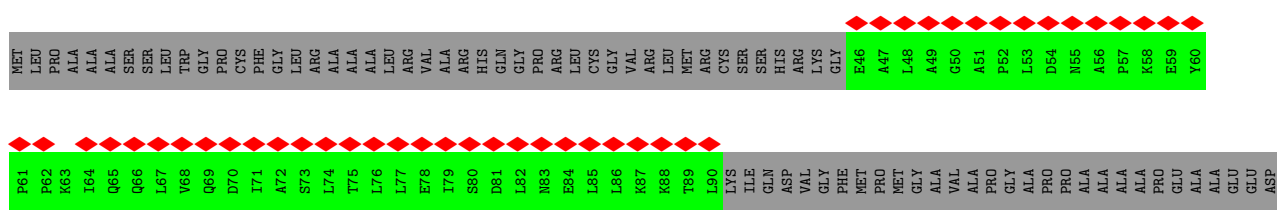
• Molecule 84: Coiled-coil-helix-coiled-coil-helix domain containing 1



• Molecule 87: 28S ribosomal protein S18b, mitochondrial



• Molecule 88: Mitochondrial ribosomal protein L12



4 Experimental information i

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15545	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.108	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	521.76, 521.76, 521.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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: ZN, GTP, SPM, 5GP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B0	0.24	0/880	0.46	0/1189
2	B1	0.23	0/2093	0.46	0/2835
3	B2	0.24	0/1586	0.47	0/2123
4	B3	0.23	0/993	0.46	0/1341
5	B4	0.24	0/481	0.59	1/653 (0.2%)
6	B5	0.24	0/917	0.51	0/1227
7	B6	0.24	0/430	0.49	0/570
8	BB	0.31	1/1595 (0.1%)	0.75	0/2475
9	B7	0.23	0/395	0.54	0/524
10	BD	0.24	0/1898	0.52	0/2555
11	BE	0.25	0/2493	0.45	0/3387
12	BF	0.23	0/2069	0.47	0/2816
13	BG	0.23	0/1510	0.45	0/2033
14	BI	0.23	0/819	0.53	0/1101
15	BJ	0.24	0/1742	0.48	0/2358
16	BK	0.25	0/1323	0.47	0/1785
17	BN	0.24	0/1487	0.44	0/2017
18	BO	0.23	0/912	0.52	0/1231
19	BP	0.25	0/2368	0.50	0/3198
20	BQ	0.24	0/1850	0.50	0/2491
21	BR	0.23	0/1262	0.50	0/1700
22	BS	0.23	0/1197	0.53	0/1624
23	BT	0.31	1/1936 (0.1%)	0.52	1/2615 (0.0%)
24	BU	0.23	0/1179	0.52	0/1578
25	BV	0.23	0/1256	0.48	0/1706
26	BW	0.24	0/1407	0.48	0/1891
27	BX	0.25	0/1211	0.51	0/1646
28	BY	0.23	0/1719	0.50	0/2329
29	Ba	0.24	0/3267	0.47	0/4455
30	Bb	0.25	0/3047	0.49	0/4139
31	Bc	0.24	0/2464	0.45	0/3330
32	Bd	0.27	0/1183	0.50	0/1594

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Be	0.26	0/1000	0.46	0/1345
34	Bf	0.24	0/851	0.57	2/1159 (0.2%)
35	Bg	0.24	0/1191	0.53	0/1614
36	B8	0.23	0/853	0.51	0/1136
37	Bh	0.24	0/2372	0.46	0/3211
38	Bi	0.24	0/2199	0.47	0/2980
39	Bj	0.23	0/1811	0.47	0/2436
40	Bk	0.24	0/1270	0.47	0/1714
41	Bl	0.25	0/1135	0.48	0/1549
42	Bm	0.23	0/917	0.44	0/1248
43	Bn	0.23	0/860	0.48	0/1150
44	Bo	0.24	0/787	0.46	0/1056
45	Bp	0.25	0/752	0.52	0/1013
46	Bq	0.24	0/692	0.52	1/936 (0.1%)
47	Bt	0.23	0/798	0.54	0/1073
48	Bu	0.23	0/1214	0.53	1/1630 (0.1%)
49	Bv	0.23	0/1157	0.49	0/1560
50	Bw	0.25	0/3206	0.46	0/4354
51	Bx	0.24	0/1364	0.49	0/1849
52	AA	0.17	0/22852	0.76	7/35580 (0.0%)
53	B9	0.24	0/342	0.53	0/450
54	AV	0.98	32/1561 (2.0%)	1.21	2/2411 (0.1%)
55	AX	1.19	3/109 (2.8%)	1.19	0/166
56	BA	0.18	0/36784	0.77	12/57270 (0.0%)
57	AB	0.24	0/1804	0.48	0/2445
58	AC	0.24	0/1105	0.49	0/1496
59	AE	0.25	0/2785	0.50	0/3735
60	AF	0.23	0/999	0.50	0/1347
61	AG	0.24	0/1763	0.45	0/2368
62	AI	0.26	0/2707	0.48	0/3636
63	AJ	0.23	0/1181	0.48	0/1597
64	AK	0.24	0/1027	0.49	0/1389
65	AL	0.25	0/858	0.52	0/1152
66	AN	0.22	0/874	0.53	0/1171
67	AO	0.23	0/1473	0.45	0/1970
68	AP	0.24	0/954	0.53	0/1284
69	AQ	0.24	0/894	0.47	0/1213
70	AR	0.24	0/802	0.43	0/1079
71	AU	0.23	0/745	0.53	0/993
73	Aa	0.23	0/2428	0.43	0/3279
74	Ab	0.25	0/1126	0.49	0/1514
75	Ac	0.25	0/1399	0.46	0/1881
76	Ad	0.24	0/1490	0.49	0/2005

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
77	Ae	0.28	0/3171	0.51	1/4292 (0.0%)
78	Af	0.24	0/790	0.48	0/1064
79	Ag	0.24	0/2945	0.45	0/3984
80	Ah	0.24	0/1045	0.40	0/1409
81	Ai	0.24	0/841	0.49	0/1121
82	Aj	0.23	0/1835	0.52	0/2484
83	Ak	0.23	0/2268	0.43	0/3069
84	Am	0.30	0/947	0.50	0/1268
85	An	0.23	0/650	0.53	0/858
86	Ao	0.24	0/4458	0.44	0/6036
87	Ap	0.24	0/1616	0.48	0/2195
88	CL	0.23	0/319	0.40	0/435
88	DL	0.22	0/212	0.44	0/286
88	EL	0.22	0/221	0.43	0/297
88	FL	0.22	0/212	0.41	0/286
88	GL	0.22	0/212	0.41	0/286
88	HL	0.22	0/204	0.41	0/275
All	All	0.24	37/183406 (0.0%)	0.61	28/260605 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	BT	0	1
77	Ae	0	1
All	All	0	2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	BB	1	G	OP3-P	-10.62	1.48	1.61
23	BT	57	PRO	N-CA	6.58	1.58	1.47
54	AV	43	U	C1'-N1	6.40	1.58	1.48
54	AV	23	U	C1'-N1	6.38	1.58	1.48
55	AX	2	U	C1'-N1	6.38	1.58	1.48
54	AV	18	U	C1'-N1	6.20	1.58	1.48
54	AV	41	U	C1'-N1	6.12	1.57	1.48
54	AV	40	U	C1'-N1	6.10	1.57	1.48
54	AV	10	U	C1'-N1	6.10	1.57	1.48
54	AV	65	U	C1'-N1	6.08	1.57	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	AV	1	U	C1'-N1	6.06	1.57	1.48
54	AV	5	U	C1'-N1	6.06	1.57	1.48
55	AX	3	U	C1'-N1	6.06	1.57	1.48
54	AV	52	U	C1'-N1	6.05	1.57	1.48
54	AV	42	U	C1'-N1	6.04	1.57	1.48
54	AV	11	U	C1'-N1	6.03	1.57	1.48
54	AV	54	U	C1'-N1	5.97	1.57	1.48
54	AV	45	U	C1'-N1	5.97	1.57	1.48
54	AV	4	U	C1'-N1	5.97	1.57	1.48
54	AV	19	U	C1'-N1	5.96	1.57	1.48
54	AV	34	U	C1'-N1	5.94	1.57	1.48
54	AV	48	U	C1'-N1	5.91	1.57	1.48
54	AV	63	U	C1'-N1	5.90	1.57	1.48
54	AV	14	U	C1'-N1	5.89	1.57	1.48
54	AV	6	U	C1'-N1	5.86	1.57	1.48
54	AV	32	U	C1'-N1	5.81	1.57	1.48
55	AX	4	U	C1'-N1	5.78	1.57	1.48
54	AV	27	U	C1'-N1	5.70	1.57	1.48
54	AV	20	U	C1'-N1	5.69	1.57	1.48
54	AV	16	U	C1'-N1	5.67	1.57	1.48
54	AV	49	U	C1'-N1	5.67	1.57	1.48
54	AV	2	U	C1'-N1	5.66	1.57	1.48
54	AV	39	U	C1'-N1	5.63	1.57	1.48
54	AV	28	U	C1'-N1	5.58	1.57	1.48
54	AV	26	U	C1'-N1	5.55	1.57	1.48
54	AV	68	U	C1'-N1	5.33	1.56	1.48
54	AV	15	U	C1'-N1	5.27	1.56	1.48

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	AA	825	C	OP1-P-OP2	11.42	136.73	119.60
52	AA	824	G	OP2-P-O3'	-10.46	82.19	105.20
52	AA	824	G	OP1-P-O3'	-9.45	84.41	105.20
52	AA	119	C	C2-N1-C1'	7.97	127.57	118.80
34	Bf	80	PRO	N-CA-CB	6.65	111.28	103.30
77	Ae	342	PRO	N-CA-CB	6.56	111.17	103.30
23	BT	58	PRO	CA-N-CD	-6.44	102.48	111.50
34	Bf	78	PRO	N-CA-CB	6.43	111.01	103.30
48	Bu	167	PRO	N-CA-CB	6.42	111.00	103.30
56	BA	1527	U	C2-N1-C1'	6.03	124.94	117.70
56	BA	394	C	N1-C2-O2	5.97	122.48	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BA	825	C	C2-N1-C1'	5.94	125.33	118.80
46	Bq	59	PRO	N-CA-CB	5.91	110.40	103.30
52	AA	536	C	C6-N1-C2	-5.81	117.98	120.30
52	AA	119	C	C6-N1-C1'	-5.75	113.90	120.80
54	AV	61	U	C2-N1-C1'	5.72	124.56	117.70
5	B4	87	PRO	N-CA-CB	5.67	110.11	103.30
54	AV	61	U	C6-N1-C1'	-5.60	113.35	121.20
56	BA	848	C	C2-N1-C1'	5.55	124.90	118.80
56	BA	890	C	N1-C2-O2	5.50	122.20	118.90
56	BA	48	U	OP1-P-O3'	5.48	117.25	105.20
56	BA	890	C	C2-N1-C1'	5.46	124.80	118.80
56	BA	825	C	N1-C2-O2	5.44	122.16	118.90
56	BA	1527	U	N1-C2-O2	5.41	126.59	122.80
56	BA	48	U	P-O3'-C3'	5.26	126.01	119.70
56	BA	1527	U	N3-C2-O2	-5.21	118.55	122.20
56	BA	847	U	C2-N1-C1'	5.08	123.80	117.70
52	AA	745	C	C2-N1-C1'	5.05	124.36	118.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
77	Ae	90	LEU	Peptide
23	BT	59	LYS	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	B0	108/148 (73%)	107 (99%)	1 (1%)	0	100	100
2	B1	242/256 (94%)	241 (100%)	1 (0%)	0	100	100
3	B2	177/252 (70%)	176 (99%)	1 (1%)	0	100	100
4	B3	116/161 (72%)	113 (97%)	3 (3%)	0	100	100
5	B4	60/126 (48%)	55 (92%)	5 (8%)	0	100	100
6	B5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
7	B6	50/65 (77%)	50 (100%)	0	0	100	100
9	B7	44/95 (46%)	44 (100%)	0	0	100	100
10	BD	238/306 (78%)	230 (97%)	8 (3%)	0	100	100
11	BE	305/399 (76%)	292 (96%)	13 (4%)	0	100	100
12	BF	248/294 (84%)	244 (98%)	4 (2%)	0	100	100
13	BG	191/257 (74%)	172 (90%)	19 (10%)	0	100	100
14	BI	96/268 (36%)	96 (100%)	0	0	100	100
15	BJ	210/262 (80%)	200 (95%)	10 (5%)	0	100	100
16	BK	174/192 (91%)	172 (99%)	2 (1%)	0	100	100
17	BN	175/178 (98%)	171 (98%)	4 (2%)	0	100	100
18	BO	113/145 (78%)	111 (98%)	2 (2%)	0	100	100
19	BP	286/296 (97%)	276 (96%)	10 (4%)	0	100	100
20	BQ	220/251 (88%)	217 (99%)	3 (1%)	0	100	100
21	BR	151/169 (89%)	143 (95%)	8 (5%)	0	100	100
22	BS	141/180 (78%)	132 (94%)	9 (6%)	0	100	100
23	BT	226/292 (77%)	217 (96%)	8 (4%)	1 (0%)	34	72
24	BU	138/149 (93%)	138 (100%)	0	0	100	100
25	BV	153/209 (73%)	150 (98%)	3 (2%)	0	100	100
26	BW	164/210 (78%)	161 (98%)	3 (2%)	0	100	100
27	BX	147/150 (98%)	143 (97%)	4 (3%)	0	100	100
28	BY	204/216 (94%)	201 (98%)	3 (2%)	0	100	100
29	Ba	391/423 (92%)	380 (97%)	11 (3%)	0	100	100
30	Bb	352/380 (93%)	338 (96%)	14 (4%)	0	100	100
31	Bc	293/334 (88%)	282 (96%)	11 (4%)	0	100	100
32	Bd	136/206 (66%)	130 (96%)	6 (4%)	0	100	100
33	Be	120/135 (89%)	115 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Bf	106/142 (75%)	102 (96%)	2 (2%)	2 (2%)	8	40
35	Bg	146/159 (92%)	137 (94%)	9 (6%)	0	100	100
36	B8	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
37	Bh	287/332 (86%)	275 (96%)	12 (4%)	0	100	100
38	Bi	258/306 (84%)	253 (98%)	5 (2%)	0	100	100
39	Bj	211/279 (76%)	205 (97%)	6 (3%)	0	100	100
40	Bk	151/269 (56%)	149 (99%)	2 (1%)	0	100	100
41	Bl	131/166 (79%)	129 (98%)	2 (2%)	0	100	100
42	Bm	107/198 (54%)	105 (98%)	2 (2%)	0	100	100
43	Bn	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
44	Bo	95/124 (77%)	94 (99%)	1 (1%)	0	100	100
45	Bp	95/112 (85%)	92 (97%)	3 (3%)	0	100	100
46	Bq	78/138 (56%)	73 (94%)	4 (5%)	1 (1%)	12	48
47	Bt	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
48	Bu	147/205 (72%)	140 (95%)	5 (3%)	2 (1%)	11	47
49	Bv	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
50	Bw	385/433 (89%)	365 (95%)	20 (5%)	0	100	100
51	Bx	160/196 (82%)	155 (97%)	5 (3%)	0	100	100
53	B9	36/100 (36%)	36 (100%)	0	0	100	100
57	AB	218/289 (75%)	214 (98%)	4 (2%)	0	100	100
58	AC	130/167 (78%)	123 (95%)	7 (5%)	0	100	100
59	AE	341/430 (79%)	332 (97%)	9 (3%)	0	100	100
60	AF	120/276 (44%)	119 (99%)	1 (1%)	0	100	100
61	AG	206/242 (85%)	206 (100%)	0	0	100	100
62	AI	326/397 (82%)	315 (97%)	11 (3%)	0	100	100
63	AJ	138/200 (69%)	127 (92%)	11 (8%)	0	100	100
64	AK	135/196 (69%)	129 (96%)	6 (4%)	0	100	100
65	AL	107/139 (77%)	103 (96%)	4 (4%)	0	100	100
66	AN	99/128 (77%)	99 (100%)	0	0	100	100
67	AO	173/239 (72%)	166 (96%)	7 (4%)	0	100	100
68	AP	115/135 (85%)	112 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	AQ	110/130 (85%)	108 (98%)	2 (2%)	0	100	100
70	AR	95/143 (66%)	94 (99%)	1 (1%)	0	100	100
71	AU	84/87 (97%)	84 (100%)	0	0	100	100
73	Aa	290/382 (76%)	285 (98%)	5 (2%)	0	100	100
74	Ab	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
75	Ac	167/173 (96%)	165 (99%)	2 (1%)	0	100	100
76	Ad	175/205 (85%)	175 (100%)	0	0	100	100
77	Ae	386/455 (85%)	356 (92%)	27 (7%)	3 (1%)	19	60
78	Af	97/188 (52%)	93 (96%)	4 (4%)	0	100	100
79	Ag	351/410 (86%)	339 (97%)	12 (3%)	0	100	100
80	Ah	118/387 (30%)	118 (100%)	0	0	100	100
81	Ai	97/106 (92%)	97 (100%)	0	0	100	100
82	Aj	211/218 (97%)	206 (98%)	5 (2%)	0	100	100
83	Ak	273/325 (84%)	264 (97%)	9 (3%)	0	100	100
84	Am	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
85	An	70/199 (35%)	69 (99%)	1 (1%)	0	100	100
86	Ao	532/690 (77%)	518 (97%)	14 (3%)	0	100	100
87	Ap	188/258 (73%)	183 (97%)	5 (3%)	0	100	100
88	CL	43/198 (22%)	41 (95%)	2 (5%)	0	100	100
88	DL	25/198 (13%)	25 (100%)	0	0	100	100
88	EL	26/198 (13%)	26 (100%)	0	0	100	100
88	FL	25/198 (13%)	25 (100%)	0	0	100	100
88	GL	25/198 (13%)	25 (100%)	0	0	100	100
88	HL	24/198 (12%)	24 (100%)	0	0	100	100
All	All	14350/19681 (73%)	13925 (97%)	416 (3%)	9 (0%)	54	85

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	Bf	78	PRO
34	Bf	80	PRO
48	Bu	167	PRO
46	Bq	64	ASP
77	Ae	136	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	BT	58	PRO
77	Ae	342	PRO
77	Ae	341	GLN
48	Bu	166	GLU

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	B0	90/115 (78%)	90 (100%)	0	100	100
2	B1	219/229 (96%)	218 (100%)	1 (0%)	88	93
3	B2	164/228 (72%)	162 (99%)	2 (1%)	71	84
4	B3	110/150 (73%)	110 (100%)	0	100	100
5	B4	45/114 (40%)	44 (98%)	1 (2%)	52	71
6	B5	99/163 (61%)	98 (99%)	1 (1%)	76	86
7	B6	49/60 (82%)	49 (100%)	0	100	100
9	B7	41/78 (53%)	41 (100%)	0	100	100
10	BD	193/248 (78%)	191 (99%)	2 (1%)	76	86
11	BE	263/320 (82%)	259 (98%)	4 (2%)	65	80
12	BF	217/251 (86%)	215 (99%)	2 (1%)	78	87
13	BG	173/224 (77%)	165 (95%)	8 (5%)	27	53
14	BI	88/228 (39%)	87 (99%)	1 (1%)	73	85
15	BJ	192/230 (84%)	192 (100%)	0	100	100
16	BK	129/151 (85%)	128 (99%)	1 (1%)	81	89
17	BN	156/157 (99%)	156 (100%)	0	100	100
18	BO	99/123 (80%)	99 (100%)	0	100	100
19	BP	245/249 (98%)	243 (99%)	2 (1%)	81	89
20	BQ	190/210 (90%)	189 (100%)	1 (0%)	88	93
21	BR	132/143 (92%)	131 (99%)	1 (1%)	81	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	BS	123/153 (80%)	122 (99%)	1 (1%)	81	89
23	BT	208/258 (81%)	204 (98%)	4 (2%)	57	75
24	BU	118/127 (93%)	118 (100%)	0	100	100
25	BV	136/178 (76%)	134 (98%)	2 (2%)	65	80
26	BW	144/180 (80%)	144 (100%)	0	100	100
27	BX	116/134 (87%)	116 (100%)	0	100	100
28	BY	185/192 (96%)	182 (98%)	3 (2%)	62	79
29	Ba	348/365 (95%)	346 (99%)	2 (1%)	86	92
30	Bb	310/328 (94%)	307 (99%)	3 (1%)	76	86
31	Bc	271/299 (91%)	270 (100%)	1 (0%)	91	94
32	Bd	127/181 (70%)	123 (97%)	4 (3%)	40	62
33	Be	100/108 (93%)	100 (100%)	0	100	100
34	Bf	80/133 (60%)	80 (100%)	0	100	100
35	Bg	128/136 (94%)	126 (98%)	2 (2%)	62	79
36	B8	87/162 (54%)	86 (99%)	1 (1%)	73	85
37	Bh	251/284 (88%)	250 (100%)	1 (0%)	91	94
38	Bi	236/275 (86%)	234 (99%)	2 (1%)	81	89
39	Bj	190/242 (78%)	187 (98%)	3 (2%)	62	79
40	Bk	135/226 (60%)	134 (99%)	1 (1%)	84	90
41	Bl	122/147 (83%)	120 (98%)	2 (2%)	62	79
42	Bm	103/178 (58%)	103 (100%)	0	100	100
43	Bn	88/113 (78%)	87 (99%)	1 (1%)	73	85
44	Bo	77/97 (79%)	77 (100%)	0	100	100
45	Bp	79/88 (90%)	78 (99%)	1 (1%)	69	82
46	Bq	70/114 (61%)	65 (93%)	5 (7%)	14	41
47	Bt	75/82 (92%)	75 (100%)	0	100	100
48	Bu	126/177 (71%)	126 (100%)	0	100	100
49	Bv	115/183 (63%)	115 (100%)	0	100	100
50	Bw	340/373 (91%)	338 (99%)	2 (1%)	86	92
51	Bx	149/173 (86%)	147 (99%)	2 (1%)	69	82
53	B9	36/77 (47%)	35 (97%)	1 (3%)	43	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	AB	187/233 (80%)	187 (100%)	0	100	100
58	AC	115/142 (81%)	113 (98%)	2 (2%)	60	78
59	AE	282/351 (80%)	273 (97%)	9 (3%)	39	62
60	AF	107/210 (51%)	105 (98%)	2 (2%)	57	75
61	AG	181/205 (88%)	180 (99%)	1 (1%)	86	92
62	AI	273/333 (82%)	269 (98%)	4 (2%)	65	80
63	AJ	130/180 (72%)	130 (100%)	0	100	100
64	AK	103/151 (68%)	103 (100%)	0	100	100
65	AL	92/116 (79%)	92 (100%)	0	100	100
66	AN	92/114 (81%)	90 (98%)	2 (2%)	52	71
67	AO	159/205 (78%)	159 (100%)	0	100	100
68	AP	97/113 (86%)	97 (100%)	0	100	100
69	AQ	97/114 (85%)	97 (100%)	0	100	100
70	AR	89/127 (70%)	87 (98%)	2 (2%)	52	71
71	AU	77/78 (99%)	76 (99%)	1 (1%)	69	82
73	Aa	258/330 (78%)	253 (98%)	5 (2%)	57	75
74	Ab	113/162 (70%)	113 (100%)	0	100	100
75	Ac	152/155 (98%)	150 (99%)	2 (1%)	69	82
76	Ad	149/168 (89%)	144 (97%)	5 (3%)	37	60
77	Ae	325/393 (83%)	315 (97%)	10 (3%)	40	62
78	Af	86/160 (54%)	85 (99%)	1 (1%)	71	84
79	Ag	312/361 (86%)	308 (99%)	4 (1%)	69	82
80	Ah	109/346 (32%)	108 (99%)	1 (1%)	78	87
81	Ai	86/93 (92%)	85 (99%)	1 (1%)	71	84
82	Aj	188/190 (99%)	187 (100%)	1 (0%)	88	93
83	Ak	249/289 (86%)	248 (100%)	1 (0%)	91	94
84	Am	100/102 (98%)	92 (92%)	8 (8%)	12	38
85	An	66/174 (38%)	66 (100%)	0	100	100
86	Ao	478/541 (88%)	473 (99%)	5 (1%)	76	86
87	Ap	170/225 (76%)	168 (99%)	2 (1%)	71	84
88	CL	30/157 (19%)	30 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
88	DL	26/157 (17%)	26 (100%)	0	100	100
88	EL	27/157 (17%)	27 (100%)	0	100	100
88	FL	26/157 (17%)	26 (100%)	0	100	100
88	GL	26/157 (17%)	26 (100%)	0	100	100
88	HL	25/157 (16%)	25 (100%)	0	100	100
All	All	12649/16737 (76%)	12509 (99%)	140 (1%)	74	85

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B1	126	THR
3	B2	92	LEU
3	B2	197	ASN
5	B4	48	THR
6	B5	153	THR
10	BD	125	GLU
10	BD	240	THR
11	BE	127	CYS
11	BE	236	THR
11	BE	245	THR
11	BE	295	CYS
12	BF	74	GLN
12	BF	262	THR
13	BG	71	ARG
13	BG	103	PHE
13	BG	163	ARG
13	BG	164	GLU
13	BG	187	ARG
13	BG	189	HIS
13	BG	224	ASP
13	BG	228	GLU
14	BI	61	LYS
16	BK	167	PHE
19	BP	44	ARG
19	BP	61	THR
20	BQ	59	VAL
21	BR	144	THR
22	BS	173	ARG
23	BT	55	GLN
23	BT	58	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	BT	59	LYS
23	BT	187	LEU
25	BV	103	VAL
25	BV	113	THR
28	BY	81	ARG
28	BY	105	ARG
28	BY	186	THR
29	Ba	40	LYS
29	Ba	273	VAL
30	Bb	52	ARG
30	Bb	189	HIS
30	Bb	233	VAL
31	Bc	56	THR
32	Bd	74	ARG
32	Bd	76	GLU
32	Bd	79	SER
32	Bd	150	LEU
35	Bg	14	VAL
35	Bg	127	GLN
36	B8	163	THR
37	Bh	267	LEU
38	Bi	153	ASN
38	Bi	221	THR
39	Bj	47	LEU
39	Bj	84	TYR
39	Bj	273	ARG
40	Bk	84	THR
41	Bl	42	VAL
41	Bl	78	PRO
43	Bn	43	VAL
45	Bp	27	VAL
46	Bq	66	PHE
46	Bq	73	MET
46	Bq	77	ILE
46	Bq	78	TYR
46	Bq	101	VAL
50	Bw	131	LEU
50	Bw	370	THR
51	Bx	70	CYS
51	Bx	152	THR
53	B9	65	THR
58	AC	52	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
58	AC	138	TYR
59	AE	184	LYS
59	AE	185	MET
59	AE	186	LYS
59	AE	187	VAL
59	AE	188	LYS
59	AE	189	ARG
59	AE	289	THR
59	AE	364	ASP
59	AE	401	VAL
60	AF	105	CYS
60	AF	111	VAL
61	AG	208	GLU
62	AI	247	ARG
62	AI	249	ILE
62	AI	251	ILE
62	AI	253	SER
66	AN	35	LEU
66	AN	117	HIS
70	AR	69	CYS
70	AR	133	ASP
71	AU	52	ARG
73	Aa	129	THR
73	Aa	150	MET
73	Aa	274	ASP
73	Aa	276	ASP
73	Aa	329	LEU
75	Ac	90	VAL
75	Ac	106	LEU
76	Ad	29	THR
76	Ad	44	THR
76	Ad	109	ASN
76	Ad	145	GLU
76	Ad	169	THR
77	Ae	89	HIS
77	Ae	93	LEU
77	Ae	98	ASP
77	Ae	135	PHE
77	Ae	136	ARG
77	Ae	137	HIS
77	Ae	138	SER
77	Ae	172	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
77	Ae	234	THR
77	Ae	280	LEU
78	Af	173	LEU
79	Ag	212	ARG
79	Ag	236	THR
79	Ag	261	VAL
79	Ag	336	LEU
80	Ah	276	LYS
81	Ai	49	TYR
82	Aj	40	THR
83	Ak	227	LEU
84	Am	37	ARG
84	Am	38	ARG
84	Am	39	GLU
84	Am	40	LYS
84	Am	64	GLU
84	Am	66	CYS
84	Am	96	LEU
84	Am	98	SER
86	Ao	115	ASN
86	Ao	349	TYR
86	Ao	387	SER
86	Ao	436	TYR
86	Ao	489	PHE
87	Ap	115	VAL
87	Ap	179	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B0	41	ASN
11	BE	154	HIS
12	BF	83	HIS
15	BJ	93	ASN
15	BJ	101	HIS
23	BT	55	GLN
29	Ba	360	ASN
36	B8	154	GLN
37	Bh	69	HIS
39	Bj	212	HIS
40	Bk	158	GLN
42	Bm	151	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	Bw	87	GLN
50	Bw	352	GLN
51	Bx	184	ASN
57	AB	238	ASN
62	AI	327	HIS
66	AN	60	ASN
73	Aa	334	GLN
75	Ac	51	ASN
75	Ac	95	ASN
80	Ah	370	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	AA	959/962 (99%)	176 (18%)	3 (0%)
54	AV	70/71 (98%)	28 (40%)	0
55	AX	4/5 (80%)	1 (25%)	0
56	BA	1542/1571 (98%)	412 (26%)	2 (0%)
8	BB	64/73 (87%)	17 (26%)	0
All	All	2639/2682 (98%)	634 (24%)	5 (0%)

All (634) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	BB	3	U
8	BB	5	A
8	BB	7	G
8	BB	8	U
8	BB	9	A
8	BB	13	U
8	BB	21	C
8	BB	23	A
8	BB	29	G
8	BB	34	U
8	BB	43	C
8	BB	44	U
8	BB	46	G
8	BB	47	A
8	BB	48	U
8	BB	69	C
8	BB	70	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	AA	5	A
52	AA	10	U
52	AA	27	U
52	AA	34	U
52	AA	42	A
52	AA	43	U
52	AA	54	A
52	AA	58	U
52	AA	63	G
52	AA	65	C
52	AA	75	A
52	AA	81	U
52	AA	83	C
52	AA	102	G
52	AA	115	A
52	AA	120	A
52	AA	127	A
52	AA	147	G
52	AA	152	A
52	AA	161	C
52	AA	164	C
52	AA	165	G
52	AA	170	A
52	AA	171	C
52	AA	173	G
52	AA	175	A
52	AA	186	U
52	AA	191	C
52	AA	194	U
52	AA	212	A
52	AA	216	A
52	AA	217	U
52	AA	219	U
52	AA	222	A
52	AA	223	U
52	AA	224	U
52	AA	231	G
52	AA	235	A
52	AA	238	C
52	AA	244	C
52	AA	247	G
52	AA	253	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	AA	256	G
52	AA	257	U
52	AA	258	C
52	AA	273	A
52	AA	281	G
52	AA	287	C
52	AA	288	G
52	AA	294	A
52	AA	296	G
52	AA	297	A
52	AA	308	A
52	AA	309	A
52	AA	310	A
52	AA	314	A
52	AA	315	U
52	AA	316	C
52	AA	317	A
52	AA	320	A
52	AA	328	A
52	AA	337	C
52	AA	345	U
52	AA	354	C
52	AA	355	U
52	AA	361	A
52	AA	362	A
52	AA	368	A
52	AA	372	C
52	AA	395	C
52	AA	399	A
52	AA	407	U
52	AA	417	C
52	AA	421	A
52	AA	433	U
52	AA	455	A
52	AA	457	C
52	AA	458	C
52	AA	461	A
52	AA	464	A
52	AA	471	U
52	AA	472	A
52	AA	477	A
52	AA	479	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	AA	498	U
52	AA	502	A
52	AA	503	A
52	AA	518	A
52	AA	531	U
52	AA	532	G
52	AA	534	U
52	AA	536	C
52	AA	538	C
52	AA	540	U
52	AA	561	U
52	AA	566	U
52	AA	571	A
52	AA	574	C
52	AA	576	C
52	AA	589	C
52	AA	592	A
52	AA	593	C
52	AA	596	U
52	AA	597	U
52	AA	604	U
52	AA	616	C
52	AA	618	G
52	AA	619	C
52	AA	625	U
52	AA	633	C
52	AA	639	A
52	AA	644	A
52	AA	645	A
52	AA	646	C
52	AA	647	A
52	AA	649	U
52	AA	665	A
52	AA	681	A
52	AA	682	G
52	AA	696	U
52	AA	698	A
52	AA	699	U
52	AA	707	A
52	AA	708	A
52	AA	709	A
52	AA	711	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	AA	720	A
52	AA	722	A
52	AA	731	A
52	AA	732	U
52	AA	739	A
52	AA	743	A
52	AA	746	A
52	AA	771	A
52	AA	775	A
52	AA	780	A
52	AA	781	G
52	AA	790	A
52	AA	791	G
52	AA	802	A
52	AA	803	U
52	AA	807	G
52	AA	808	U
52	AA	823	G
52	AA	825	C
52	AA	838	A
52	AA	841	C
52	AA	842	A
52	AA	854	C
52	AA	863	G
52	AA	869	A
52	AA	870	G
52	AA	876	A
52	AA	877	A
52	AA	883	C
52	AA	885	U
52	AA	886	A
52	AA	893	A
52	AA	894	U
52	AA	897	C
52	AA	899	C
52	AA	902	C
52	AA	910	G
52	AA	918	A
52	AA	919	A
52	AA	923	G
52	AA	925	A
52	AA	928	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	AA	930	G
52	AA	932	U
52	AA	943	G
52	AA	946	A
52	AA	955	G
52	AA	956	G
52	AA	959	U
52	AA	960	A
54	AV	6	U
54	AV	8	U
54	AV	9	U
54	AV	10	U
54	AV	11	U
54	AV	12	U
54	AV	13	U
54	AV	14	U
54	AV	16	U
54	AV	17	U
54	AV	18	U
54	AV	24	U
54	AV	30	U
54	AV	38	U
54	AV	43	U
54	AV	44	U
54	AV	45	U
54	AV	46	U
54	AV	49	U
54	AV	55	U
54	AV	56	U
54	AV	60	U
54	AV	62	U
54	AV	64	U
54	AV	65	U
54	AV	68	U
54	AV	69	C
54	AV	71	A
55	AX	3	U
56	BA	4	A
56	BA	7	G
56	BA	11	G
56	BA	15	A
56	BA	19	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	BA	20	A
56	BA	21	C
56	BA	22	U
56	BA	26	C
56	BA	27	A
56	BA	31	A
56	BA	32	C
56	BA	36	A
56	BA	37	A
56	BA	40	C
56	BA	41	A
56	BA	45	A
56	BA	46	A
56	BA	49	A
56	BA	56	A
56	BA	57	A
56	BA	59	A
56	BA	60	U
56	BA	63	A
56	BA	66	U
56	BA	67	A
56	BA	68	A
56	BA	82	G
56	BA	83	A
56	BA	96	U
56	BA	97	A
56	BA	105	G
56	BA	109	U
56	BA	118	U
56	BA	119	A
56	BA	122	G
56	BA	129	A
56	BA	130	A
56	BA	132	G
56	BA	135	G
56	BA	139	G
56	BA	140	A
56	BA	141	A
56	BA	142	U
56	BA	143	A
56	BA	146	A
56	BA	147	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	BA	163	C
56	BA	164	A
56	BA	168	A
56	BA	172	C
56	BA	178	C
56	BA	180	A
56	BA	182	C
56	BA	190	U
56	BA	192	A
56	BA	205	A
56	BA	218	A
56	BA	219	A
56	BA	223	A
56	BA	225	C
56	BA	229	A
56	BA	231	C
56	BA	237	A
56	BA	238	C
56	BA	239	C
56	BA	243	A
56	BA	245	A
56	BA	254	G
56	BA	263	G
56	BA	265	G
56	BA	271	U
56	BA	272	A
56	BA	273	A
56	BA	275	A
56	BA	277	A
56	BA	295	G
56	BA	309	A
56	BA	311	A
56	BA	313	U
56	BA	322	G
56	BA	323	A
56	BA	324	G
56	BA	329	A
56	BA	330	A
56	BA	331	A
56	BA	336	A
56	BA	337	A
56	BA	338	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	BA	340	A
56	BA	351	A
56	BA	352	G
56	BA	359	G
56	BA	366	A
56	BA	368	A
56	BA	369	G
56	BA	373	U
56	BA	374	U
56	BA	376	A
56	BA	389	A
56	BA	390	A
56	BA	393	A
56	BA	394	C
56	BA	398	A
56	BA	404	C
56	BA	409	A
56	BA	413	C
56	BA	414	A
56	BA	417	G
56	BA	427	G
56	BA	428	A
56	BA	432	A
56	BA	433	G
56	BA	446	C
56	BA	447	A
56	BA	448	G
56	BA	459	A
56	BA	460	C
56	BA	467	A
56	BA	468	A
56	BA	472	U
56	BA	473	G
56	BA	474	A
56	BA	479	A
56	BA	480	G
56	BA	488	U
56	BA	490	U
56	BA	491	U
56	BA	492	A
56	BA	493	A
56	BA	494	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	BA	497	U
56	BA	498	A
56	BA	499	C
56	BA	500	C
56	BA	501	A
56	BA	503	A
56	BA	505	U
56	BA	509	C
56	BA	514	A
56	BA	515	A
56	BA	516	G
56	BA	517	C
56	BA	518	A
56	BA	526	A
56	BA	527	U
56	BA	530	A
56	BA	532	A
56	BA	533	A
56	BA	541	A
56	BA	547	A
56	BA	548	A
56	BA	549	C
56	BA	550	A
56	BA	551	A
56	BA	553	U
56	BA	554	U
56	BA	557	C
56	BA	560	A
56	BA	561	C
56	BA	562	A
56	BA	563	U
56	BA	570	A
56	BA	574	A
56	BA	576	U
56	BA	578	A
56	BA	579	U
56	BA	584	A
56	BA	586	C
56	BA	592	G
56	BA	595	C
56	BA	596	A
56	BA	618	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	BA	625	A
56	BA	626	G
56	BA	631	A
56	BA	633	U
56	BA	634	G
56	BA	640	A
56	BA	648	C
56	BA	649	A
56	BA	654	G
56	BA	660	C
56	BA	665	C
56	BA	673	C
56	BA	674	U
56	BA	675	U
56	BA	683	U
56	BA	684	A
56	BA	689	A
56	BA	694	A
56	BA	695	U
56	BA	697	C
56	BA	704	U
56	BA	707	A
56	BA	713	A
56	BA	719	C
56	BA	720	C
56	BA	722	A
56	BA	723	A
56	BA	724	A
56	BA	725	C
56	BA	727	A
56	BA	728	C
56	BA	737	G
56	BA	744	A
56	BA	745	A
56	BA	746	U
56	BA	747	U
56	BA	748	A
56	BA	763	C
56	BA	764	A
56	BA	774	A
56	BA	777	A
56	BA	778	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	BA	780	G
56	BA	782	A
56	BA	783	A
56	BA	784	G
56	BA	814	C
56	BA	819	A
56	BA	825	C
56	BA	835	A
56	BA	847	U
56	BA	848	C
56	BA	852	C
56	BA	854	U
56	BA	855	U
56	BA	856	A
56	BA	859	A
56	BA	864	U
56	BA	872	A
56	BA	878	G
56	BA	883	G
56	BA	889	C
56	BA	892	G
56	BA	894	U
56	BA	895	U
56	BA	896	A
56	BA	897	A
56	BA	899	G
56	BA	900	G
56	BA	902	C
56	BA	909	U
56	BA	910	U
56	BA	922	A
56	BA	923	A
56	BA	924	G
56	BA	925	G
56	BA	926	U
56	BA	931	U
56	BA	933	A
56	BA	935	C
56	BA	938	U
56	BA	939	U
56	BA	947	A
56	BA	948	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	BA	950	U
56	BA	958	U
56	BA	959	G
56	BA	960	U
56	BA	962	U
56	BA	964	A
56	BA	965	A
56	BA	967	G
56	BA	970	C
56	BA	977	G
56	BA	983	U
56	BA	986	U
56	BA	987	G
56	BA	992	U
56	BA	1015	C
56	BA	1016	C
56	BA	1018	U
56	BA	1025	A
56	BA	1026	A
56	BA	1027	G
56	BA	1028	A
56	BA	1038	A
56	BA	1041	A
56	BA	1045	U
56	BA	1050	C
56	BA	1055	A
56	BA	1056	G
56	BA	1057	A
56	BA	1063	U
56	BA	1064	G
56	BA	1071	U
56	BA	1072	A
56	BA	1074	U
56	BA	1075	U
56	BA	1081	U
56	BA	1089	G
56	BA	1091	U
56	BA	1092	A
56	BA	1093	A
56	BA	1127	A
56	BA	1129	C
56	BA	1138	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	BA	1140	A
56	BA	1146	G
56	BA	1167	C
56	BA	1168	A
56	BA	1169	A
56	BA	1180	G
56	BA	1183	U
56	BA	1194	U
56	BA	1195	A
56	BA	1204	A
56	BA	1206	U
56	BA	1207	C
56	BA	1217	A
56	BA	1218	U
56	BA	1219	A
56	BA	1220	A
56	BA	1221	C
56	BA	1222	A
56	BA	1226	C
56	BA	1231	U
56	BA	1233	A
56	BA	1237	A
56	BA	1238	A
56	BA	1239	A
56	BA	1240	A
56	BA	1241	U
56	BA	1242	U
56	BA	1246	A
56	BA	1247	U
56	BA	1249	A
56	BA	1252	G
56	BA	1253	G
56	BA	1254	A
56	BA	1258	A
56	BA	1264	C
56	BA	1270	G
56	BA	1271	A
56	BA	1287	G
56	BA	1288	U
56	BA	1291	U
56	BA	1294	A
56	BA	1298	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	BA	1299	C
56	BA	1314	U
56	BA	1321	C
56	BA	1323	U
56	BA	1325	G
56	BA	1326	A
56	BA	1328	G
56	BA	1332	G
56	BA	1336	A
56	BA	1341	A
56	BA	1342	C
56	BA	1352	G
56	BA	1357	C
56	BA	1358	G
56	BA	1385	U
56	BA	1386	U
56	BA	1387	A
56	BA	1388	A
56	BA	1389	A
56	BA	1390	G
56	BA	1395	A
56	BA	1396	C
56	BA	1405	A
56	BA	1407	U
56	BA	1409	C
56	BA	1420	A
56	BA	1425	A
56	BA	1426	G
56	BA	1429	C
56	BA	1432	U
56	BA	1433	U
56	BA	1436	U
56	BA	1438	U
56	BA	1445	U
56	BA	1448	A
56	BA	1451	U
56	BA	1455	C
56	BA	1457	A
56	BA	1464	A
56	BA	1468	A
56	BA	1473	A
56	BA	1474	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	BA	1475	A
56	BA	1476	A
56	BA	1493	A
56	BA	1494	A
56	BA	1498	C
56	BA	1504	A
56	BA	1505	G
56	BA	1509	U
56	BA	1514	A
56	BA	1518	A
56	BA	1521	U
56	BA	1522	A
56	BA	1526	U
56	BA	1527	U
56	BA	1528	A
56	BA	1529	A
56	BA	1531	C
56	BA	1532	U
56	BA	1533	A
56	BA	1536	U
56	BA	1548	A
56	BA	1549	A
56	BA	1551	C
56	BA	1552	C
56	BA	1553	A
56	BA	1558	U
56	BA	1559	A
56	BA	1569	A
56	BA	1571	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	AA	535	U
52	AA	824	G
52	AA	918	A
56	BA	48	U
56	BA	1241	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 338 ligands modelled in this entry, 333 are monoatomic - leaving 5 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
93	GTP	Ag	500	89	26,34,34	1.10	2 (7%)	32,54,54	1.61	7 (21%)
92	5GP	BA	1792	89	22,26,26	1.24	2 (9%)	26,40,40	1.24	4 (15%)
91	SPM	BA	1793	-	13,13,13	0.35	0	12,12,12	0.77	0
91	SPM	BA	1794	-	13,13,13	0.34	0	12,12,12	0.79	0
91	SPM	AA	3001	-	13,13,13	0.34	0	12,12,12	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
93	GTP	Ag	500	89	-	3/18/38/38	0/3/3/3
92	5GP	BA	1792	89	-	0/6/26/26	0/3/3/3
91	SPM	BA	1793	-	-	2/11/11/11	-
91	SPM	BA	1794	-	-	3/11/11/11	-
91	SPM	AA	3001	-	-	2/11/11/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
92	BA	1792	5GP	C5-C6	-4.12	1.39	1.47
93	Ag	500	GTP	C5-C6	-3.92	1.39	1.47
92	BA	1792	5GP	C6-N1	-2.51	1.34	1.37
93	Ag	500	GTP	C2-N3	2.17	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
93	Ag	500	GTP	PA-O3A-PB	-3.92	119.36	132.83
93	Ag	500	GTP	PB-O3B-PG	-3.36	121.31	132.83
93	Ag	500	GTP	C5-C6-N1	3.27	119.72	113.95
93	Ag	500	GTP	C3'-C2'-C1'	3.25	105.86	100.98
92	BA	1792	5GP	C5-C6-N1	3.08	119.38	113.95
93	Ag	500	GTP	C8-N7-C5	2.96	108.63	102.99
93	Ag	500	GTP	C2-N1-C6	-2.92	119.72	125.10
92	BA	1792	5GP	C8-N7-C5	2.33	107.44	102.99
92	BA	1792	5GP	C2-N1-C6	-2.30	120.86	125.10
93	Ag	500	GTP	O6-C6-C5	-2.14	120.20	124.37
92	BA	1792	5GP	O6-C6-C5	-2.07	120.32	124.37

There are no chirality outliers.

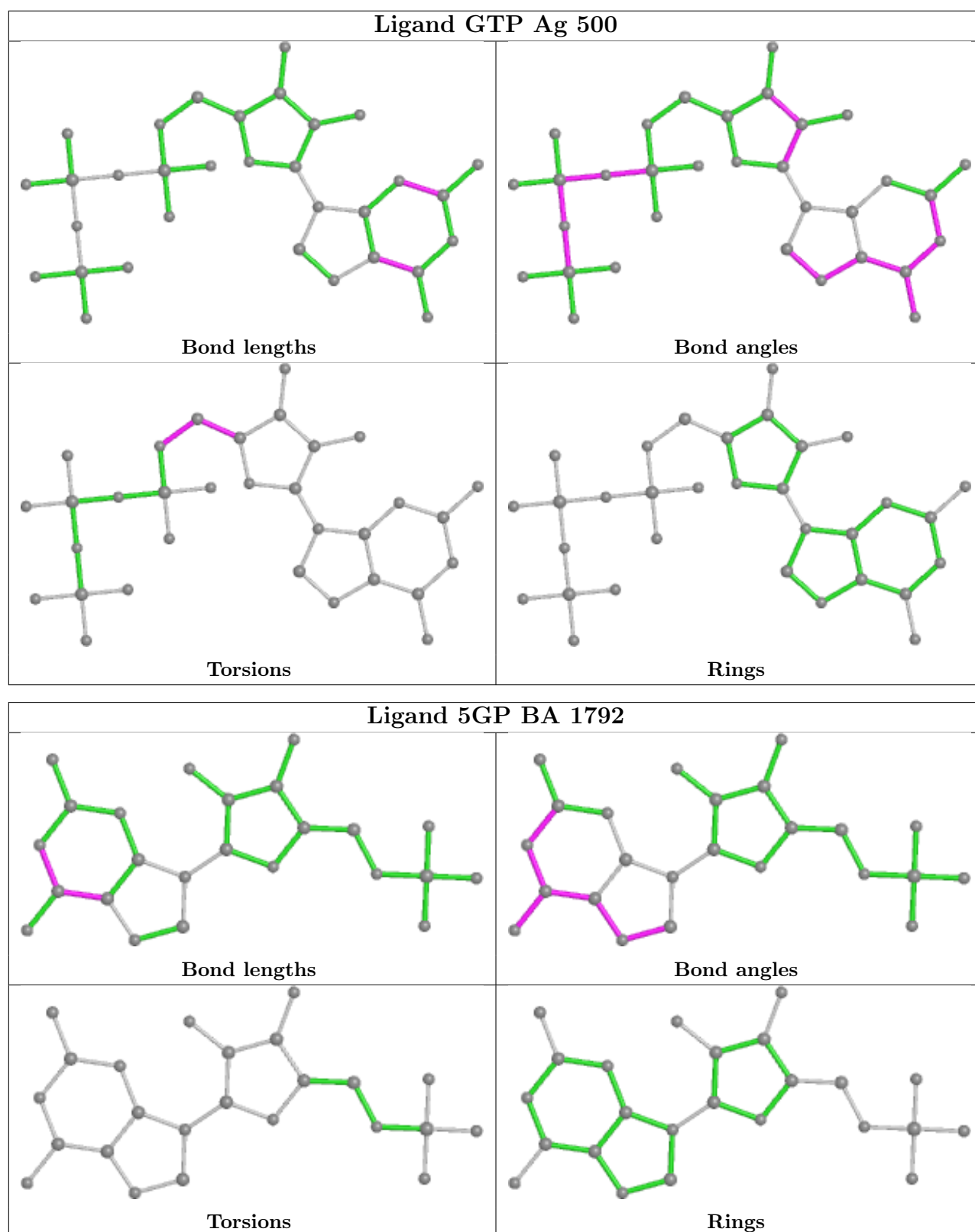
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
91	BA	1794	SPM	N5-C6-C7-C8
91	AA	3001	SPM	C8-C9-N10-C11
91	BA	1794	SPM	C8-C9-N10-C11
91	BA	1793	SPM	C6-C7-C8-C9
91	BA	1794	SPM	C6-C7-C8-C9
91	BA	1793	SPM	C7-C8-C9-N10
91	AA	3001	SPM	C6-C7-C8-C9
93	Ag	500	GTP	C4'-C5'-O5'-PA
93	Ag	500	GTP	O4'-C4'-C5'-O5'
93	Ag	500	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
86	Ao	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ao	234:UNK	C	240:THR	N	7.63

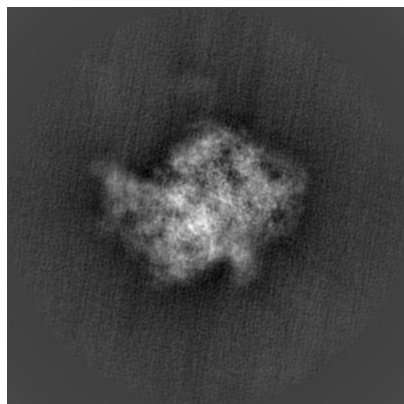
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12568. These allow visual inspection of the internal detail of the map and identification of artifacts.

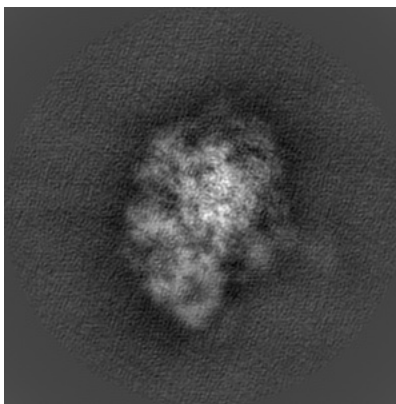
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

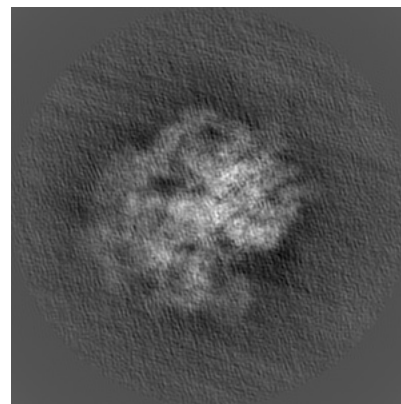
6.1.1 Primary map



X

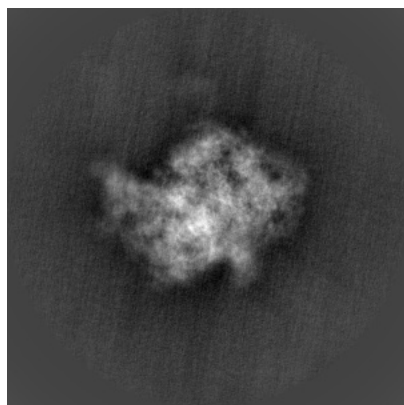


Y

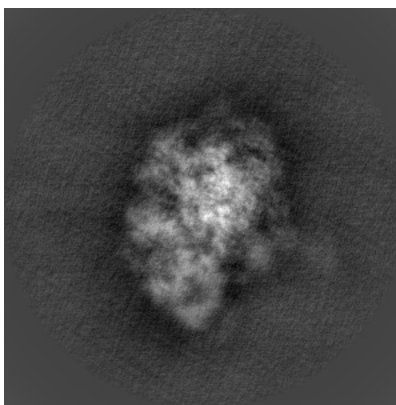


Z

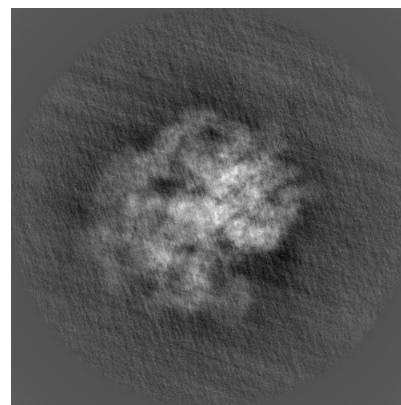
6.1.2 Raw map



X



Y

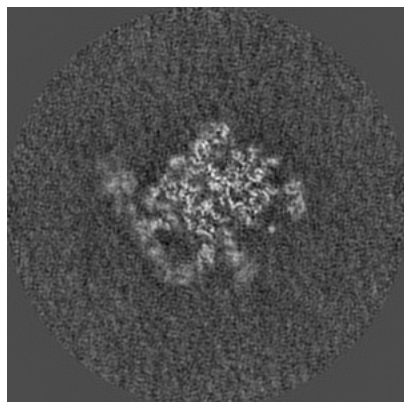


Z

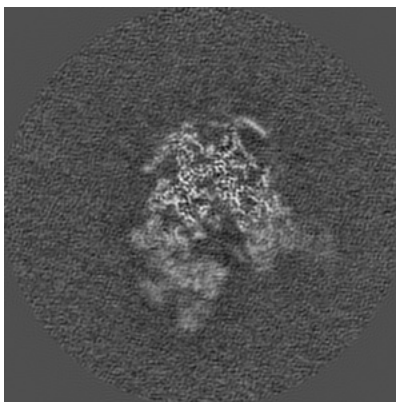
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

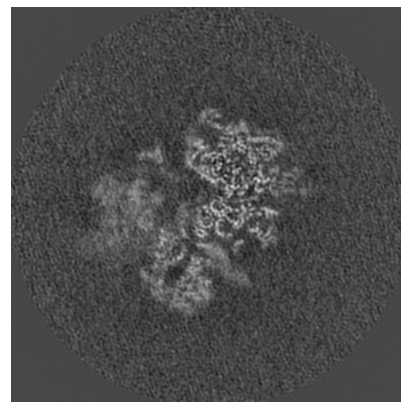
6.2.1 Primary map



X Index: 240

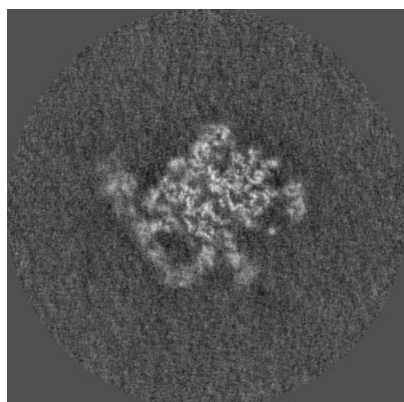


Y Index: 240

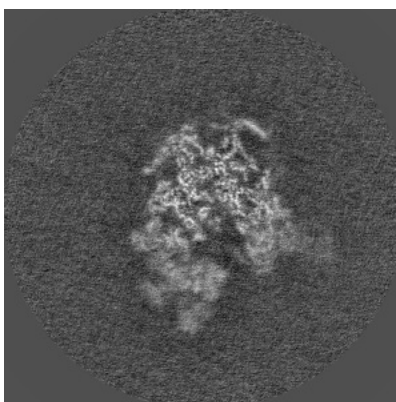


Z Index: 240

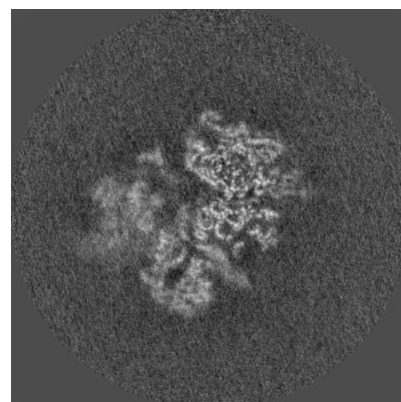
6.2.2 Raw map



X Index: 240



Y Index: 240

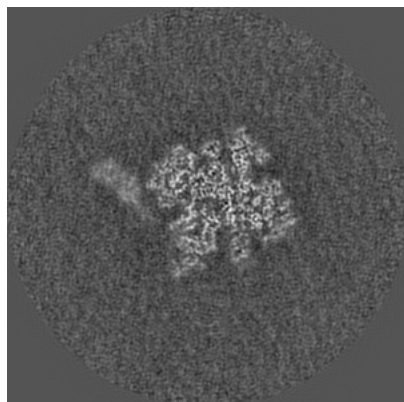


Z Index: 240

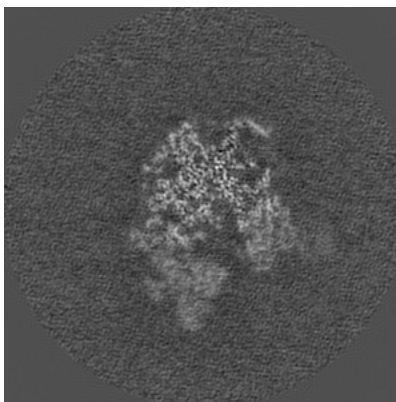
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

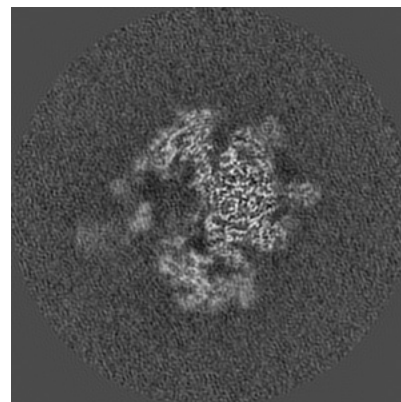
6.3.1 Primary map



X Index: 268

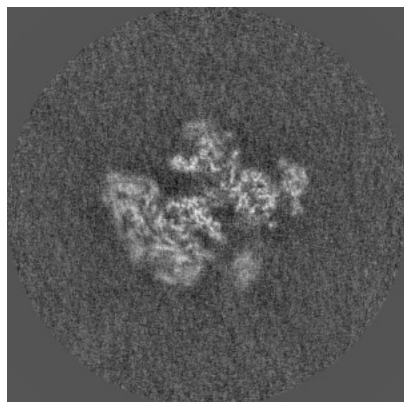


Y Index: 238

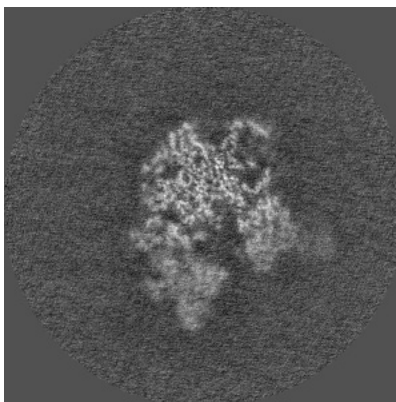


Z Index: 262

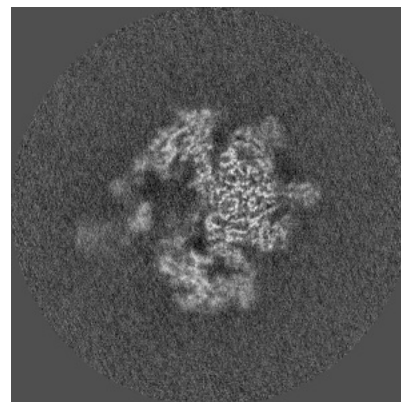
6.3.2 Raw map



X Index: 228



Y Index: 237

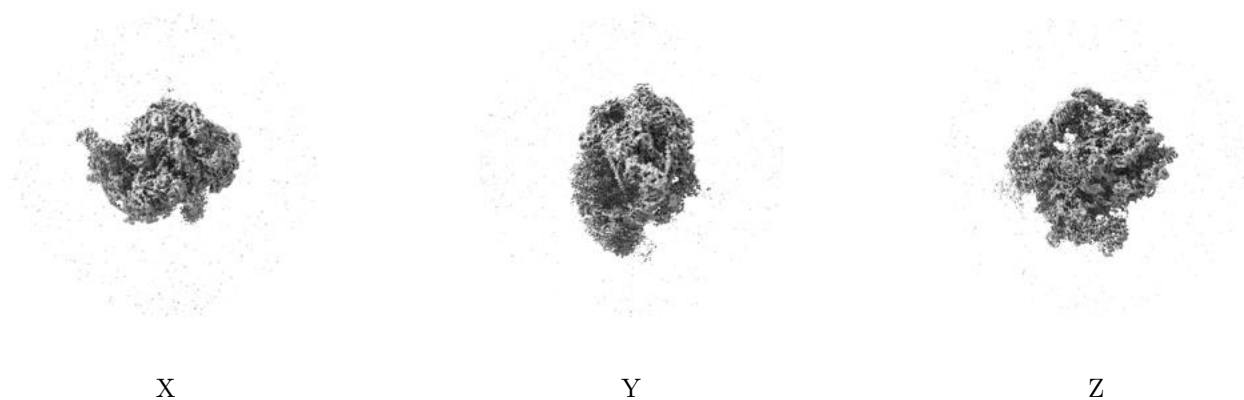


Z Index: 262

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

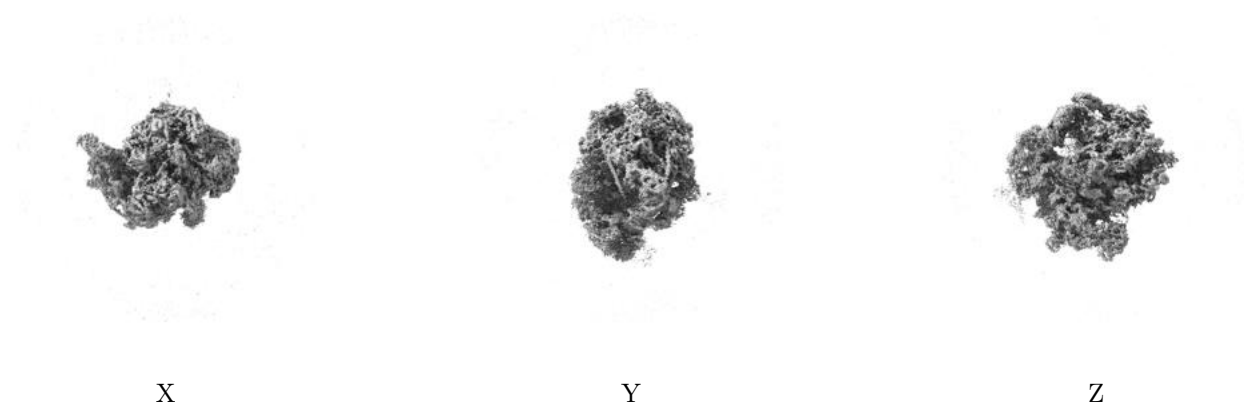
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

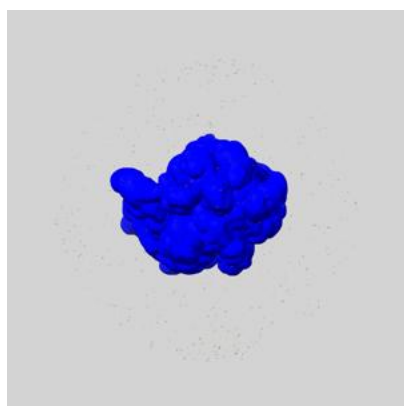
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

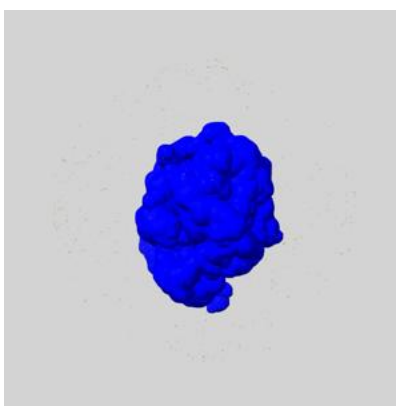
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

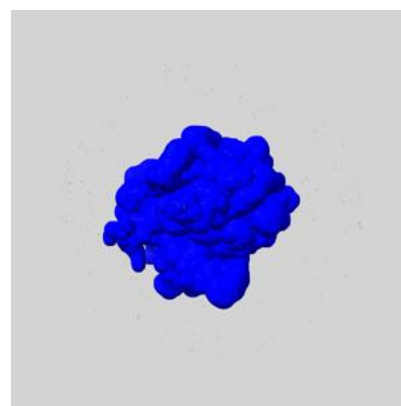
6.5.1 emd_12568_msk_1.map [i](#)



X



Y

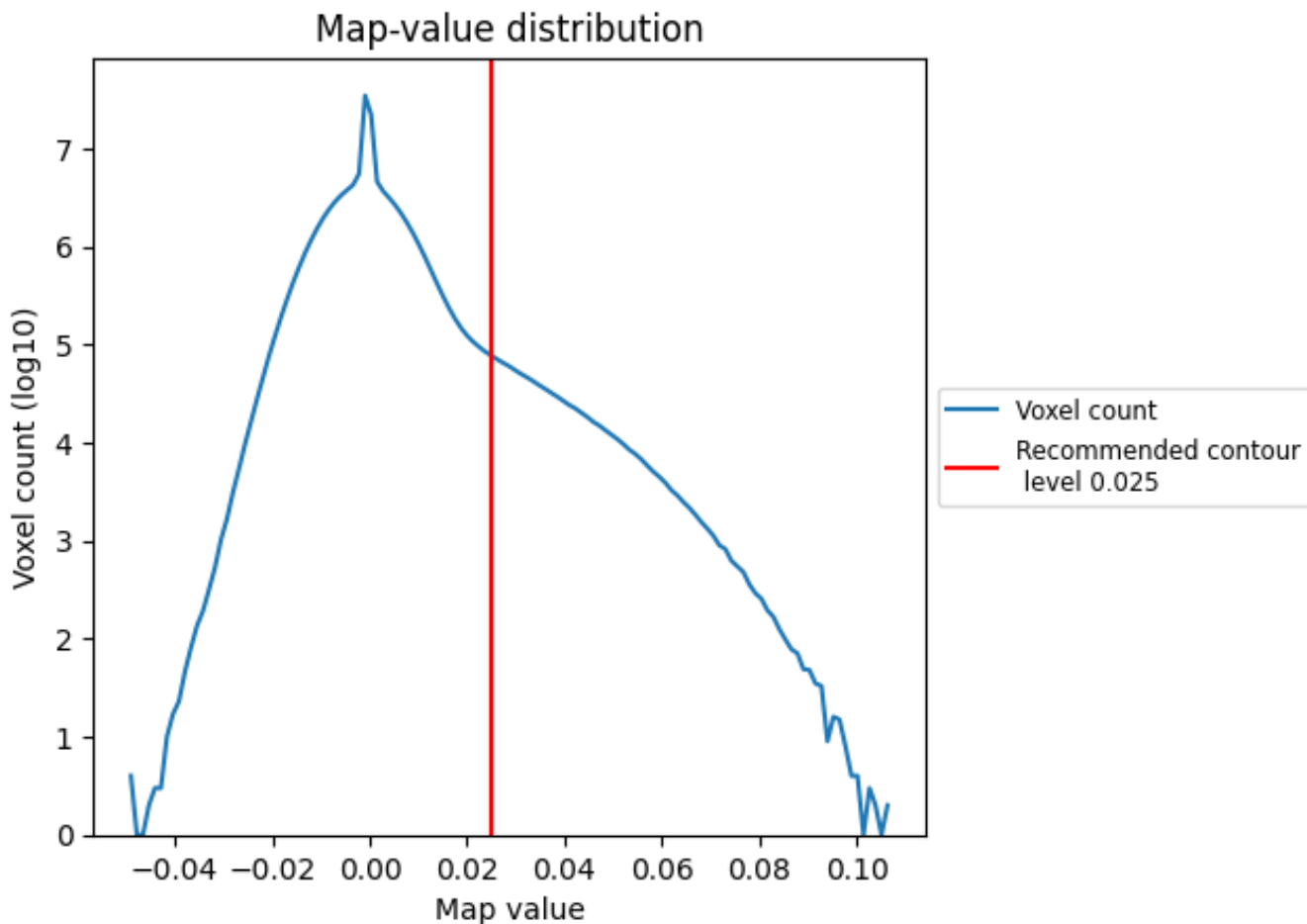


Z

7 Map analysis [i](#)

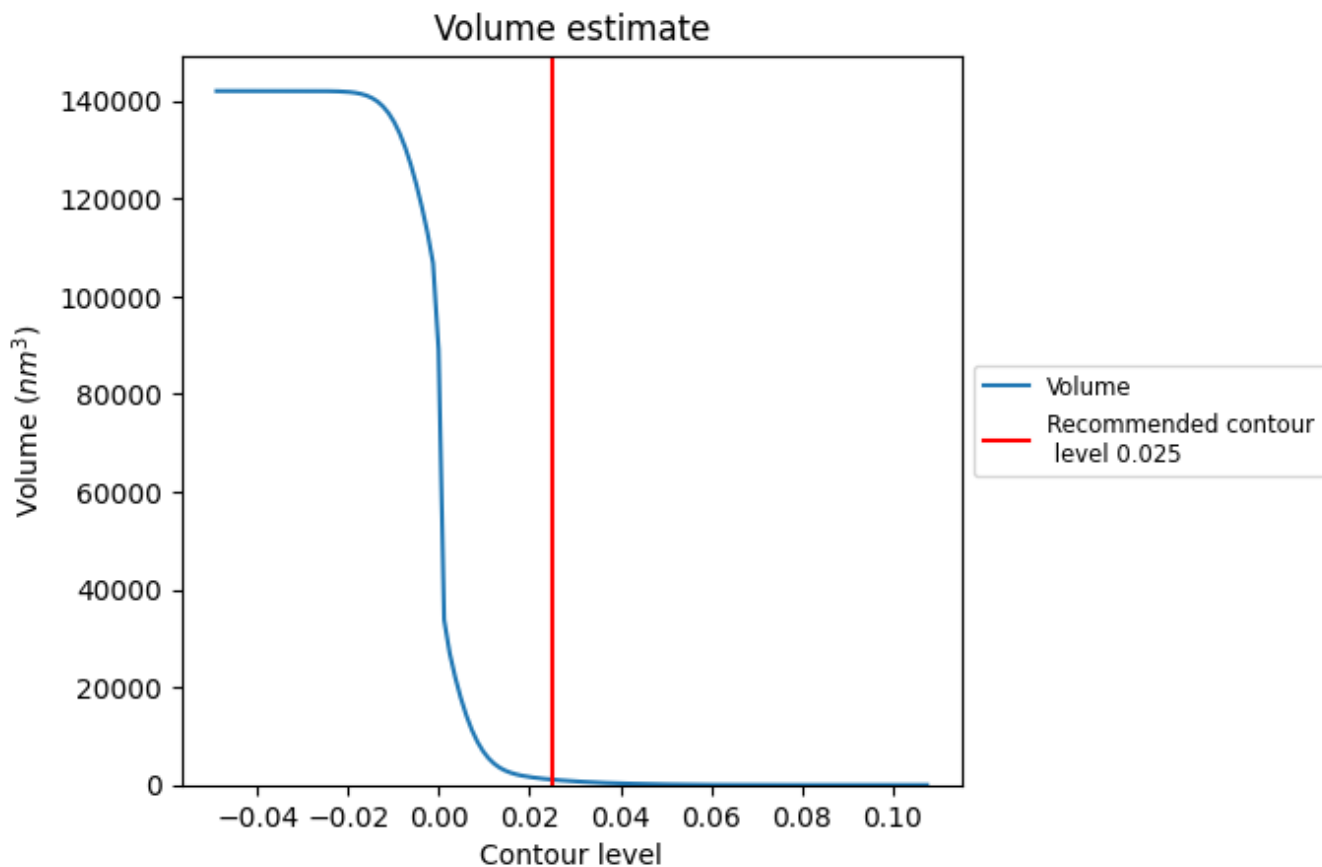
This section contains the results of statistical analysis of the map.

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.

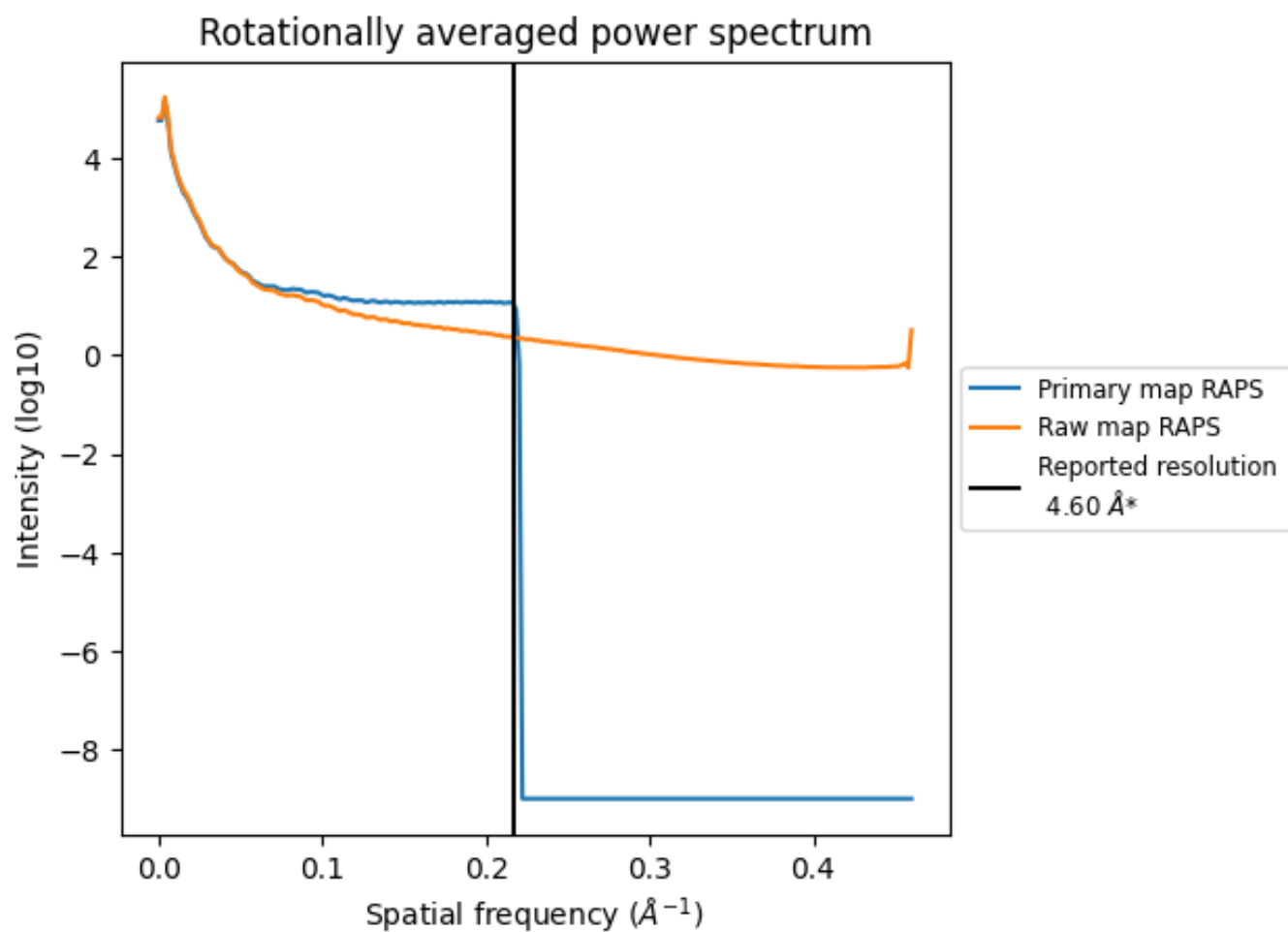
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1096 nm^3 ; this corresponds to an approximate mass of 990 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

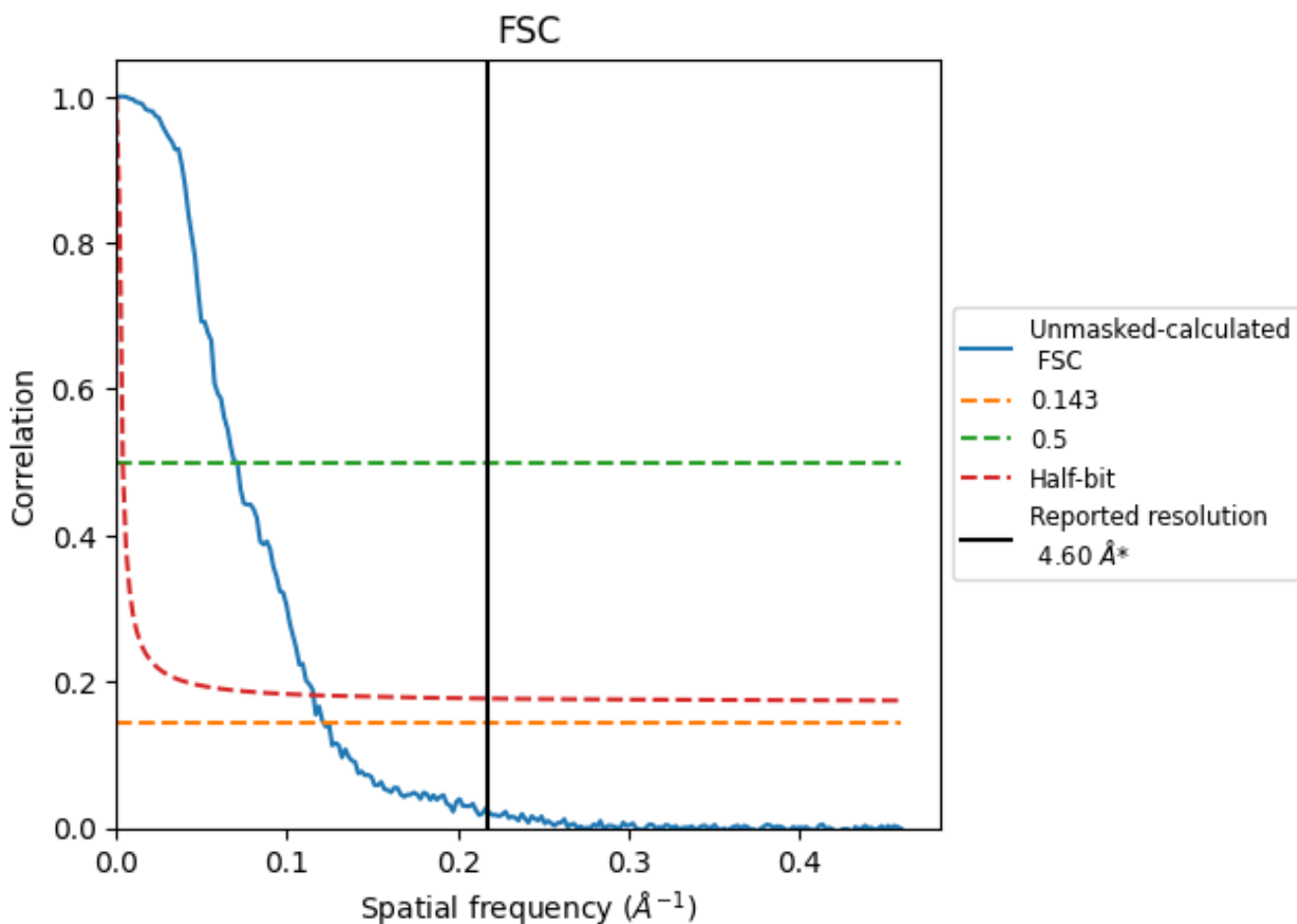


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

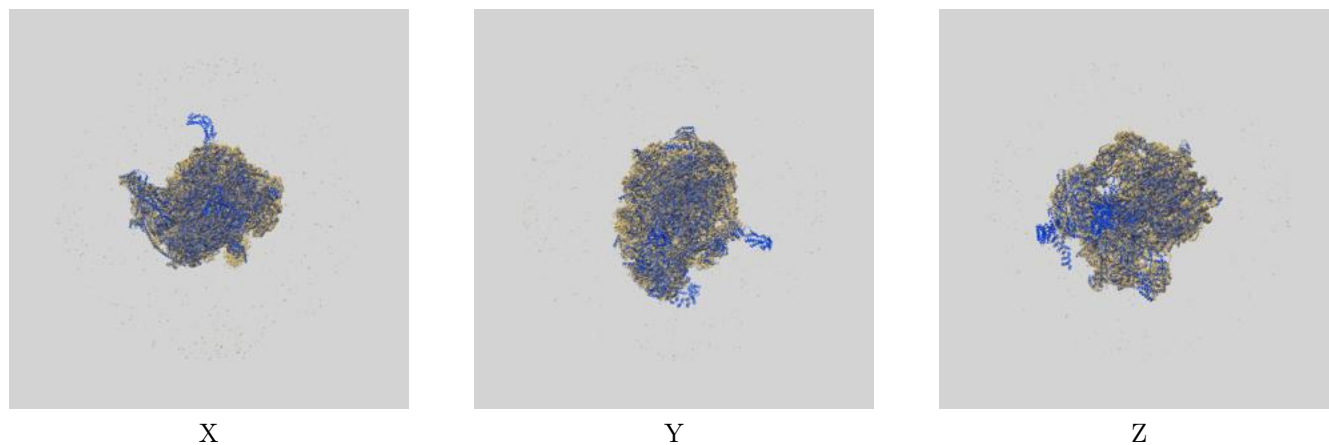
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.23	14.27	8.67

*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 8.23 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

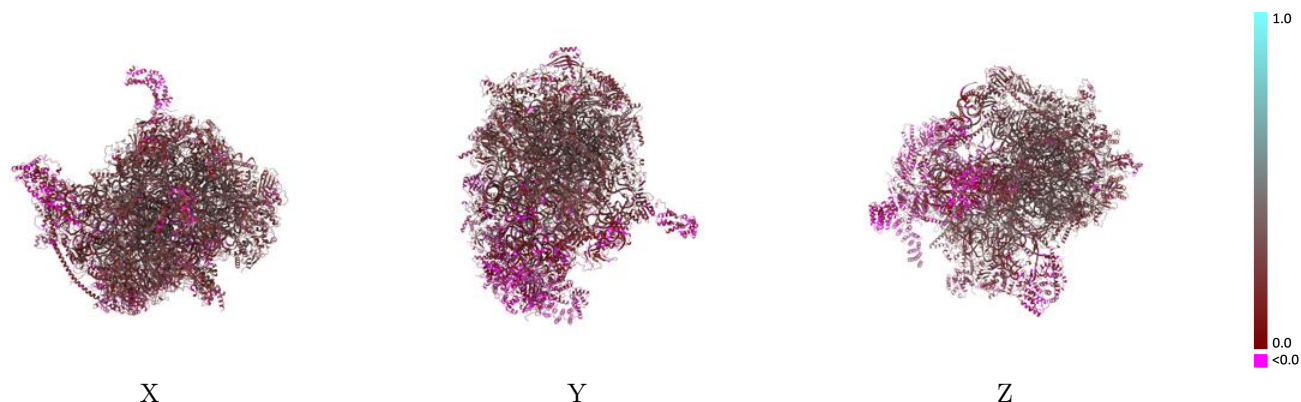
This section contains information regarding the fit between EMDB map EMD-12568 and PDB model 7NSI. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)



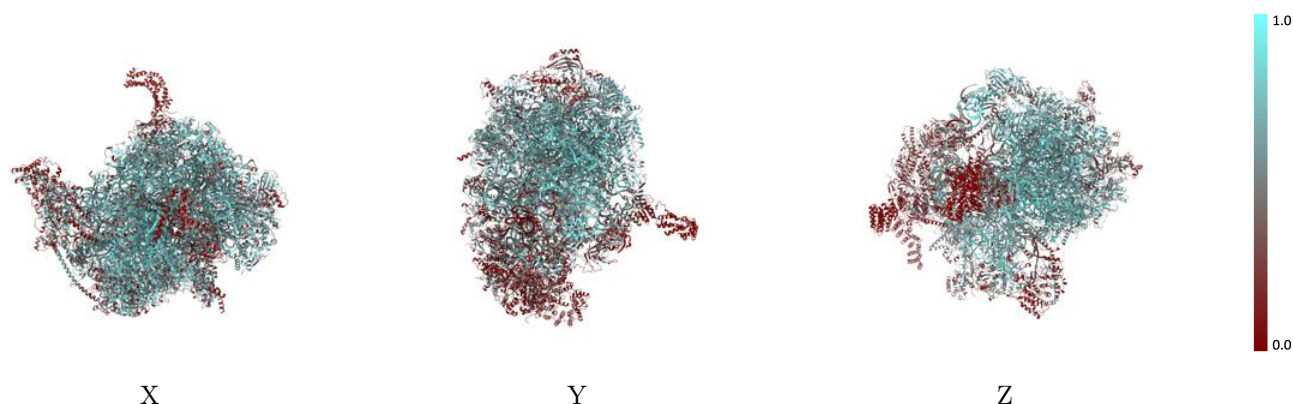
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



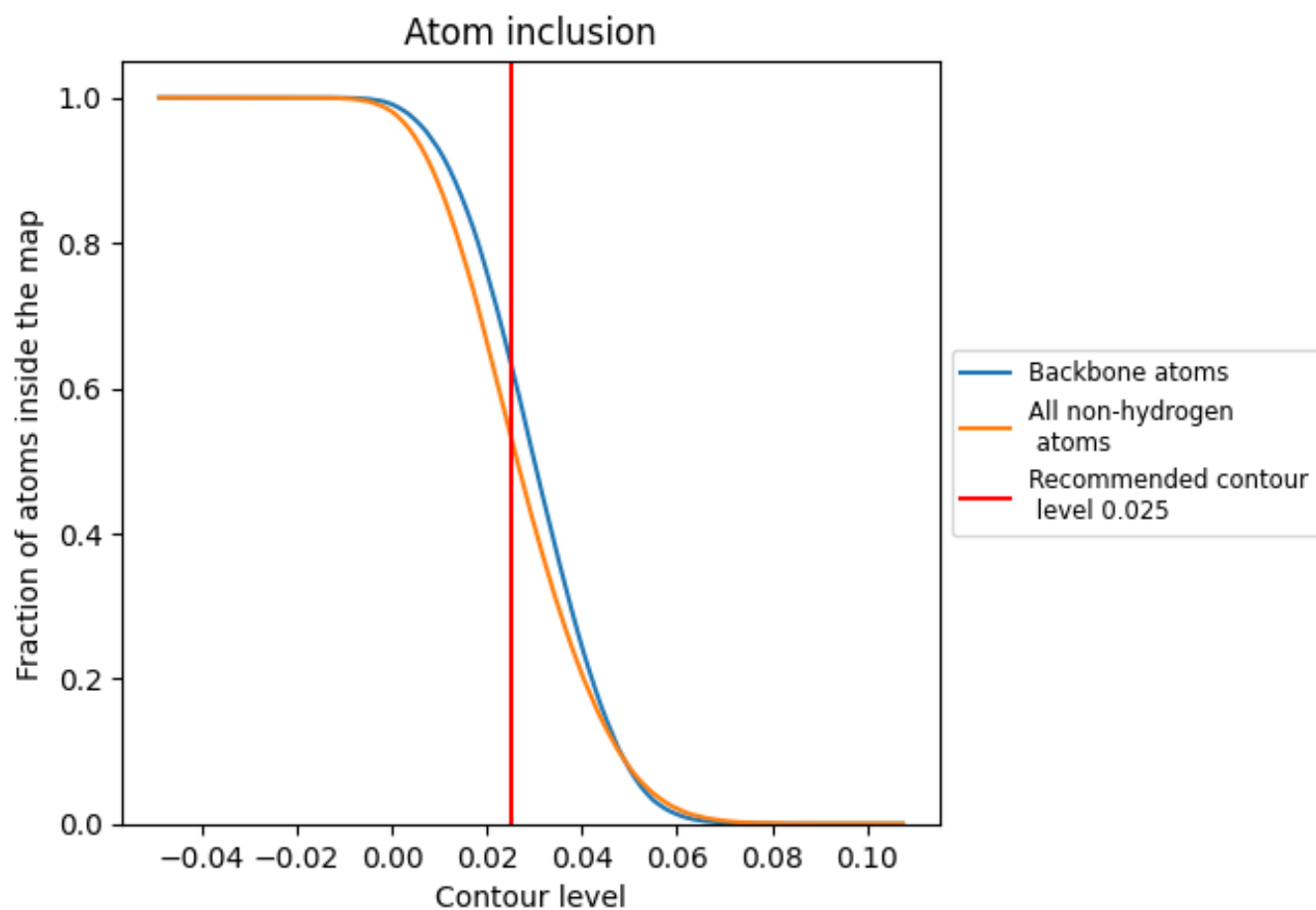
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 53% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5337	0.2280
AA	0.6892	0.2170
AB	0.5253	0.2150
AC	0.1830	0.0880
AE	0.3340	0.1870
AF	0.3365	0.1520
AG	0.1938	0.0770
AI	0.3062	0.1310
AJ	0.1530	0.0960
AK	0.3259	0.1580
AL	0.5043	0.2670
AN	0.2896	0.0890
AO	0.3609	0.1490
AP	0.3993	0.1650
AQ	0.5058	0.2070
AR	0.4075	0.1650
AU	0.4599	0.2290
AV	0.0507	0.0580
AX	0.2574	0.1710
AZ	0.2000	0.0460
Aa	0.3466	0.1680
Ab	0.4286	0.1700
Ac	0.4959	0.2360
Ad	0.4523	0.1500
Ae	0.2285	0.0670
Af	0.3914	0.1710
Ag	0.2107	0.0390
Ah	0.1470	0.0680
Ai	0.1952	0.0780
Aj	0.2813	0.1280
Ak	0.1717	0.0830
Am	0.2306	0.1380
An	0.4164	0.2230
Ao	0.0283	0.0320
Ap	0.4141	0.1650





































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
B0	 0.6790	 0.3260
B1	 0.5263	 0.2690
B2	 0.6333	 0.2840
B3	 0.6337	 0.3080
B4	 0.3495	 0.1400
B5	 0.6051	 0.3010
B6	 0.4423	 0.2420
B7	 0.6396	 0.3080
B8	 0.6198	 0.3330
B9	 0.6604	 0.2820
BA	 0.8145	 0.3280
BB	 0.6639	 0.1730
BD	 0.6245	 0.2940
BE	 0.6579	 0.3080
BF	 0.6027	 0.3000
BG	 0.1479	 0.2050
BI	 0.4647	 0.2480
BJ	 0.2340	 0.1720
BK	 0.1282	 0.1290
BN	 0.6506	 0.3100
BO	 0.6161	 0.3250
BP	 0.6081	 0.3050
BQ	 0.6151	 0.3010
BR	 0.6367	 0.3100
BS	 0.6536	 0.2770
BT	 0.5809	 0.2740
BU	 0.6341	 0.2990
BV	 0.6294	 0.3150
BW	 0.5914	 0.3220
BX	 0.5567	 0.2900
BY	 0.3044	 0.2500
Ba	 0.6316	 0.2600
Bb	 0.6533	 0.2620
Bc	 0.5881	 0.2640
Bd	 0.3452	 0.1410
Be	 0.4979	 0.2550
Bf	 0.5560	 0.2740
Bg	 0.6360	 0.3140
Bh	 0.6061	 0.2640
Bi	 0.2919	 0.1930
Bj	 0.3546	 0.1100
Bk	 0.3358	 0.1580

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Bl	 0.6258	 0.2970
Bm	 0.2144	 0.2230
Bn	 0.6030	 0.3070
Bo	 0.6471	 0.2850
Bp	 0.2735	 0.1740
Bq	 0.2071	 0.1870
Bt	 0.6711	 0.3010
Bu	 0.4749	 0.2240
Bv	 0.5023	 0.2260
Bw	 0.6088	 0.2720
Bx	 0.6022	 0.2640
CL	 0.0222	 0.1070
DL	 0.0047	 0.0340
EL	 0.0000	 -0.0180
FL	 0.0000	 -0.0030
GL	 0.0000	 0.0180
HL	 0.0000	 -0.0550