



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 03:36 AM EDT

PDB ID : 9PS0 / pdb_00009ps0
EMDB ID : EMD-71818
Title : In situ structure of the human mitoribosome in the A/P-P/E state from TACO1-knockout cells
Authors : Wang, S.; Xiong, Y.; Zhang, Y.
Deposited on : 2025-07-24
Resolution : 3.29 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

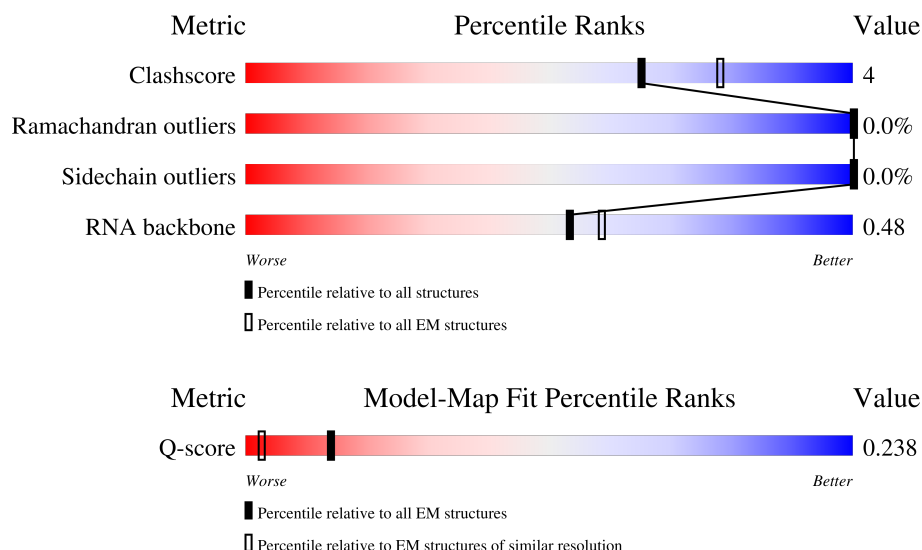
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.29 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14466 (2.79 - 3.79)

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	0	188	
2	1	65	
3	2	92	

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Mol	Chain	Length	Quality of chain
4	3	188	
5	4	103	
6	5	423	
7	6	380	
8	7	338	
9	8	206	
10	9	137	
11	A	1558	
12	A0	217	
13	A1	323	
14	A2	118	
15	A3	199	
16	A4	689	
17	AA	954	
18	AB	296	
19	AC	167	
20	AD	430	
21	AE	125	
22	AF	242	
23	AG	396	
24	AH	201	
25	AI	194	
26	AJ	138	
27	AK	128	
28	AL	257	

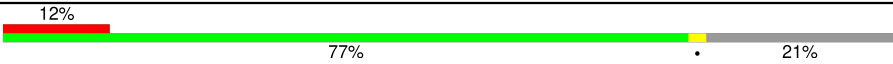
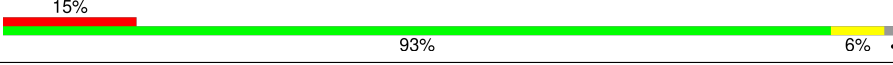
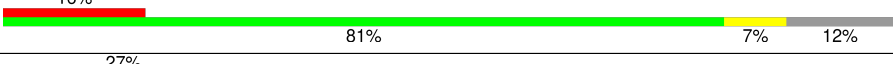
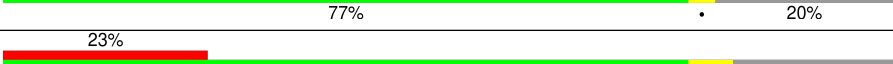
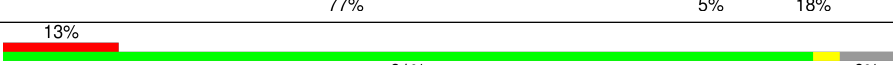
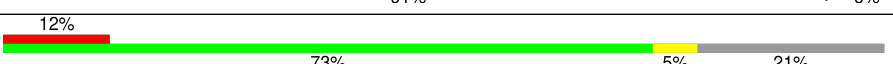
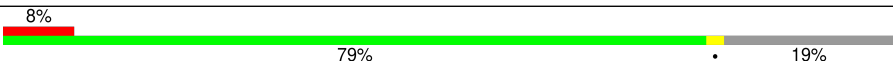
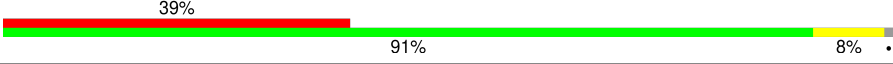
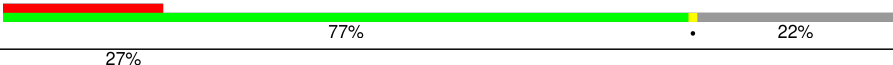
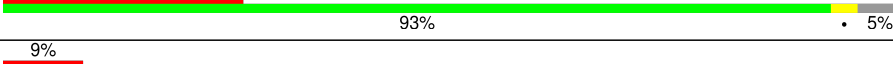
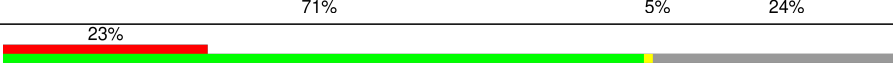
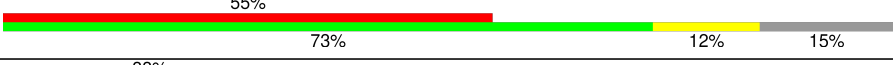
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Mol	Chain	Length	Quality of chain
29	AM	137	
30	AN	130	
31	AO	258	
32	AP	142	
33	AQ	87	
34	AR	360	
35	AS	190	
36	AT	173	
37	AU	205	
38	AV	414	
39	AW	187	
40	AX	398	
41	AY	395	
42	AZ	106	
43	Aw	76	
44	Ax	76	
45	Az	34	
46	B	72	
47	D	305	
48	E	348	
49	F	311	
50	H	267	
51	I	261	
52	J	192	
53	K	178	

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Mol	Chain	Length	Quality of chain
54	L	145	
55	M	296	
56	N	251	
57	O	175	
58	OX	435	
59	P	180	
60	Q	292	
61	R	149	
62	S	205	
63	T	206	
64	U	153	
65	V	216	
66	W	148	
67	X	256	
68	Y	250	
69	Z	161	
70	a	142	
71	b	215	
72	c	332	
73	d	306	
74	e	279	
75	f	212	
76	g	166	
77	h	158	
78	i	128	

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Mol	Chain	Length	Quality of chain
79	j	123	
80	k	112	
81	l	138	
82	m	128	
83	n	43	
84	o	102	
85	p	206	
86	q	222	
87	r	196	
88	s	439	
89	t	198	
89	u	198	
90	z	325	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
101	VAL	B	101	-	-	X	-

2 Entry composition

There are 101 unique types of molecules in this entry. The entry contains 179893 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 L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	110	Total	C	N	O	S	0	0
			898	554	176	162	6		

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	56	Total	C	N	O	S	0	0
			464	296	89	77	2		

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	233	83	60	1		

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	95	Total	C	N	O	S	0	0
			832	539	162	128	3		

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	354	Total	C	N	O	S	0	0
			2948	1881	525	533	9		

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	294	Total	C	N	O	S	0	0
			2390	1529	405	438	18		

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	157	Total	C	N	O	S	0	0
			1327	844	235	246	2		

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 11 is a RNA chain called 16S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1558	Total	C	N	O	P	0	0
			33070	14843	5963	10706	1558		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	A	deletion	GB 2756414513
A	?	-	C	deletion	GB 2756414513
A	?	-	U	deletion	GB 2756414513

- Molecule 12 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A0	215	Total	C	N	O	S	0	0
			1787	1130	339	313	5		

- Molecule 13 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A1	279	Total	C	N	O	S	0	0
			2265	1435	387	432	11		

- Molecule 14 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A2	118	Total	C	N	O	S	0	0
			935	579	182	166	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1	ACE	-	acetylation	UNP Q96BP2

- Molecule 15 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A3	70	Total	C	N	O	S	0	0
			625	401	134	89	1		

- Molecule 16 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A4	588	Total	C	N	O	S	0	0
			4768	3053	808	879	28		

- Molecule 17 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AA	954	Total	C	N	O	P	0	0
			20260	9088	3647	6571	954		

- Molecule 18 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AB	225	Total	C	N	O	S	0	0
			1828	1164	331	323	10		

- Molecule 19 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AC	132	Total	C	N	O	S	0	0
			1083	699	195	185	4		

- Molecule 20 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AD	343	Total	C	N	O	S	0	0
			2731	1713	518	487	13		

- Molecule 21 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AE	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 22 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AF	208	Total	C	N	O	S	0	0
			1725	1104	312	298	11		

- Molecule 23 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AG	327	Total	C	N	O	S	0	0
			2688	1710	477	487	14		

- Molecule 24 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AH	140	Total	C	N	O	S	0	0
			1152	745	194	210	3		

- Molecule 25 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AI	137	Total	C	N	O	S	0	0
			1019	641	193	181	4		

- Molecule 26 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AJ	108	Total	C	N	O	S	0	0
			839	521	169	143	6		

- Molecule 27 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AK	101	Total	C	N	O	S	0	0
			862	537	179	141	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AL	174	Total	C	N	O	S	0	0
			1453	925	270	251	7		

- Molecule 29 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AM	119	Total	C	N	O	S	0	0
			942	594	185	157	6		

- Molecule 30 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AN	110	Total	C	N	O	S	0	0
			868	562	156	147	3		

- Molecule 31 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AO	193	Total	C	N	O	S	0	0
			1592	1014	294	277	7		

- Molecule 32 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AP	97	Total	C	N	O	S	0	0
			781	501	134	138	8		

- Molecule 33 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AQ	87	Total	C	N	O	S	0	0
			744	460	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	1	ACE	-	acetylation	UNP P82921
AQ	50	ARG	CYS	variant	UNP P82921

- Molecule 34 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AR	295	Total	C	N	O	S	0	0
			2409	1533	413	455	8		

- Molecule 35 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AS	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

- Molecule 36 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AT	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

- Molecule 37 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AU	176	Total	C	N	O	S	0	0
			1488	916	301	267	4		

- Molecule 38 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	AV	362	Total	C	N	O	S	0	0
			2969	1904	495	558	12		

- Molecule 39 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AW	100	Total	C	N	O	S	0	0
			789	498	141	146	4		

- Molecule 40 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AX	352	Total	C	N	O	S	0	0
			2849	1822	499	517	11		

- Molecule 41 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AY	119	Total	C	N	O	S	0	0
			1010	654	166	188	2		

- Molecule 42 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AZ	100	Total	C	N	O	S	0	0
			839	534	153	148	4		

- Molecule 43 is a RNA chain called A/P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Aw	68	Total	C	N	O	P	0	0
			1434	646	248	472	68		

- Molecule 44 is a RNA chain called P/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ax	70	Total	C	N	O	P	0	0
			1482	665	260	487	70		

- Molecule 45 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Az	34	Total	C	N	O	P	0	0
			719	324	123	238	34		

- Molecule 46 is a RNA chain called mitochondrial tRNA^{Val}.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	B	72	Total	C	N	O	P	0	0
			1524	685	269	498	72		

- Molecule 47 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	D	238	Total	C	N	O	S	0	0
			1859	1157	376	317	9		

- Molecule 48 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	E	305	Total	C	N	O	S	0	0
			2406	1545	418	432	11		

- Molecule 49 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	F	252	Total	C	N	O	S	0	0
			2031	1305	370	350	6		

- Molecule 50 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	H	202	Total	C	N	O	S	0	0
			1661	1067	304	286	4		

- Molecule 51 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	I	181	Total	C	N	O	S	0	0
			1446	932	260	244	10		

- Molecule 52 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 53 is a protein called Large ribosomal subunit protein uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	K	178	Total	C	N	O	S	0	0
			1455	936	259	253	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ACE	-	acetylation	UNP H2QWN0
K	132	TYR	ASP	conflict	UNP H2QWN0

- Molecule 54 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	L	115	Total	C	N	O	S	0	0
			890	559	171	155	5		

- Molecule 55 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	M	291	Total	C	N	O	S	0	0
			2327	1483	430	408	6		

- Molecule 56 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	N	222	Total	C	N	O	S	0	0
			1786	1143	326	307	10		

- Molecule 57 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	O	154	Total	C	N	O	S	0	0
			1259	792	241	219	7		

- Molecule 58 is a protein called Mitochondrial inner membrane protein OXA1L.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	OX	55	Total	C	N	O	S	0	0
			468	292	93	81	2		

- Molecule 59 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	P	144	Total	C	N	O	S	0	0
			1173	733	224	211	5		

- Molecule 60 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Q	239	Total	C	N	O	S	0	0
			1990	1277	353	351	9		

- Molecule 61 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	R	140	Total	C	N	O	S	0	0
			1154	732	231	187	4		

- Molecule 62 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	S	161	Total	C	N	O	S	0	0
			1293	835	227	227	4		

- Molecule 63 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	T	166	Total	C	N	O	S	0	0
			1369	875	254	233	7		

- Molecule 64 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	U	152	Total	C	N	O	S	0	0
			1248	786	234	225	3		

- Molecule 65 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	V	205	Total	C	N	O	S	0	0
			1676	1068	298	302	8		

- Molecule 66 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	W	116	Total	C	N	O	S	0	0
			904	577	171	153	3		

- Molecule 67 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	X	244	Total	C	N	O	S	0	0
			2044	1322	352	365	5		

- Molecule 68 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Y	181	Total	C	N	O	S	0	0
			1556	995	298	259	4		

- Molecule 69 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Z	122	Total	C	N	O	S	0	0
			996	636	186	171	3		

- Molecule 70 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	a	103	Total	C	N	O	S	0	0
			865	543	155	162	5		

- Molecule 71 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	b	150	Total	C	N	O	S	0	0
			1193	742	231	217	3		

- Molecule 72 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	c	286	Total	C	N	O	S	0	0
			2299	1470	397	423	9		

- Molecule 73 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	d	259	Total	C	N	O	S	0	0
			2124	1357	369	384	14		

- Molecule 74 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	e	238	Total	C	N	O	S	0	0
			1931	1222	339	364	6		

- Molecule 75 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	f	157	Total	C	N	O	S	0	0
			1252	799	207	242	4		

- Molecule 76 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	g	134	Total	C	N	O	S	0	0
			1113	719	193	199	2		

- Molecule 77 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 78 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	i	97	Total	C	N	O	S	0	0
			828	532	165	127	4		

- Molecule 79 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	j	94	Total	C	N	O	S	0	0
			745	463	144	136	2		

- Molecule 80 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	k	102	Total	C	N	O	S	0	0
			774	479	148	142	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	1	ACE	-	acetylation	UNP Q96EL3

- Molecule 81 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	l	82	Total	C	N	O	S	0	0
			688	437	120	128	3		

- Molecule 82 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	m	92	Total	C	N	O	S	0	0
			791	488	159	142	2		

- Molecule 83 is a protein called Nascent polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	n	43	Total	C	N	O	0	0
			215	129	43	43		

- Molecule 84 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	o	94	Total	C	N	O	S	0	0
			798	501	165	129	3		

- Molecule 85 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	p	147	Total	C	N	O	S	0	0
			1205	748	228	225	4		

- Molecule 86 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	q	177	Total	C	N	O	S	0	0
			1495	929	292	269	5		

- Molecule 87 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	r	162	Total	C	N	O	S	0	0
			1322	839	252	223	8		

- Molecule 88 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	s	385	Total	C	N	O	S	0	0
			3148	2018	558	558	14		

- Molecule 89 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
89	t	46	Total	C	N	O	0	0
			354	228	56	70		
89	u	32	Total	C	N	O	0	0
			257	168	40	49		

- Molecule 90 is a protein called Large ribosomal subunit protein uL1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	z	252	Total	C	N	O	S	0	0
			2027	1304	336	381	6		

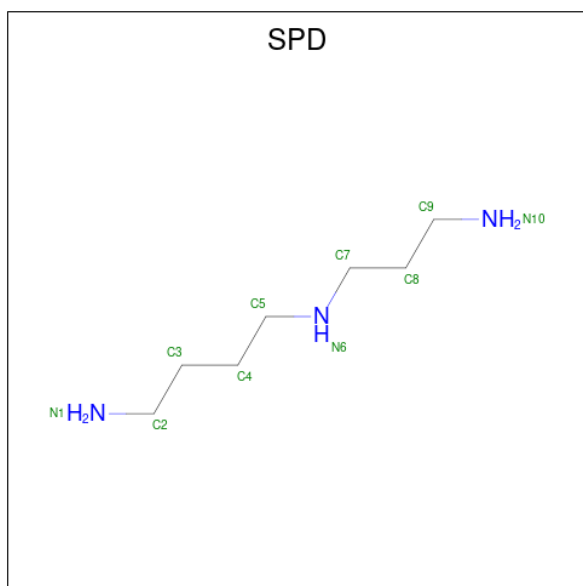
- Molecule 91 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
91	0	1	Total	Zn	0
			1	1	
91	4	1	Total	Zn	0
			1	1	
91	AO	1	Total	Zn	0
			1	1	

- Molecule 92 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
92	6	1	Total	K	0
			1	1	
92	A	29	Total	K	0
			29	29	
92	AA	17	Total	K	0
			17	17	
92	D	1	Total	K	0
			1	1	
92	M	1	Total	K	0
			1	1	
92	N	1	Total	K	0
			1	1	
92	W	1	Total	K	0
			1	1	
92	o	1	Total	K	0
			1	1	

- Molecule 93 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



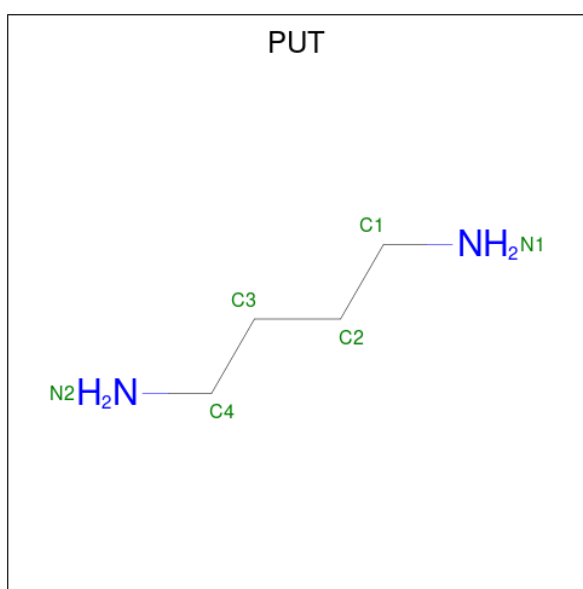
Mol	Chain	Residues	Atoms			AltConf
93	A	1	Total	C	N	0
			10	7	3	
93	A	1	Total	C	N	0
			10	7	3	
93	A	1	Total	C	N	0
			10	7	3	

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Mol	Chain	Residues	Atoms			AltConf
93	A	1	Total	C	N	0
			10	7	3	
93	AA	1	Total	C	N	0
			10	7	3	
93	AA	1	Total	C	N	0
			10	7	3	
93	O	1	Total	C	N	0
			10	7	3	

- Molecule 94 is 1,4-DIAMINO BUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
94	A	1	Total	C	N	0
			6	4	2	

- Molecule 95 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

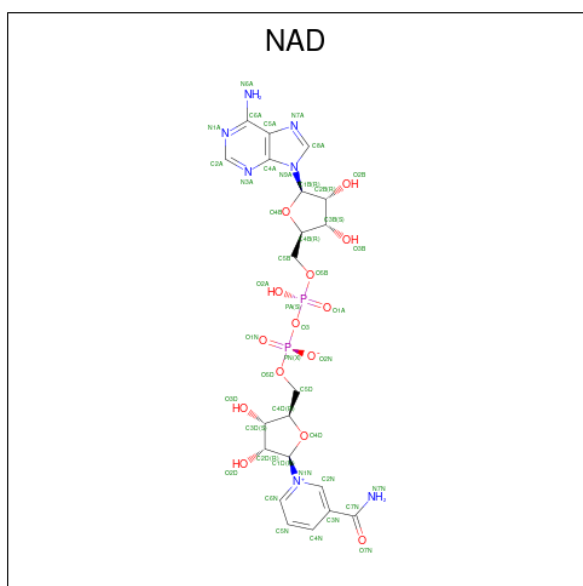
Mol	Chain	Residues	Atoms		AltConf
95	A	138	Total	Mg	0
			138	138	
95	A3	1	Total	Mg	0
			1	1	
95	AA	60	Total	Mg	0
			60	60	
95	AB	1	Total	Mg	0
			1	1	

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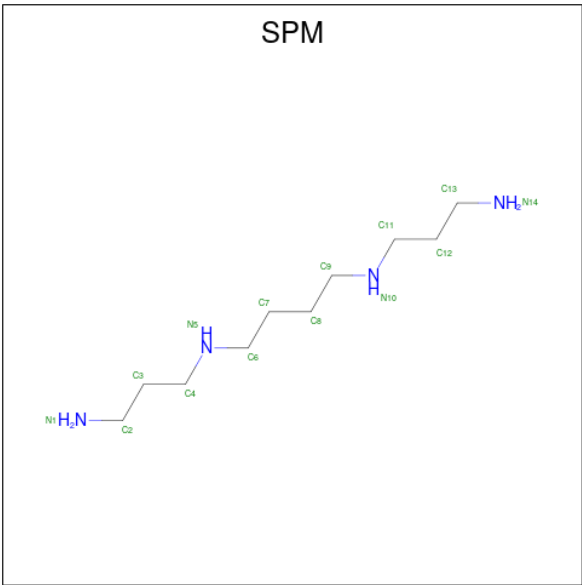
Mol	Chain	Residues	Atoms		AltConf
95	AX	1	Total	Mg	0
			1	1	
95	D	2	Total	Mg	0
			2	2	
95	g	1	Total	Mg	0
			1	1	

- Molecule 96 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



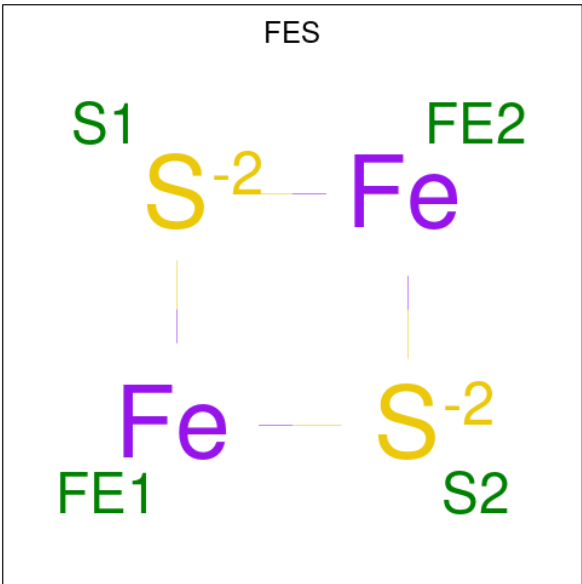
Mol	Chain	Residues	Atoms					AltConf
96	AA	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 97 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
97	AA	1	Total	C	N	0
			14	10	4	
97	AA	1	Total	C	N	0
			14	10	4	

- Molecule 98 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).



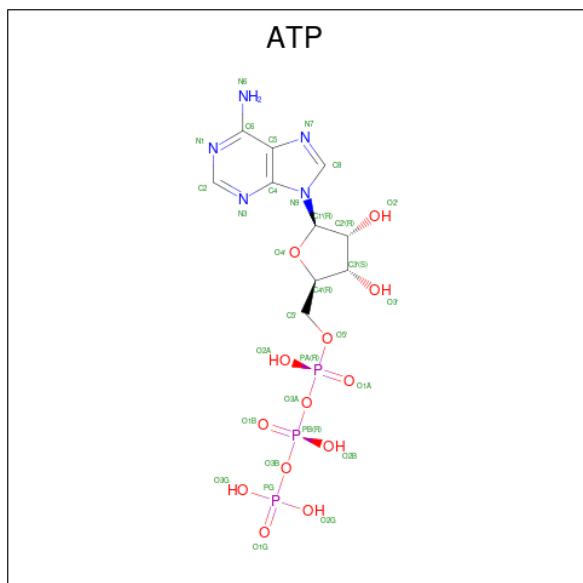
Mol	Chain	Residues	Atoms			AltConf
98	AP	1	Total	Fe	S	0
			4	2	2	

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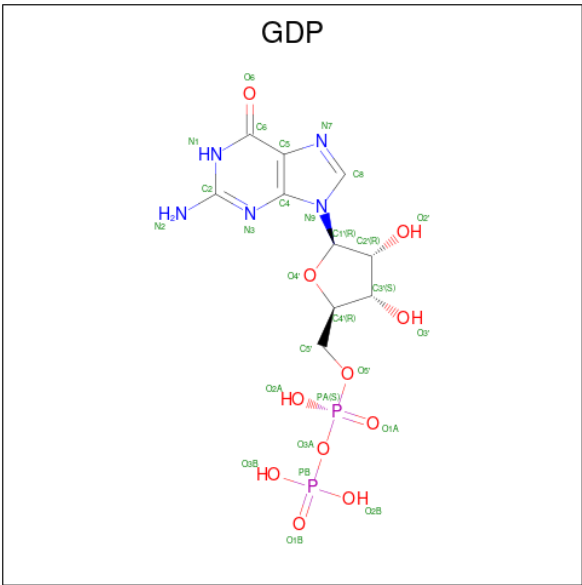
Mol	Chain	Residues	Atoms			AltConf
98	AT	1	Total	Fe	S	0
			4	2	2	
98	r	1	Total	Fe	S	0
			4	2	2	

- Molecule 99 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



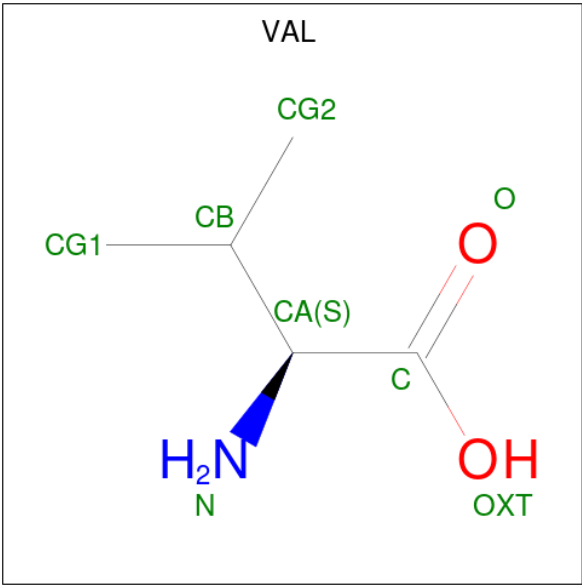
Mol	Chain	Residues	Atoms					AltConf
99	AX	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 100 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
100	AX	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 101 is VALINE (CCD ID: VAL) (formula: C₅H₁₁NO₂).

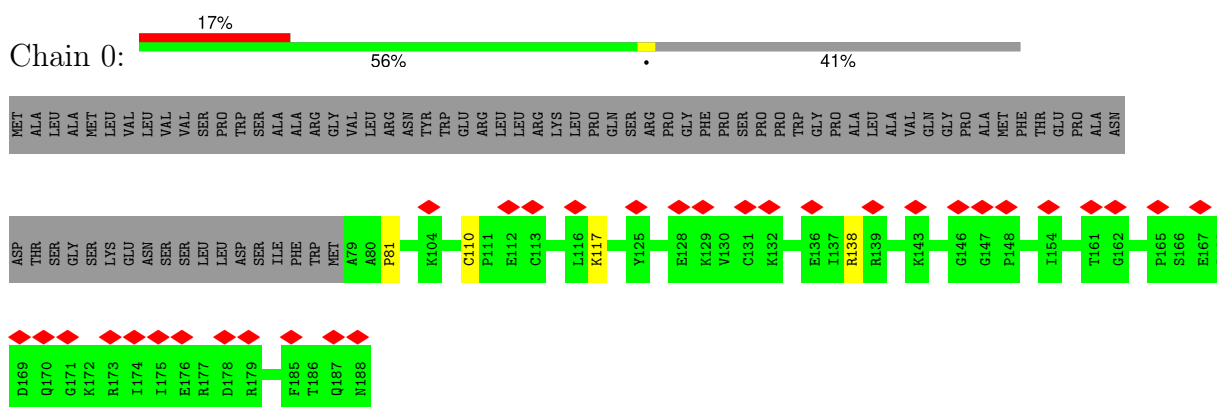


Mol	Chain	Residues	Atoms				AltConf
101	B	1	Total	C	N	O	0
			7	5	1	1	

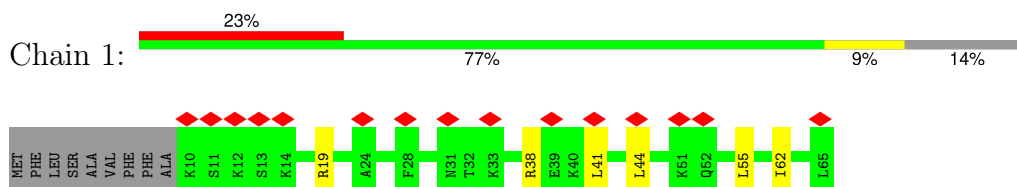
3 Residue-property plots [i](#)

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.

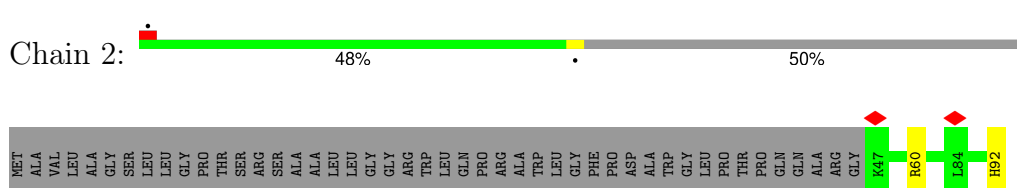
- Molecule 1: 39S ribosomal protein L32, mitochondrial



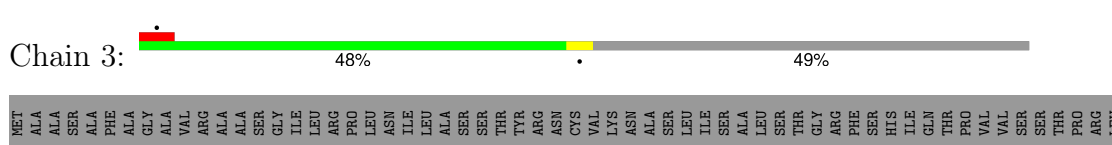
- Molecule 2: 39S ribosomal protein L33, mitochondrial

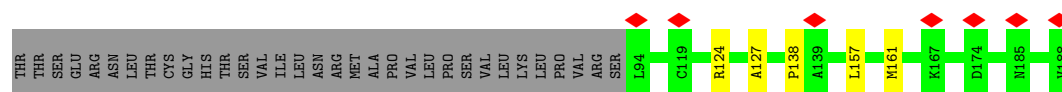


- Molecule 3: 39S ribosomal protein L34, mitochondrial

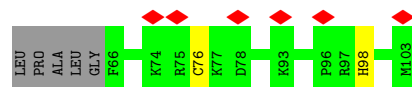
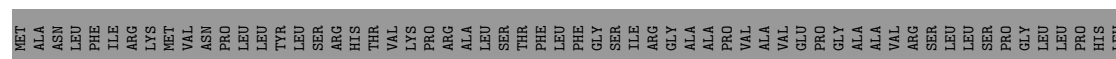


- Molecule 4: 39S ribosomal protein L35, mitochondrial

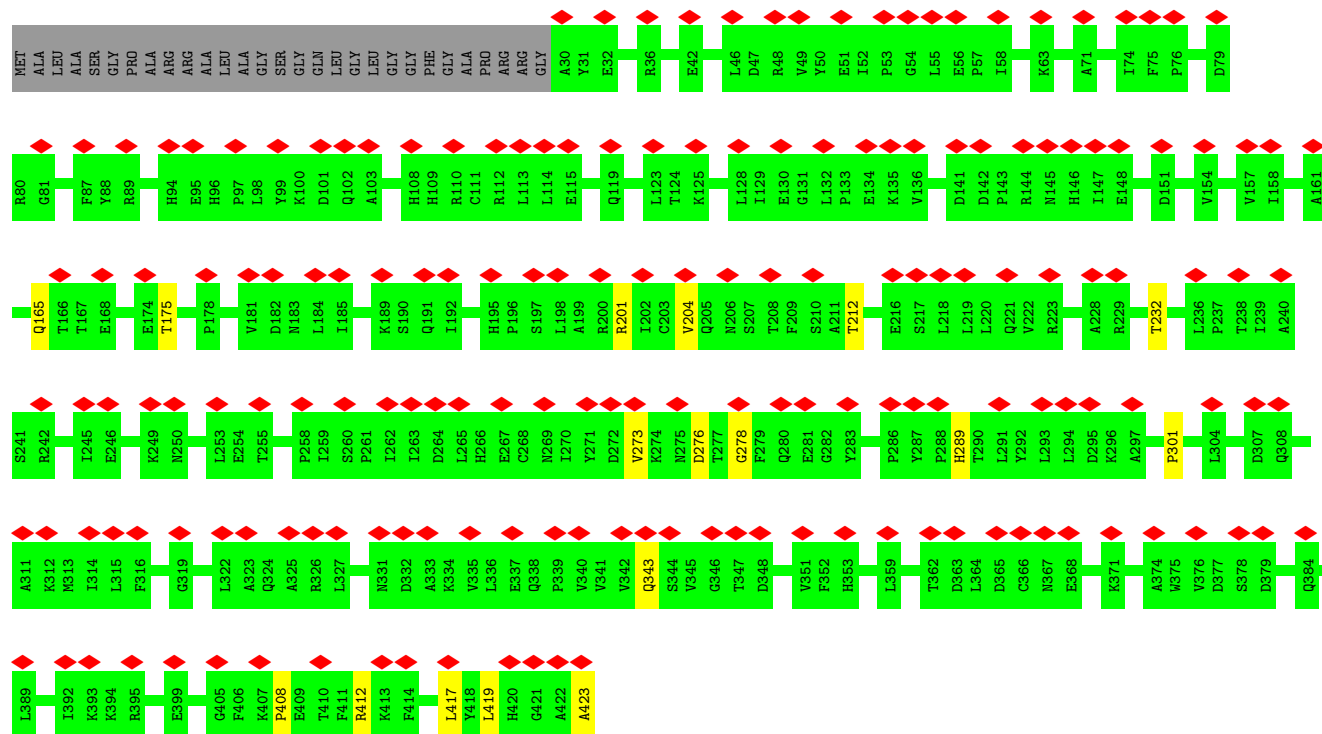
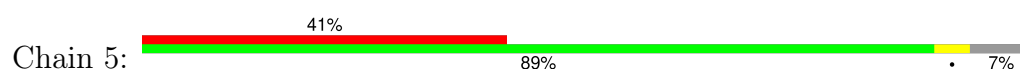




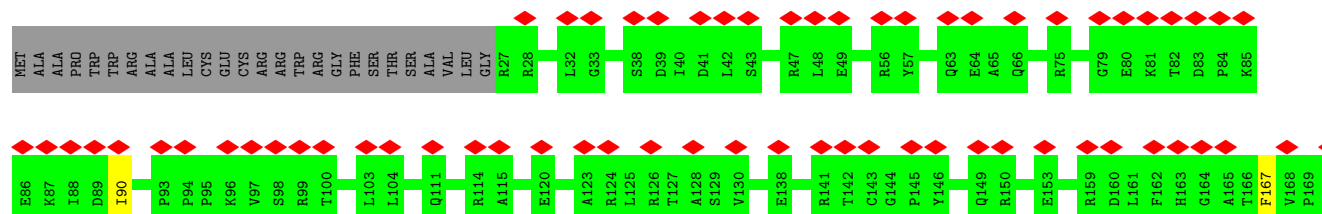
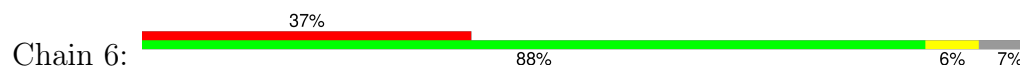
- Molecule 5: 39S ribosomal protein L36, mitochondrial

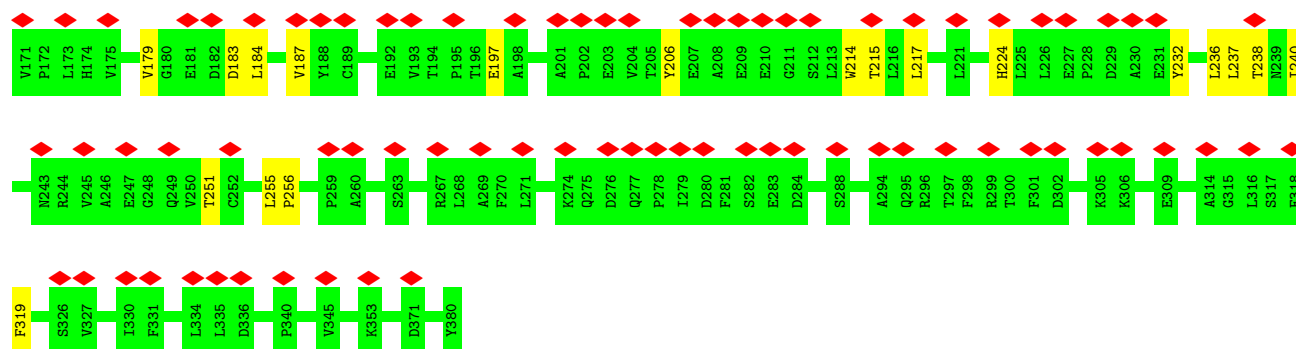


- Molecule 6: 39S ribosomal protein L37, mitochondrial

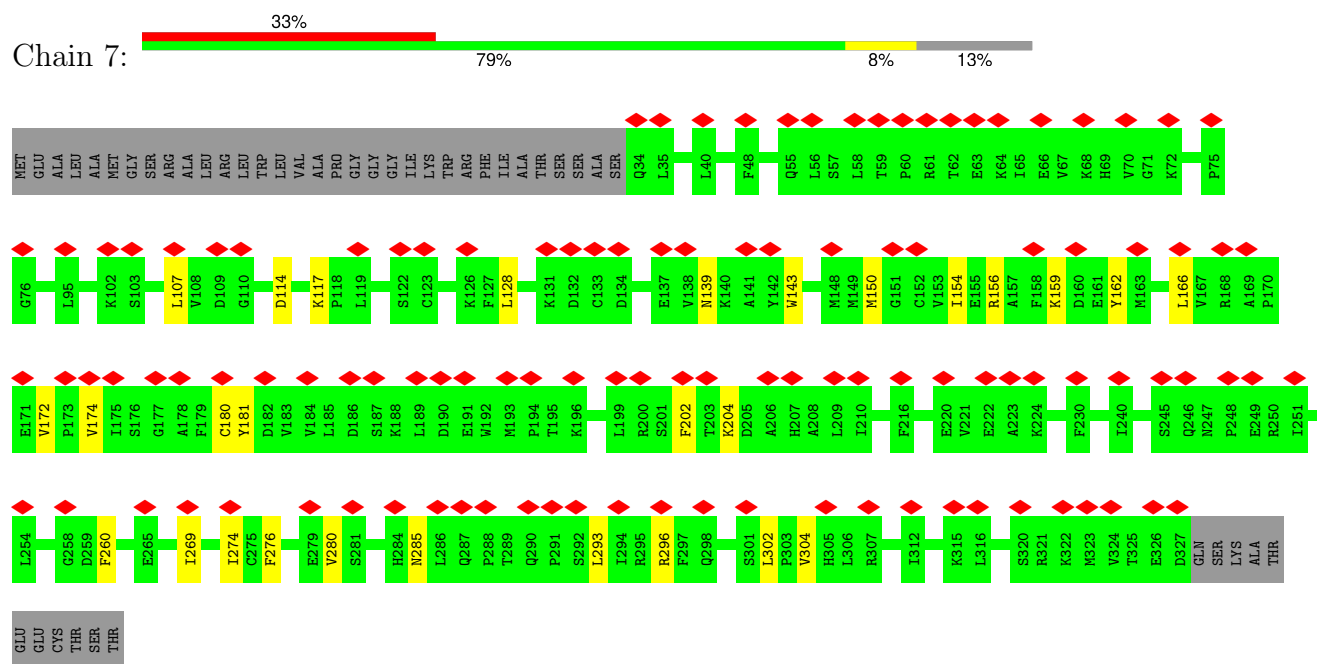


- Molecule 7: 39S ribosomal protein L38, mitochondrial

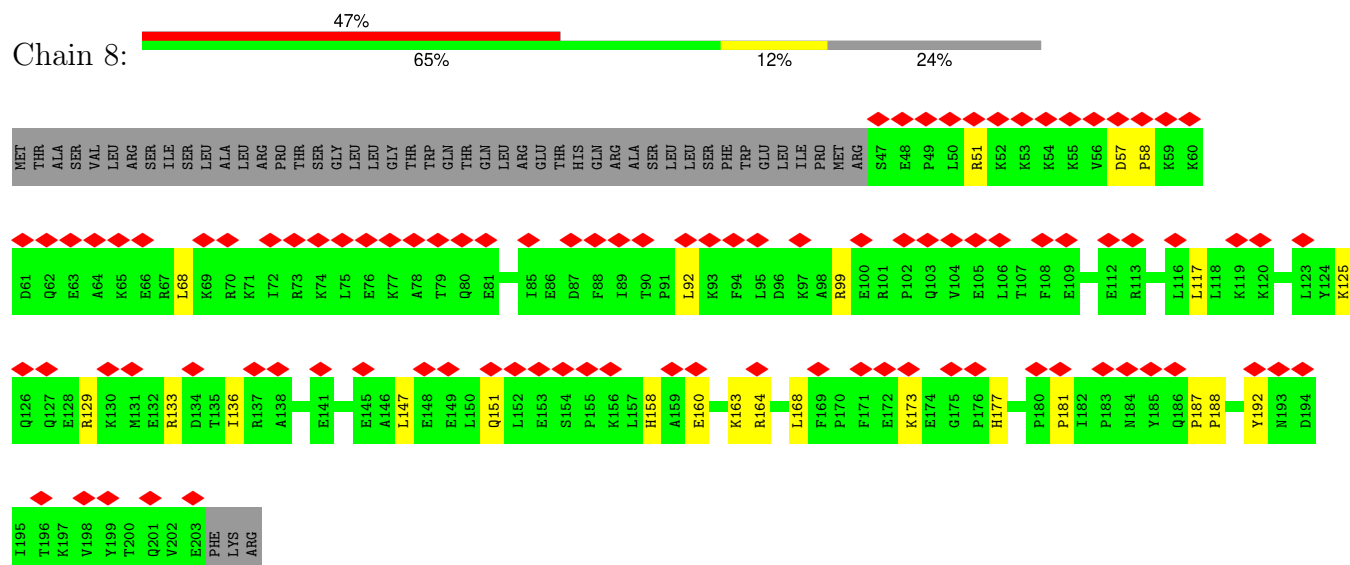




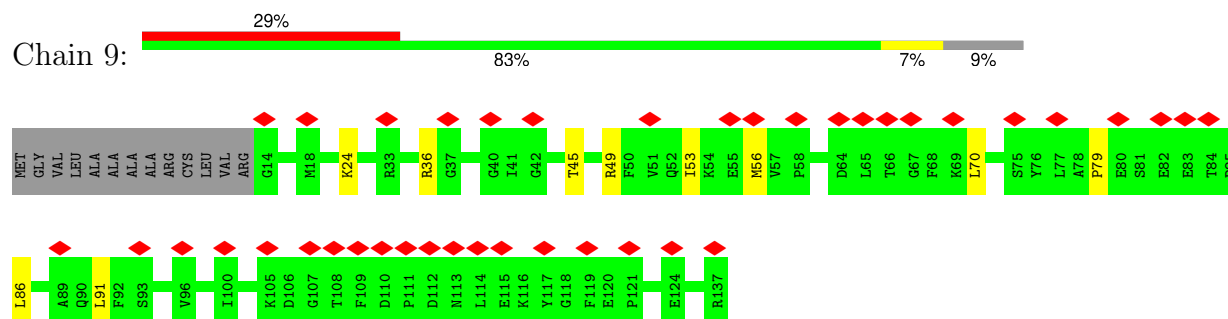
- Molecule 8: 39S ribosomal protein L39, mitochondrial



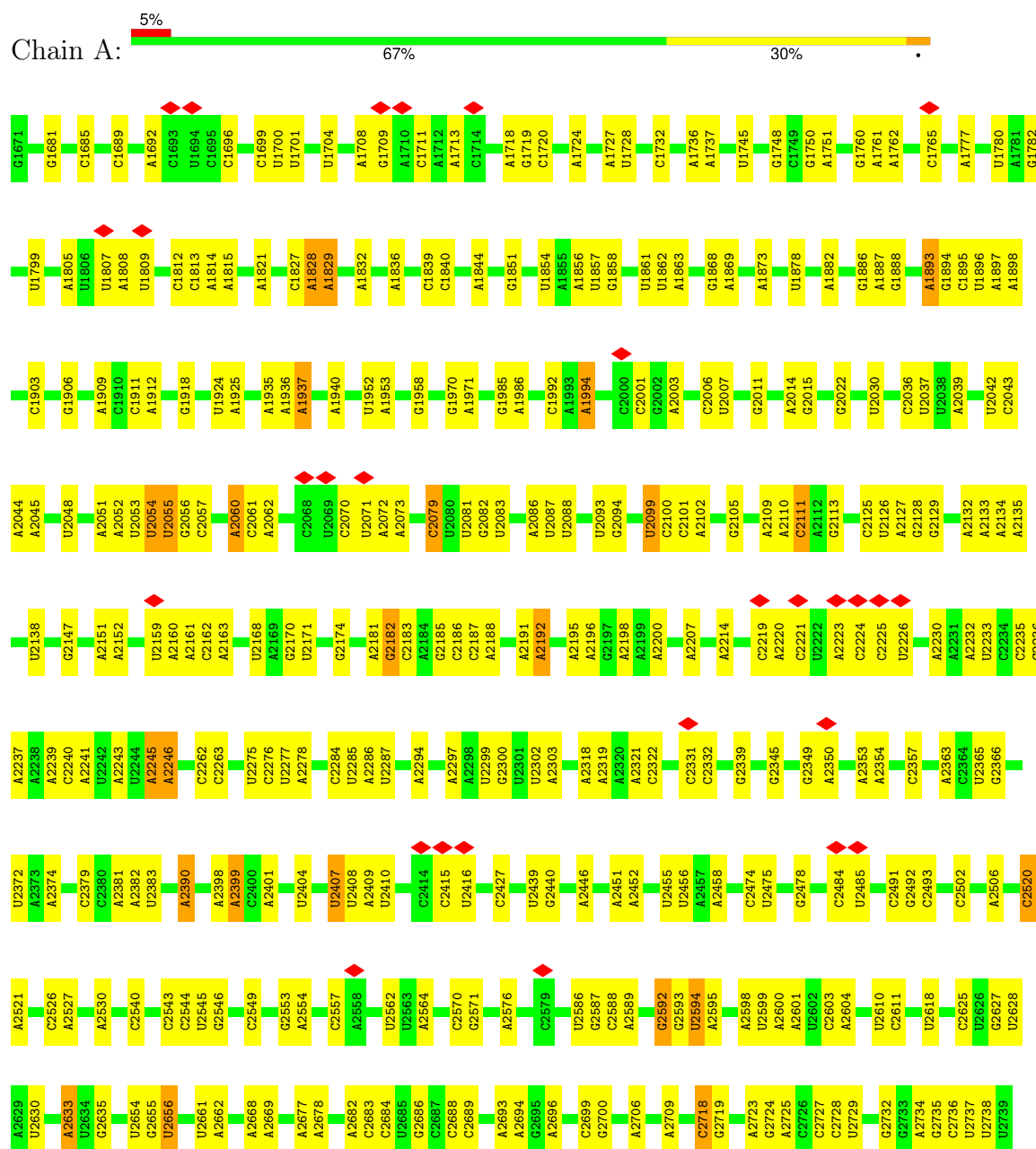
- Molecule 9: 39S ribosomal protein L40, mitochondrial

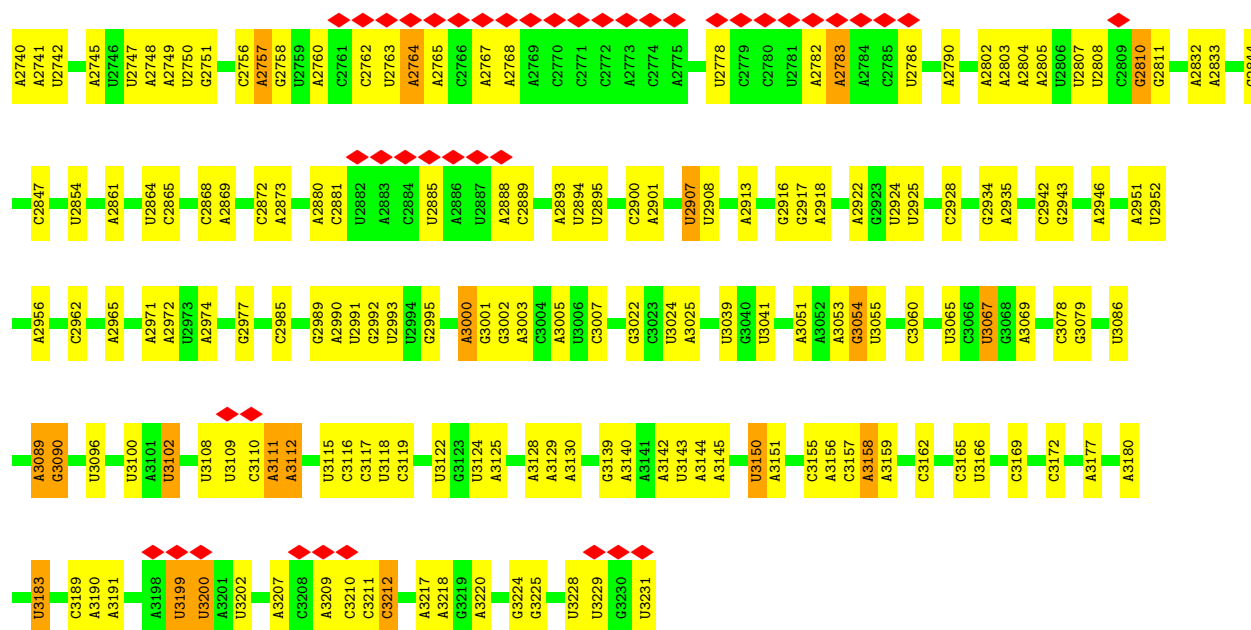


- Molecule 10: 39S ribosomal protein L41, mitochondrial

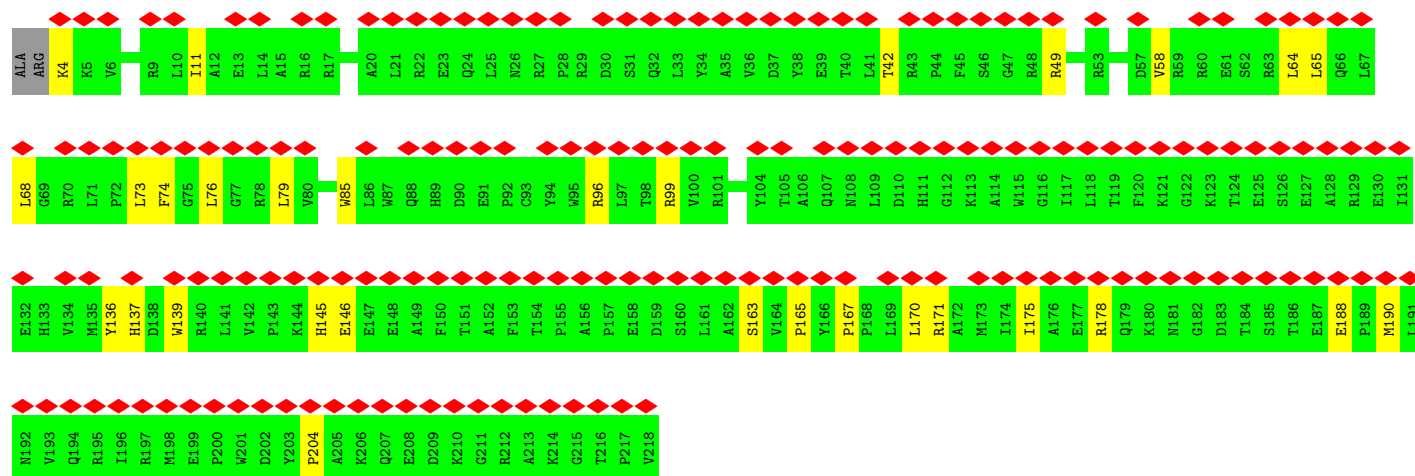
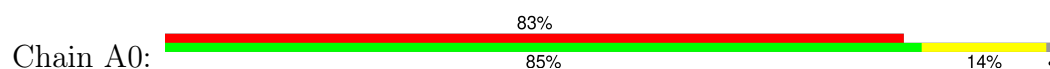


- Molecule 11: 16S mitochondrial rRNA

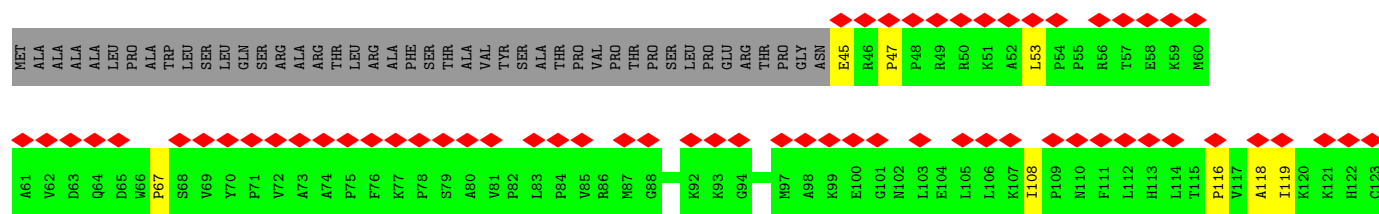
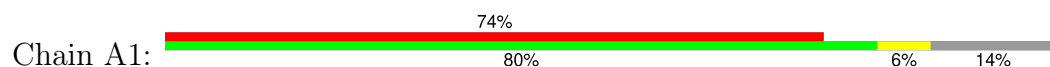


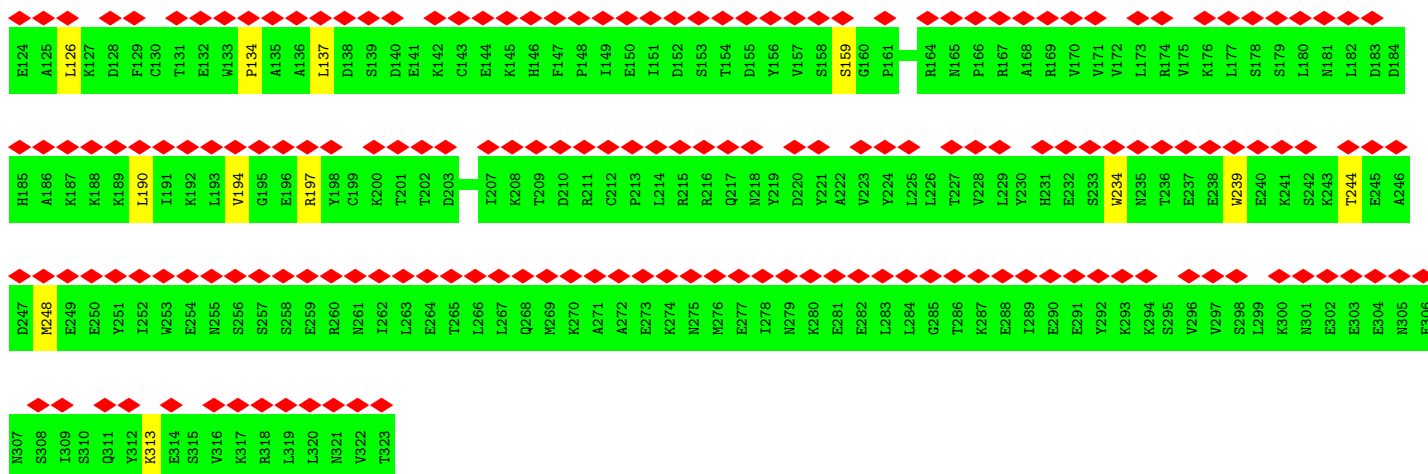


• Molecule 12: Small ribosomal subunit protein mS34

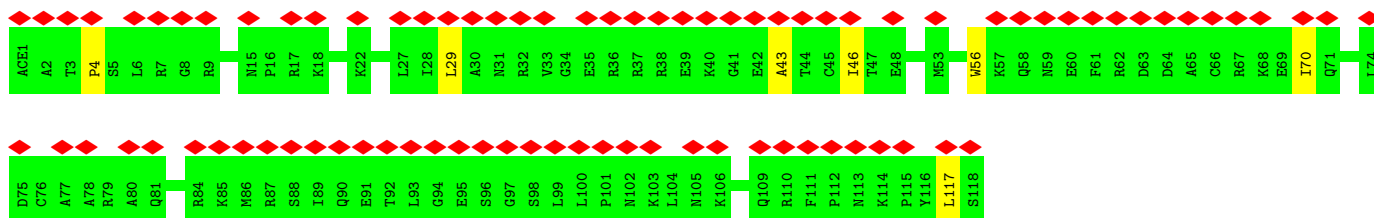
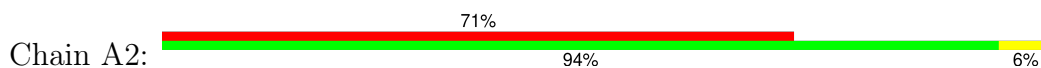


• Molecule 13: 28S ribosomal protein S35, mitochondrial

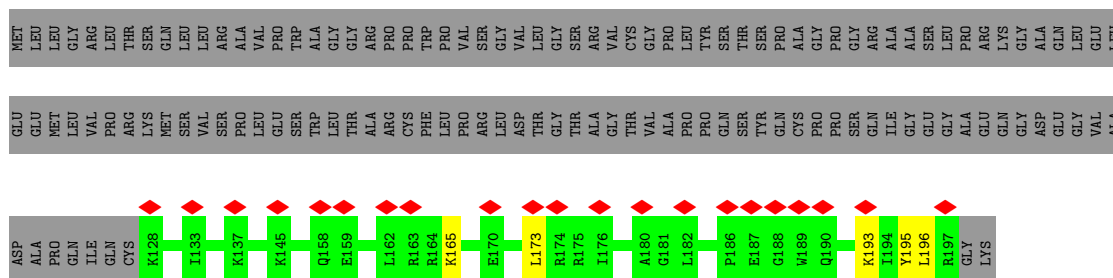




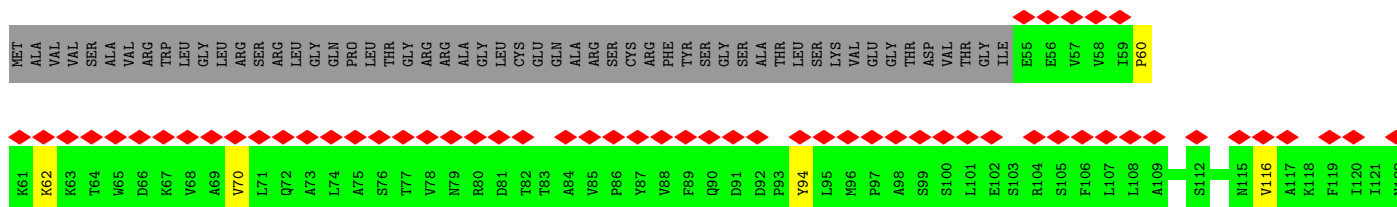
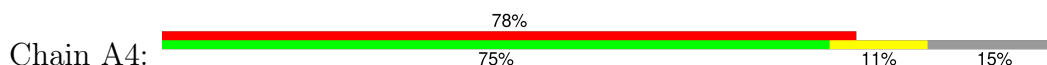
- Molecule 14: Small ribosomal subunit protein mS37

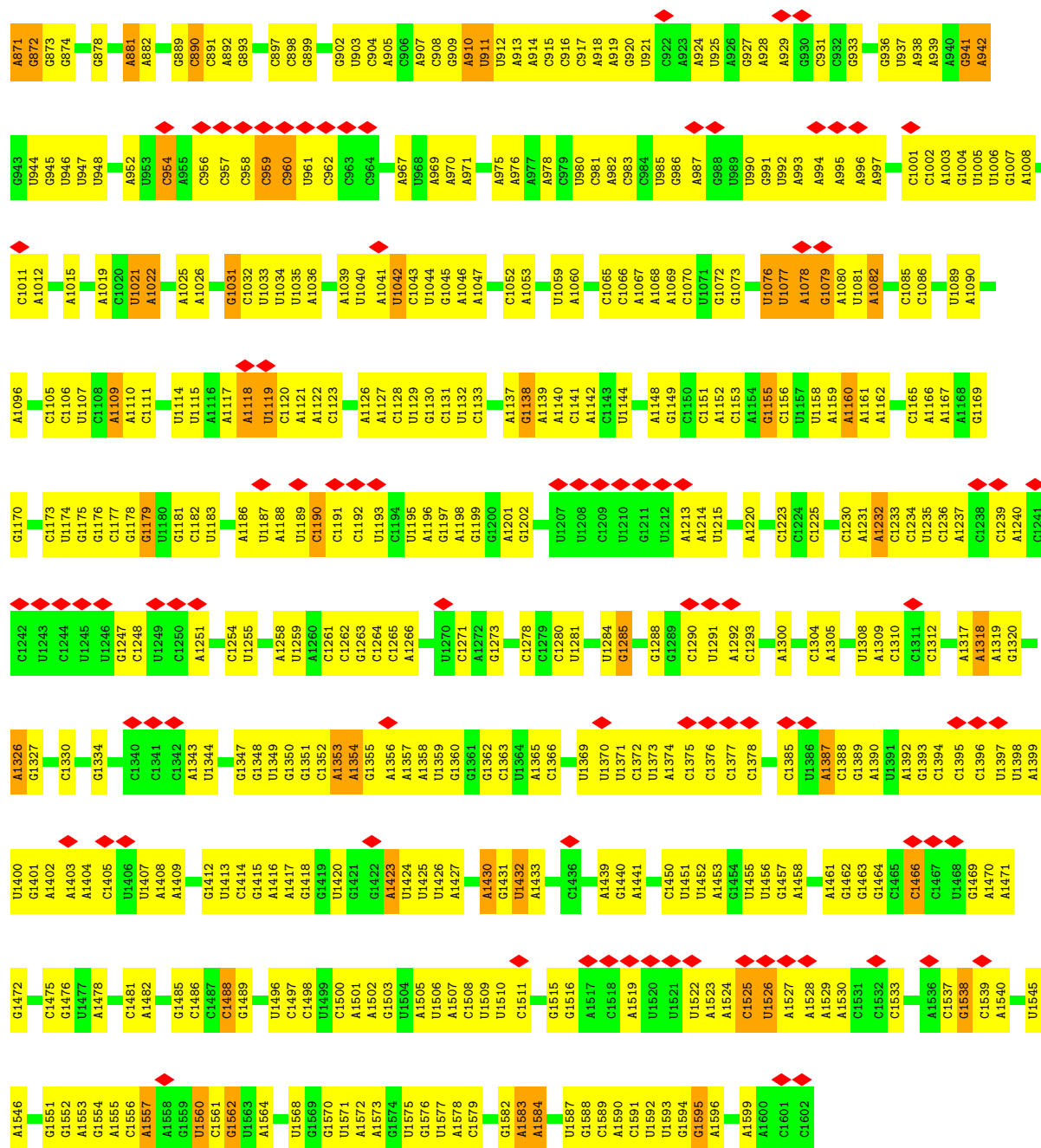


- Molecule 15: Aurora kinase A-interacting protein

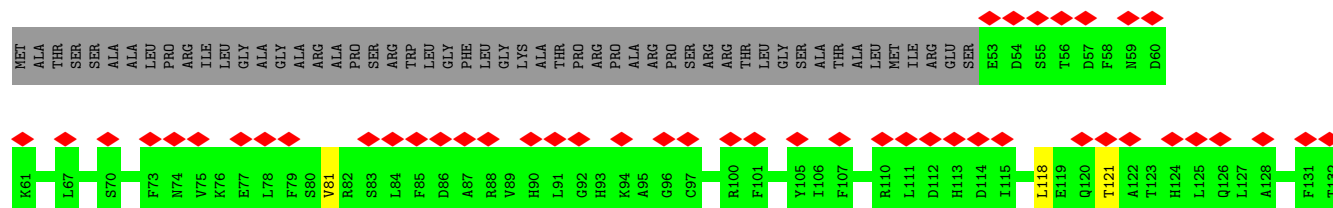
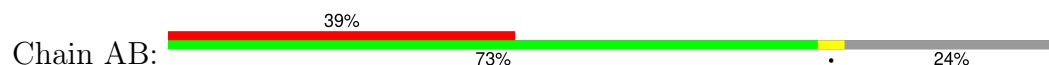


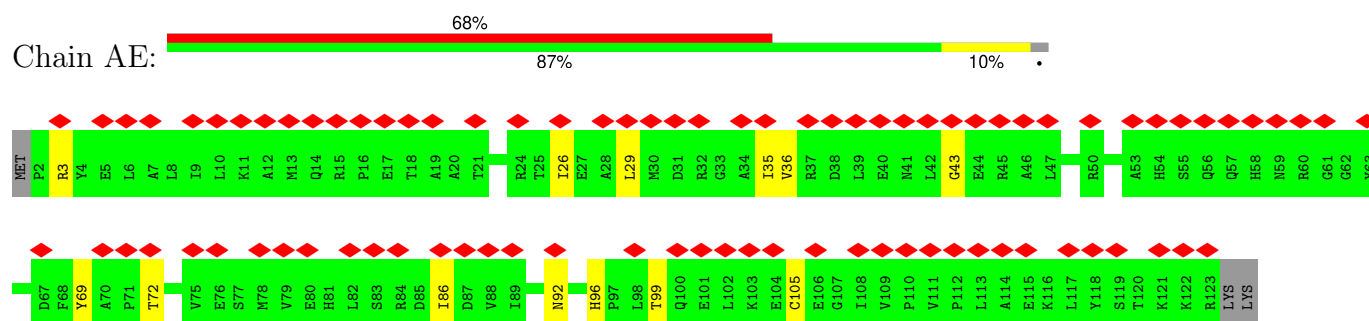
- Molecule 16: Pentatricopeptide repeat domain-containing protein 3, mitochondrial



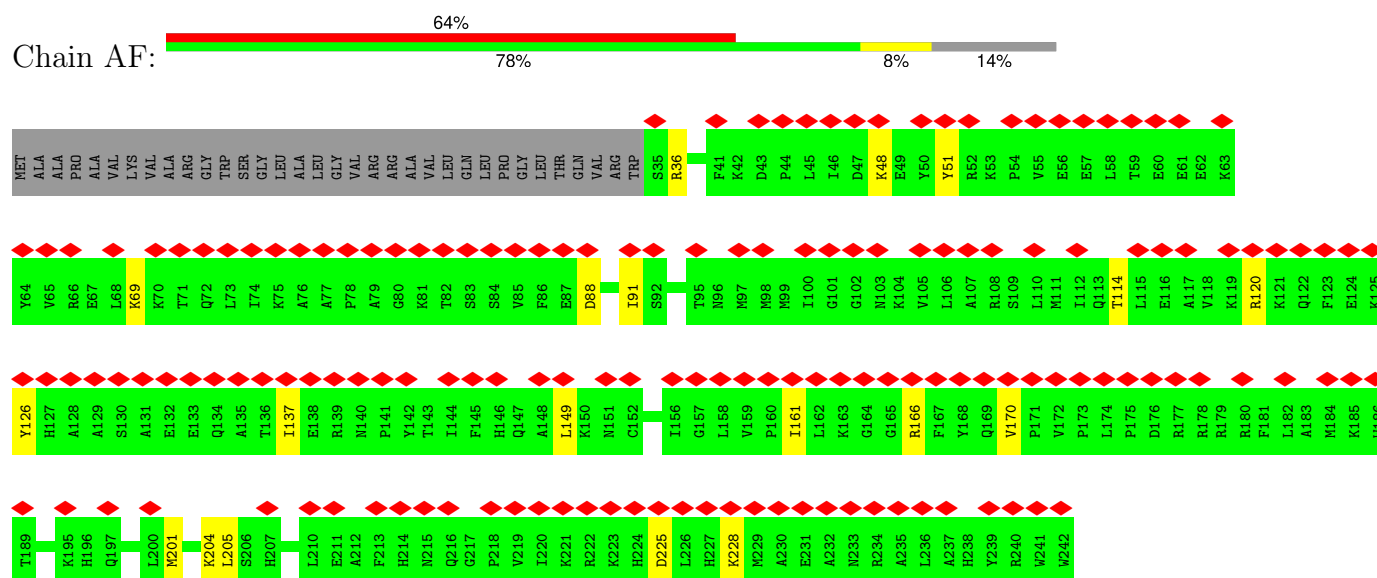


• Molecule 18: 28S ribosomal protein S2, mitochondrial

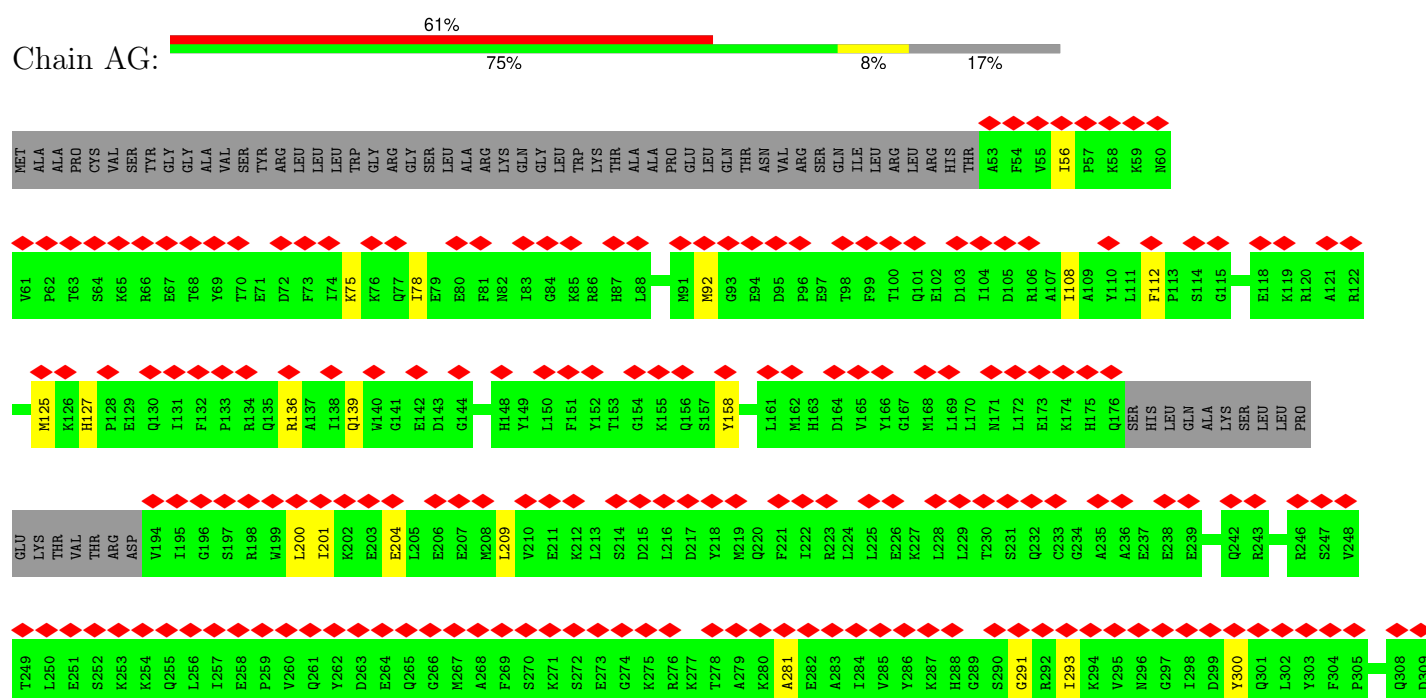




- Molecule 22: 28S ribosomal protein S7, mitochondrial



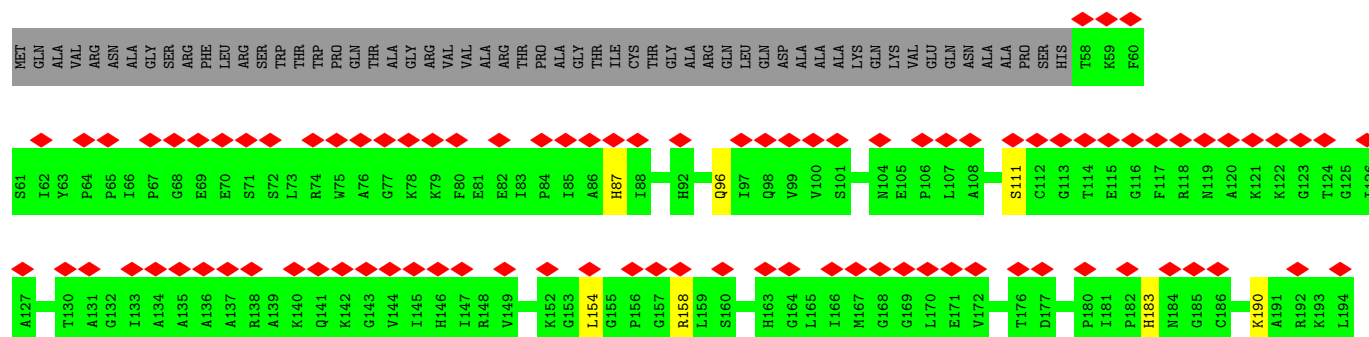
- Molecule 23: 28S ribosomal protein S9, mitochondrial



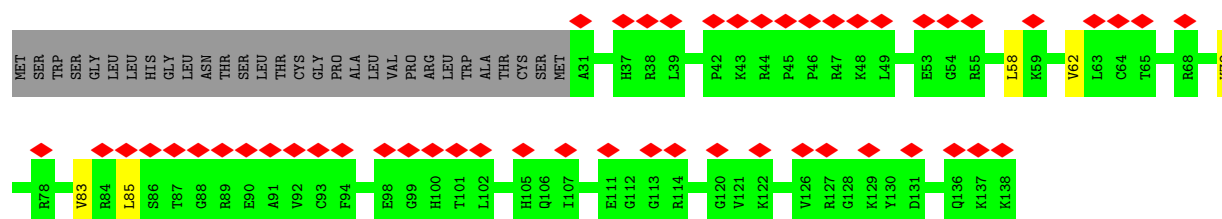
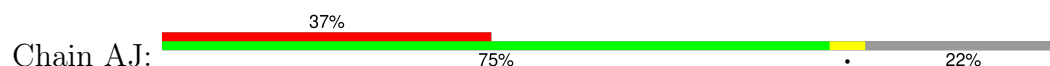
- Molecule 24: 28S ribosomal protein S10, mitochondrial



- Molecule 25: 28S ribosomal protein S11, mitochondrial

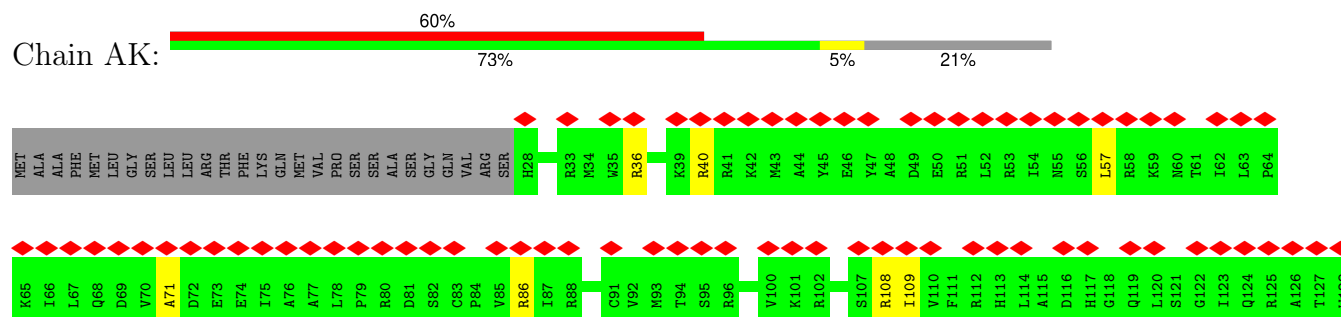


- Molecule 26: 28S ribosomal protein S12, mitochondrial



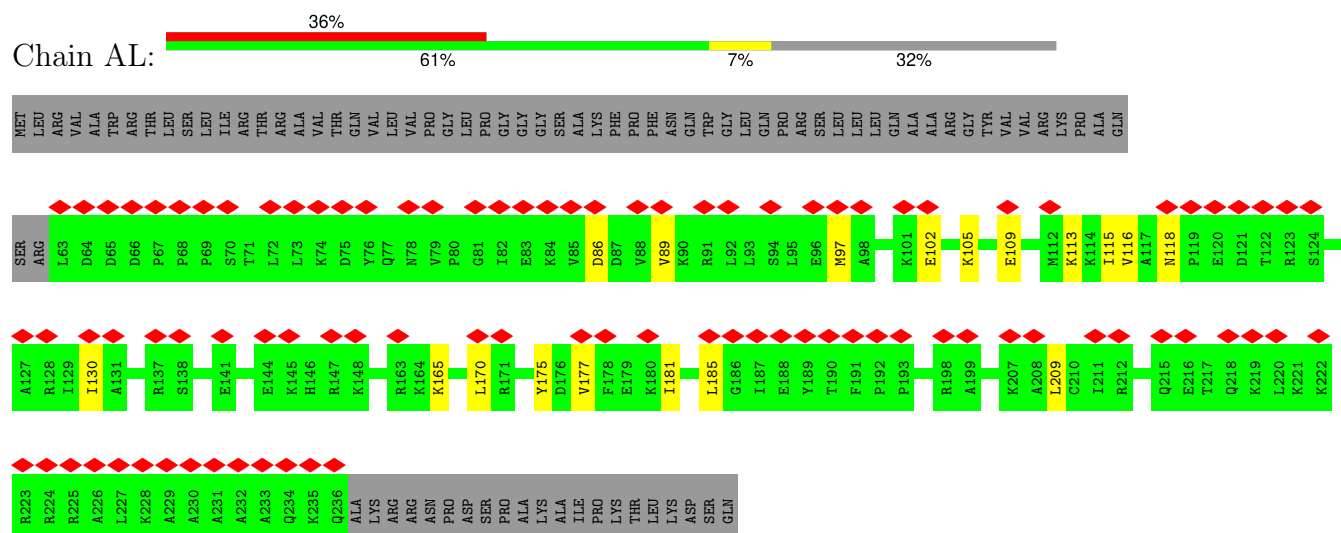
- Molecule 27: 28S ribosomal protein S14, mitochondrial

Chain AK:



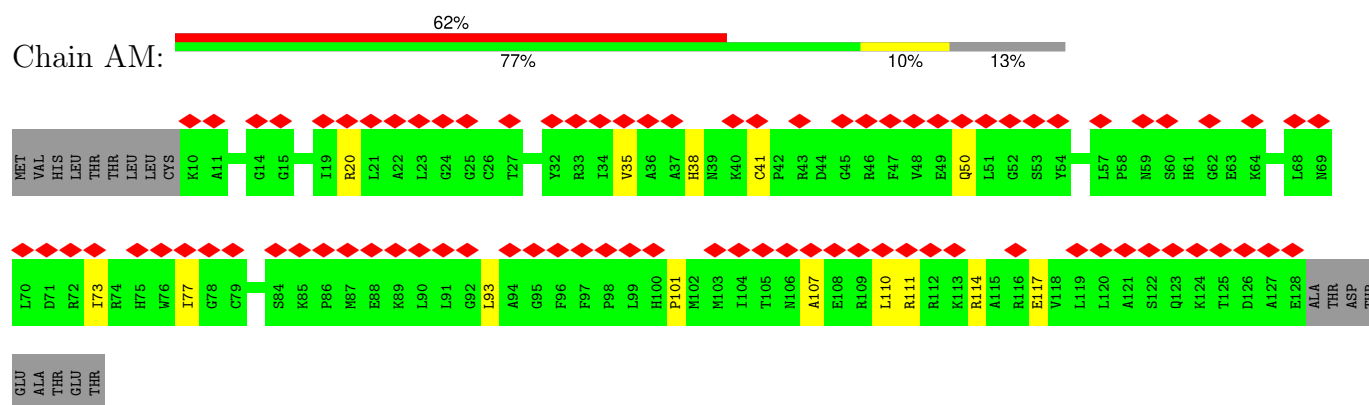
- Molecule 28: 28S ribosomal protein S15, mitochondrial

Chain AL:



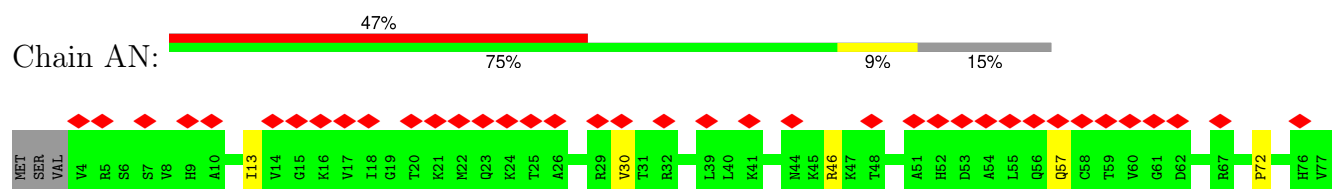
- Molecule 29: 28S ribosomal protein S16, mitochondrial

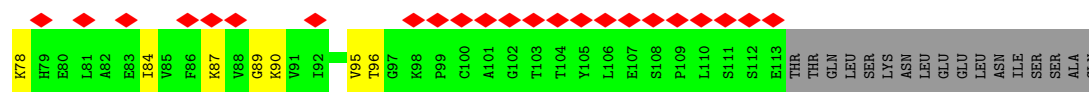
Chain AM:



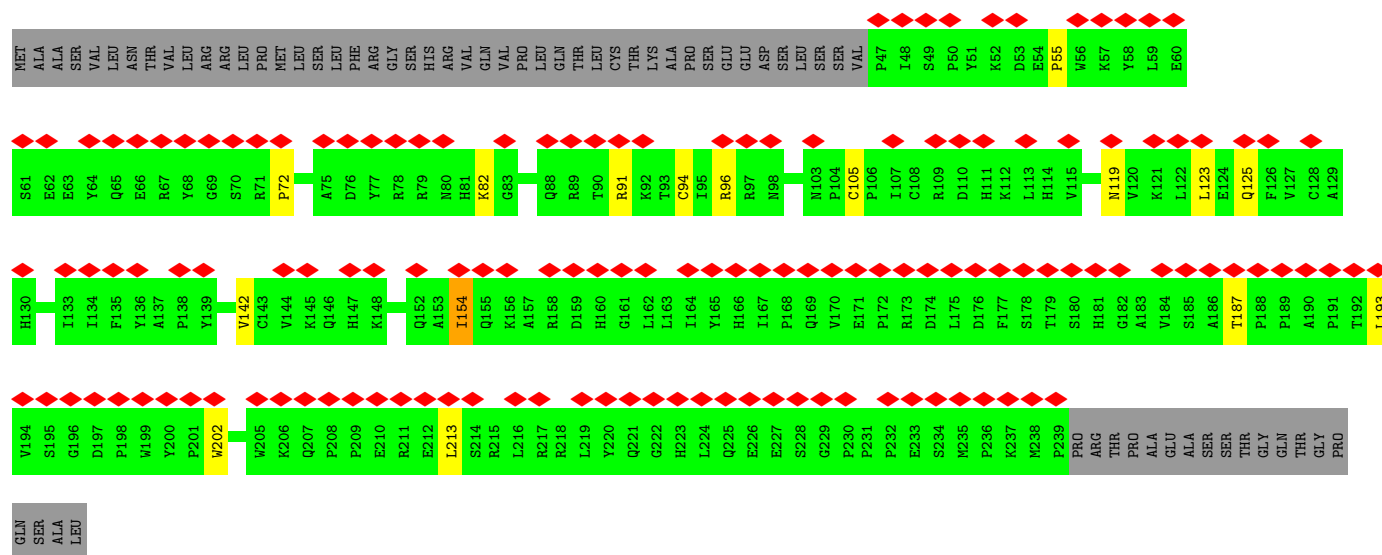
- Molecule 30: 28S ribosomal protein S17, mitochondrial

Chain AN:

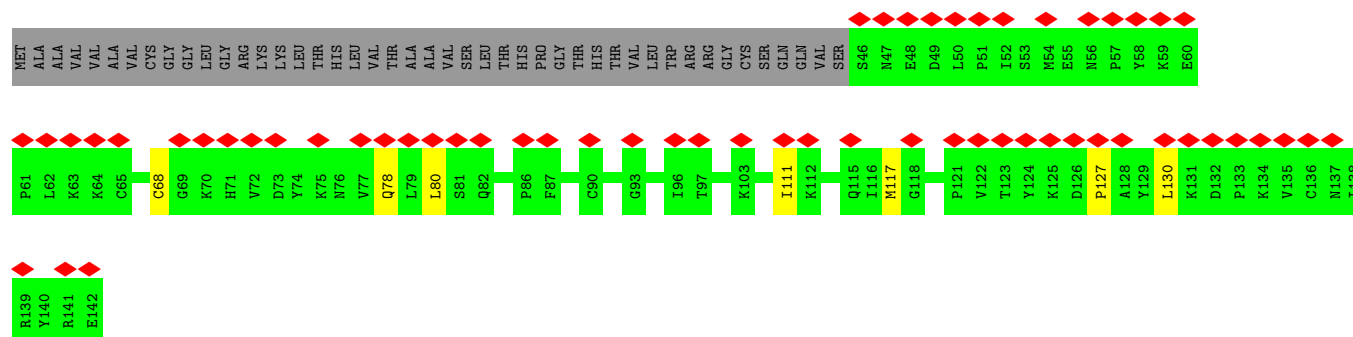
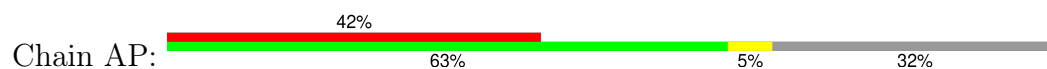




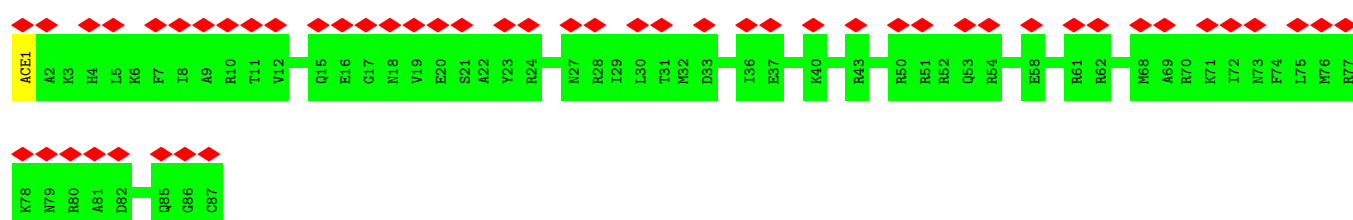
- Molecule 31: 28S ribosomal protein S18b, mitochondrial



- Molecule 32: 28S ribosomal protein S18c, mitochondrial

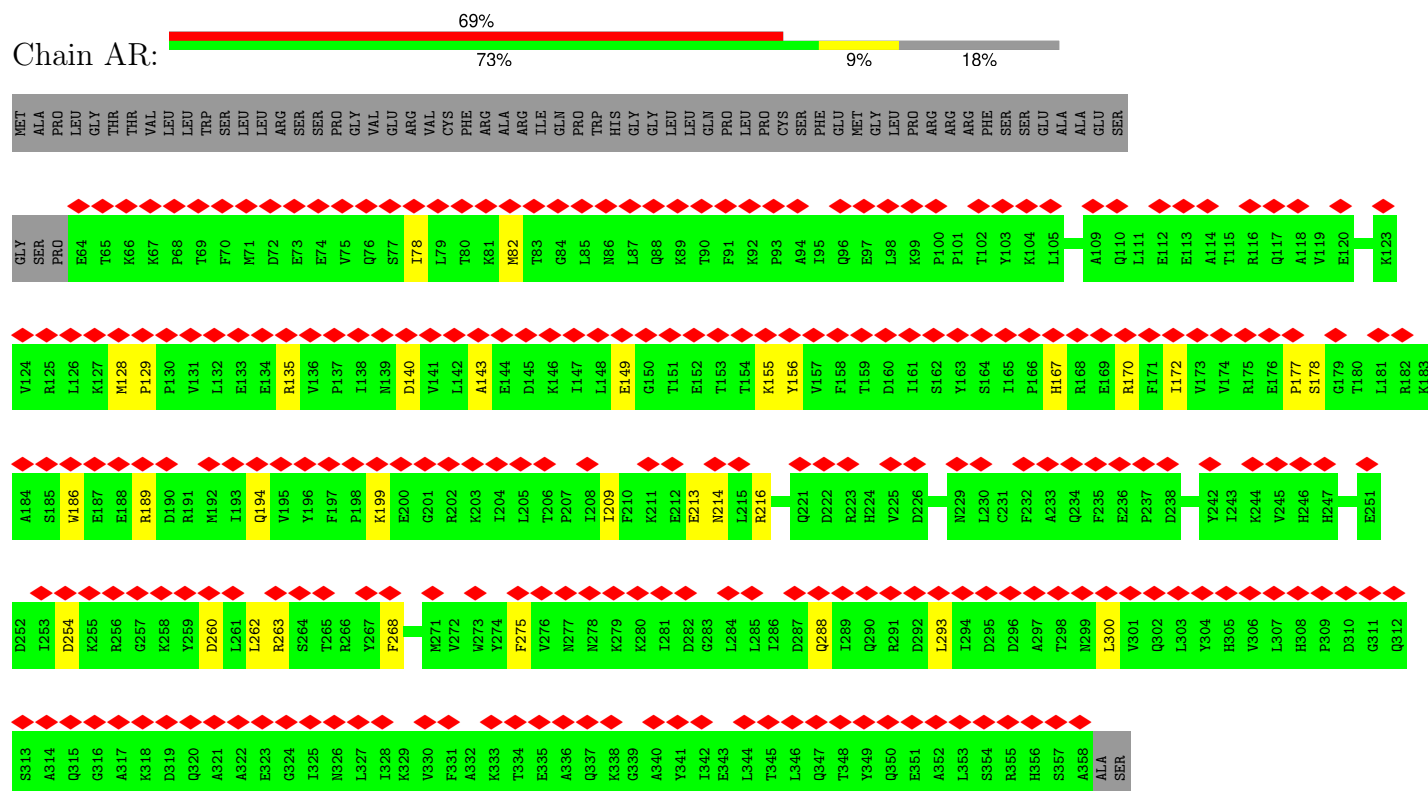


- Molecule 33: Small ribosomal subunit protein bS21m



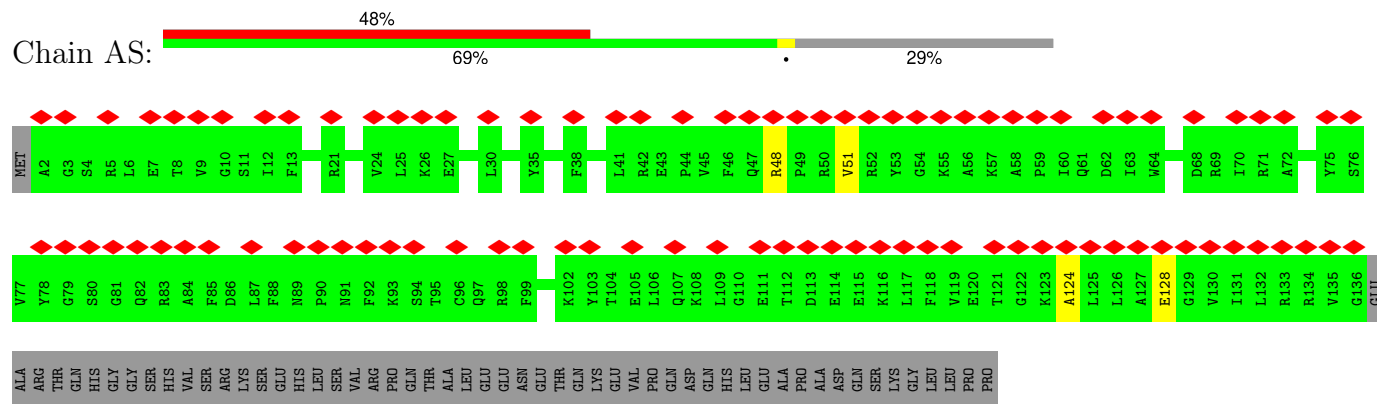
- Molecule 34: 28S ribosomal protein S22, mitochondrial

Chain AR:



- Molecule 35: 28S ribosomal protein S23, mitochondrial

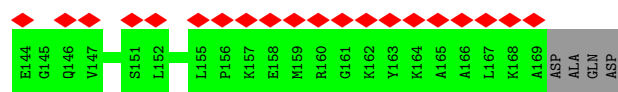
Chain AS:



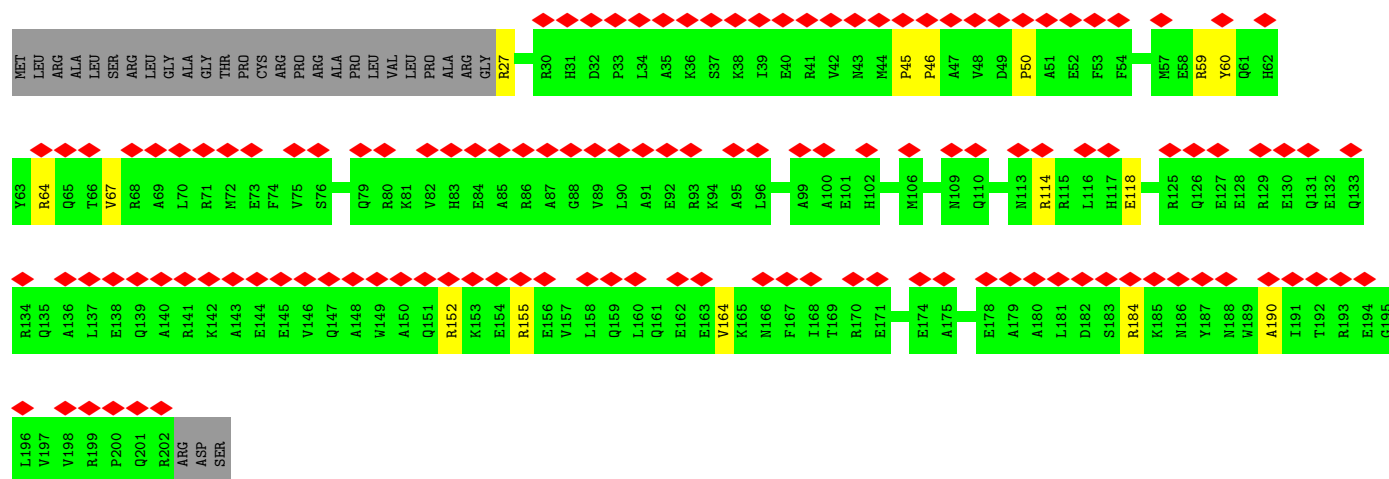
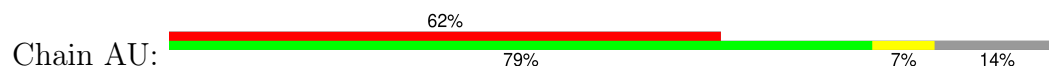
- Molecule 36: 28S ribosomal protein S25, mitochondrial

Chain AT:

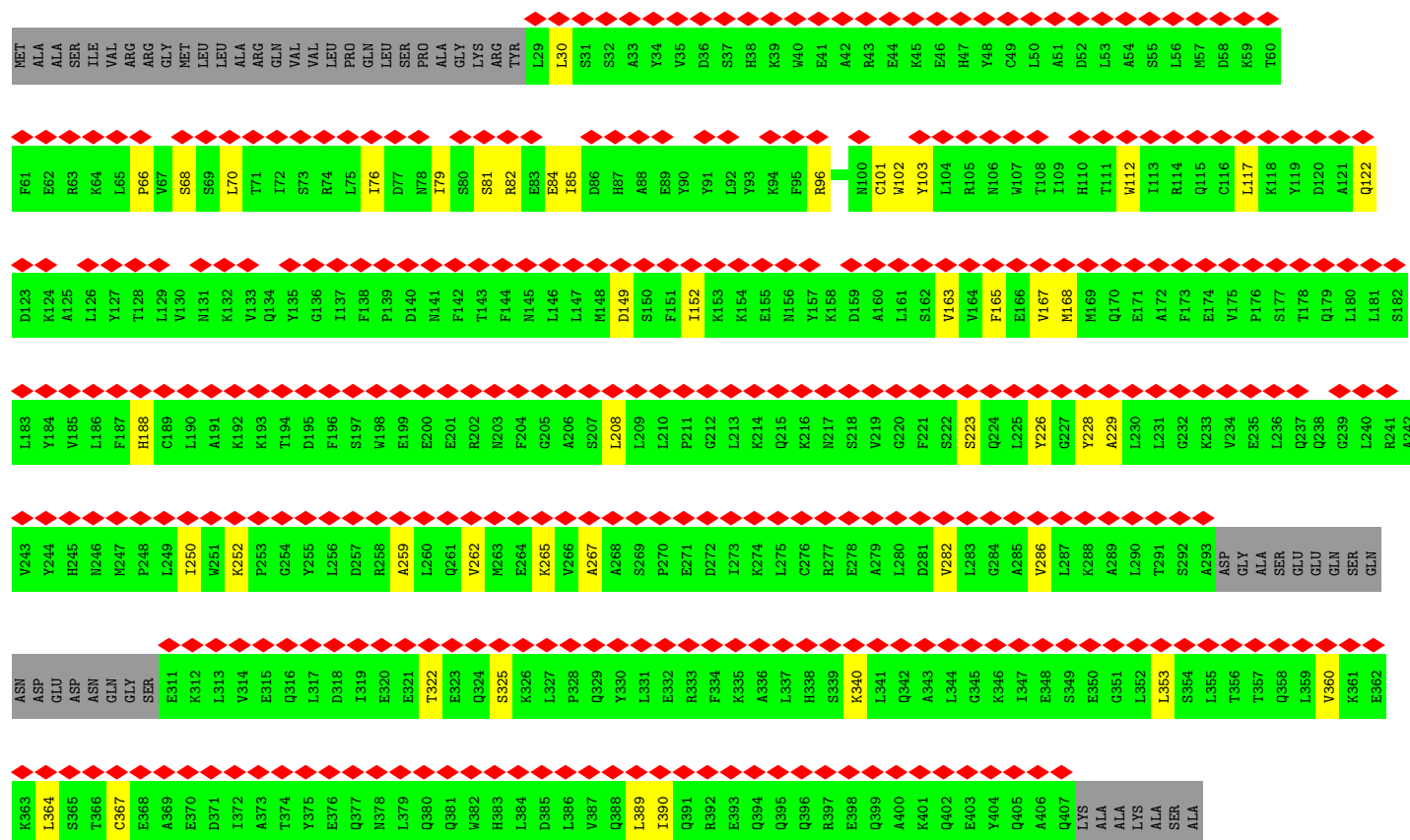
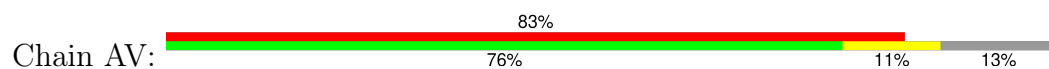




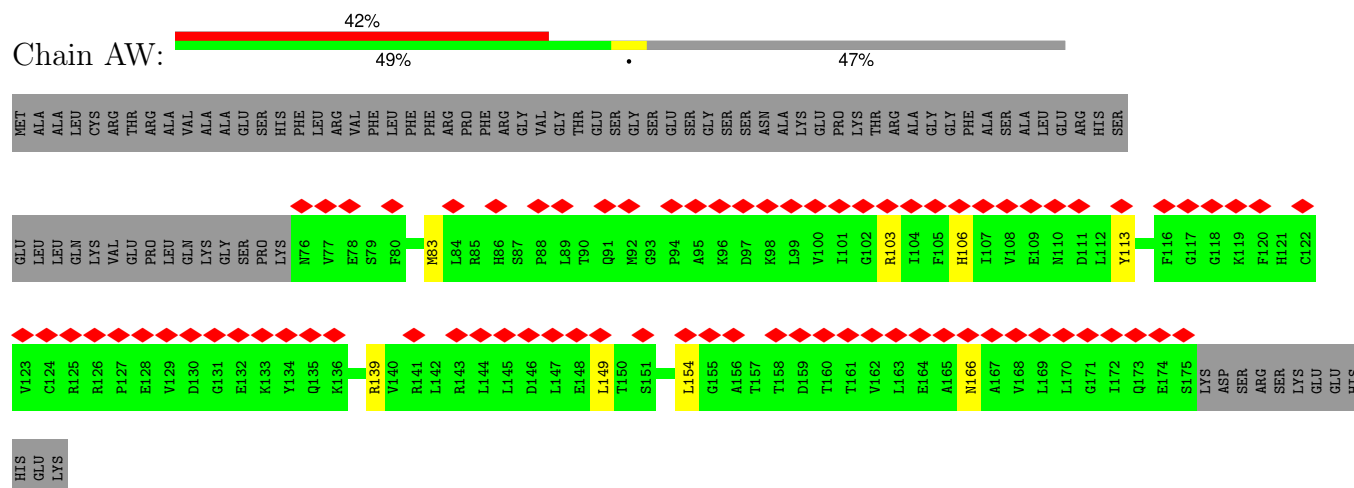
- Molecule 37: 28S ribosomal protein S26, mitochondrial



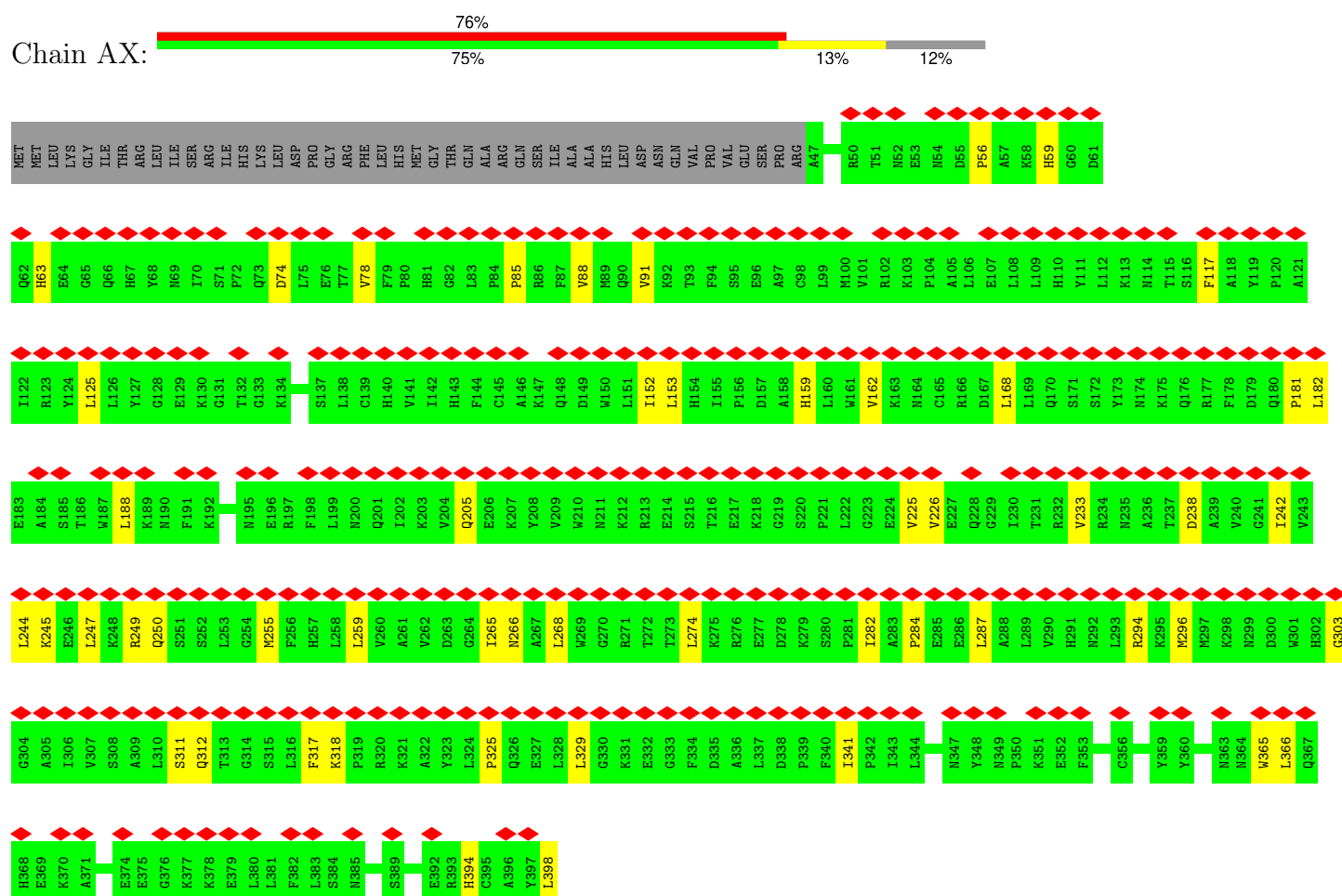
- Molecule 38: 28S ribosomal protein S27, mitochondrial



- Molecule 39: 28S ribosomal protein S28, mitochondrial



- Molecule 40: 28S ribosomal protein S29, mitochondrial

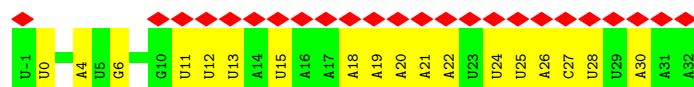
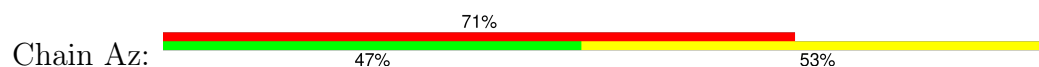


- Molecule 41: 28S ribosomal protein S31, mitochondrial

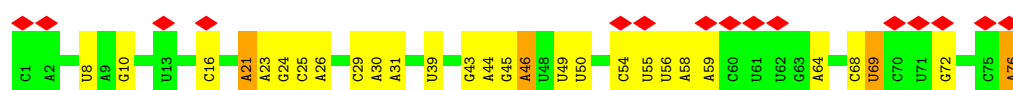




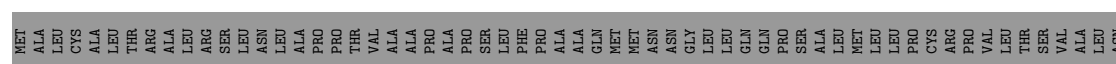
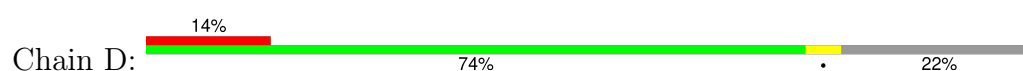
• Molecule 45: mRNA



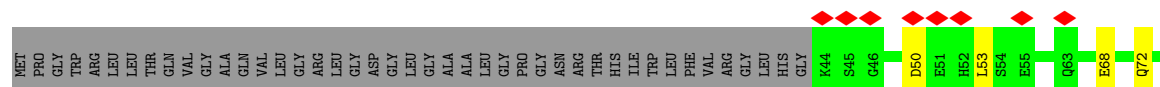
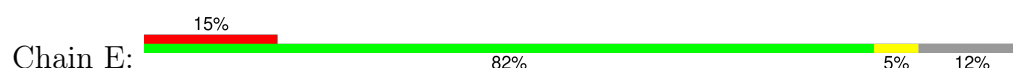
• Molecule 46: mitochondrial tRNAVal



• Molecule 47: 39S ribosomal protein L2, mitochondrial



• Molecule 48: 39S ribosomal protein L3, mitochondrial



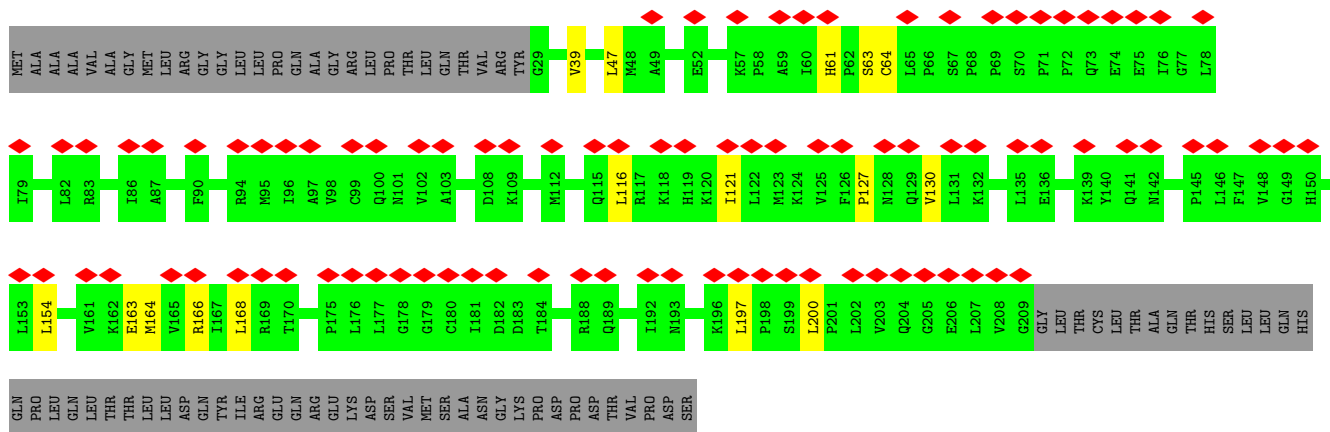
• Molecule 49: 39S ribosomal protein L4, mitochondrial



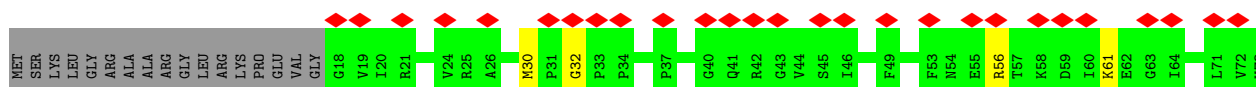
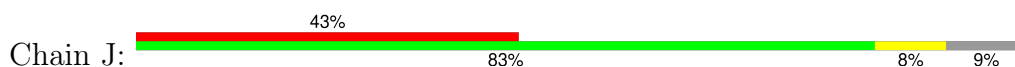
- Molecule 50: 39S ribosomal protein L9, mitochondrial

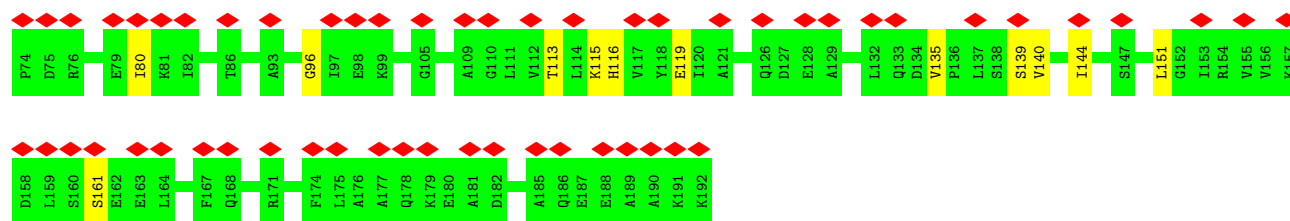


- Molecule 51: 39S ribosomal protein L10, mitochondrial

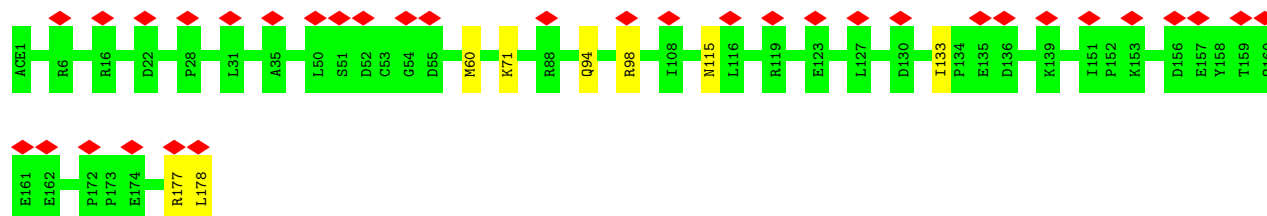


- Molecule 52: 39S ribosomal protein L11, mitochondrial

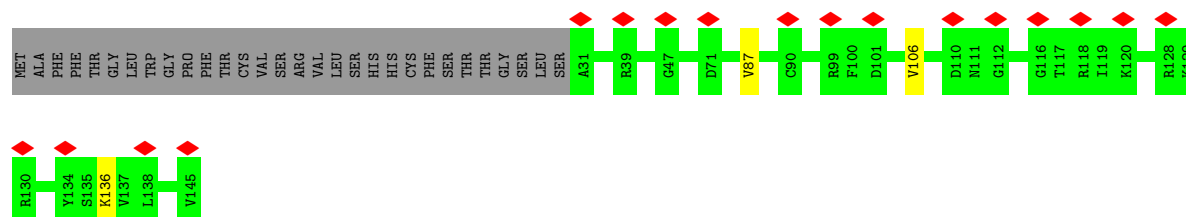
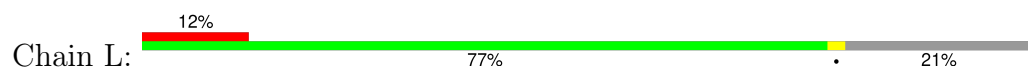




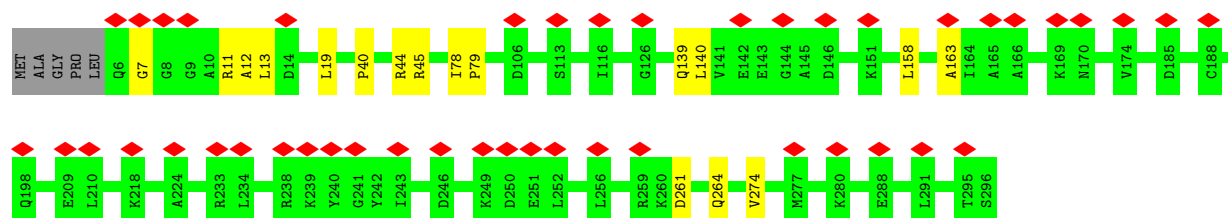
- Molecule 53: Large ribosomal subunit protein uL13m



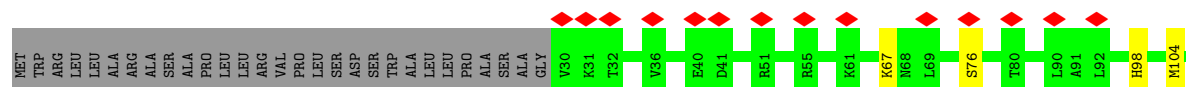
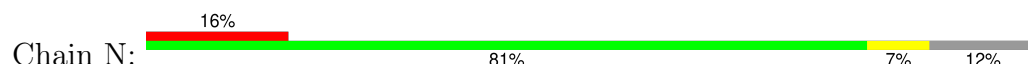
- Molecule 54: 39S ribosomal protein L14, mitochondrial



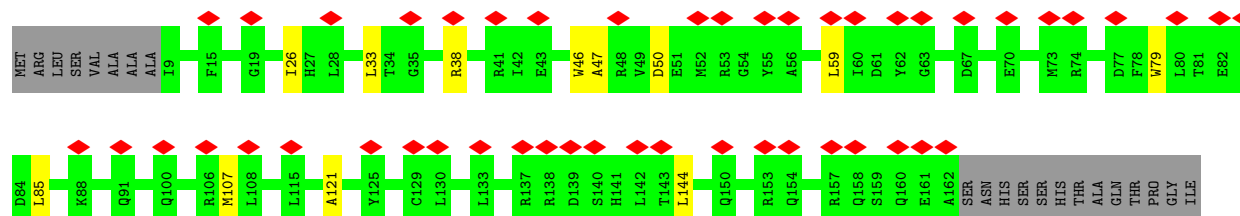
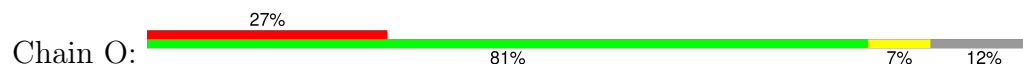
- Molecule 55: 39S ribosomal protein L15, mitochondrial



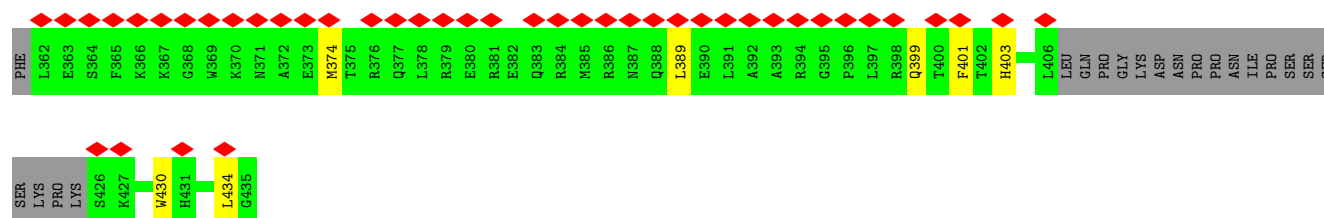
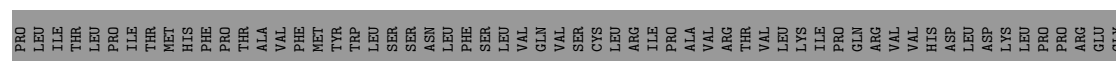
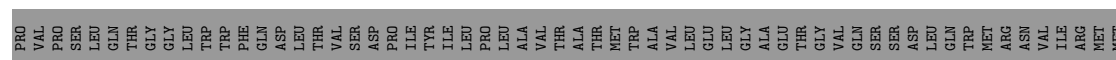
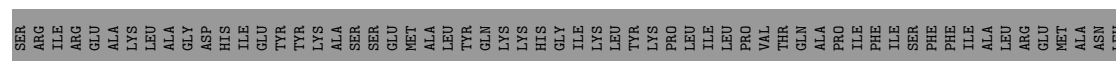
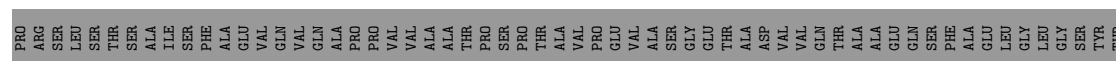
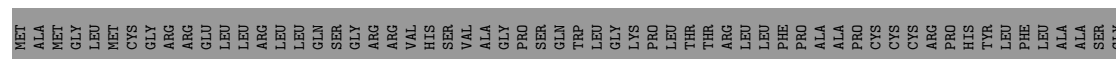
- Molecule 56: 39S ribosomal protein L16, mitochondrial



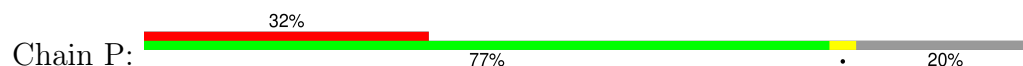
- Molecule 57: 39S ribosomal protein L17, mitochondrial

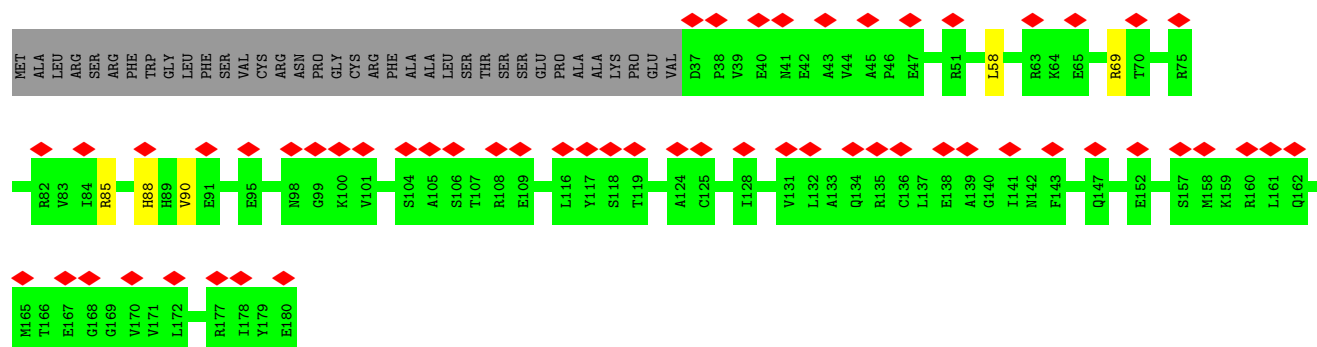


- Molecule 58: Mitochondrial inner membrane protein OXA1L

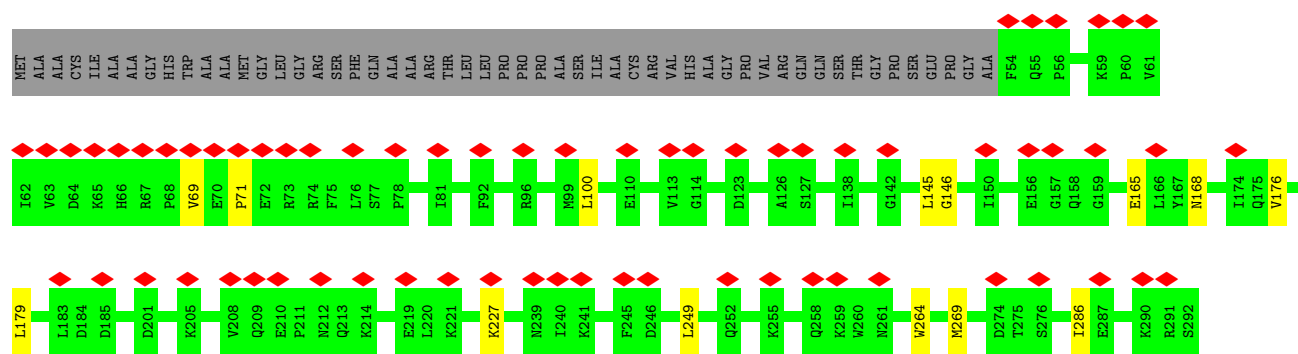
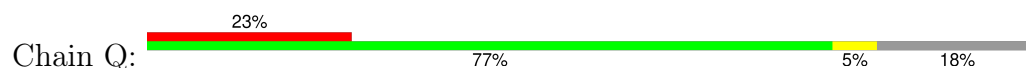


- Molecule 59: 39S ribosomal protein L18, mitochondrial

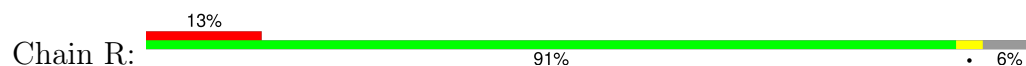




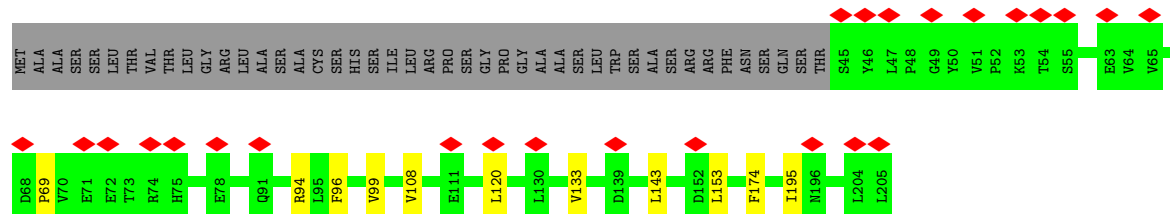
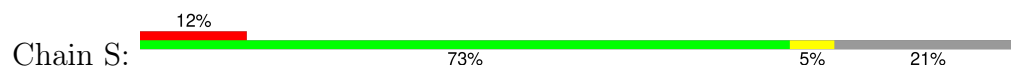
- Molecule 60: 39S ribosomal protein L19, mitochondrial



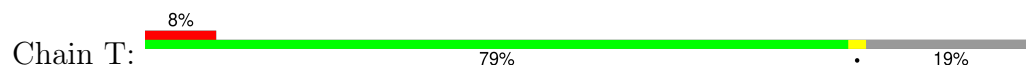
- Molecule 61: 39S ribosomal protein L20, mitochondrial

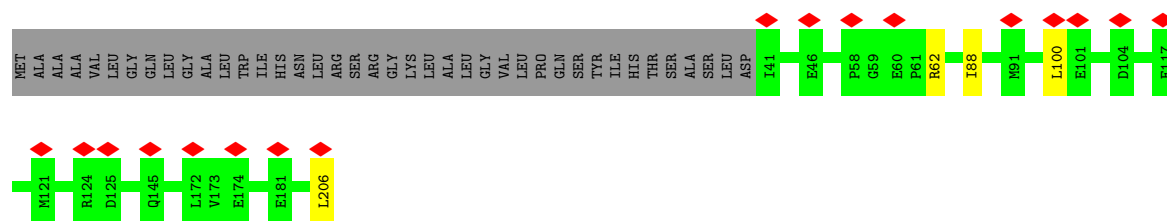


- Molecule 62: 39S ribosomal protein L21, mitochondrial

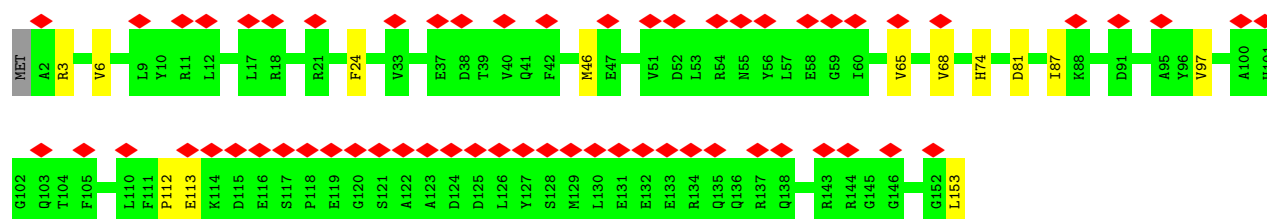
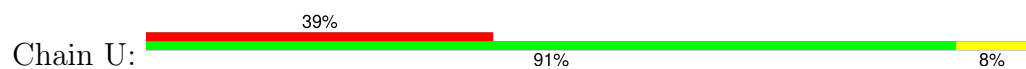


- Molecule 63: 39S ribosomal protein L22, mitochondrial

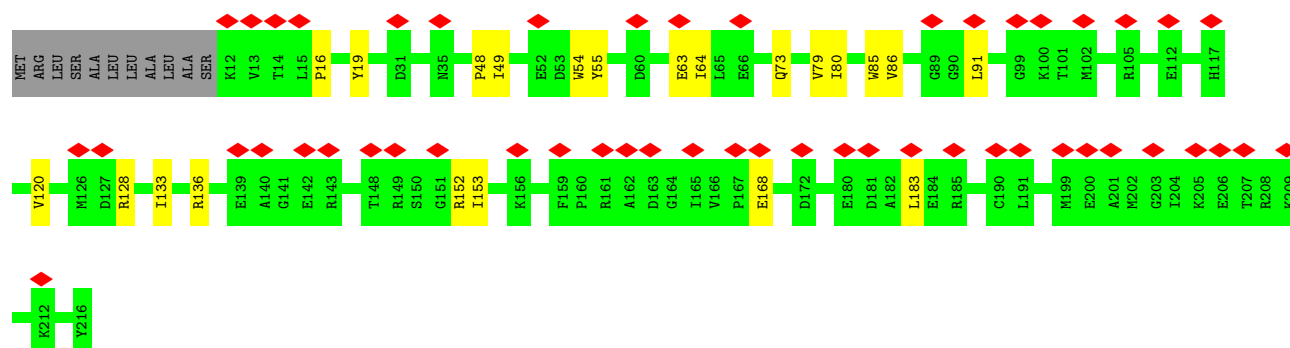
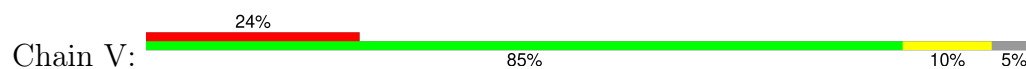




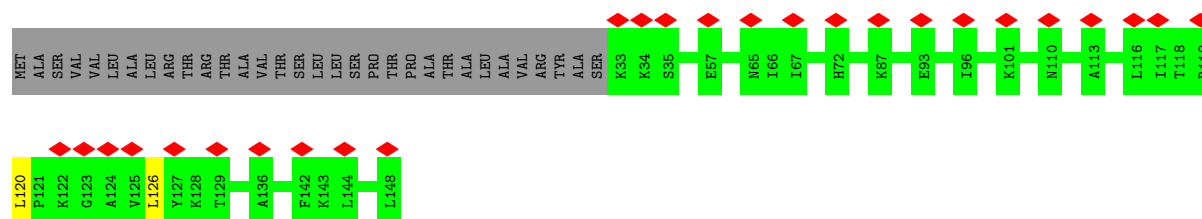
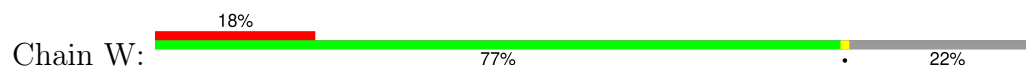
- Molecule 64: 39S ribosomal protein L23, mitochondrial



- Molecule 65: 39S ribosomal protein L24, mitochondrial



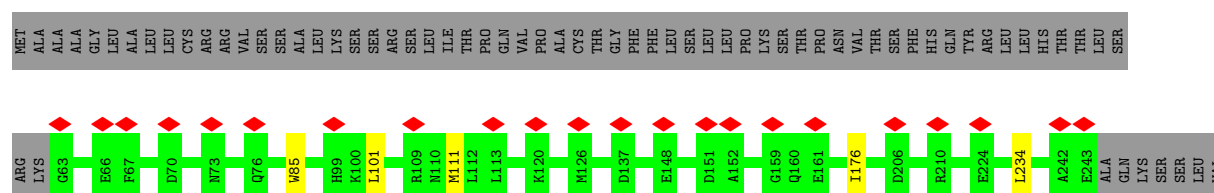
- Molecule 66: 39S ribosomal protein L27, mitochondrial



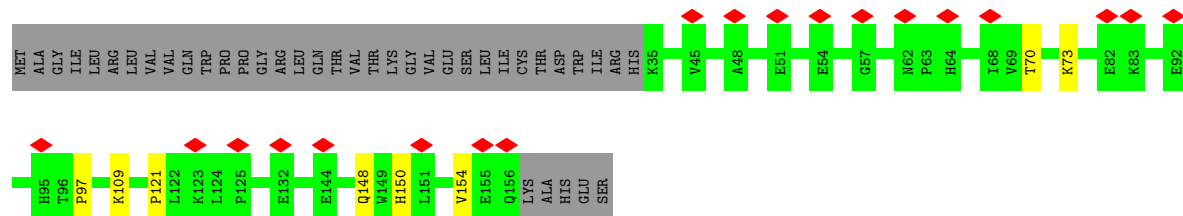
- Molecule 67: 39S ribosomal protein L28, mitochondrial



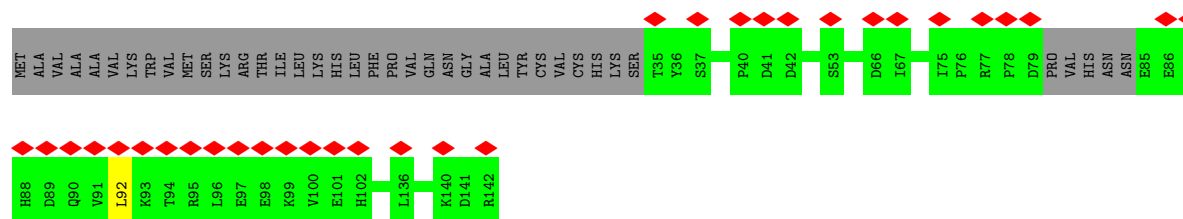
- Molecule 68: 39S ribosomal protein L47, mitochondrial



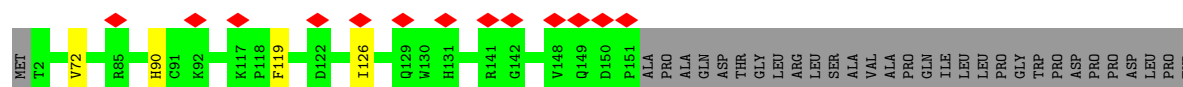
- Molecule 69: 39S ribosomal protein L30, mitochondrial



- Molecule 70: 39S ribosomal protein L42, mitochondrial

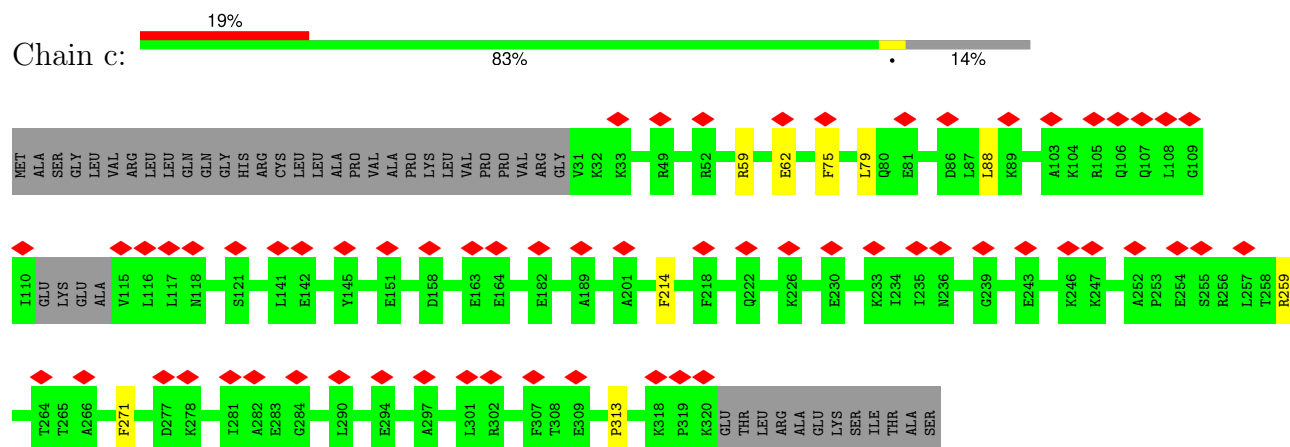


- Molecule 71: 39S ribosomal protein L43, mitochondrial

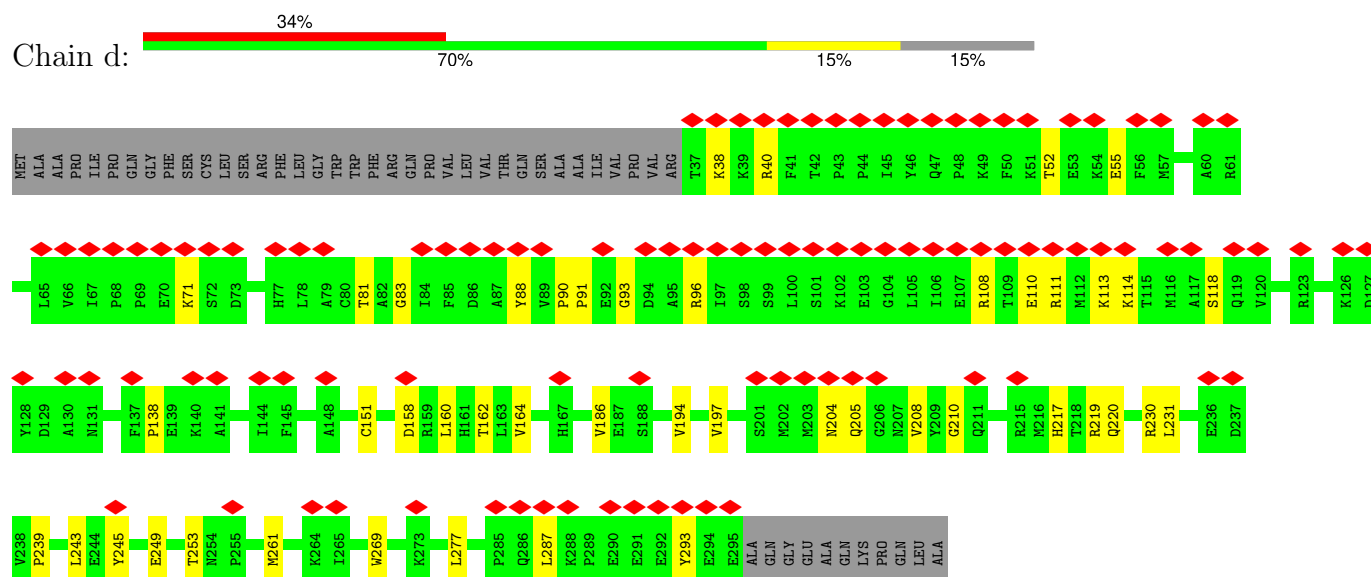


VAL ASP
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ALA
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MET
LEU
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SER
VAL
SER
SER
CYS
LEU
PRO
ILE
VAL
PRO
ALA
LEU
THR
VAL
CYS
SER
ALA

- Molecule 72: 39S ribosomal protein L44, mitochondrial



- Molecule 73: 39S ribosomal protein L45, mitochondrial



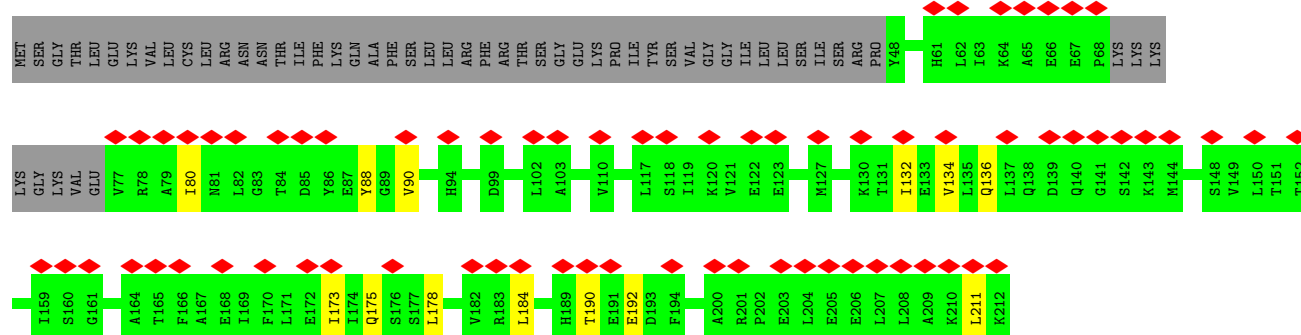
- Molecule 74: 39S ribosomal protein L46, mitochondrial





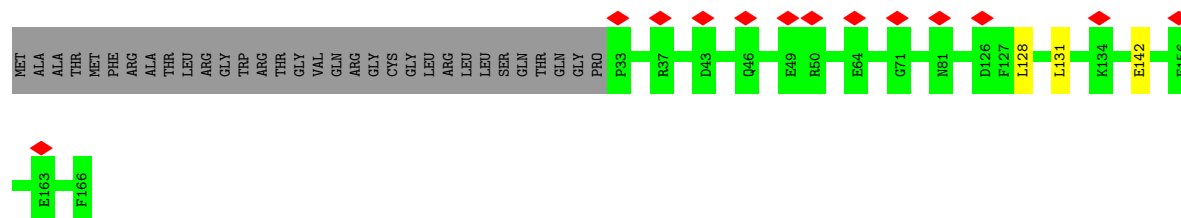
- Molecule 75: 39S ribosomal protein L48, mitochondrial

Chain f: 33% 68% 6% 26%



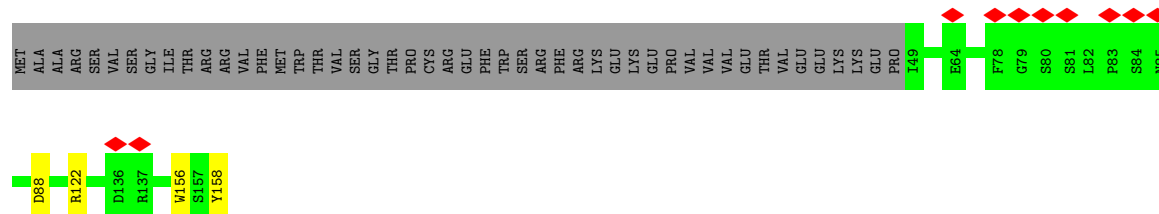
- Molecule 76: 39S ribosomal protein L49, mitochondrial

Chain g: 8% 79% 19%



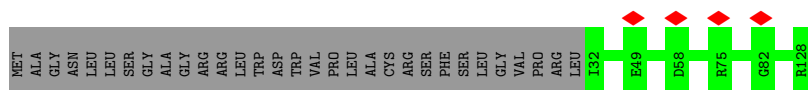
- Molecule 77: 39S ribosomal protein L50, mitochondrial

Chain h: 6% 67% 30%

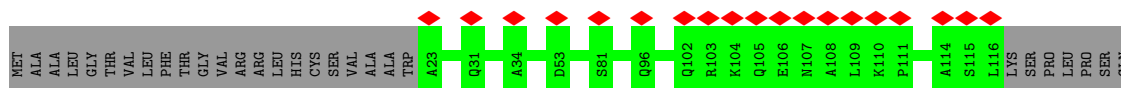
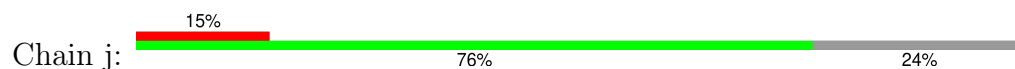


- Molecule 78: 39S ribosomal protein L51, mitochondrial

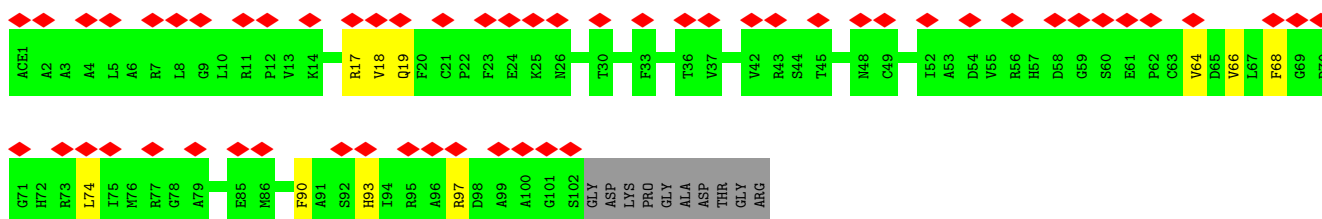
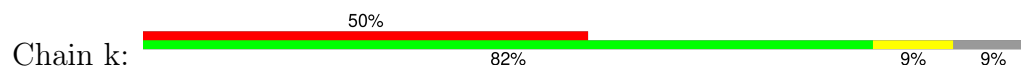
Chain i: 76% 24%



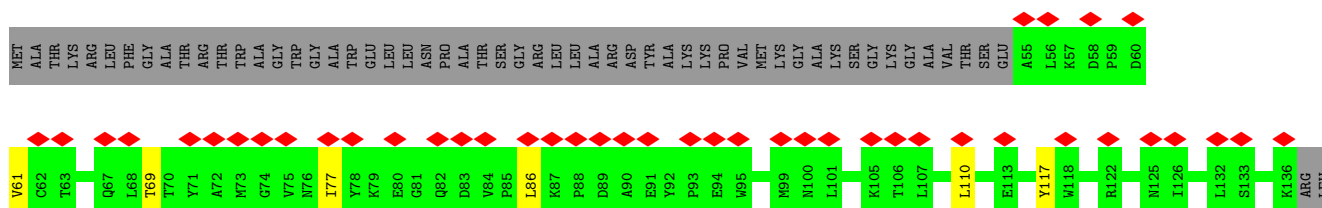
- Molecule 79: 39S ribosomal protein L52, mitochondrial



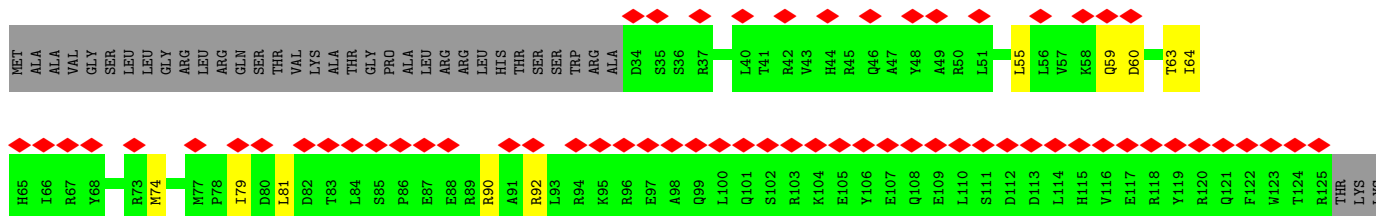
- Molecule 80: Large ribosomal subunit protein mL53



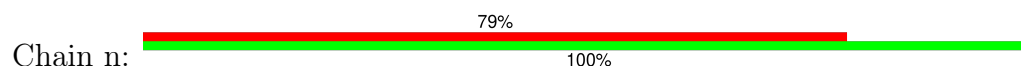
- Molecule 81: 39S ribosomal protein L54, mitochondrial

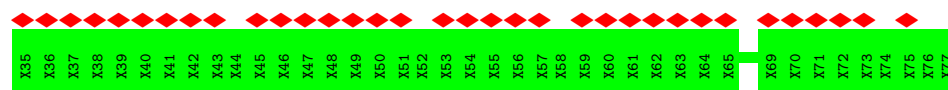


- Molecule 82: 39S ribosomal protein L55, mitochondrial

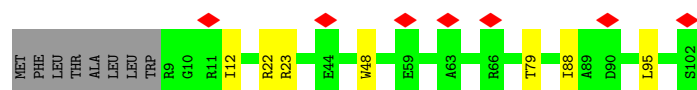
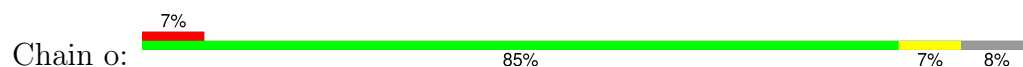


- Molecule 83: Nascent polypeptide

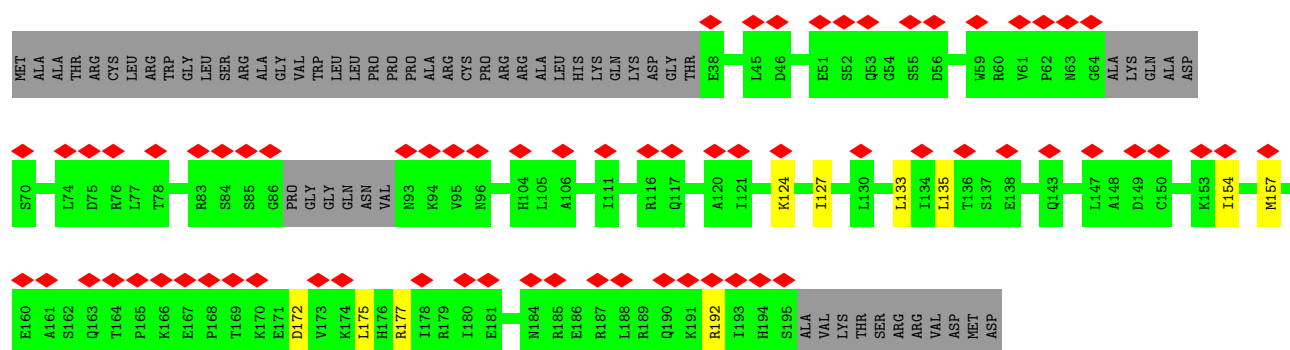




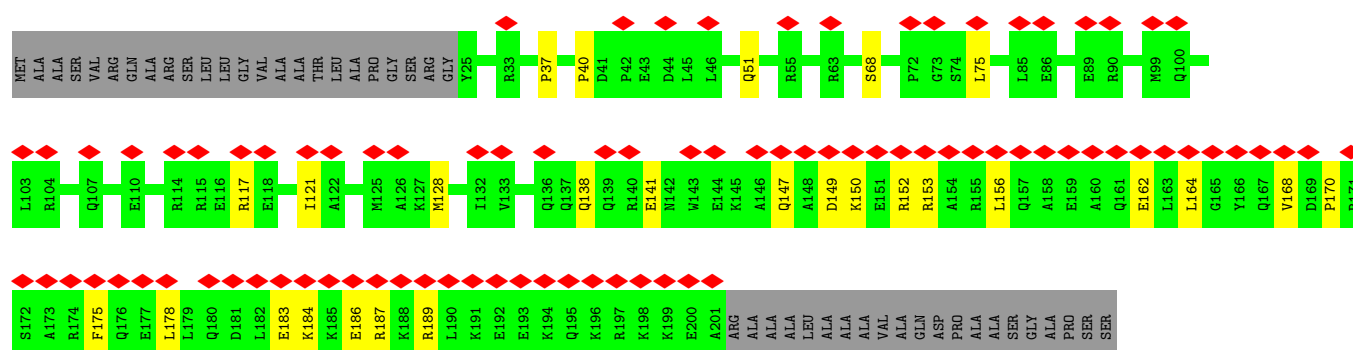
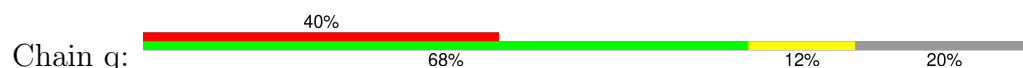
- Molecule 84: Ribosomal protein 63, mitochondrial



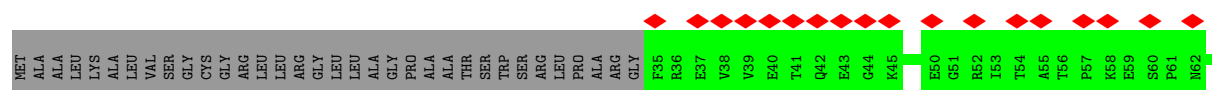
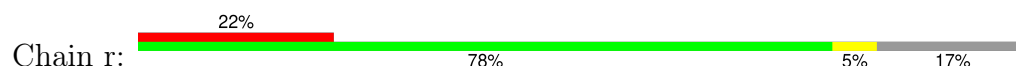
- Molecule 85: Peptidyl-tRNA hydrolase ICT1, mitochondrial

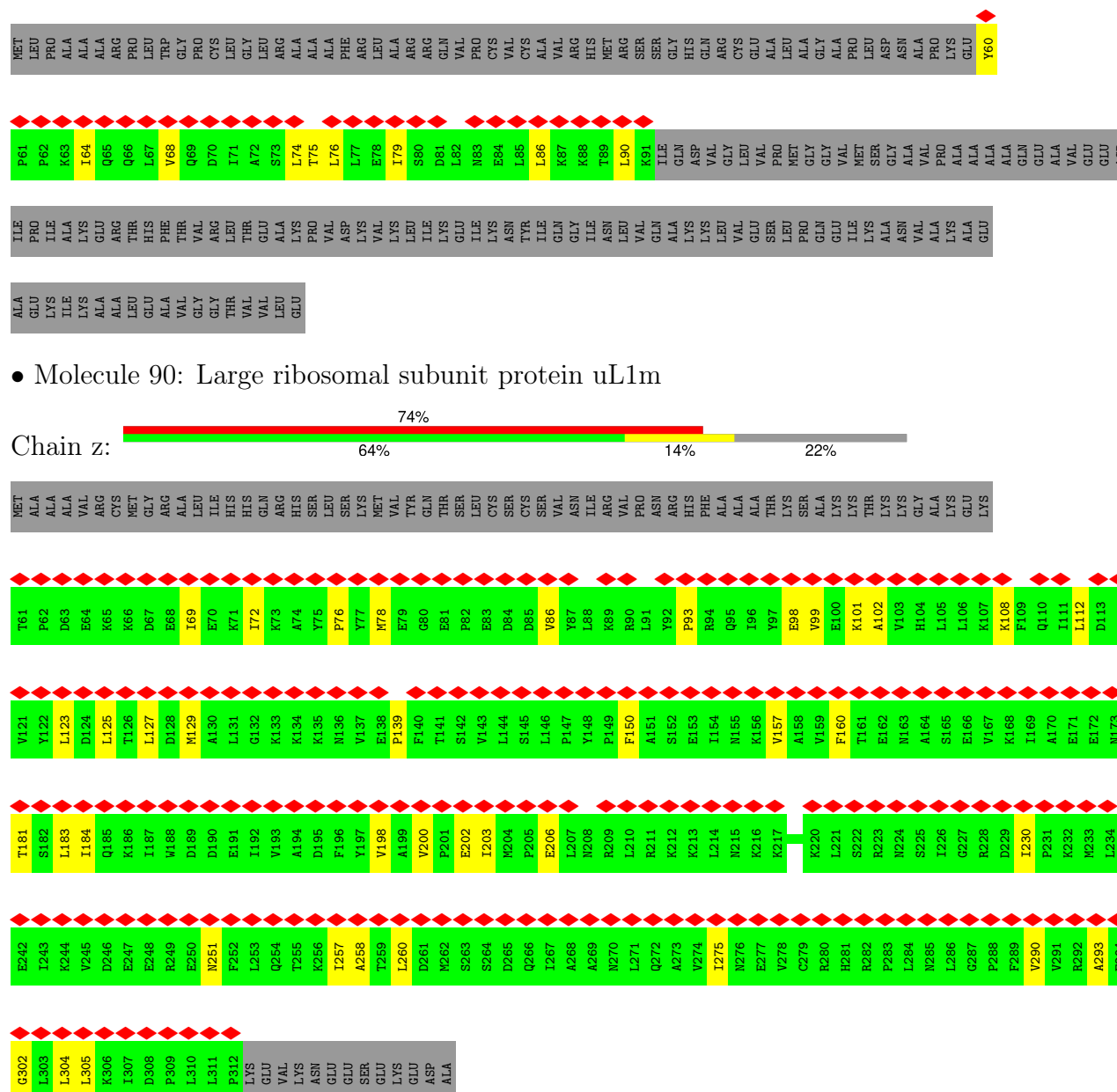


- Molecule 86: Growth arrest and DNA damage-inducible proteins-interacting protein 1



- Molecule 87: 39S ribosomal protein S18a, mitochondrial





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10517	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.029	Depositor
Map size (Å)	512.63995, 512.63995, 512.63995	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	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: 2MG, SPM, GDP, 5MU, ACE, PSU, NAD, SPD, 5MC, MG, ATP, 1MA, FES, PUT, ZN, OMG, B8T, K, MA6, OMU

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	0	0.15	0/913	0.30	0/1224
2	1	0.14	0/469	0.26	0/621
3	2	0.15	0/383	0.26	0/507
4	3	0.16	0/853	0.25	0/1136
5	4	0.15	0/350	0.22	0/461
6	5	0.14	0/3305	0.28	0/4502
7	6	0.13	0/3043	0.28	0/4140
8	7	0.14	0/2447	0.30	0/3310
9	8	0.15	0/1354	0.35	0/1819
10	9	0.13	0/1025	0.26	0/1379
11	A	0.17	0/36876	0.30	0/57402
12	A0	0.14	0/1834	0.29	0/2484
13	A1	0.13	0/2313	0.29	0/3129
14	A2	0.13	0/947	0.27	0/1266
15	A3	0.12	0/636	0.25	0/839
16	A4	0.14	0/4877	0.32	0/6598
17	AA	0.17	0/22537	0.29	0/35085
18	AB	0.13	0/1871	0.26	0/2531
19	AC	0.14	0/1113	0.27	0/1505
20	AD	0.13	0/2783	0.25	0/3724
21	AE	0.13	0/989	0.28	0/1335
22	AF	0.12	0/1767	0.25	0/2373
23	AG	0.13	0/2746	0.27	0/3681
24	AH	0.14	0/1178	0.29	0/1598
25	AI	0.12	0/1039	0.26	0/1400
26	AJ	0.12	0/855	0.27	0/1148
27	AK	0.13	0/880	0.26	0/1182
28	AL	0.12	0/1477	0.23	0/1974
29	AM	0.14	0/963	0.31	0/1295
30	AN	0.14	0/886	0.30	0/1199
31	AO	0.13	0/1648	0.30	0/2243

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	AP	0.13	0/798	0.26	0/1070
33	AQ	0.11	0/754	0.24	0/1003
34	AR	0.13	0/2456	0.30	0/3317
35	AS	0.11	0/1138	0.22	0/1533
36	AT	0.12	0/1402	0.27	0/1883
37	AU	0.14	0/1510	0.27	0/2025
38	AV	0.15	0/3030	0.34	0/4093
39	AW	0.12	0/801	0.26	0/1079
40	AX	0.14	0/2921	0.33	0/3954
41	AY	0.12	0/1040	0.26	0/1402
42	AZ	0.12	0/857	0.30	0/1141
43	Aw	0.16	0/1600	0.39	0/2476
44	Ax	0.18	0/1654	0.40	0/2565
45	Az	0.16	0/804	0.37	0/1248
46	B	0.14	0/1626	0.27	0/2523
47	D	0.14	0/1896	0.27	0/2549
48	E	0.15	0/2475	0.30	0/3355
49	F	0.16	0/2090	0.29	0/2842
50	H	0.12	0/1698	0.29	0/2292
51	I	0.14	0/1478	0.33	0/1999
52	J	0.14	0/1348	0.30	0/1813
53	K	0.16	0/1497	0.26	0/2031
54	L	0.13	0/905	0.27	0/1218
55	M	0.16	0/2381	0.28	0/3212
56	N	0.16	0/1833	0.27	0/2468
57	O	0.15	0/1283	0.27	0/1727
58	OX	0.16	0/478	0.43	0/639
59	P	0.13	0/1199	0.26	0/1623
60	Q	0.13	0/2039	0.26	0/2750
61	R	0.15	0/1175	0.26	0/1572
62	S	0.16	0/1320	0.29	0/1789
63	T	0.14	0/1403	0.26	0/1886
64	U	0.15	0/1279	0.32	0/1730
65	V	0.14	0/1721	0.27	0/2333
66	W	0.16	0/926	0.26	0/1244
67	X	0.13	0/2099	0.25	0/2837
68	Y	0.14	0/1593	0.25	0/2136
69	Z	0.17	0/1021	0.28	0/1378
70	a	0.14	0/891	0.32	0/1208
71	b	0.16	0/1218	0.29	0/1649
72	c	0.13	0/2347	0.27	0/3171
73	d	0.14	0/2181	0.33	0/2949
74	e	0.14	0/1970	0.34	0/2658

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	f	0.14	0/1273	0.34	0/1716
76	g	0.14	0/1151	0.27	0/1569
77	h	0.12	0/918	0.25	0/1249
78	i	0.16	0/850	0.28	0/1135
79	j	0.14	0/760	0.24	0/1023
80	k	0.11	0/783	0.24	0/1057
81	l	0.12	0/707	0.31	0/960
82	m	0.11	0/805	0.33	0/1081
84	o	0.15	0/819	0.26	0/1097
85	p	0.12	0/1223	0.25	0/1641
86	q	0.13	0/1529	0.28	0/2055
87	r	0.14	0/1362	0.28	0/1846
88	s	0.15	0/3231	0.29	0/4389
89	t	0.15	0/358	0.33	0/486
89	u	0.20	0/259	0.44	0/350
90	z	0.14	0/2067	0.36	0/2793
All	All	0.15	0/188587	0.29	0/267907

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
25	AI	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	AI	183	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	898	0	916	3	0
2	1	464	0	511	4	0
3	2	377	0	406	1	0
4	3	832	0	883	4	0
5	4	342	0	361	1	0
6	5	3210	0	3206	10	0
7	6	2948	0	2841	12	0
8	7	2390	0	2397	15	0
9	8	1327	0	1368	25	0
10	9	997	0	987	8	0
11	A	33070	0	16793	203	0
12	A0	1787	0	1796	19	0
13	A1	2265	0	2294	16	0
14	A2	935	0	971	5	0
15	A3	625	0	699	3	0
16	A4	4768	0	4766	47	0
17	AA	20260	0	10288	399	0
18	AB	1828	0	1815	7	0
19	AC	1083	0	1088	11	0
20	AD	2731	0	2804	15	0
21	AE	972	0	1000	10	0
22	AF	1725	0	1769	13	0
23	AG	2688	0	2687	19	0
24	AH	1152	0	1183	24	0
25	AI	1019	0	1059	4	0
26	AJ	839	0	887	3	0
27	AK	862	0	885	5	0
28	AL	1453	0	1540	12	0
29	AM	942	0	965	10	0
30	AN	868	0	928	8	0
31	AO	1592	0	1557	12	0
32	AP	781	0	806	5	0
33	AQ	744	0	758	1	0
34	AR	2409	0	2428	20	0
35	AS	1111	0	1115	4	0
36	AT	1371	0	1393	4	0
37	AU	1488	0	1499	12	0
38	AV	2969	0	2961	29	0
39	AW	789	0	802	6	0
40	AX	2849	0	2843	34	0
41	AY	1010	0	957	2	0
42	AZ	839	0	858	4	0
43	Aw	1434	0	728	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Ax	1482	0	753	30	0
45	Az	719	0	360	3	0
46	B	1524	0	779	13	0
47	D	1859	0	1919	7	0
48	E	2406	0	2415	11	0
49	F	2031	0	2065	5	0
50	H	1661	0	1734	22	0
51	I	1446	0	1532	11	0
52	J	1330	0	1407	12	0
53	K	1455	0	1452	6	0
54	L	890	0	941	2	0
55	M	2327	0	2395	12	0
56	N	1786	0	1817	11	0
57	O	1259	0	1294	8	0
58	OX	468	0	464	7	0
59	P	1173	0	1165	4	0
60	Q	1990	0	2031	9	0
61	R	1154	0	1214	5	0
62	S	1293	0	1365	8	0
63	T	1369	0	1410	5	0
64	U	1248	0	1228	9	0
65	V	1676	0	1687	14	0
66	W	904	0	934	1	0
67	X	2044	0	2060	7	0
68	Y	1556	0	1597	5	0
69	Z	996	0	1044	6	0
70	a	865	0	829	1	0
71	b	1193	0	1191	4	0
72	c	2299	0	2320	5	0
73	d	2124	0	2125	30	0
74	e	1931	0	1916	27	0
75	f	1252	0	1269	11	0
76	g	1113	0	1097	2	0
77	h	895	0	881	2	0
78	i	828	0	857	0	0
79	j	745	0	746	0	0
80	k	774	0	784	6	0
81	l	688	0	674	5	0
82	m	791	0	796	9	0
83	n	215	0	52	0	0
84	o	798	0	804	7	0
85	p	1205	0	1223	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	q	1495	0	1492	18	0
87	r	1322	0	1348	8	0
88	s	3148	0	3131	13	0
89	t	354	0	377	1	0
89	u	257	0	283	7	0
90	z	2027	0	2076	30	0
91	0	1	0	0	0	0
91	4	1	0	0	0	0
91	AO	1	0	0	0	0
92	6	1	0	0	0	0
92	A	29	0	0	0	0
92	AA	17	0	0	0	0
92	D	1	0	0	0	0
92	M	1	0	0	0	0
92	N	1	0	0	0	0
92	W	1	0	0	0	0
92	o	1	0	0	0	0
93	A	40	0	76	0	0
93	AA	20	0	38	0	0
93	O	10	0	19	0	0
94	A	6	0	12	0	0
95	A	138	0	0	0	0
95	A3	1	0	0	0	0
95	AA	60	0	0	0	0
95	AB	1	0	0	0	0
95	AX	1	0	0	0	0
95	D	2	0	0	0	0
95	g	1	0	0	0	0
96	AA	44	0	26	2	0
97	AA	28	0	52	1	0
98	AP	4	0	0	0	0
98	AT	4	0	0	0	0
98	r	4	0	0	0	0
99	AX	31	0	12	0	0
100	AX	28	0	12	2	0
101	B	7	0	8	4	0
All	All	179893	0	152386	1326	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 1326 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:57:ASP:HB2	43:Aw:23:A:H1'	1.62	0.81
17:AA:1528:A:H2'	17:AA:1529:A:H8	1.47	0.80
12:A0:99:ARG:HD3	17:AA:1526:U:H2'	1.64	0.79
17:AA:1197:G:H1	17:AA:1425:U:H3	1.33	0.76
17:AA:976:A:H5''	33:AQ:1:ACE:H1	1.68	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	108/188 (57%)	108 (100%)	0	0	100	100
2	1	54/65 (83%)	54 (100%)	0	0	100	100
3	2	44/92 (48%)	44 (100%)	0	0	100	100
4	3	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
5	4	36/103 (35%)	36 (100%)	0	0	100	100
6	5	392/423 (93%)	387 (99%)	5 (1%)	0	100	100
7	6	352/380 (93%)	342 (97%)	10 (3%)	0	100	100
8	7	292/338 (86%)	283 (97%)	9 (3%)	0	100	100
9	8	155/206 (75%)	150 (97%)	5 (3%)	0	100	100
10	9	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
12	A0	213/217 (98%)	204 (96%)	9 (4%)	0	100	100
13	A1	277/323 (86%)	266 (96%)	11 (4%)	0	100	100
14	A2	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
15	A3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
16	A4	584/689 (85%)	568 (97%)	16 (3%)	0	100	100
18	AB	223/296 (75%)	216 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AC	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
20	AD	341/430 (79%)	331 (97%)	10 (3%)	0	100	100
21	AE	120/125 (96%)	117 (98%)	3 (2%)	0	100	100
22	AF	206/242 (85%)	203 (98%)	3 (2%)	0	100	100
23	AG	323/396 (82%)	314 (97%)	9 (3%)	0	100	100
24	AH	138/201 (69%)	132 (96%)	5 (4%)	1 (1%)	18	49
25	AI	135/194 (70%)	130 (96%)	5 (4%)	0	100	100
26	AJ	106/138 (77%)	105 (99%)	1 (1%)	0	100	100
27	AK	99/128 (77%)	99 (100%)	0	0	100	100
28	AL	172/257 (67%)	170 (99%)	2 (1%)	0	100	100
29	AM	117/137 (85%)	113 (97%)	4 (3%)	0	100	100
30	AN	108/130 (83%)	103 (95%)	5 (5%)	0	100	100
31	AO	191/258 (74%)	184 (96%)	7 (4%)	0	100	100
32	AP	95/142 (67%)	94 (99%)	1 (1%)	0	100	100
33	AQ	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
34	AR	293/360 (81%)	285 (97%)	8 (3%)	0	100	100
35	AS	133/190 (70%)	133 (100%)	0	0	100	100
36	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
37	AU	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
38	AV	358/414 (86%)	348 (97%)	10 (3%)	0	100	100
39	AW	98/187 (52%)	95 (97%)	3 (3%)	0	100	100
40	AX	350/398 (88%)	341 (97%)	9 (3%)	0	100	100
41	AY	117/395 (30%)	116 (99%)	1 (1%)	0	100	100
42	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
47	D	236/305 (77%)	229 (97%)	7 (3%)	0	100	100
48	E	303/348 (87%)	294 (97%)	9 (3%)	0	100	100
49	F	250/311 (80%)	247 (99%)	3 (1%)	0	100	100
50	H	200/267 (75%)	194 (97%)	6 (3%)	0	100	100
51	I	179/261 (69%)	176 (98%)	3 (2%)	0	100	100
52	J	173/192 (90%)	171 (99%)	2 (1%)	0	100	100
53	K	176/178 (99%)	173 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	L	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
55	M	289/296 (98%)	283 (98%)	6 (2%)	0	100	100
56	N	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
57	O	152/175 (87%)	146 (96%)	6 (4%)	0	100	100
58	OX	51/435 (12%)	48 (94%)	3 (6%)	0	100	100
59	P	142/180 (79%)	139 (98%)	3 (2%)	0	100	100
60	Q	237/292 (81%)	234 (99%)	3 (1%)	0	100	100
61	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
62	S	159/205 (78%)	155 (98%)	4 (2%)	0	100	100
63	T	164/206 (80%)	162 (99%)	2 (1%)	0	100	100
64	U	150/153 (98%)	148 (99%)	2 (1%)	0	100	100
65	V	203/216 (94%)	200 (98%)	3 (2%)	0	100	100
66	W	114/148 (77%)	112 (98%)	2 (2%)	0	100	100
67	X	242/256 (94%)	239 (99%)	3 (1%)	0	100	100
68	Y	179/250 (72%)	174 (97%)	5 (3%)	0	100	100
69	Z	120/161 (74%)	118 (98%)	2 (2%)	0	100	100
70	a	99/142 (70%)	98 (99%)	1 (1%)	0	100	100
71	b	148/215 (69%)	143 (97%)	5 (3%)	0	100	100
72	c	282/332 (85%)	278 (99%)	4 (1%)	0	100	100
73	d	257/306 (84%)	240 (93%)	17 (7%)	0	100	100
74	e	236/279 (85%)	228 (97%)	8 (3%)	0	100	100
75	f	153/212 (72%)	146 (95%)	7 (5%)	0	100	100
76	g	132/166 (80%)	130 (98%)	2 (2%)	0	100	100
77	h	108/158 (68%)	104 (96%)	4 (4%)	0	100	100
78	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
79	j	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
80	k	100/112 (89%)	99 (99%)	1 (1%)	0	100	100
81	l	80/138 (58%)	77 (96%)	3 (4%)	0	100	100
82	m	90/128 (70%)	87 (97%)	3 (3%)	0	100	100
84	o	92/102 (90%)	90 (98%)	2 (2%)	0	100	100
85	p	141/206 (68%)	139 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
86	q	175/222 (79%)	175 (100%)	0	0	100	100
87	r	160/196 (82%)	159 (99%)	1 (1%)	0	100	100
88	s	381/439 (87%)	374 (98%)	7 (2%)	0	100	100
89	t	44/198 (22%)	44 (100%)	0	0	100	100
89	u	30/198 (15%)	30 (100%)	0	0	100	100
90	z	250/325 (77%)	236 (94%)	14 (6%)	0	100	100
All	All	14617/19127 (76%)	14271 (98%)	345 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	AH	126	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	99/164 (60%)	99 (100%)	0	100	100
2	1	53/60 (88%)	53 (100%)	0	100	100
3	2	40/72 (56%)	40 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	37/89 (42%)	37 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100
7	6	313/332 (94%)	313 (100%)	0	100	100
8	7	270/303 (89%)	270 (100%)	0	100	100
9	8	146/190 (77%)	146 (100%)	0	100	100
10	9	104/112 (93%)	104 (100%)	0	100	100
12	A0	188/189 (100%)	188 (100%)	0	100	100
13	A1	257/291 (88%)	257 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	A2	100/100 (100%)	100 (100%)	0	100	100
15	A3	65/166 (39%)	65 (100%)	0	100	100
16	A4	526/609 (86%)	526 (100%)	0	100	100
18	AB	198/249 (80%)	198 (100%)	0	100	100
19	AC	115/143 (80%)	115 (100%)	0	100	100
20	AD	286/357 (80%)	286 (100%)	0	100	100
21	AE	104/107 (97%)	104 (100%)	0	100	100
22	AF	185/209 (88%)	185 (100%)	0	100	100
23	AG	285/342 (83%)	285 (100%)	0	100	100
24	AH	130/180 (72%)	130 (100%)	0	100	100
25	AI	105/147 (71%)	105 (100%)	0	100	100
26	AJ	93/118 (79%)	93 (100%)	0	100	100
27	AK	91/113 (80%)	91 (100%)	0	100	100
28	AL	158/226 (70%)	158 (100%)	0	100	100
29	AM	97/113 (86%)	97 (100%)	0	100	100
30	AN	96/115 (84%)	96 (100%)	0	100	100
31	AO	174/230 (76%)	173 (99%)	1 (1%)	78	81
32	AP	88/123 (72%)	88 (100%)	0	100	100
33	AQ	78/78 (100%)	78 (100%)	0	100	100
34	AR	264/318 (83%)	264 (100%)	0	100	100
35	AS	116/164 (71%)	116 (100%)	0	100	100
36	AT	153/157 (98%)	153 (100%)	0	100	100
37	AU	152/174 (87%)	152 (100%)	0	100	100
38	AV	325/364 (89%)	325 (100%)	0	100	100
39	AW	87/158 (55%)	87 (100%)	0	100	100
40	AX	311/351 (89%)	311 (100%)	0	100	100
41	AY	110/357 (31%)	110 (100%)	0	100	100
42	AZ	90/95 (95%)	90 (100%)	0	100	100
47	D	192/245 (78%)	192 (100%)	0	100	100
48	E	260/290 (90%)	260 (100%)	0	100	100
49	F	219/262 (84%)	219 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	H	182/228 (80%)	182 (100%)	0	100	100
51	I	165/232 (71%)	165 (100%)	0	100	100
52	J	138/150 (92%)	138 (100%)	0	100	100
53	K	155/155 (100%)	155 (100%)	0	100	100
54	L	98/124 (79%)	98 (100%)	0	100	100
55	M	246/249 (99%)	246 (100%)	0	100	100
56	N	189/211 (90%)	189 (100%)	0	100	100
57	O	134/150 (89%)	134 (100%)	0	100	100
58	OX	49/372 (13%)	49 (100%)	0	100	100
59	P	126/155 (81%)	126 (100%)	0	100	100
60	Q	221/256 (86%)	221 (100%)	0	100	100
61	R	118/126 (94%)	118 (100%)	0	100	100
62	S	146/180 (81%)	146 (100%)	0	100	100
63	T	146/176 (83%)	146 (100%)	0	100	100
64	U	134/135 (99%)	134 (100%)	0	100	100
65	V	183/191 (96%)	183 (100%)	0	100	100
66	W	94/119 (79%)	94 (100%)	0	100	100
67	X	220/229 (96%)	220 (100%)	0	100	100
68	Y	163/223 (73%)	163 (100%)	0	100	100
69	Z	113/147 (77%)	113 (100%)	0	100	100
70	a	99/133 (74%)	99 (100%)	0	100	100
71	b	132/186 (71%)	132 (100%)	0	100	100
72	c	251/288 (87%)	251 (100%)	0	100	100
73	d	237/274 (86%)	237 (100%)	0	100	100
74	e	207/236 (88%)	207 (100%)	0	100	100
75	f	139/188 (74%)	139 (100%)	0	100	100
76	g	124/148 (84%)	124 (100%)	0	100	100
77	h	104/148 (70%)	104 (100%)	0	100	100
78	i	86/110 (78%)	86 (100%)	0	100	100
79	j	74/97 (76%)	74 (100%)	0	100	100
80	k	83/89 (93%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
81	l	76/116 (66%)	76 (100%)	0	100	100
82	m	85/113 (75%)	85 (100%)	0	100	100
84	o	80/87 (92%)	80 (100%)	0	100	100
85	p	135/181 (75%)	135 (100%)	0	100	100
86	q	153/178 (86%)	153 (100%)	0	100	100
87	r	147/169 (87%)	147 (100%)	0	100	100
88	s	339/381 (89%)	339 (100%)	0	100	100
89	t	40/158 (25%)	40 (100%)	0	100	100
89	u	31/158 (20%)	31 (100%)	0	100	100
90	z	226/287 (79%)	226 (100%)	0	100	100
All	All	13069/16529 (79%)	13068 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	AO	154	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
50	H	196	ASN
72	c	168	HIS
53	K	117	HIS
68	Y	88	GLN
76	g	93	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1556/1558 (99%)	274 (17%)	2 (0%)
17	AA	953/954 (99%)	176 (18%)	1 (0%)
43	Aw	64/76 (84%)	30 (46%)	0
44	Ax	67/76 (88%)	27 (40%)	0
45	Az	33/34 (97%)	14 (42%)	0
46	B	70/72 (97%)	15 (21%)	0
All	All	2743/2770 (99%)	536 (19%)	3 (0%)

5 of 536 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1681	G
11	A	1685	C
11	A	1689	C
11	A	1692	A
11	A	1699	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	2245	A
11	A	2484	C
17	AA	828	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

13 non-standard protein/DNA/RNA residues are modelled in this entry.

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
11	PSU	A	3067	11	18,21,22	1.07	2 (11%)	21,30,33	0.79	1 (4%)
17	5MU	AA	1076	17	19,22,23	0.41	0	27,32,35	0.68	0
11	OMG	A	2815	92,11	23,26,27	0.34	0	32,38,41	0.40	0
17	MA6	AA	1584	17	23,26,27	0.31	0	33,38,41	0.74	1 (3%)
46	1MA	B	9	46	21,25,26	0.38	0	30,37,40	0.65	0
46	PSU	B	39	46	18,21,22	1.03	1 (5%)	21,30,33	0.71	0
11	OMU	A	3039	92,11	19,22,23	0.32	0	25,31,34	0.75	1 (4%)
17	B8T	AA	1486	17,95	19,22,23	0.39	0	25,31,34	0.31	0
46	2MG	B	10	46	23,26,27	0.36	0	33,38,41	0.40	0
17	MA6	AA	1583	17	23,26,27	0.32	0	33,38,41	0.73	1 (3%)
11	OMG	A	3040	11	23,26,27	0.34	0	32,38,41	0.41	0
17	5MC	AA	1488	17	19,22,23	0.82	1 (5%)	26,32,35	0.49	0
11	1MA	A	2617	11	21,25,26	0.39	0	30,37,40	0.59	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PSU	A	3067	11	-	0/7/25/26	0/2/2/2
17	5MU	AA	1076	17	-	5/7/25/26	0/2/2/2
11	OMG	A	2815	92,11	-	0/9/27/28	0/3/3/3
17	MA6	AA	1584	17	-	1/11/29/30	0/3/3/3
46	1MA	B	9	46	-	0/7/25/26	0/3/3/3
46	PSU	B	39	46	-	0/7/25/26	0/2/2/2
11	OMU	A	3039	92,11	-	0/9/27/28	0/2/2/2
17	B8T	AA	1486	17,95	-	0/7/27/28	0/2/2/2
46	2MG	B	10	46	-	0/9/27/28	0/3/3/3
17	MA6	AA	1583	17	-	0/11/29/30	0/3/3/3
11	OMG	A	3040	11	-	0/9/27/28	0/3/3/3
17	5MC	AA	1488	17	-	0/7/25/26	0/2/2/2
11	1MA	A	2617	11	-	0/7/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	B	39	PSU	C6-C5	3.66	1.39	1.35
11	A	3067	PSU	C6-C5	3.63	1.39	1.35
17	AA	1488	5MC	C5-C4	-3.19	1.41	1.44
11	A	3067	PSU	O4'-C1'	-2.22	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AA	1583	MA6	C2-N1-C6	2.95	119.04	111.83
17	AA	1584	MA6	C2-N1-C6	2.92	118.97	111.83
11	A	3039	OMU	C2'-C1'-N1	-2.72	109.07	114.24
11	A	3067	PSU	O4'-C1'-C2'	2.41	108.49	105.15

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	AA	1076	5MU	C3'-C4'-C5'-O5'
17	AA	1076	5MU	O4'-C4'-C5'-O5'
17	AA	1584	MA6	C4'-C5'-O5'-P
17	AA	1076	5MU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
17	AA	1076	5MU	C2'-C1'-N1-C2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	3067	PSU	1	0
17	AA	1076	5MU	2	0
17	AA	1486	B8T	1	0
17	AA	1583	MA6	2	0
17	AA	1488	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 276 ligands modelled in this entry, 259 are monoatomic - leaving 17 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	$\# Z > 2$
101	VAL	B	101	46	4,6,7	0.82	0	6,7,9	1.02	1 (16%)
93	SPD	AA	1782	-	9,9,9	0.15	0	8,8,8	0.17	0
99	ATP	AX	501	95	32,33,33	0.49	0	48,52,52	0.34	0
93	SPD	O	301	-	9,9,9	0.15	0	8,8,8	0.19	0
93	SPD	A	3471	-	9,9,9	0.15	0	8,8,8	0.19	0
97	SPM	AA	1702	-	13,13,13	0.15	0	12,12,12	0.24	0
98	FES	AP	201	32,21	0,4,4	-	-	-	-	-
94	PUT	A	3302	-	5,5,5	0.15	0	4,4,4	0.23	0
93	SPD	AA	1703	-	9,9,9	0.16	0	8,8,8	0.31	0
93	SPD	A	3301	-	9,9,9	0.15	0	8,8,8	0.22	0
98	FES	AT	201	29,36	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
100	GDP	AX	503	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
93	SPD	A	3472	-	9,9,9	0.15	0	8,8,8	0.32	0
97	SPM	AA	1780	-	13,13,13	0.15	0	12,12,12	0.18	0
96	NAD	AA	1701	95	46,48,48	1.24	3 (6%)	64,73,73	0.81	2 (3%)
93	SPD	A	3340	95	9,9,9	0.15	0	8,8,8	0.17	0
98	FES	r	201	51,87	0,4,4	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
101	VAL	B	101	46	-	2/5/6/8	-
93	SPD	AA	1782	-	-	0/7/7/7	-
99	ATP	AX	501	95	-	0/22/38/38	0/3/3/3
93	SPD	O	301	-	-	1/7/7/7	-
93	SPD	A	3471	-	-	0/7/7/7	-
97	SPM	AA	1702	-	-	0/11/11/11	-
100	GDP	AX	503	-	-	2/16/32/32	0/3/3/3
94	PUT	A	3302	-	-	0/3/3/3	-
93	SPD	AA	1703	-	-	0/7/7/7	-
93	SPD	A	3301	-	-	2/7/7/7	-
98	FES	AP	201	32,21	-	-	0/1/1/1
98	FES	AT	201	29,36	-	-	0/1/1/1
93	SPD	A	3472	-	-	1/7/7/7	-
97	SPM	AA	1780	-	-	2/11/11/11	-
96	NAD	AA	1701	95	-	11/30/62/62	0/5/5/5
93	SPD	A	3340	95	-	1/7/7/7	-
98	FES	r	201	51,87	-	-	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
96	AA	1701	NAD	PA-O3	5.45	1.65	1.59
96	AA	1701	NAD	PN-O3	3.67	1.63	1.59
100	AX	503	GDP	C5-C4	3.12	1.47	1.38
96	AA	1701	NAD	O4D-C1D	-2.53	1.37	1.40
100	AX	503	GDP	C6-N1	-2.47	1.34	1.38

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
100	AX	503	GDP	C5-C4-N3	-5.99	118.86	128.39
100	AX	503	GDP	C2-N3-C4	4.96	120.85	112.30
100	AX	503	GDP	N9-C4-N3	4.53	135.02	125.95
100	AX	503	GDP	C6-C5-N7	3.32	136.33	130.29
100	AX	503	GDP	C4-C5-N7	-2.48	106.74	110.67

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

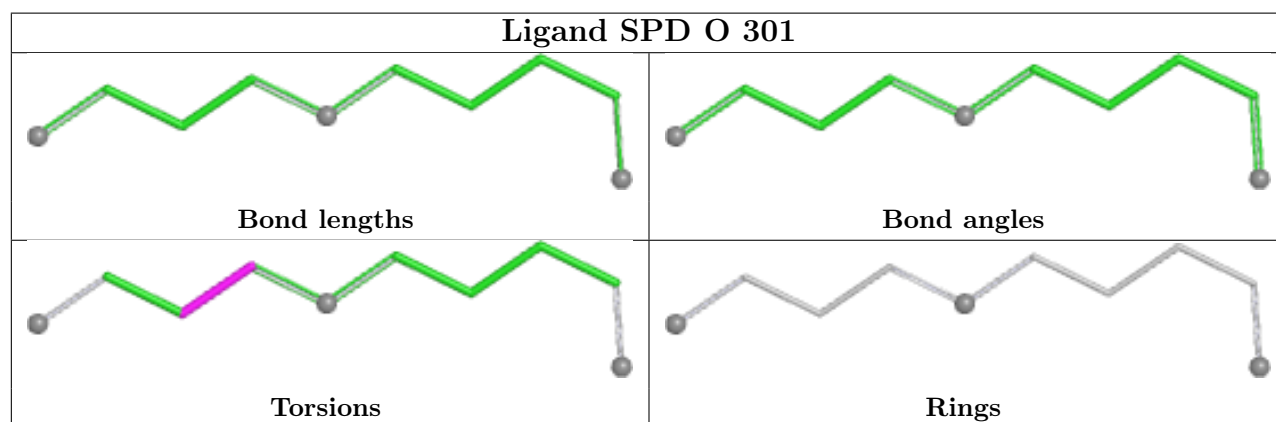
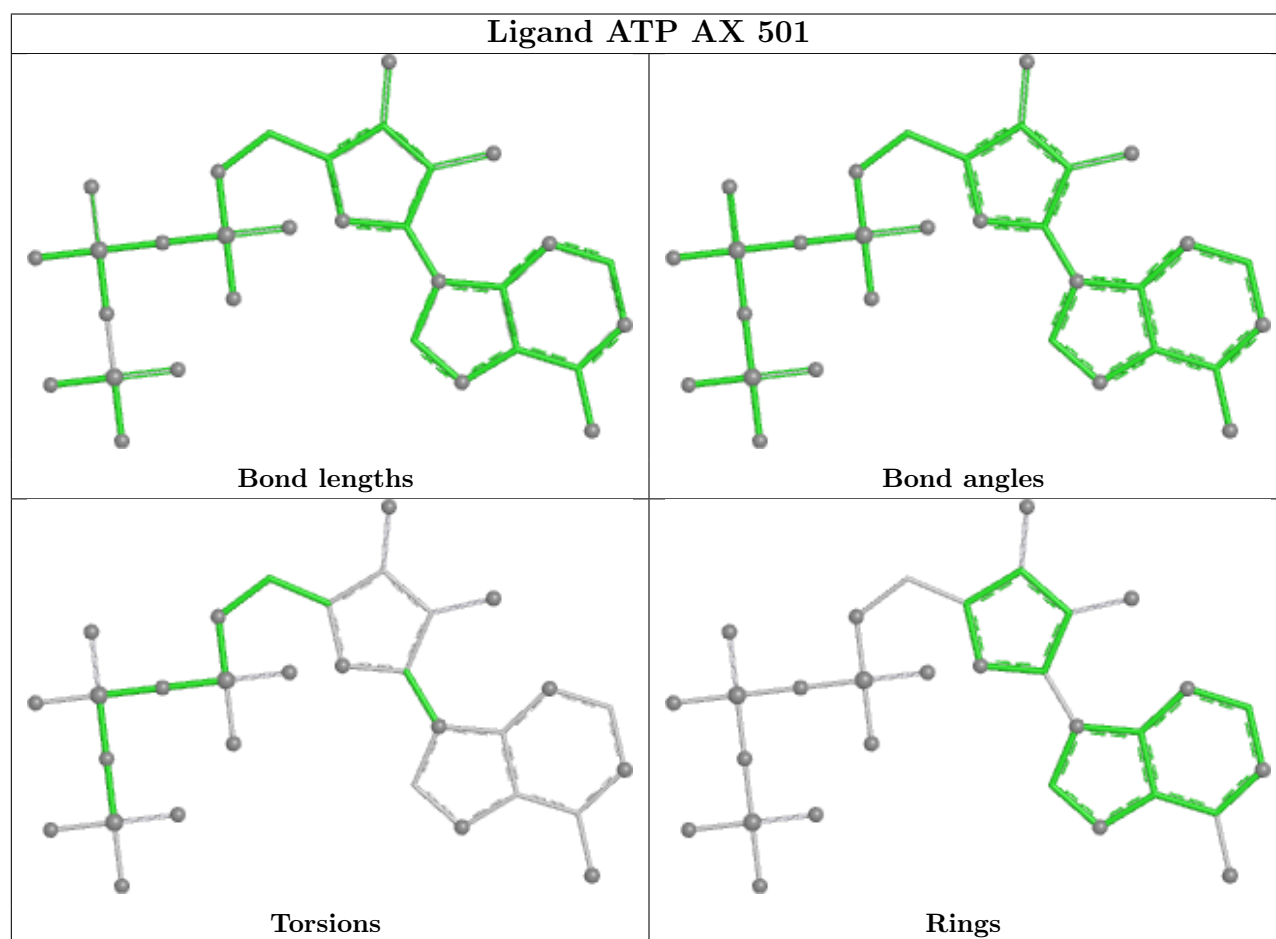
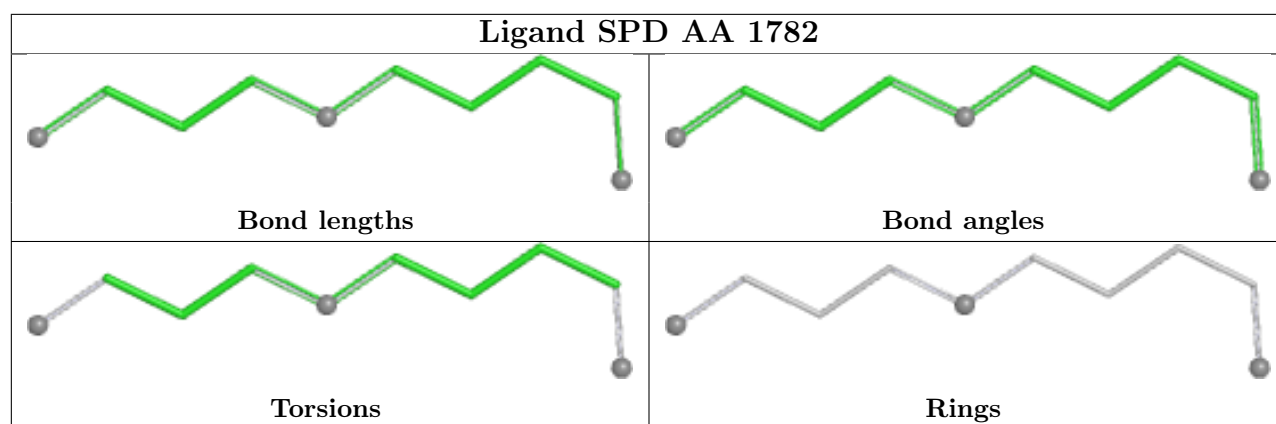
Mol	Chain	Res	Type	Atoms
96	AA	1701	NAD	C5B-O5B-PA-O1A
100	AX	503	GDP	C5'-O5'-PA-O3A
100	AX	503	GDP	C5'-O5'-PA-O1A
101	B	101	VAL	O-C-CA-CB
101	B	101	VAL	C-CA-CB-CG2

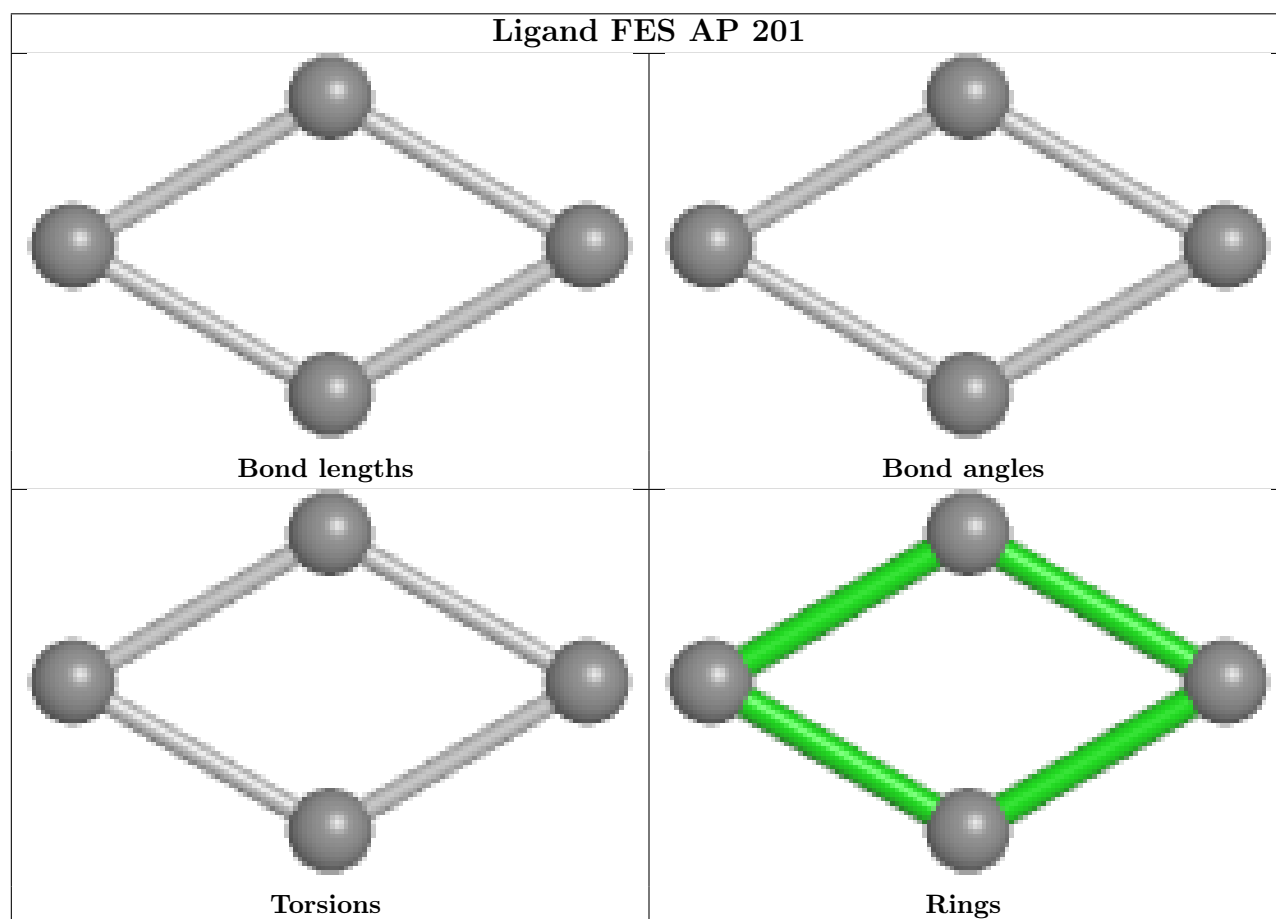
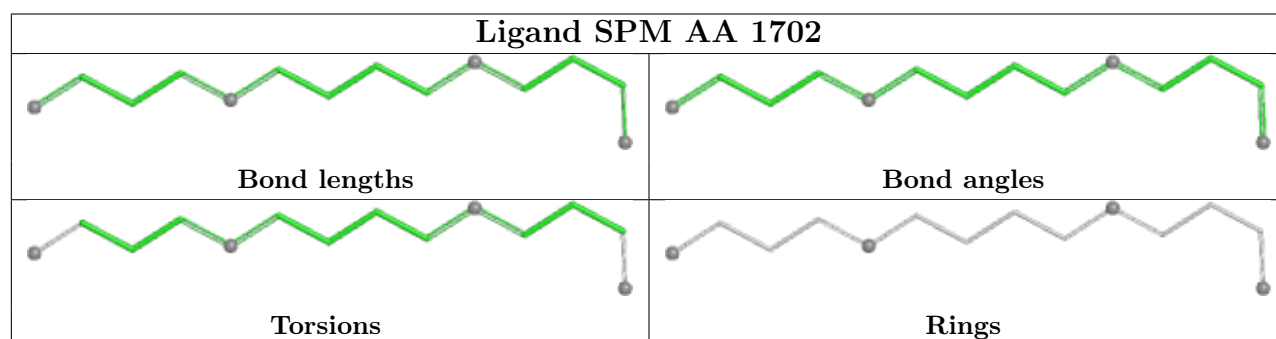
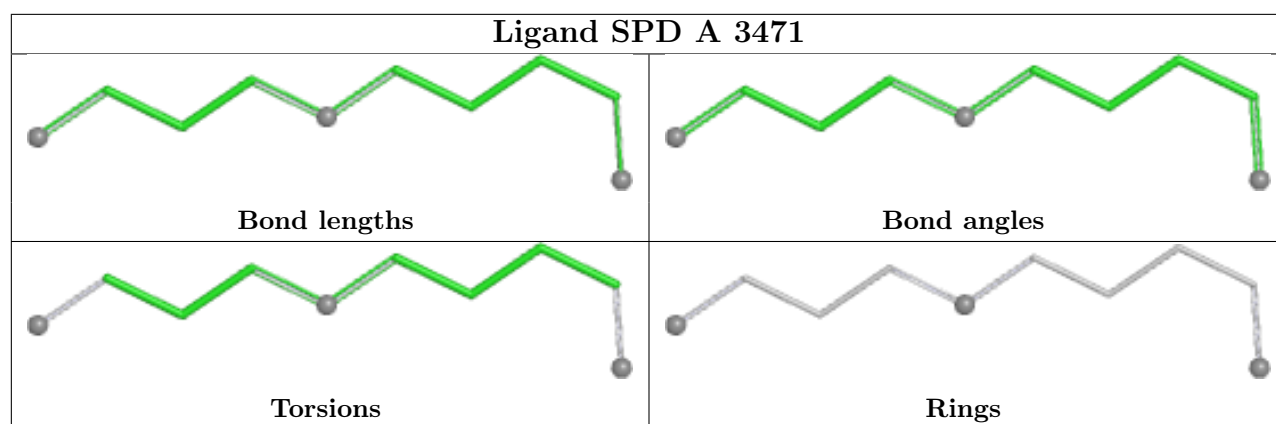
There are no ring outliers.

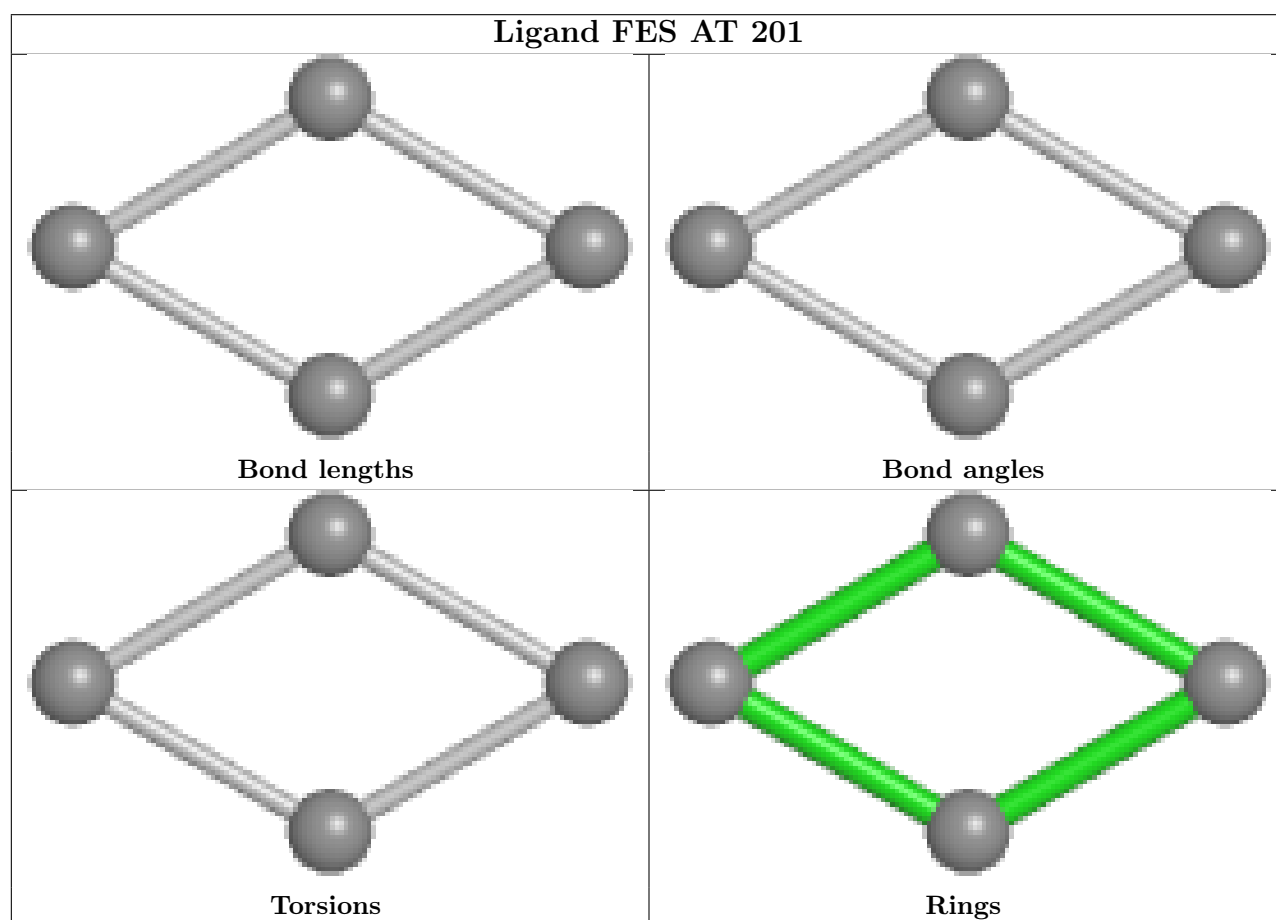
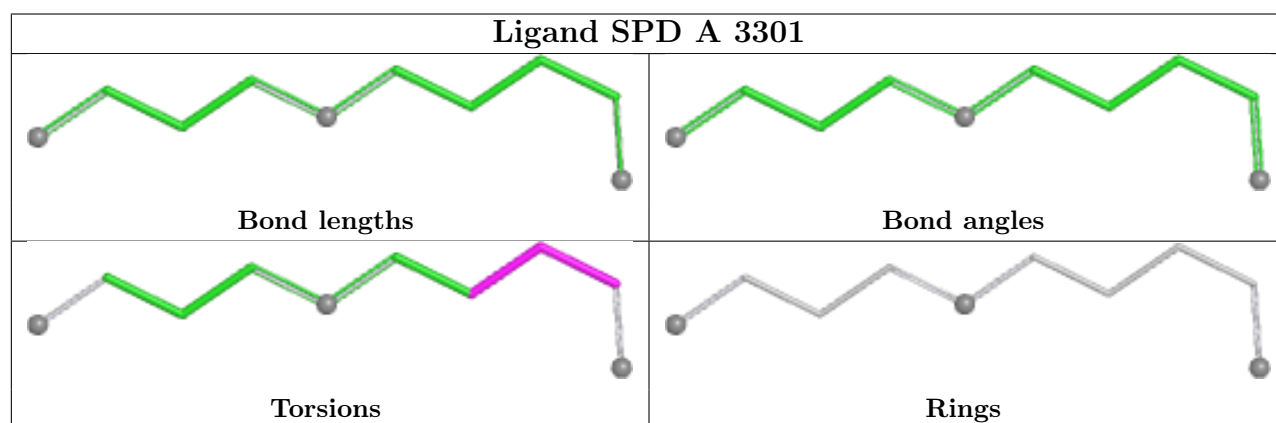
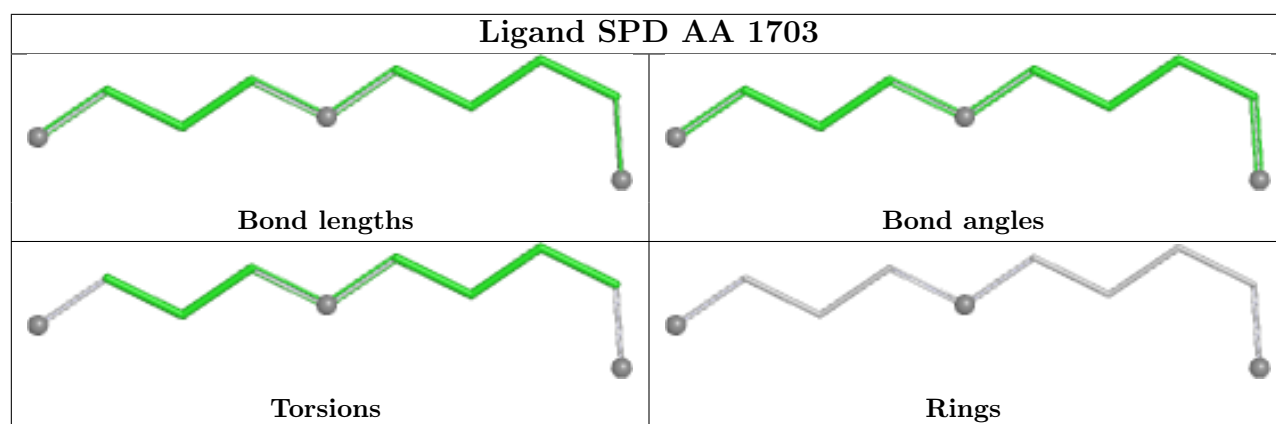
4 monomers are involved in 9 short contacts:

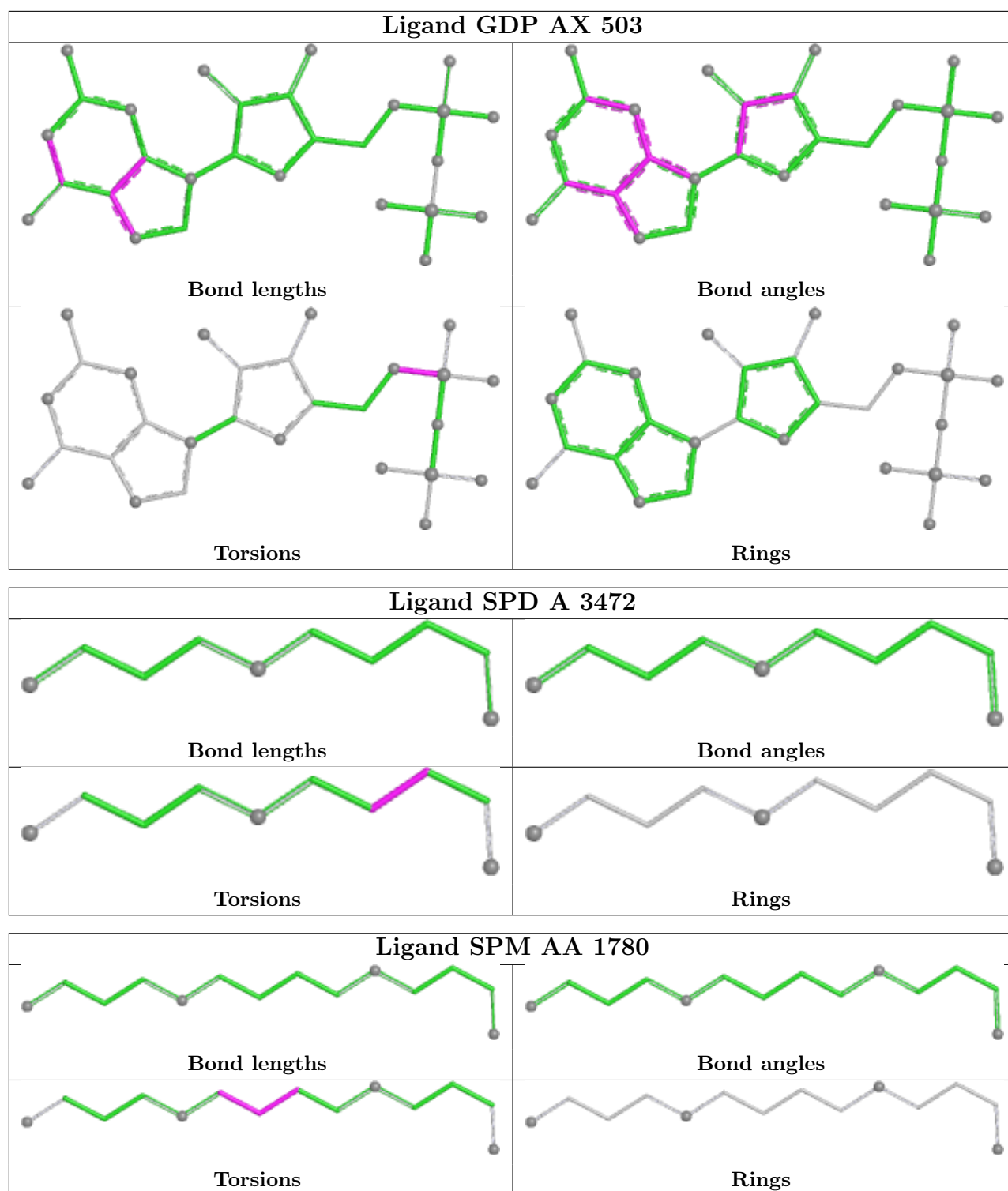
Mol	Chain	Res	Type	Clashes	Symm-Clashes
101	B	101	VAL	4	0
100	AX	503	GDP	2	0
97	AA	1780	SPM	1	0
96	AA	1701	NAD	2	0

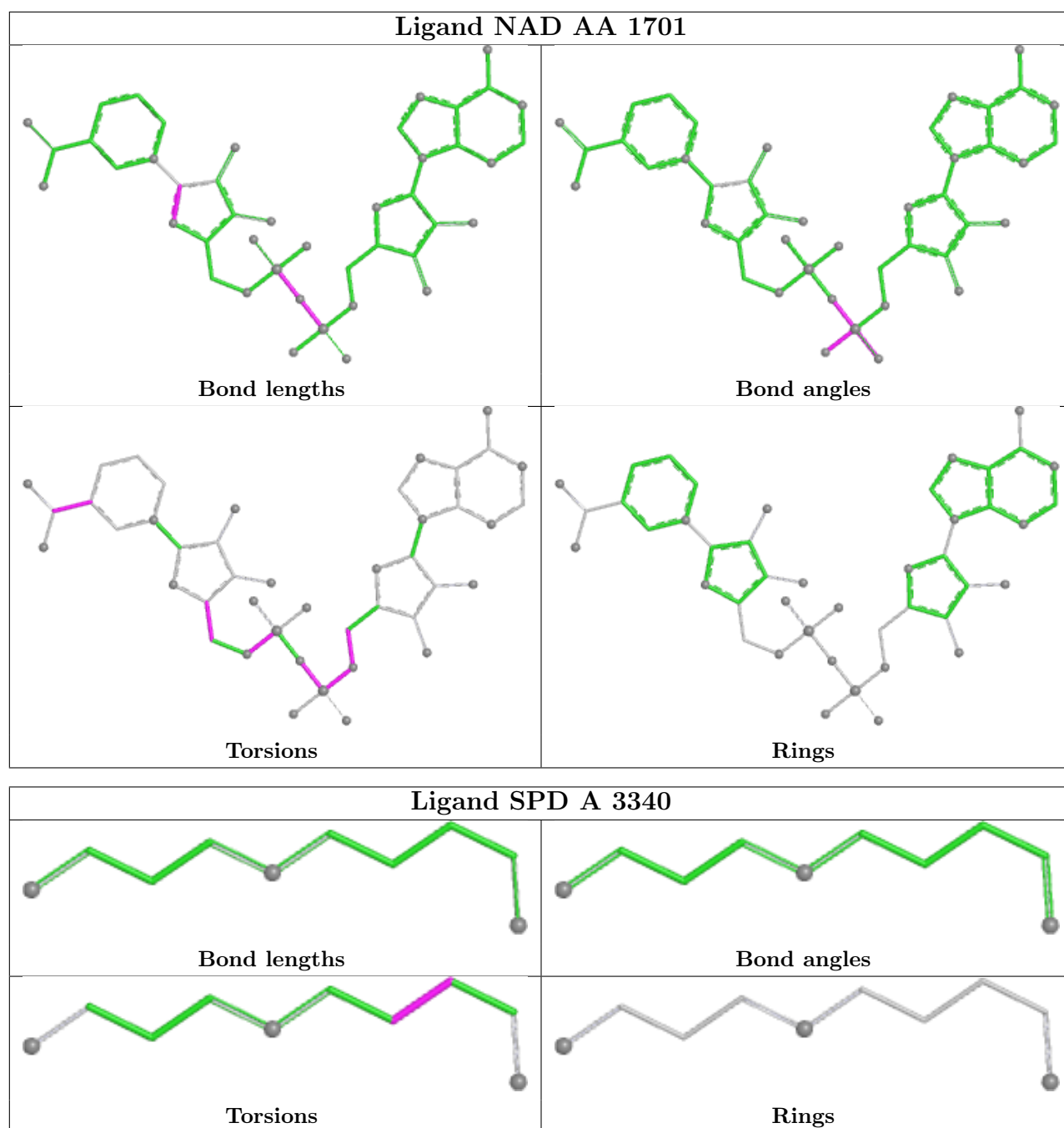
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

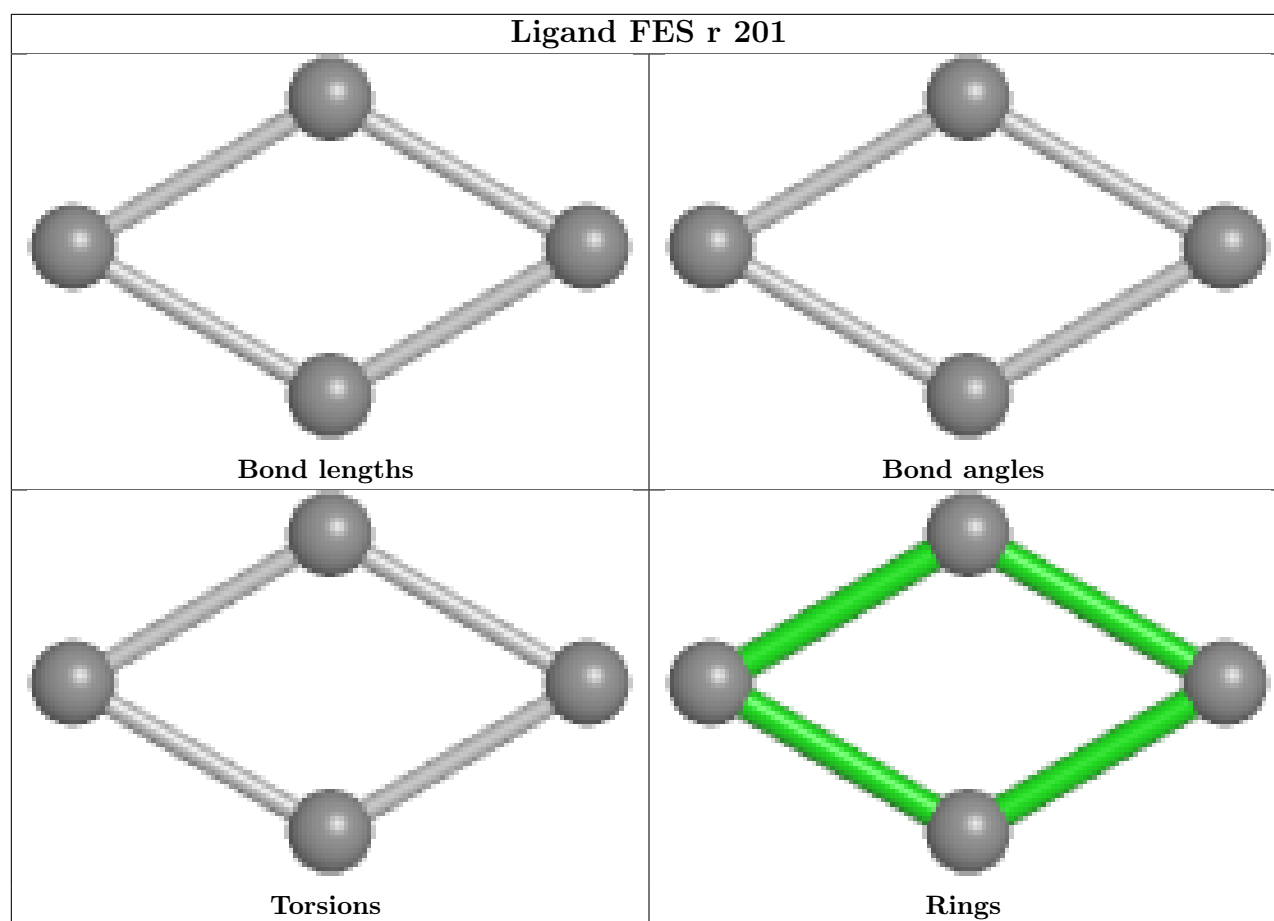












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	A	1
46	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2357:C	O3'	2361:G	P	8.65
1	B	46:A	O3'	48:U	P	4.61

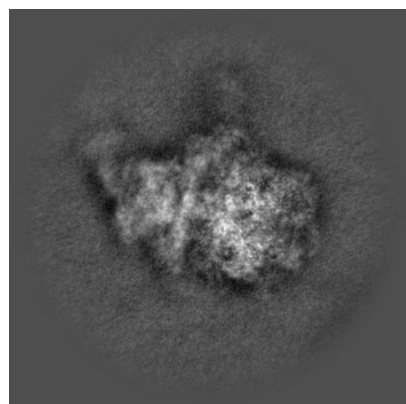
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71818. These allow visual inspection of the internal detail of the map and identification of artifacts.

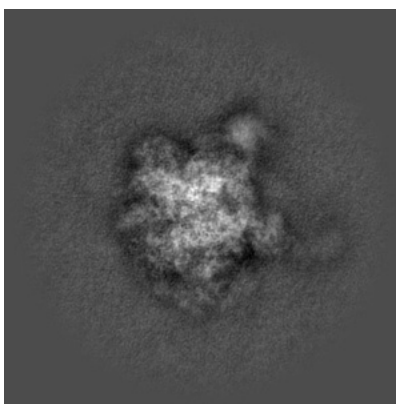
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

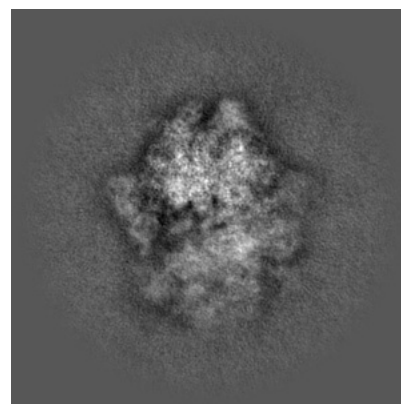
6.1.1 Primary map



X

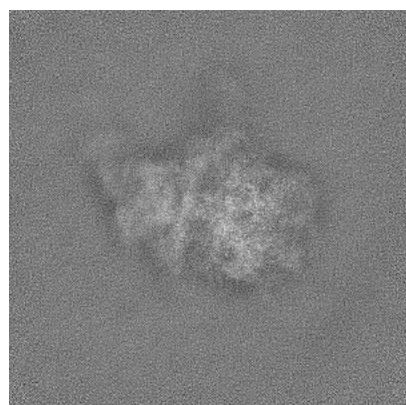


Y

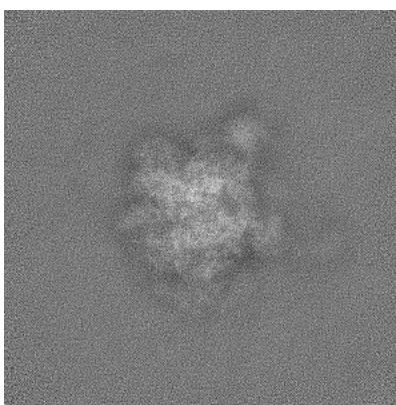


Z

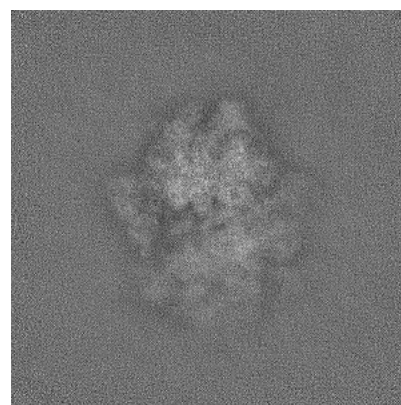
6.1.2 Raw map



X



Y

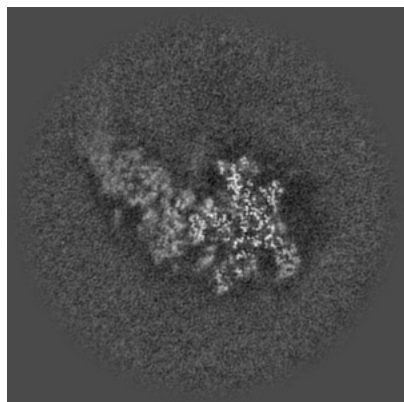


Z

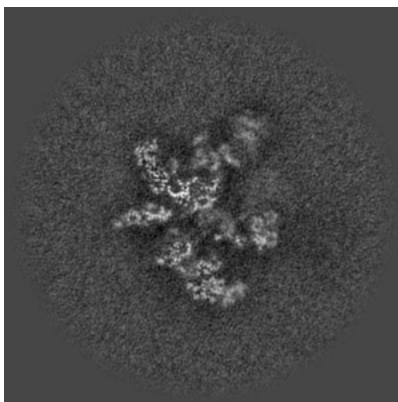
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

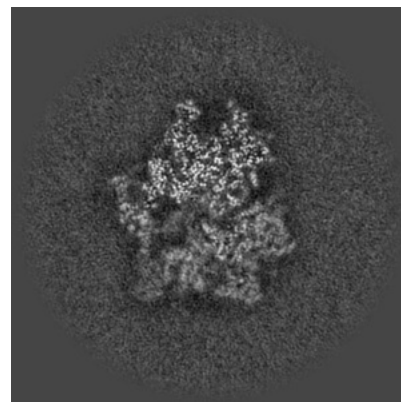
6.2.1 Primary map



X Index: 240

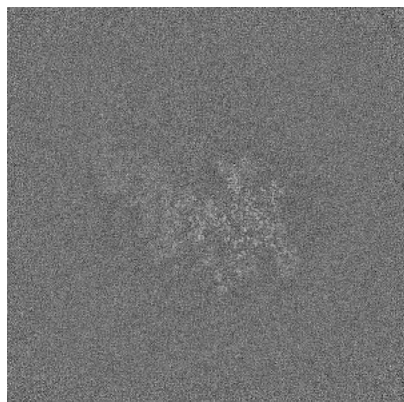


Y Index: 240

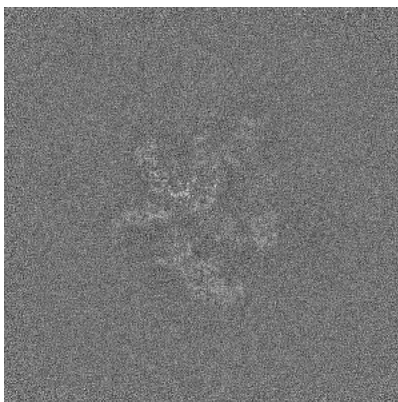


Z Index: 240

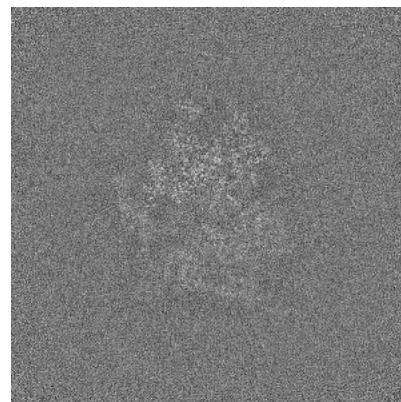
6.2.2 Raw map



X Index: 240



Y Index: 240

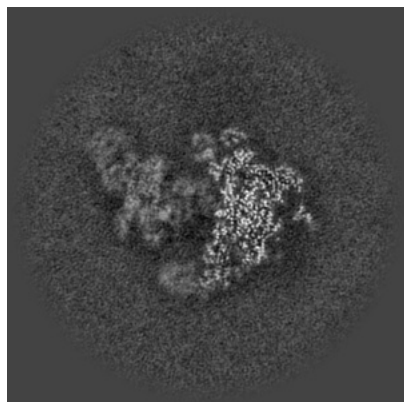


Z Index: 240

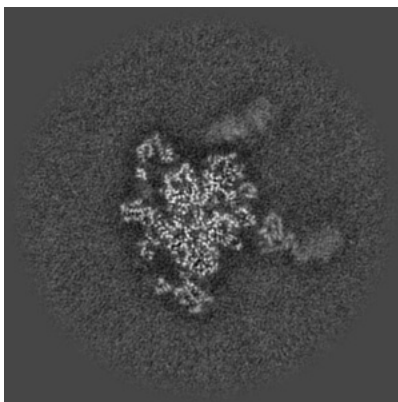
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

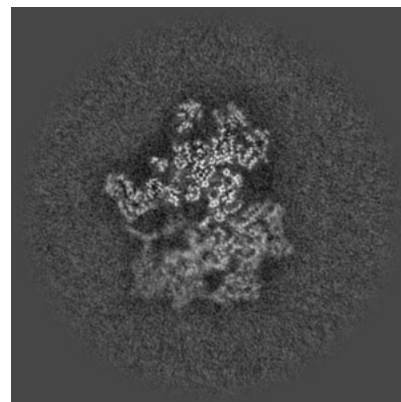
6.3.1 Primary map



X Index: 224

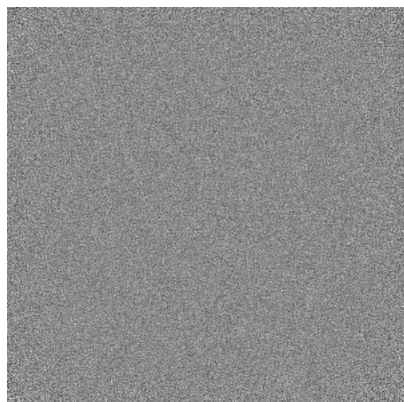


Y Index: 263

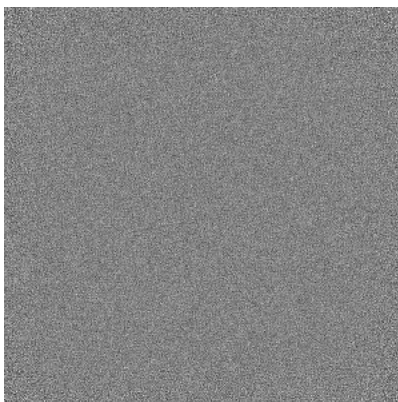


Z Index: 231

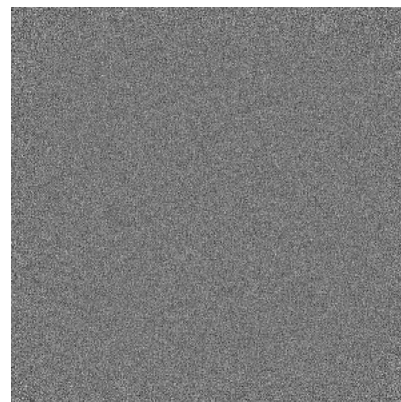
6.3.2 Raw map



X Index: 0



Y Index: 0

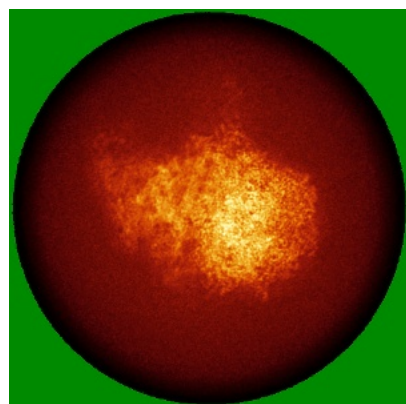


Z Index: 0

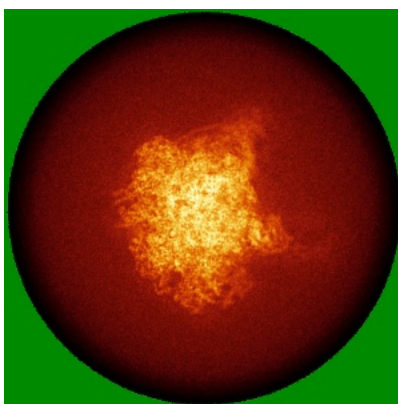
The images above show the largest variance slices of the map in three orthogonal directions.

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

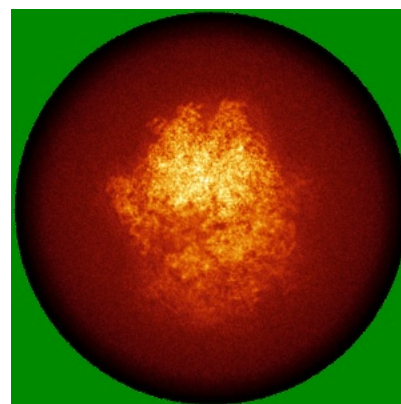
6.4.1 Primary map



X

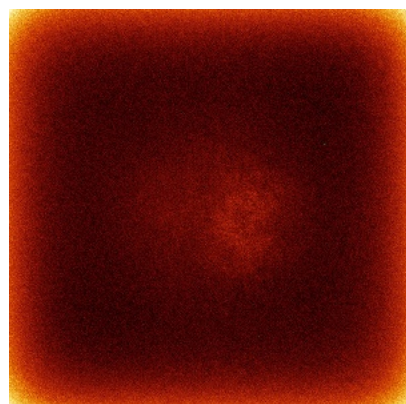


Y

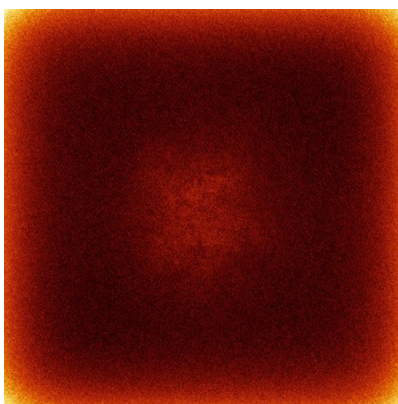


Z

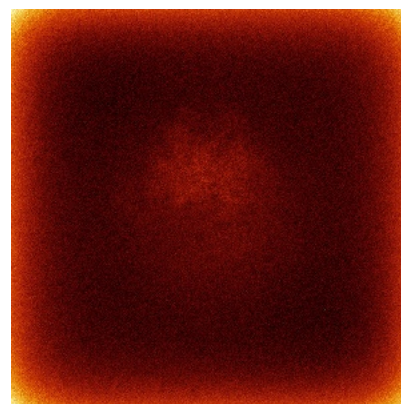
6.4.2 Raw map



X



Y

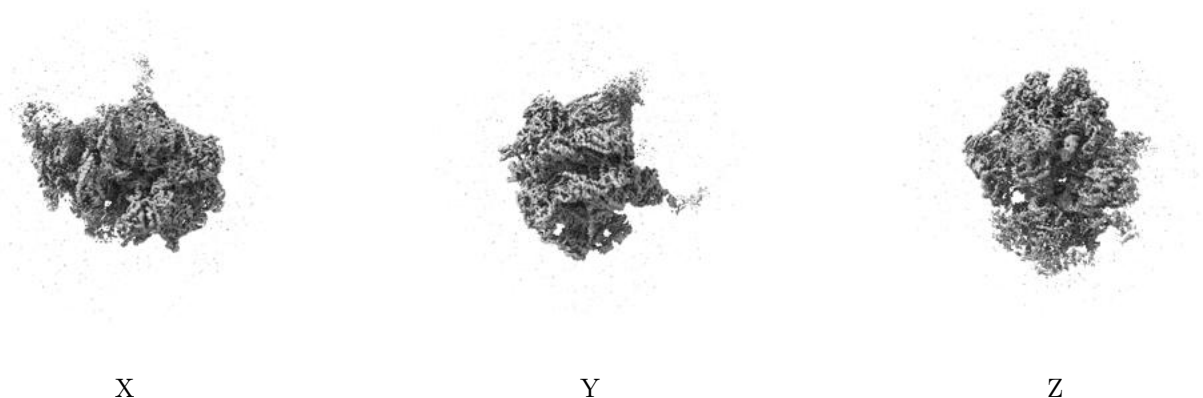


Z

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

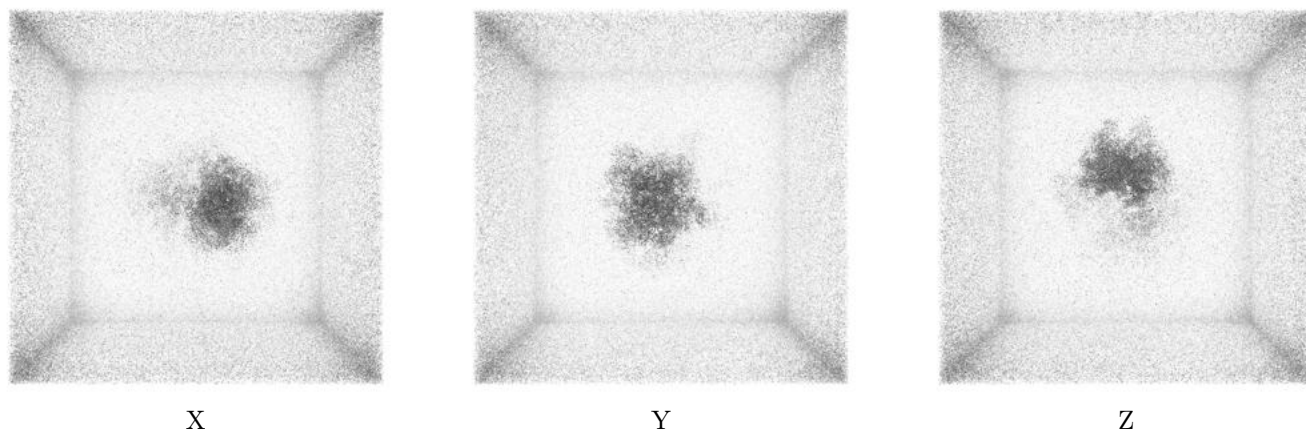
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.029. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

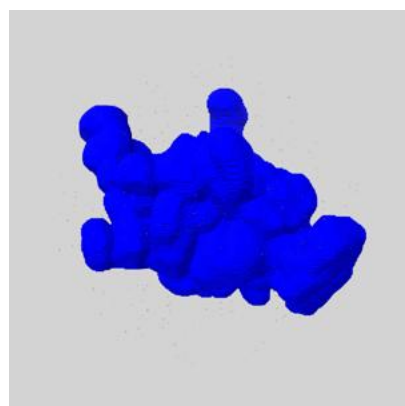
6.6 Mask visualisation [i](#)

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

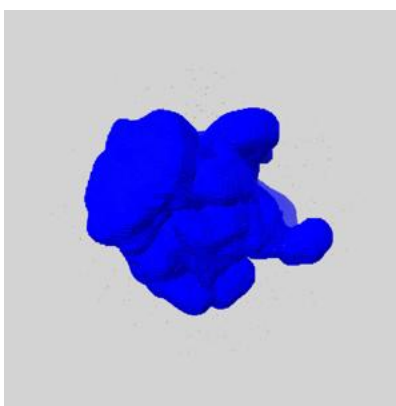
A mask typically either:

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

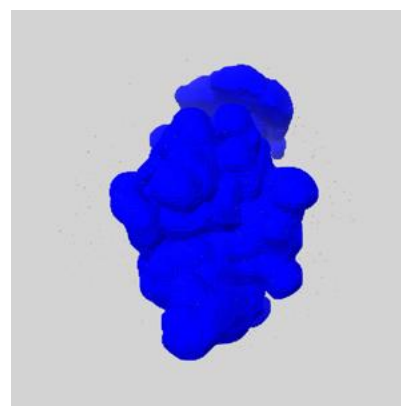
6.6.1 emd_71818_msk_1.map [i](#)



X



Y

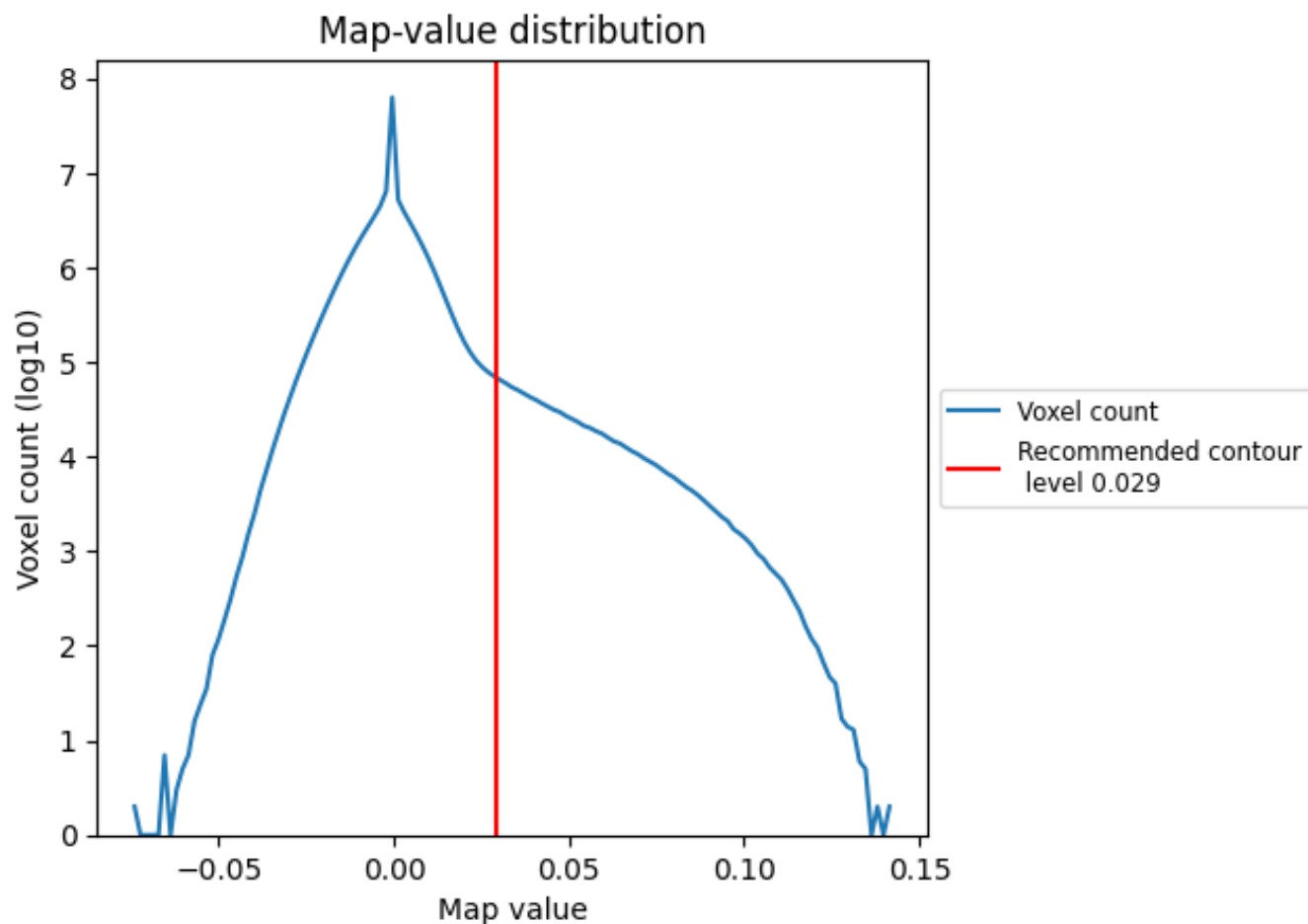


Z

7 Map analysis [i](#)

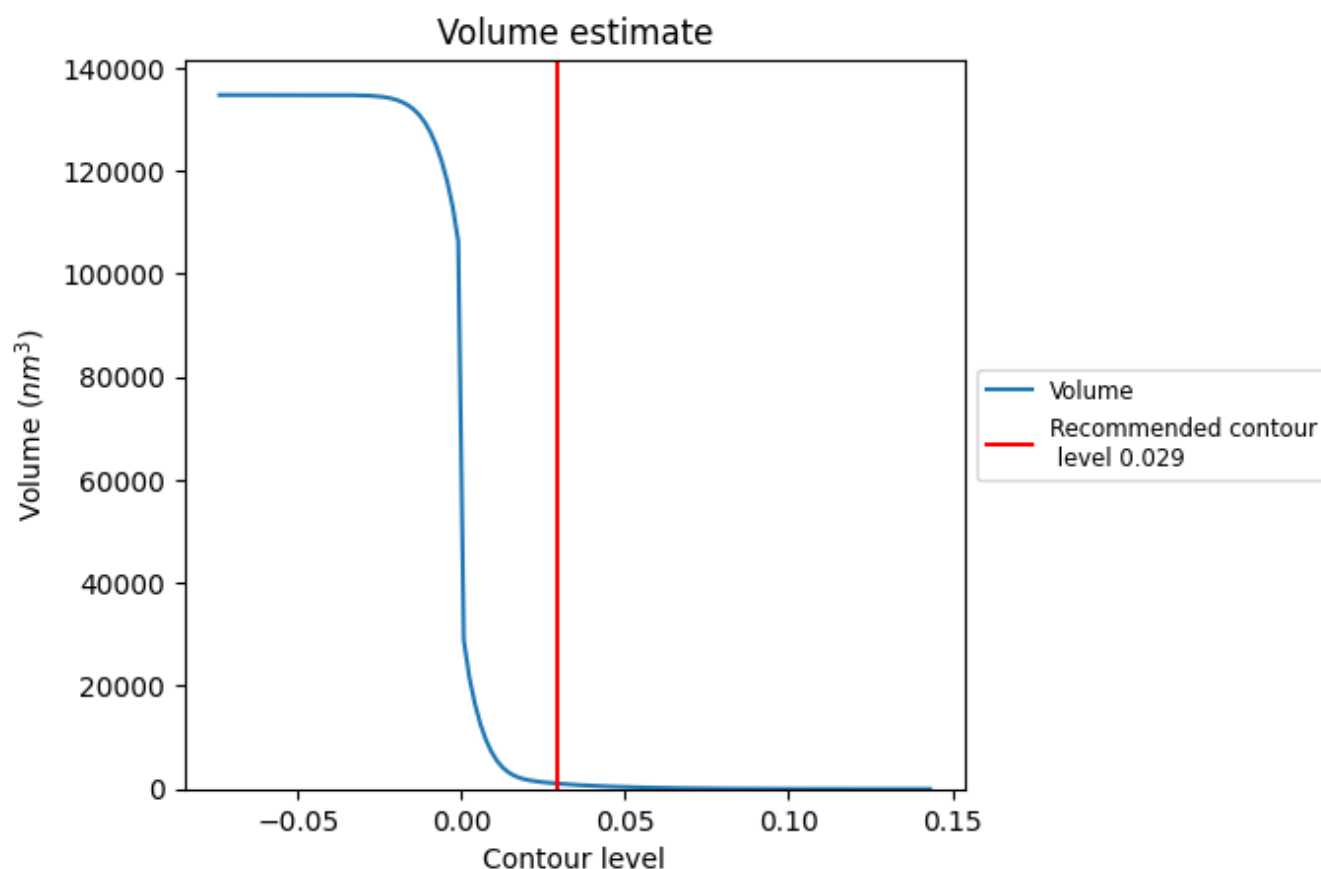
This section contains the results of statistical analysis of the map.

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.

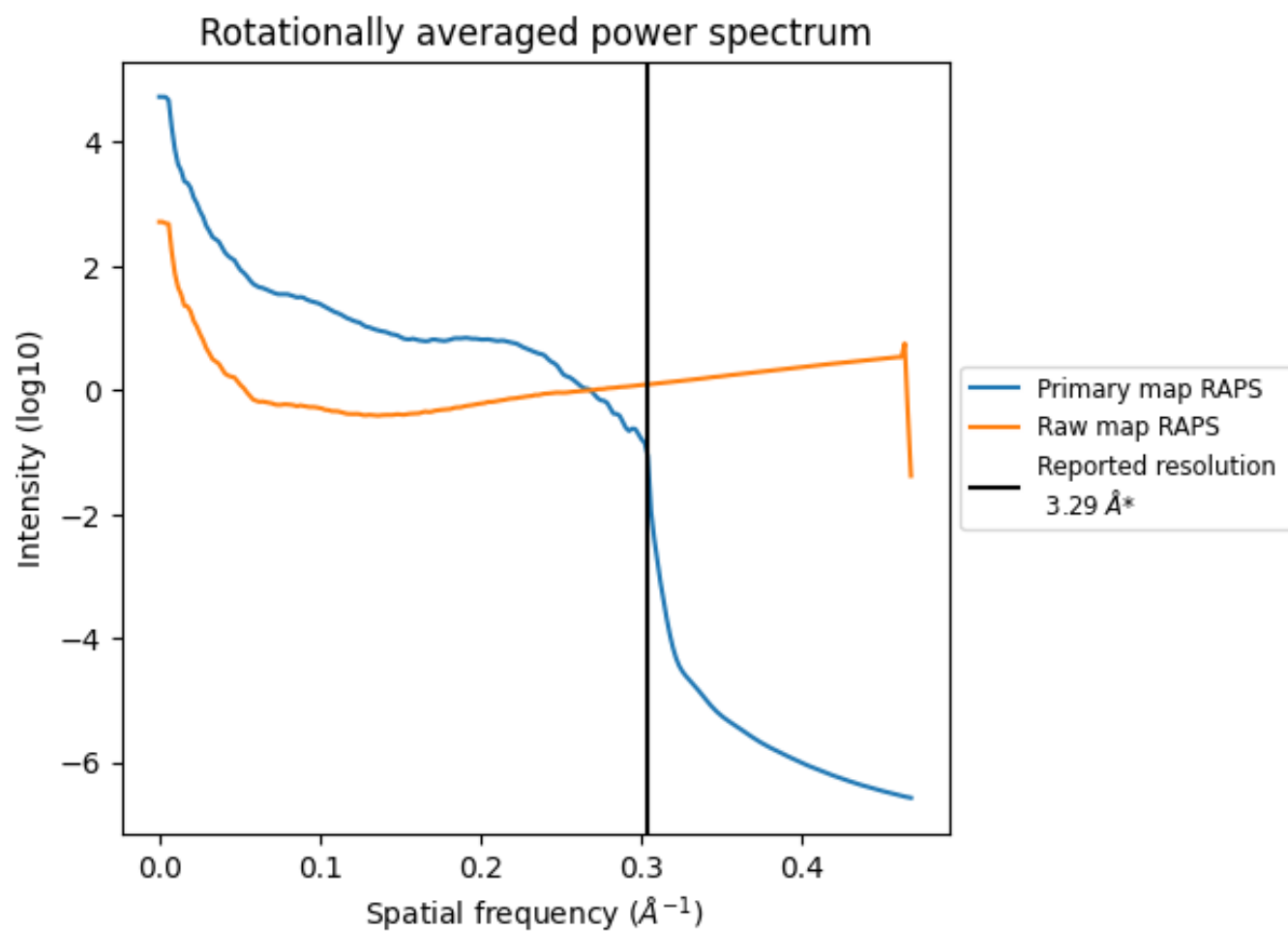
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1060 nm³; this corresponds to an approximate mass of 958 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

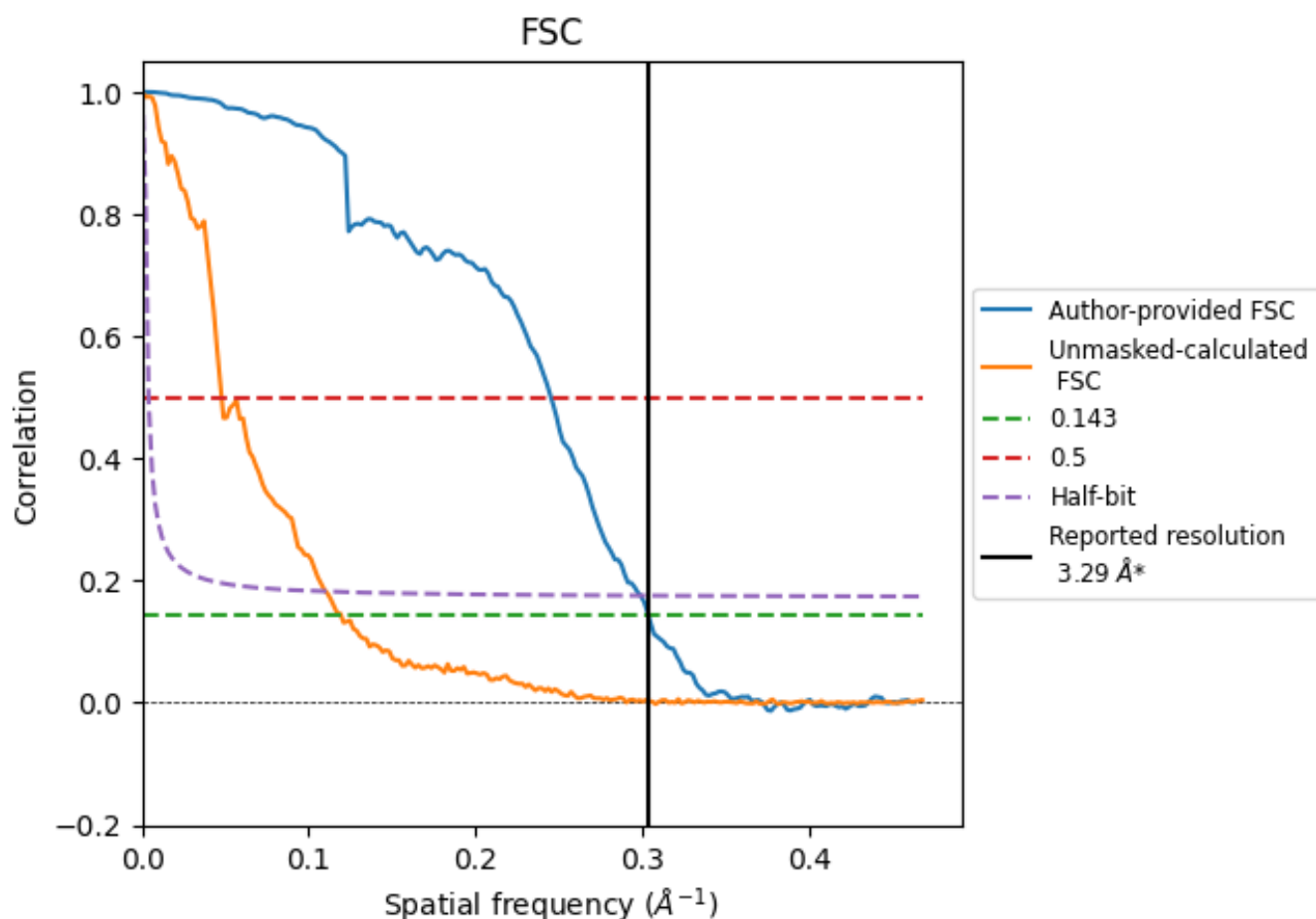


*Reported resolution corresponds to spatial frequency of 0.304 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.304 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

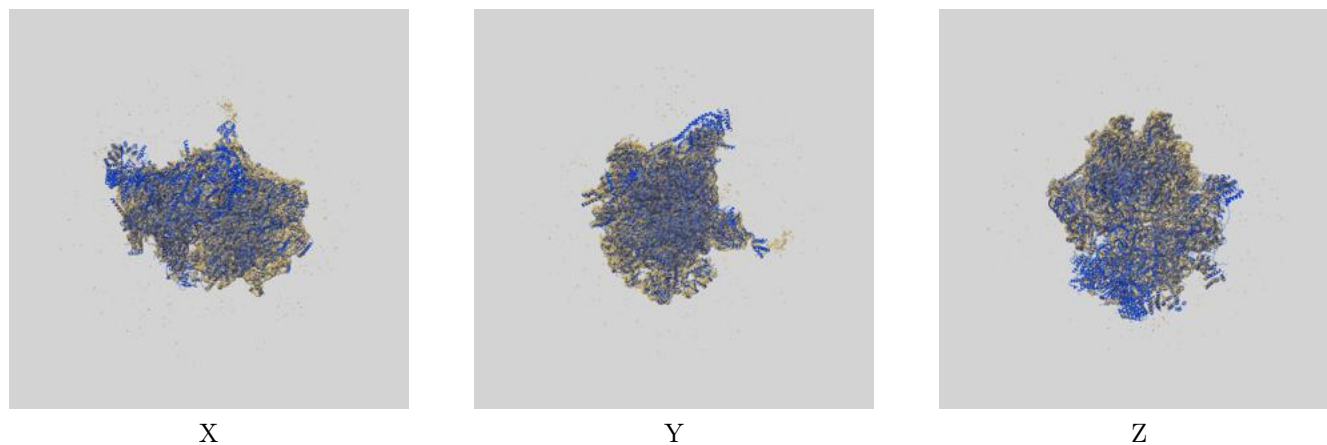
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	3.29	4.07	3.34
Unmasked-calculated*	8.38	20.96	9.07

*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 8.38 differs from the reported value 3.29 by more than 10 %

9 Map-model fit [i](#)

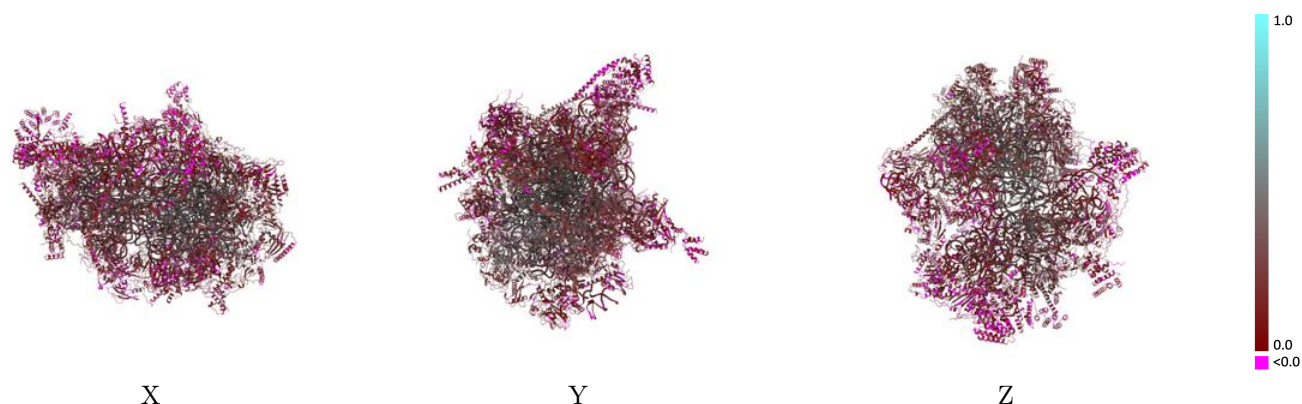
This section contains information regarding the fit between EMDB map EMD-71818 and PDB model 9PS0. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



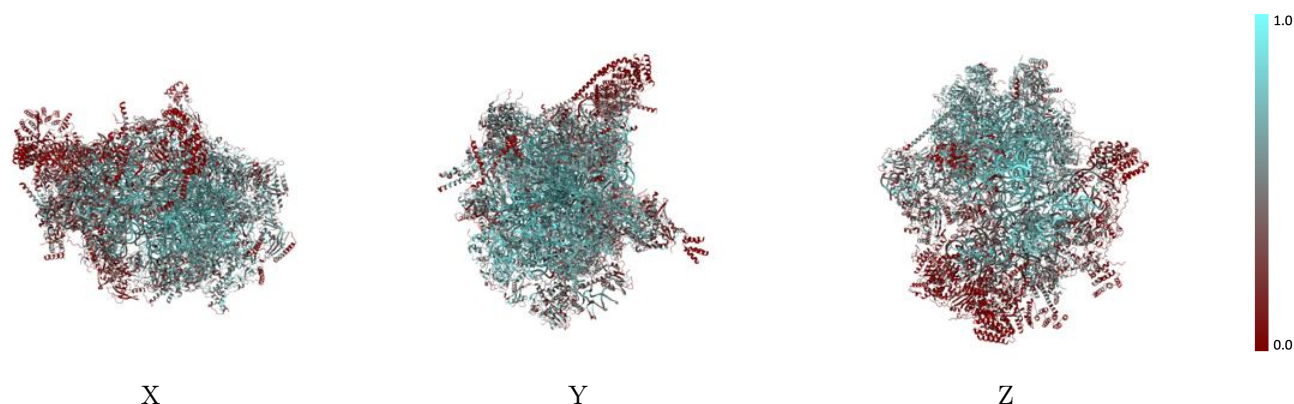
The images above show the 3D surface view of the map at the recommended contour level 0.029 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



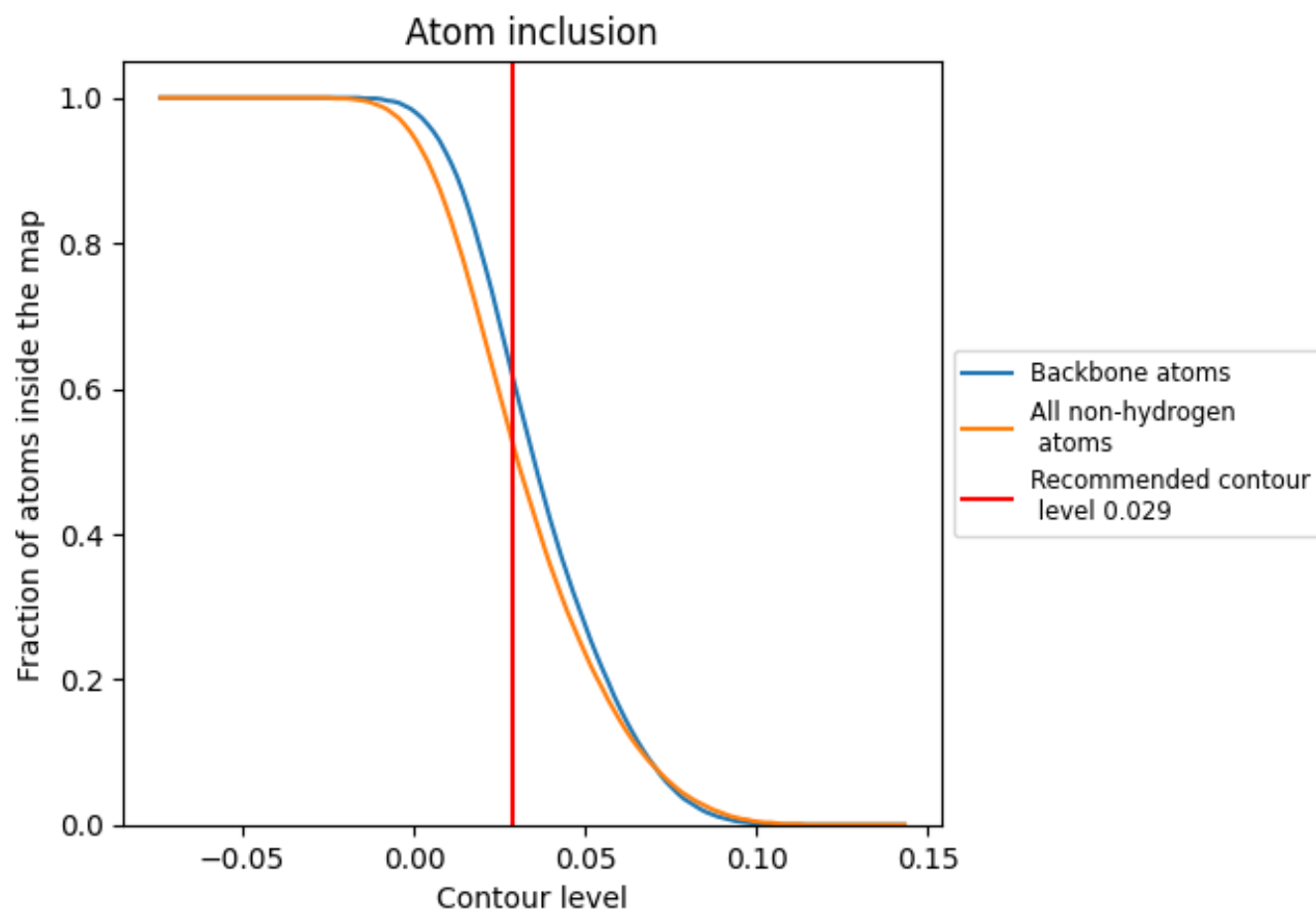
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.029).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 52% 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 (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5220	 0.2380
0	 0.5560	 0.2370
1	 0.5630	 0.2130
2	 0.7310	 0.3580
3	 0.6850	 0.3640
4	 0.6420	 0.2840
5	 0.4770	 0.1520
6	 0.4920	 0.1720
7	 0.4850	 0.1560
8	 0.3290	 0.1430
9	 0.5340	 0.2060
A	 0.8350	 0.3510
A0	 0.1680	 0.0990
A1	 0.1620	 0.1210
A2	 0.2620	 0.2050
A3	 0.5150	 0.2960
A4	 0.1020	 0.0920
AA	 0.7040	 0.2750
AB	 0.3990	 0.2270
AC	 0.2420	 0.1750
AD	 0.3460	 0.2340
AE	 0.2900	 0.2240
AF	 0.2580	 0.1820
AG	 0.2570	 0.1720
AH	 0.1820	 0.1210
AI	 0.2930	 0.2230
AJ	 0.4030	 0.2540
AK	 0.2670	 0.1760
AL	 0.3840	 0.2260
AM	 0.2840	 0.1650
AN	 0.3630	 0.2570
AO	 0.2480	 0.1630
AP	 0.3320	 0.2340
AQ	 0.3550	 0.2600
AR	 0.1670	 0.1240



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Chain	Atom inclusion	Q-score
AS	 0.2970	 0.2040
AT	 0.3240	 0.2080
AU	 0.2840	 0.1480
AV	 0.0730	 0.0700
AW	 0.2210	 0.1790
AX	 0.1560	 0.1500
AY	 0.0990	 0.1150
AZ	 0.2040	 0.1610
Aw	 0.3020	 0.1110
Ax	 0.3930	 0.0960
Az	 0.2340	 0.1550
B	 0.6150	 0.1430
D	 0.5980	 0.2620
E	 0.5880	 0.2380
F	 0.7410	 0.4270
H	 0.2900	 0.1380
I	 0.3900	 0.1460
J	 0.4040	 0.1470
K	 0.6060	 0.2820
L	 0.6210	 0.3470
M	 0.6330	 0.3260
N	 0.6340	 0.3120
O	 0.5340	 0.2080
OX	 0.2390	 0.1590
P	 0.4690	 0.1620
Q	 0.5190	 0.2300
R	 0.6560	 0.3350
S	 0.6180	 0.3040
T	 0.6650	 0.3220
U	 0.4780	 0.2000
V	 0.5710	 0.2710
W	 0.5830	 0.2620
X	 0.5680	 0.2710
Y	 0.6300	 0.2580
Z	 0.6080	 0.3020
a	 0.5080	 0.2450
b	 0.6680	 0.3680
c	 0.5880	 0.2890
d	 0.4260	 0.2160
e	 0.3310	 0.1260
f	 0.4080	 0.1870
g	 0.6790	 0.3550

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Chain	Atom inclusion	Q-score
h	 0.6680	 0.3690
i	 0.7400	 0.4280
j	 0.5600	 0.2710
k	 0.4140	 0.1330
l	 0.4130	 0.1560
m	 0.2480	 0.1370
n	 0.2420	 0.2420
o	 0.6890	 0.3580
p	 0.4450	 0.1790
q	 0.4340	 0.2050
r	 0.5620	 0.2130
s	 0.4950	 0.1490
t	 0.1080	 0.1050
u	 0.0660	 0.0830
z	 0.0640	 0.0420