



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 05:59 PM UTC

PDB ID : 8OIR / pdb_00008oir
EMDB ID : EMD-16897
Title : 55S human mitochondrial ribosome with mtRF1 and P-site tRNA
Authors : Saurer, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.; Ban, N.
Deposited on : 2023-03-23
Resolution : 3.10 Å(reported)
Based on initial models : ., 7QI4

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:

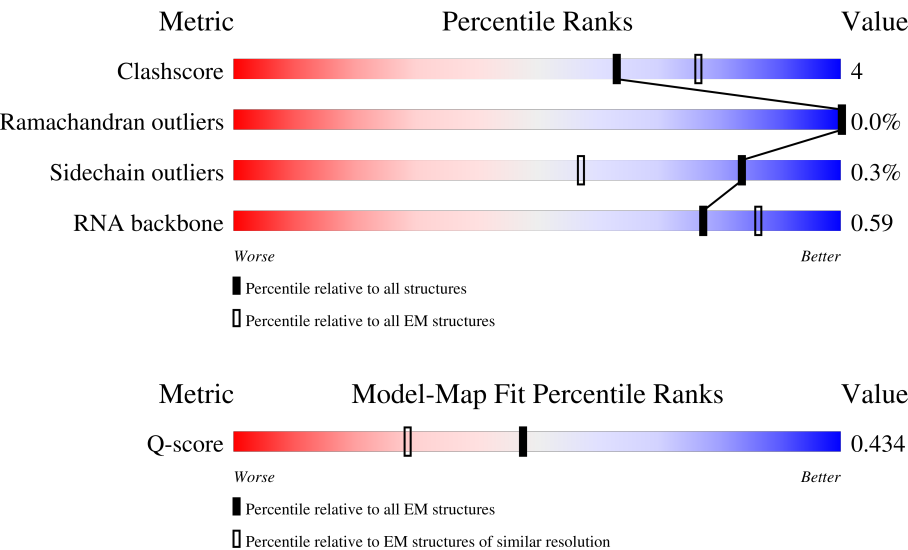
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	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	14724 (2.60 - 3.60)

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	B1	198	
1	B2	198	
1	B3	198	

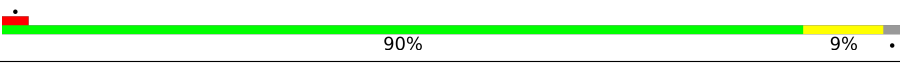
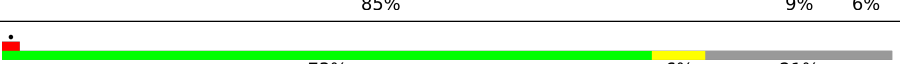
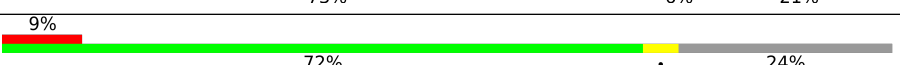
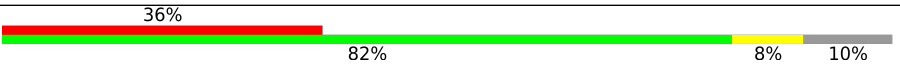
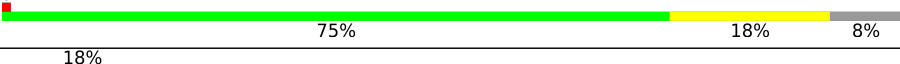
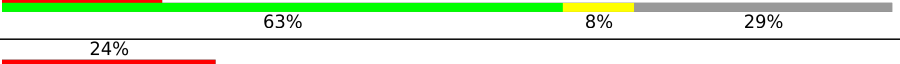
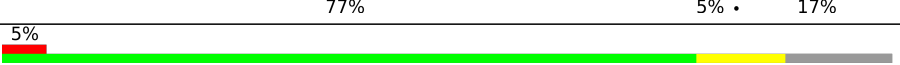
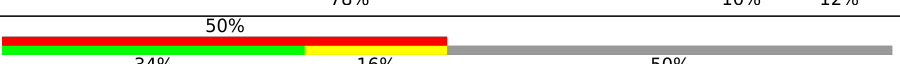
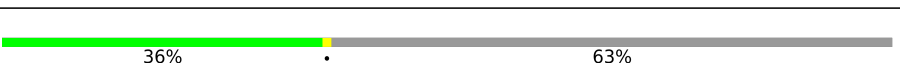
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Mol	Chain	Length	Quality of chain
1	B4	198	
1	B5	198	
1	B6	198	
2	B7	3	
3	B8	1561	
4	B9	72	
5	BA	206	
6	BB	153	
7	BC	216	
8	BD	148	
9	BE	256	
10	BF	250	
11	BG	161	
12	BH	188	
13	BI	65	
14	BJ	92	
15	BK	188	
16	BL	305	
17	BM	348	
18	BN	311	
19	BO	267	
20	BP	261	
21	BQ	192	
22	BR	178	
23	BS	145	

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Mol	Chain	Length	Quality of chain
24	BT	296	
25	BU	251	
26	BV	175	
27	BW	180	
28	BX	292	
29	BY	149	
30	BZ	205	
31	Ba	123	
32	Bb	112	
33	Bc	138	
34	Bd	128	
35	Be	102	
36	Bf	206	
37	Bg	222	
38	Bh	196	
39	Bi	439	
40	Bj	325	
41	Bl	103	
42	Bm	423	
43	Bn	380	
44	Bo	338	
45	Bp	206	
46	Bq	137	
47	Br	142	
48	Bs	215	

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Mol	Chain	Length	Quality of chain
49	Bt	332	
50	Bu	306	
51	Bv	279	
52	Bw	212	
53	Bx	166	
54	By	158	
55	Bz	128	
56	AA	955	
57	AB	323	
58	AC	167	
59	AD	199	
60	AE	125	
61	AF	242	
62	AG	71	
63	AH	201	
64	AI	33	
65	AJ	138	
66	AK	128	
67	AL	257	
68	AM	137	
69	AN	130	
70	AO	258	
71	AP	142	
72	AQ	87	
73	AR	360	

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Mol	Chain	Length	Quality of chain
74	AS	190	
75	AT	173	
76	AU	205	
77	AV	414	
78	AW	187	
79	AX	398	
80	AY	395	
81	AZ	106	
82	Aa	484	
83	Ab	296	
84	Ac	118	
85	Ad	430	
86	Ae	689	
87	Ag	396	
88	Ai	194	
89	Aj	218	

2 Entry composition

There are 98 unique types of molecules in this entry. The entry contains 181140 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 L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	B1	46	Total	C	N	O	0	0
			354	228	56	70		
1	B2	32	Total	C	N	O	0	0
			257	168	40	49		
1	B3	32	Total	C	N	O	0	0
			257	168	40	49		
1	B4	31	Total	C	N	O	0	0
			245	159	39	47		
1	B5	31	Total	C	N	O	0	0
			245	159	39	47		
1	B6	31	Total	C	N	O	0	0
			245	159	39	47		

- Molecule 2 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B7	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 3 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B8	1558	Total	C	N	O	P	0	0
			33070	14843	5963	10706	1558		

- Molecule 4 is a RNA chain called CP Val-tRNA(Val).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B9	72	Total	C	N	O	P	0	0
			1524	685	269	498	72		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B9	70	C	G	conflict	GB NC_012920.1
B9	72	A	U	conflict	GB NC_012920.1

- Molecule 5 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 6 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BB	152	Total	C	N	O	S	0	0
			1251	788	234	226	3		

- Molecule 7 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 8 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 9 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 10 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 11 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 12 is a protein called 39S ribosomal protein L32, mitochondrial.

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

- Molecule 13 is a protein called 39S ribosomal protein L33, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L34, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L35, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 17 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BP	212	Total	C	N	O	S	0	0
			1695	1088	304	292	11		

- Molecule 21 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BR	177	Total	C	N	O	S	0	0
			1455	936	259	253	7		

- Molecule 23 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BX	238	Total	C	N	O	S	0	0
			1979	1268	352	350	9		

- Molecule 29 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 30 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 31 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 32 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bb	101	Total	C	N	O	S	0	0
			774	479	148	142	5		

- Molecule 33 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 35 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 36 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 37 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bg	161	Total	C	N	O	S	0	0
			1350	841	260	244	5		

- Molecule 38 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bi	386	Total	C	N	O	S	0	0
			3155	2023	559	559	14		

- Molecule 40 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bj	164	Total	C	N	O	S	0	0
			1327	856	217	250	4		

- Molecule 41 is a protein called 39S ribosomal protein L36, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L37, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L38, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L39, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bp	147	Total	C	N	O	S	0	0
			1243	790	218	233	2		

- Molecule 46 is a protein called 39S ribosomal protein L41, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Br	100	Total	C	N	O	S	0	0
			840	529	152	154	5		

- Molecule 48 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bs	151	Total	C	N	O	S	0	0
			1196	744	231	218	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bs	2	ACE	-	acetylation	UNP Q8N983

- Molecule 49 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 50 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bu	241	Total	C	N	O	S	0	0
			1985	1273	340	359	13		

- Molecule 51 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 52 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 53 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 54 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 55 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 56 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AA	955	Total	C	N	O	P	0	0
			20283	9098	3652	6578	955		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	62	G	A	conflict	GB OM714795.1

- Molecule 57 is a protein called 28S ribosomal protein S35, mitochondrial.

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

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

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

- Molecule 59 is a protein called Aurora kinase A-interacting protein.

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

- Molecule 60 is a protein called 28S ribosomal protein S6, mitochondrial.

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

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

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

- Molecule 62 is a RNA chain called P-site Met-tRNA(Met).

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AG	71	Total	C	N	O	P	0	0
			1504	674	264	495	71		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	69	C	-	insertion	GB NC_012920.1
AG	70	C	-	insertion	GB NC_012920.1

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

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

- Molecule 64 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AI	33	Total	C	N	O	P	0	0
			463	198	29	203	33		

- Molecule 65 is a protein called 28S ribosomal protein S12, mitochondrial.

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

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

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

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

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

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

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

- Molecule 69 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 70 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 71 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 72 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AQ	86	Total	C	N	O	S	0	0
			744	460	150	126	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	50	ARG	CYS	variant	UNP P82921

- Molecule 73 is a protein called 28S ribosomal protein S22, mitochondrial.

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

- Molecule 74 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 75 is a protein called 28S ribosomal protein S25, mitochondrial.

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

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

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

- Molecule 77 is a protein called 28S ribosomal protein S27, mitochondrial.

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

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

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

- Molecule 79 is a protein called 28S ribosomal protein S29, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AY	149	Total	C	N	O	S	0	0
			1246	801	207	234	4		

- Molecule 81 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 82 is a protein called Peptide chain release factor 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Aa	381	Total	C	N	O	S	0	0
			3114	1940	569	592	13		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	311	ALA	GLY	engineered mutation	UNP O75570
Aa	312	ALA	GLY	engineered mutation	UNP O75570
Aa	446	GLY	-	expression tag	UNP O75570
Aa	447	GLY	-	expression tag	UNP O75570
Aa	448	SER	-	expression tag	UNP O75570
Aa	449	GLY	-	expression tag	UNP O75570

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Chain	Residue	Modelled	Actual	Comment	Reference
Aa	450	GLY	-	expression tag	UNP O75570
Aa	451	SER	-	expression tag	UNP O75570
Aa	452	GLY	-	expression tag	UNP O75570
Aa	453	GLY	-	expression tag	UNP O75570
Aa	454	SER	-	expression tag	UNP O75570
Aa	455	GLY	-	expression tag	UNP O75570
Aa	456	GLY	-	expression tag	UNP O75570
Aa	457	SER	-	expression tag	UNP O75570
Aa	458	GLY	-	expression tag	UNP O75570
Aa	459	GLY	-	expression tag	UNP O75570
Aa	460	SER	-	expression tag	UNP O75570
Aa	461	GLY	-	expression tag	UNP O75570
Aa	462	GLY	-	expression tag	UNP O75570
Aa	463	ASP	-	expression tag	UNP O75570
Aa	464	TYR	-	expression tag	UNP O75570
Aa	465	LYS	-	expression tag	UNP O75570
Aa	466	ASP	-	expression tag	UNP O75570
Aa	467	HIS	-	expression tag	UNP O75570
Aa	468	ASP	-	expression tag	UNP O75570
Aa	469	GLY	-	expression tag	UNP O75570
Aa	470	ASP	-	expression tag	UNP O75570
Aa	471	TYR	-	expression tag	UNP O75570
Aa	472	LYS	-	expression tag	UNP O75570
Aa	473	ASP	-	expression tag	UNP O75570
Aa	474	HIS	-	expression tag	UNP O75570
Aa	475	ASP	-	expression tag	UNP O75570
Aa	476	ILE	-	expression tag	UNP O75570
Aa	477	ASP	-	expression tag	UNP O75570
Aa	478	TYR	-	expression tag	UNP O75570
Aa	479	LYS	-	expression tag	UNP O75570
Aa	480	ASP	-	expression tag	UNP O75570
Aa	481	ASP	-	expression tag	UNP O75570
Aa	482	ASP	-	expression tag	UNP O75570
Aa	483	ASP	-	expression tag	UNP O75570
Aa	484	LYS	-	expression tag	UNP O75570

- Molecule 83 is a protein called 28S ribosomal protein S2, mitochondrial.

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

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

1.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Ac	117	Total	C	N	O	S	0	0
			935	579	182	166	8		

- Molecule 85 is a protein called 28S ribosomal protein S5, mitochondrial.

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

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

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

- Molecule 87 is a protein called 28S ribosomal protein S9, mitochondrial.

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

- Molecule 88 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Ai	137	Total	C	N	O	S	0	0
			1020	642	192	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ai	184	5F0	ASN	conflict	UNP P82912

- Molecule 89 is a protein called 28S ribosomal protein S34, mitochondrial.

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

- Molecule 90 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
90	B8	30	Total 30	K 30	0
90	BL	1	Total 1	K 1	0
90	BT	1	Total 1	K 1	0
90	Be	1	Total 1	K 1	0
90	Bn	1	Total 1	K 1	0
90	AA	16	Total 16	K 16	0
90	Ae	1	Total 1	K 1	0

- Molecule 91 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

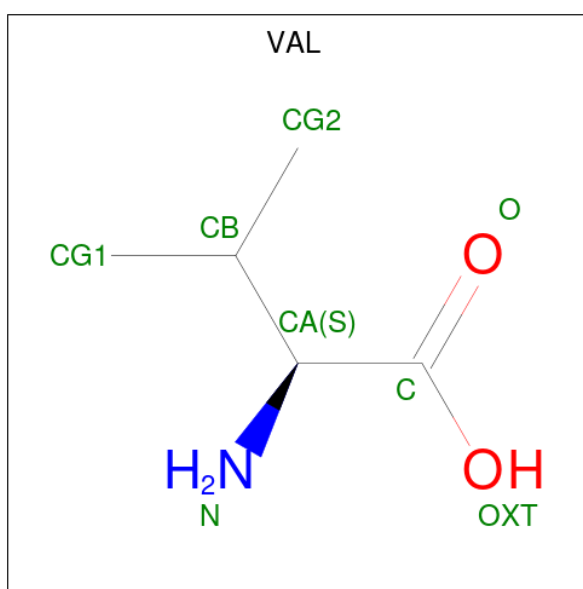
Mol	Chain	Residues	Atoms		AltConf
91	B8	216	Total 216	Mg 216	0
91	BD	1	Total 1	Mg 1	0
91	BL	3	Total 3	Mg 3	0
91	BN	1	Total 1	Mg 1	0
91	BO	1	Total 1	Mg 1	0
91	BR	1	Total 1	Mg 1	0
91	BT	1	Total 1	Mg 1	0
91	BV	1	Total 1	Mg 1	0
91	Bx	1	Total 1	Mg 1	0
91	AA	120	Total 120	Mg 120	0
91	AD	1	Total 1	Mg 1	0
91	AG	2	Total 2	Mg 2	0
91	AU	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
91	AX	1	Total	Mg	0
			1	1	
91	Aa	1	Total	Mg	0
			1	1	
91	Ab	1	Total	Mg	0
			1	1	
91	Ad	1	Total	Mg	0
			1	1	

- Molecule 92 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).

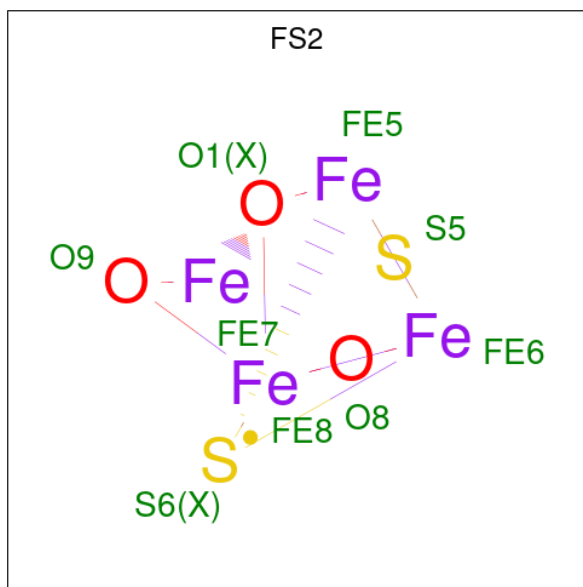


Mol	Chain	Residues	Atoms				AltConf
92	B9	1	Total	C	N	O	0
			7	5	1	1	

- Molecule 93 is ZINC ION (CCD ID: ZN) (formula: Zn).

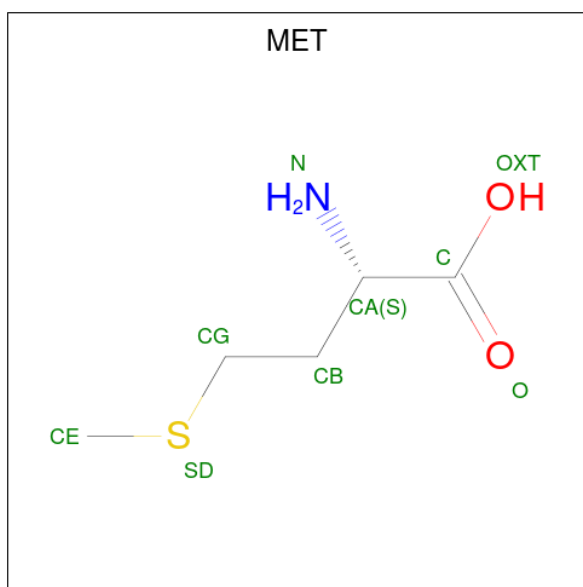
Mol	Chain	Residues	Atoms		AltConf
93	BH	1	Total	Zn	0
			1	1	
93	Bl	1	Total	Zn	0
			1	1	
93	AO	1	Total	Zn	0
			1	1	

- Molecule 94 is FE-S-O HYBRID CLUSTER (CCD ID: FS2) (formula: $Fe_4O_3S_2$).



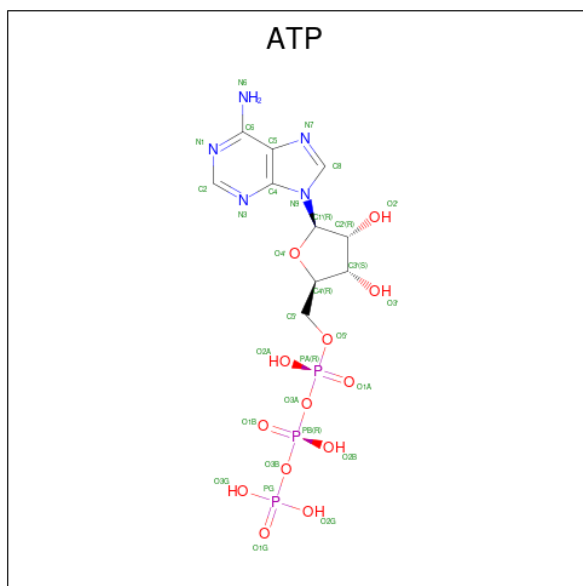
Mol	Chain	Residues	Atoms			AltConf
94	Bh	1	Total	Fe	S	0
			4	2	2	
94	AP	1	Total	Fe	S	0
			4	2	2	
94	AT	1	Total	Fe	S	0
			4	2	2	

- Molecule 95 is METHIONINE (CCD ID: MET) (formula: $C_5H_{11}NO_2S$).



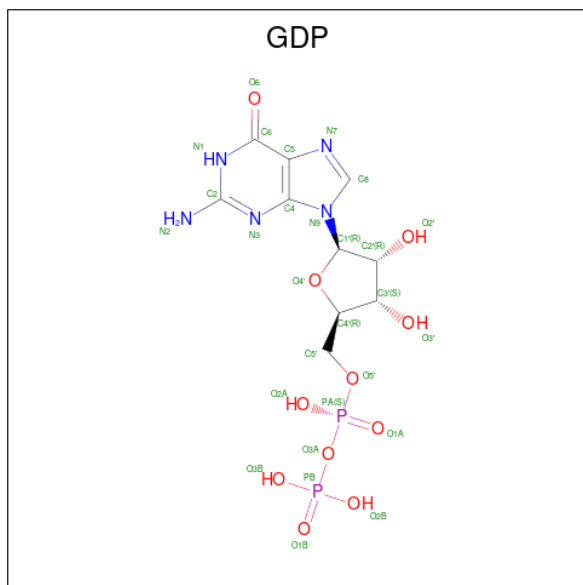
Mol	Chain	Residues	Atoms					AltConf
95	AG	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 96 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 97 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

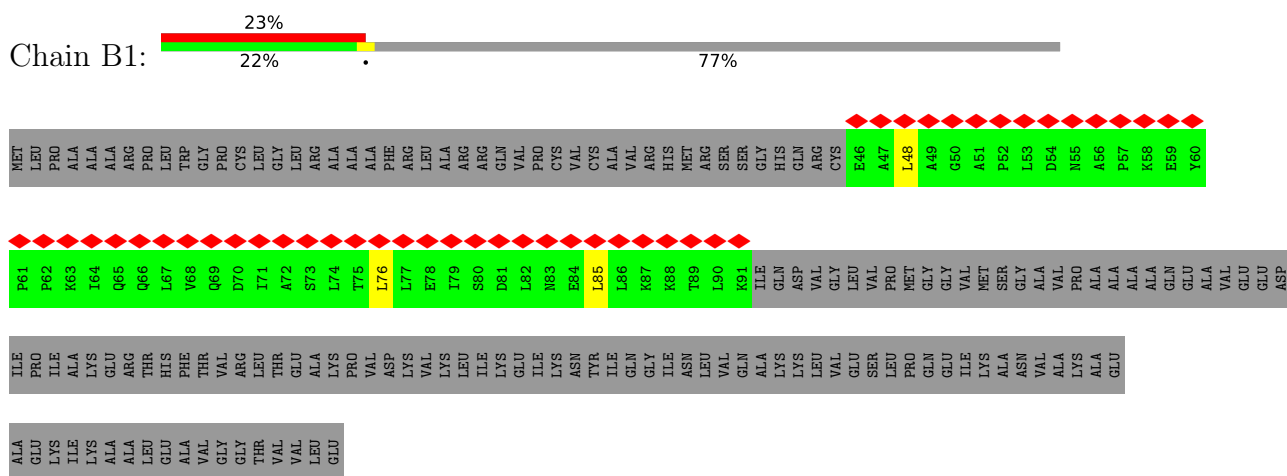
- Molecule 98 is water.

Mol	Chain	Residues	Atoms		AltConf
98	AX	3	Total 3	O 3	0

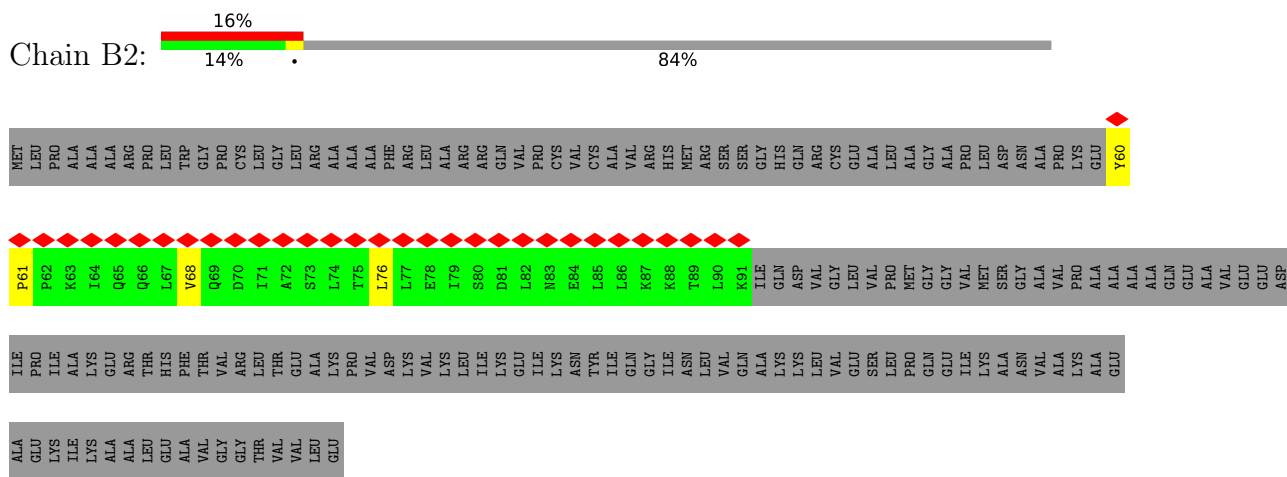
3 Residue-property plots

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

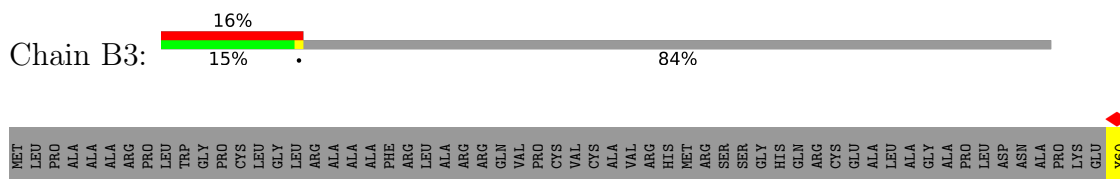
- Molecule 1: 39S ribosomal protein L12, mitochondrial



- Molecule 1: 39S ribosomal protein L12, mitochondrial

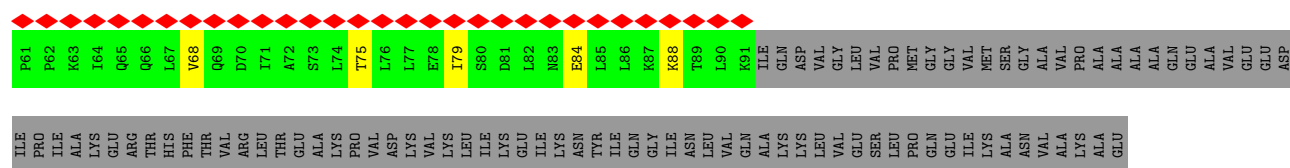
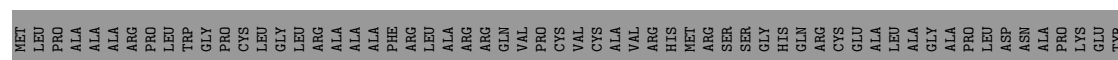


- Molecule 1: 39S ribosomal protein L12, mitochondrial



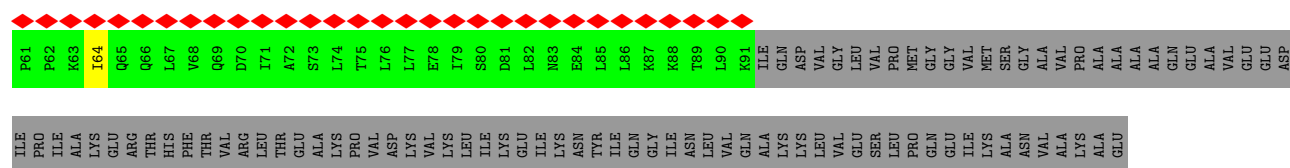
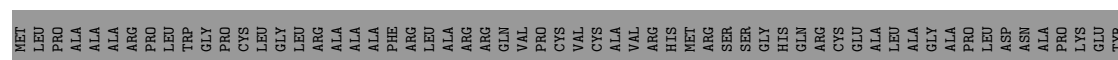
ALA
GLU
LYS
ILE
LYS
ALA
ALA
LEU
GLU
ALA
VAL
GLY
GLY
THR
VAL
VAL
LEU
GLU

- Molecule 1: 39S ribosomal protein L12, mitochondrial



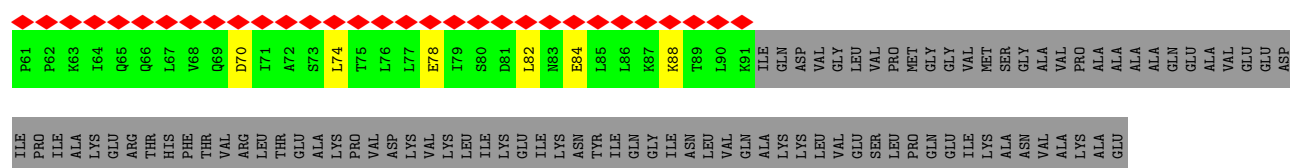
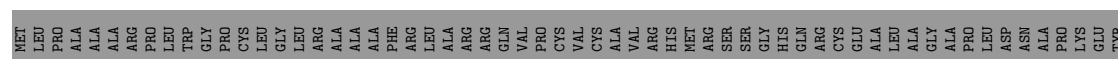
ALA
GLU
LYS
ILE
LYS
ALA
ALA
LEU
GLU
ALA
VAL
GLY
GLY
THR
VAL
VAL
LEU
GLU

- Molecule 1: 39S ribosomal protein L12, mitochondrial



ALA
GLU
LYS
ILE
LYS
ALA
ALA
LEU
GLU
ALA
VAL
GLY
GLY
THR
VAL
VAL
LEU
GLU

- Molecule 1: 39S ribosomal protein L12, mitochondrial

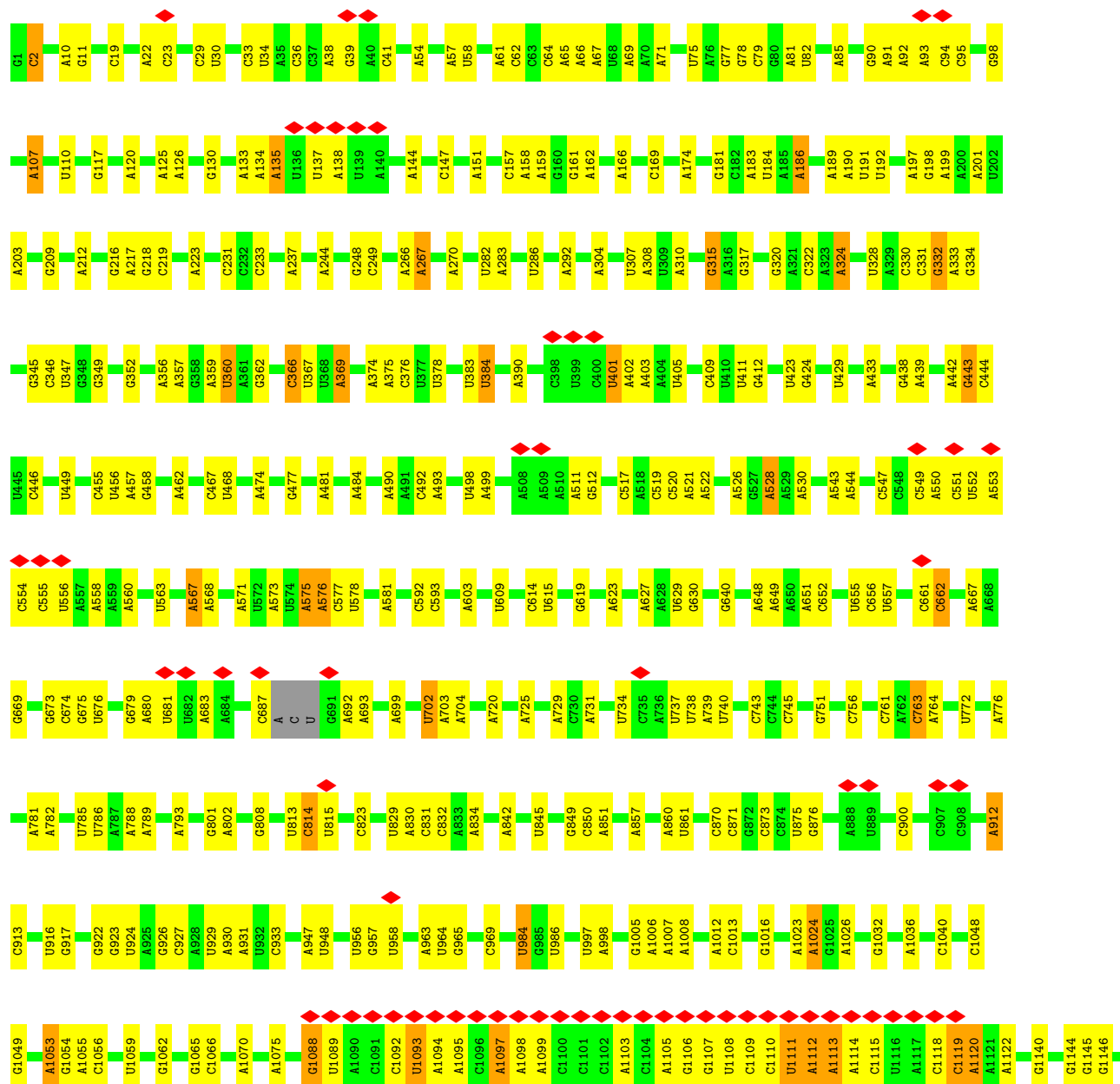


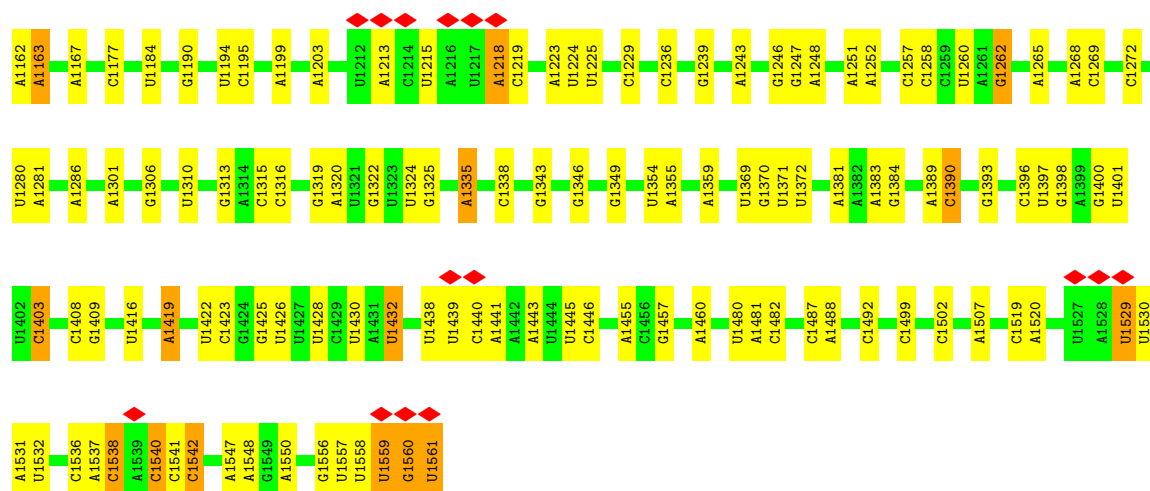
ALA	GLU
LYS	LYS
ILE	LYS
ALA	ALA
ALA	LEU
GLU	ALA
VAL	VAL
GLY	GLY
THR	THR
VAL	VAL
LEU	LEU
GLU	GLU

• Molecule 2: E-site tRNA

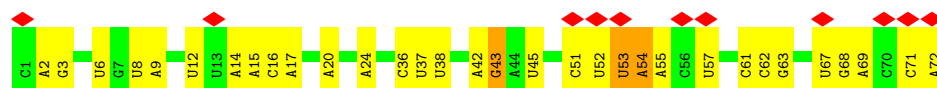


• Molecule 3: 16S rRNA

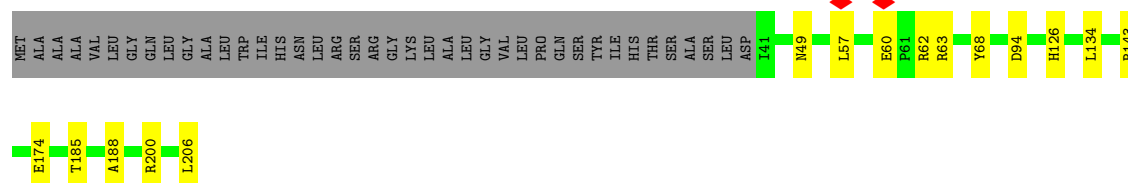
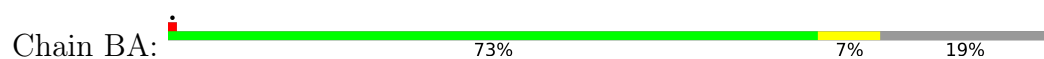




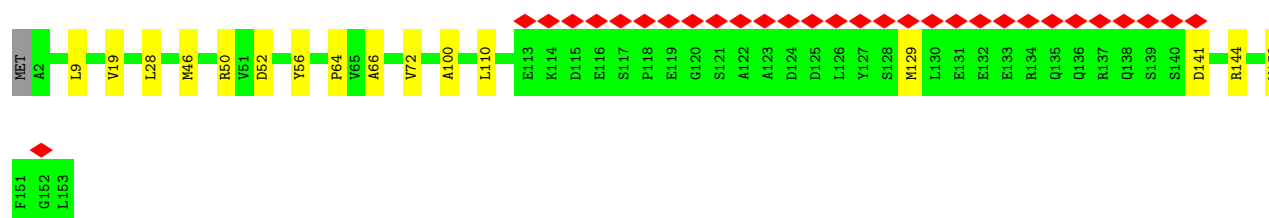
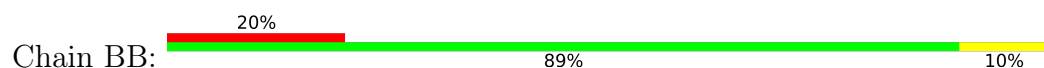
• Molecule 4: CP Val-tRNA(Val)



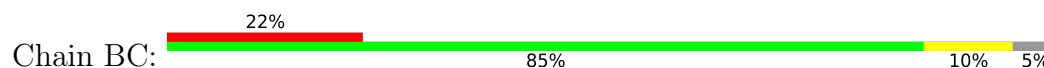
• Molecule 5: 39S ribosomal protein L22, mitochondrial

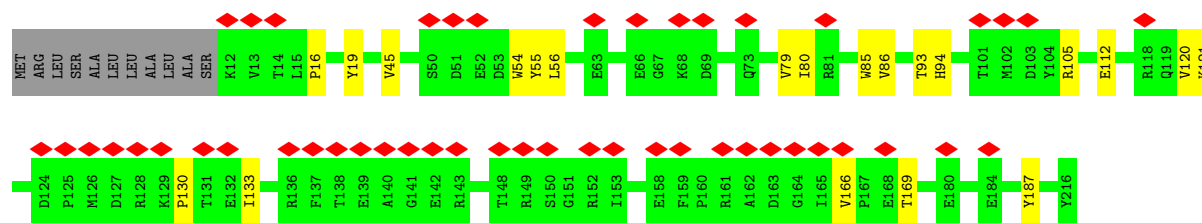


• Molecule 6: 39S ribosomal protein L23, mitochondrial

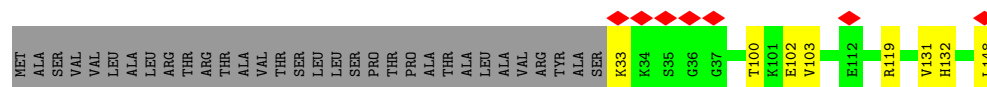
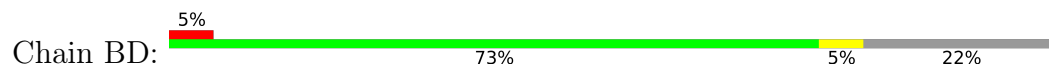


• Molecule 7: 39S ribosomal protein L24, mitochondrial

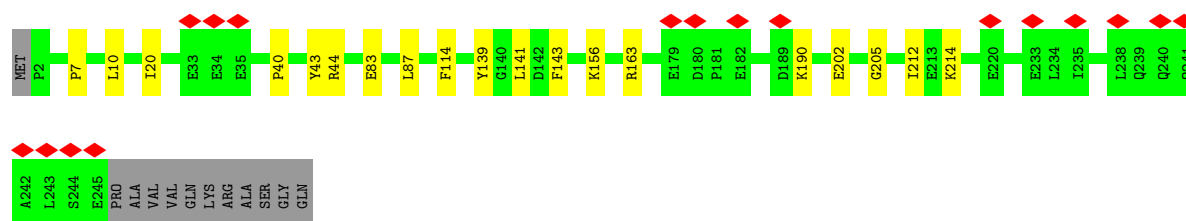
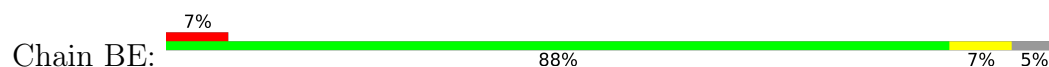




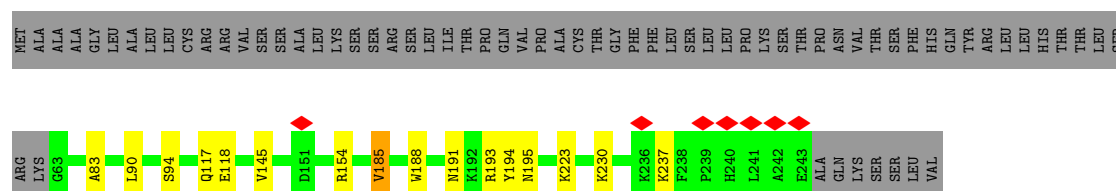
- Molecule 8: 39S ribosomal protein L27, mitochondrial



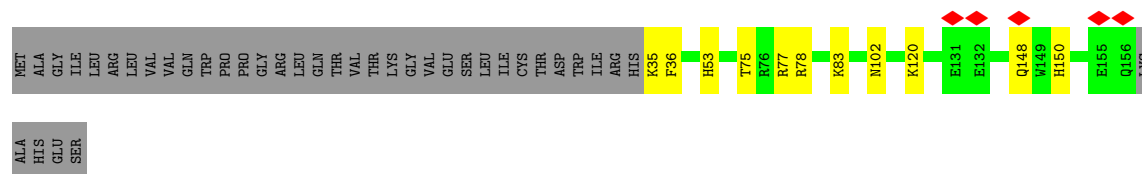
- Molecule 9: 39S ribosomal protein L28, mitochondrial



- Molecule 10: 39S ribosomal protein L47, mitochondrial



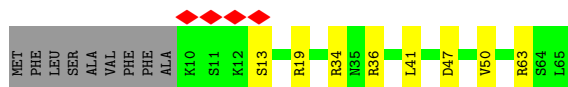
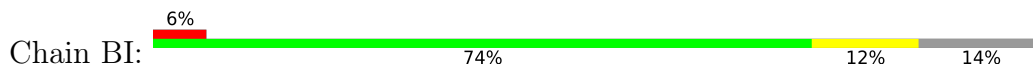
- Molecule 11: 39S ribosomal protein L30, mitochondrial



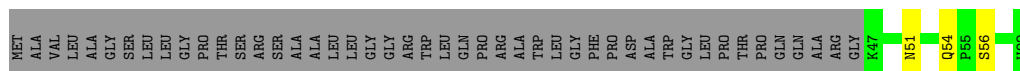
- Molecule 12: 39S ribosomal protein L32, mitochondrial



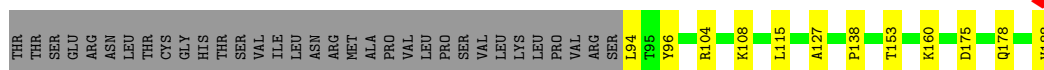
- Molecule 13: 39S ribosomal protein L33, mitochondrial



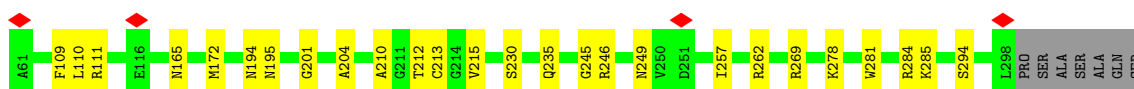
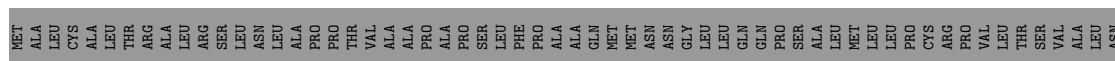
- Molecule 14: 39S ribosomal protein L34, mitochondrial



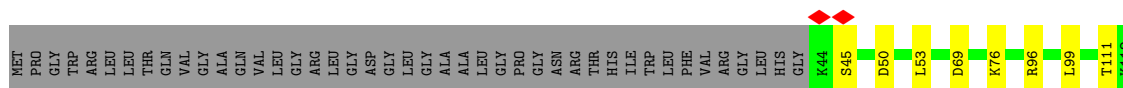
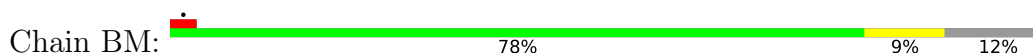
- Molecule 15: 39S ribosomal protein L35, mitochondrial



- Molecule 16: 39S ribosomal protein L2, mitochondrial



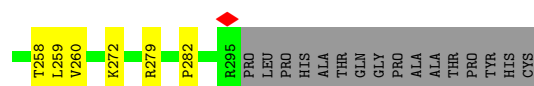
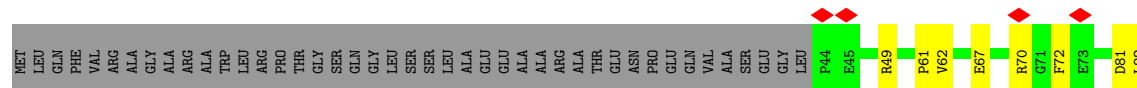
- Molecule 17: 39S ribosomal protein L3, mitochondrial





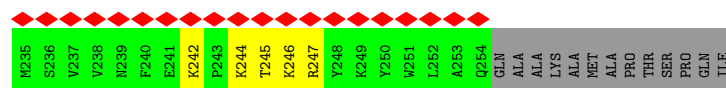
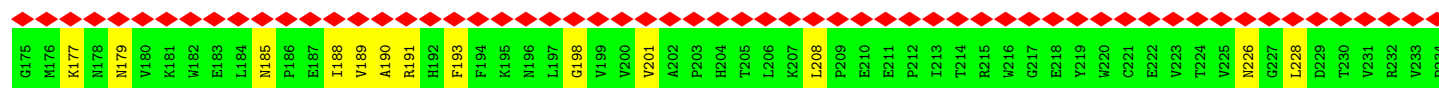
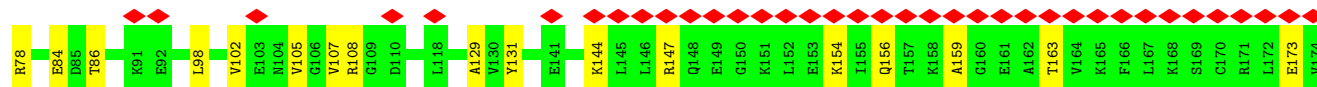
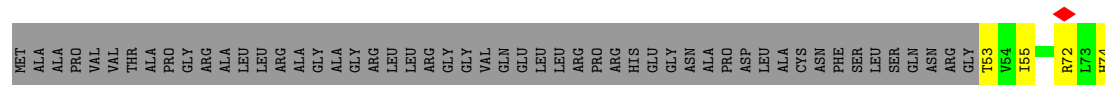
- Molecule 18: 39S ribosomal protein L4, mitochondrial

Chain BN: 67% 14% 19%



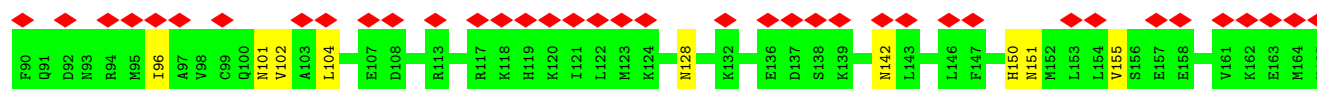
- Molecule 19: 39S ribosomal protein L9, mitochondrial

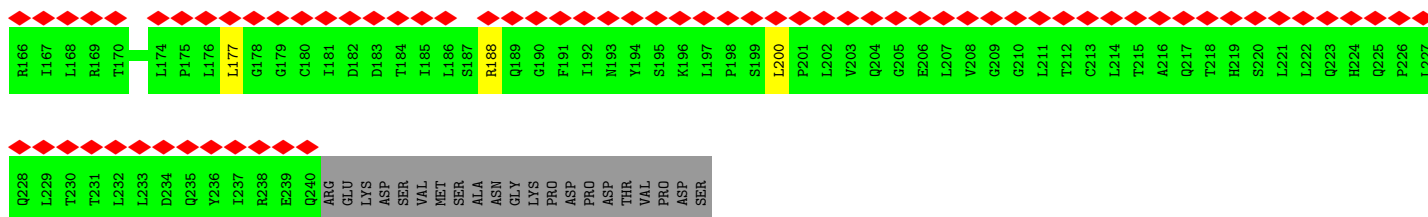
Chain BO: 44% 61% 15% 24%



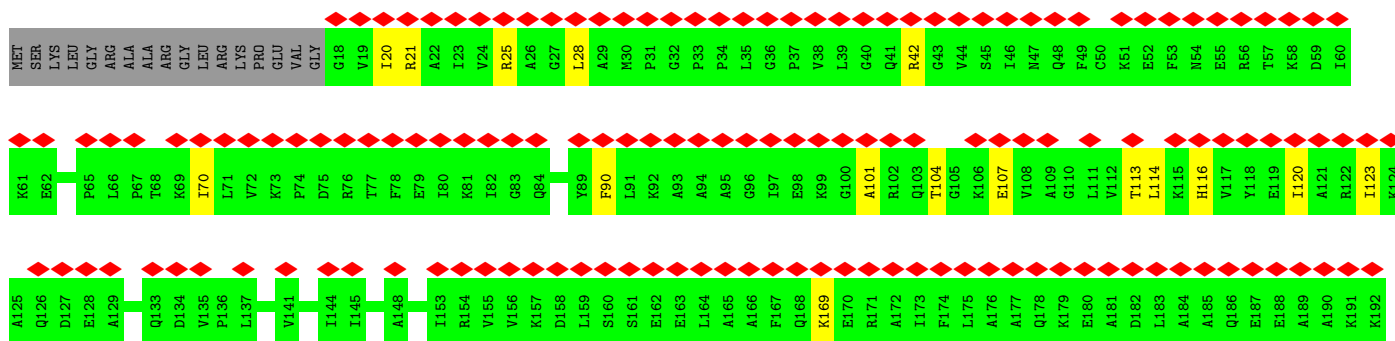
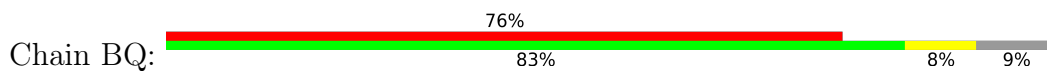
- Molecule 20: 39S ribosomal protein L10, mitochondrial

Chain BP: 48% 75% 7% 19%

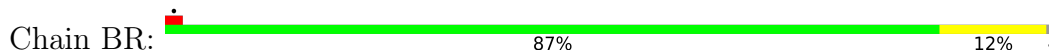




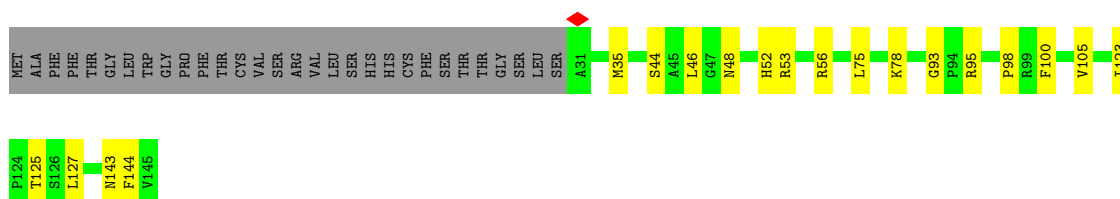
- Molecule 21: 39S ribosomal protein L11, mitochondrial



- Molecule 22: 39S ribosomal protein L13, mitochondrial

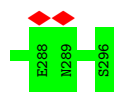


- Molecule 23: 39S ribosomal protein L14, mitochondrial



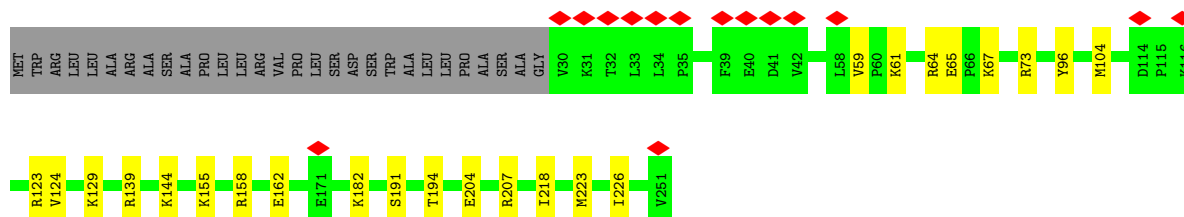
- Molecule 24: 39S ribosomal protein L15, mitochondrial





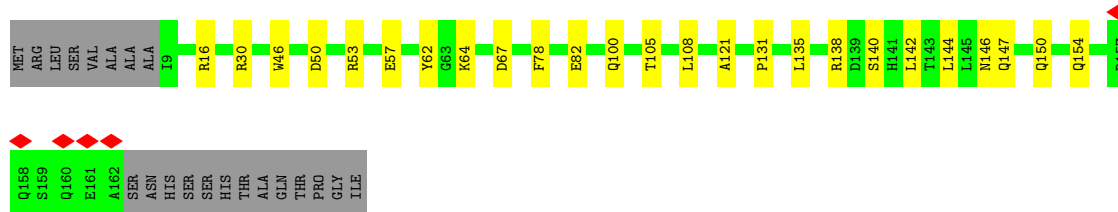
- Molecule 25: 39S ribosomal protein L16, mitochondrial

Chain BU: 6% 79% 10% 12%



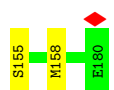
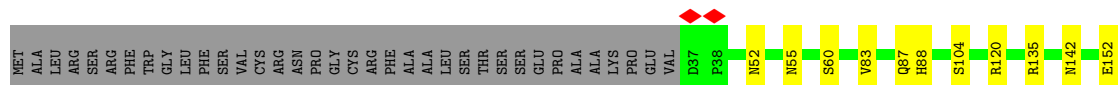
- Molecule 26: 39S ribosomal protein L17, mitochondrial

Chain BV: 74% 14% 12%



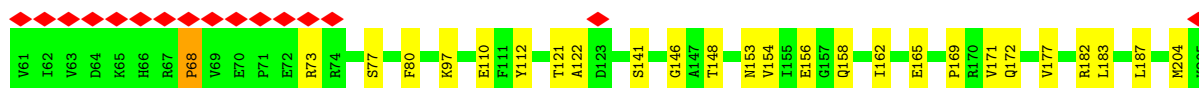
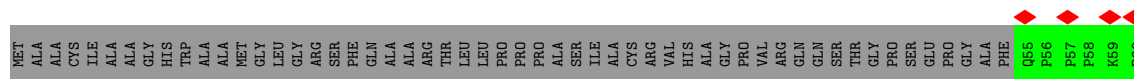
- Molecule 27: 39S ribosomal protein L18, mitochondrial

Chain BW: 73% 7% 20%



- Molecule 28: 39S ribosomal protein L19, mitochondrial

Chain BX: 9% 69% 12% 18%





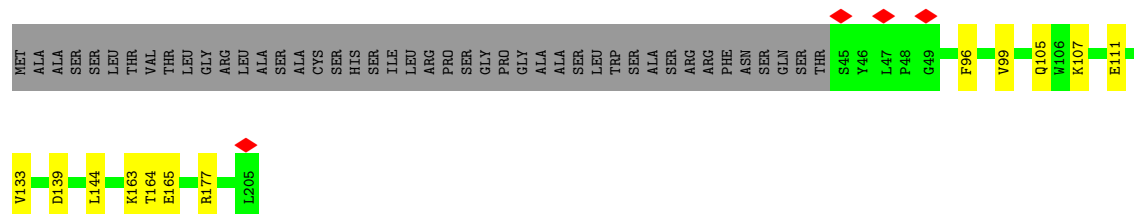
- Molecule 29: 39S ribosomal protein L20, mitochondrial

Chain BY: 85% 9% 6%



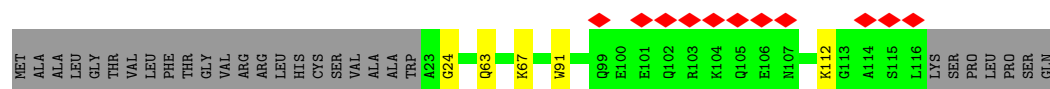
- Molecule 30: 39S ribosomal protein L21, mitochondrial

Chain BZ: 73% 6% 21%



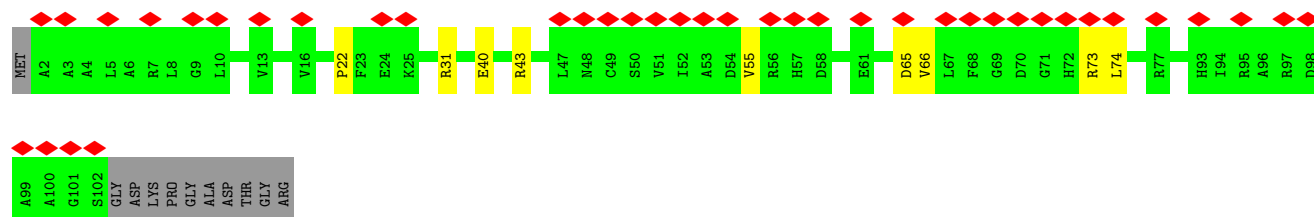
- Molecule 31: 39S ribosomal protein L52, mitochondrial

Chain Ba: 9% 72% 24%



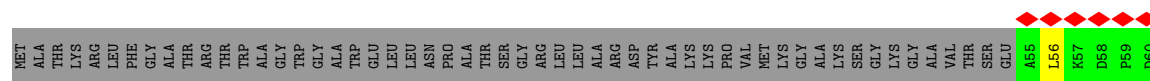
- Molecule 32: 39S ribosomal protein L53, mitochondrial

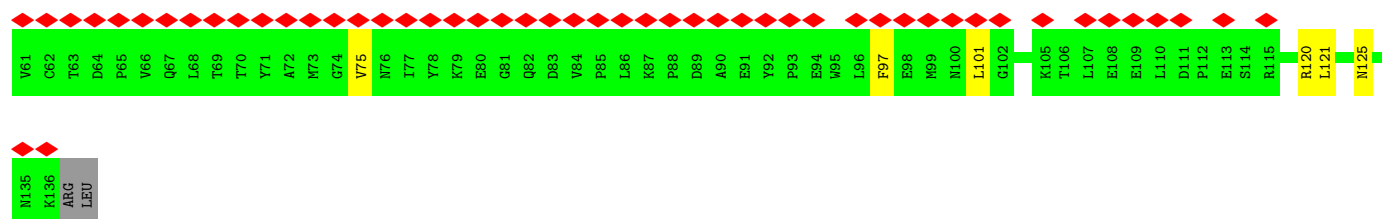
Chain Bb: 36% 82% 8% 10%



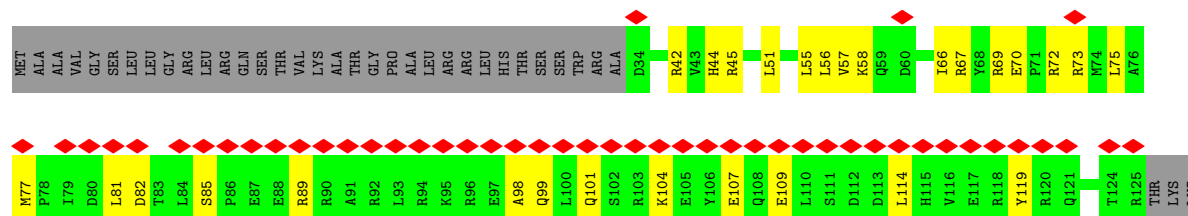
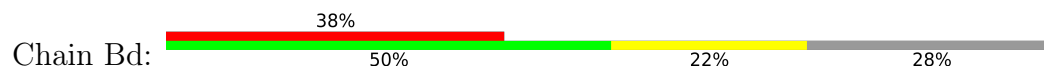
- Molecule 33: 39S ribosomal protein L54, mitochondrial

Chain Bc: 41% 54% 5% 41%

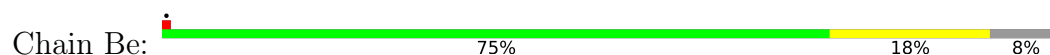




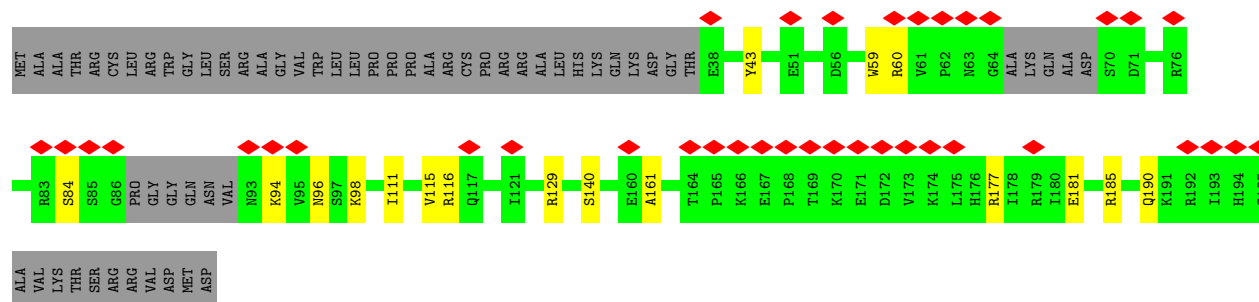
- Molecule 34: 39S ribosomal protein L55, mitochondrial



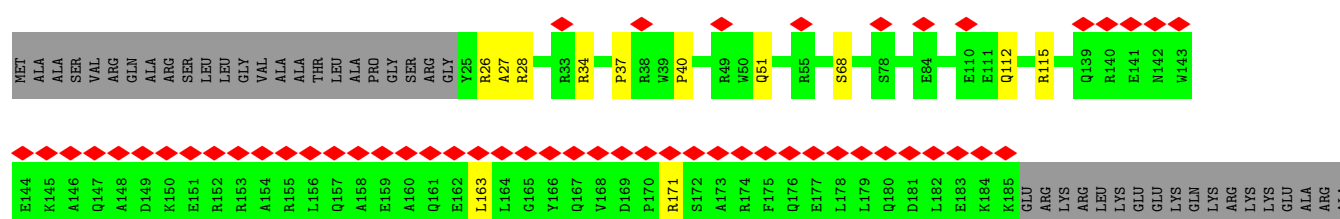
- Molecule 35: Ribosomal protein 63, mitochondrial

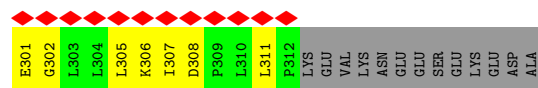


- Molecule 36: Peptidyl-tRNA hydrolase ICT1, mitochondrial



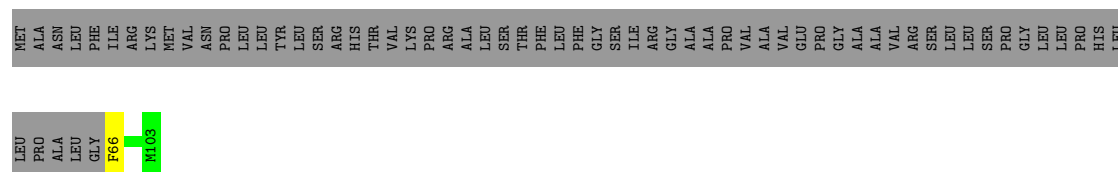
- Molecule 37: Growth arrest and DNA damage-inducible proteins-interacting protein 1





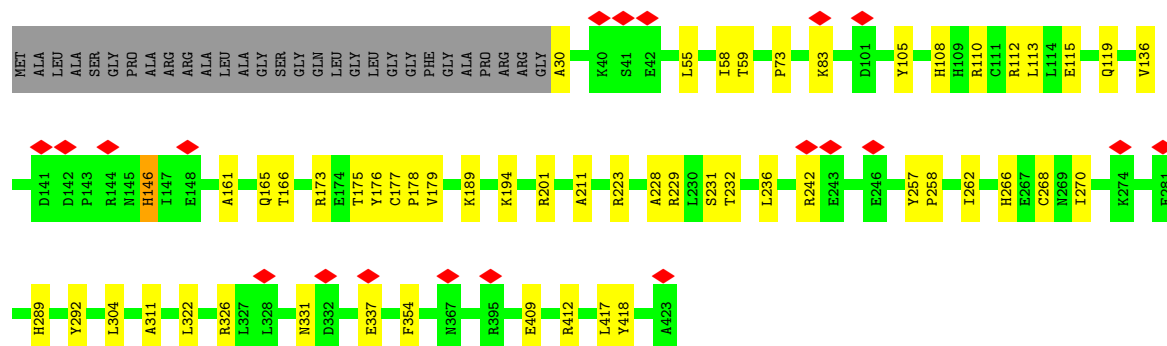
- Molecule 41: 39S ribosomal protein L36, mitochondrial

Chain Bl: 36% 63%



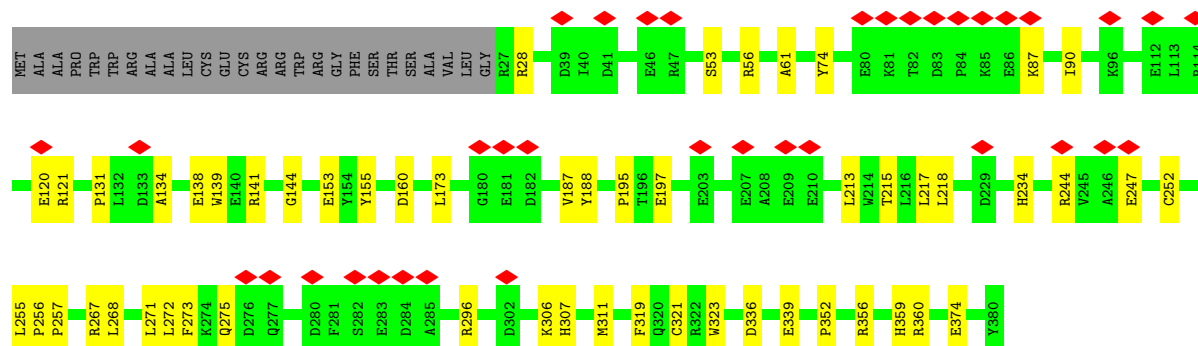
- Molecule 42: 39S ribosomal protein L37, mitochondrial

Chain Bm: 5% 80% 13% 7%



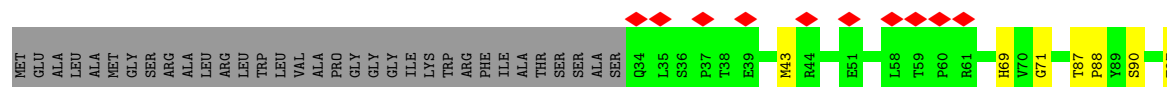
- Molecule 43: 39S ribosomal protein L38, mitochondrial

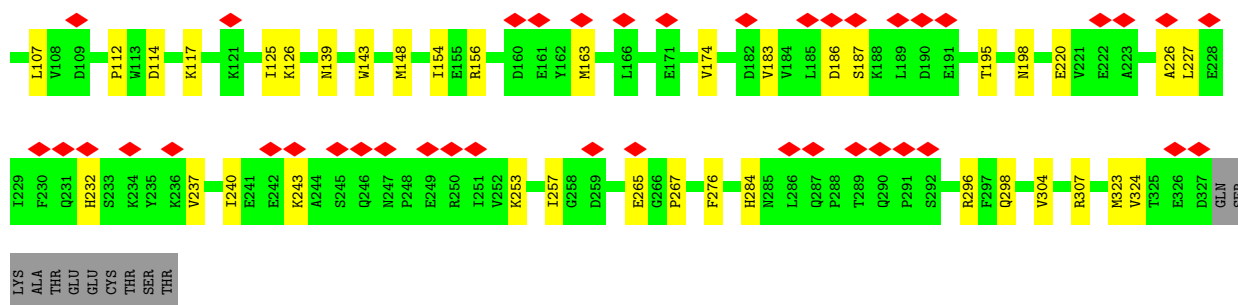
Chain Bn: 9% 79% 14% 7%



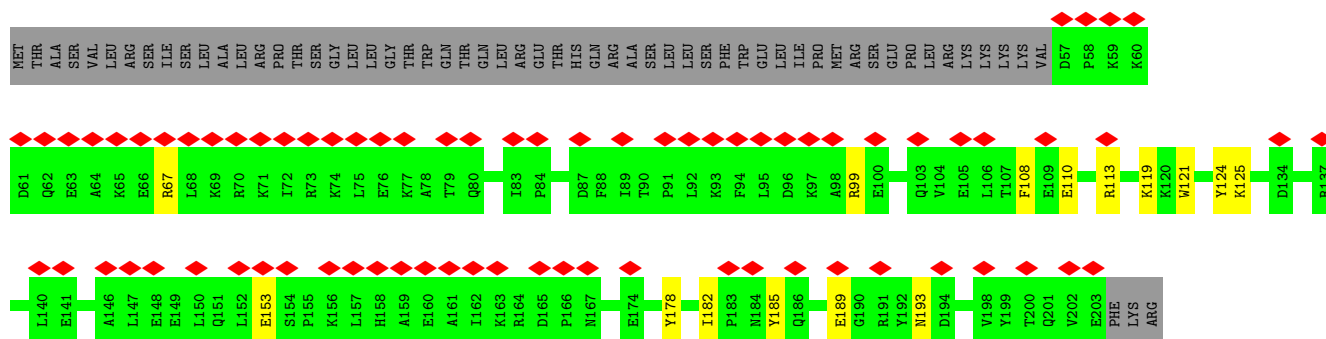
- Molecule 44: 39S ribosomal protein L39, mitochondrial

Chain Bo: 15% 74% 13% 13%

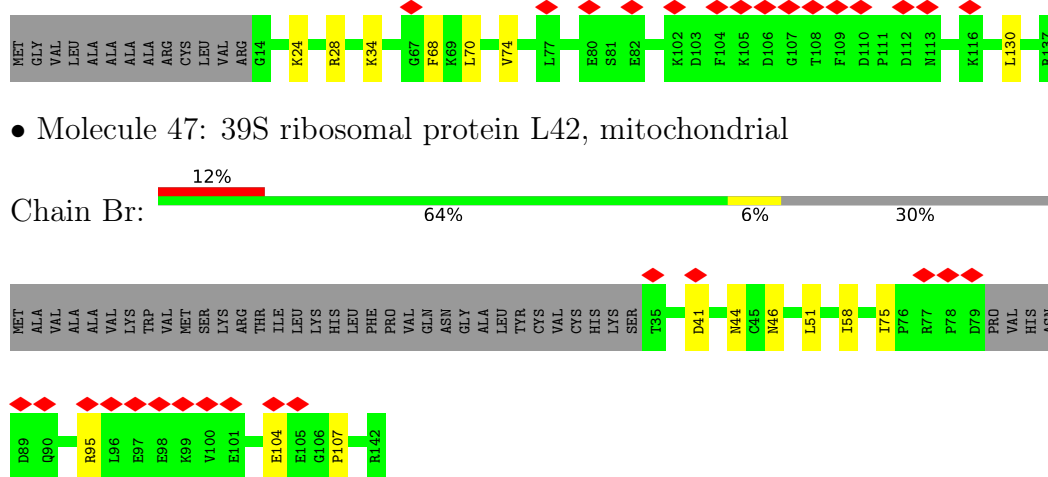
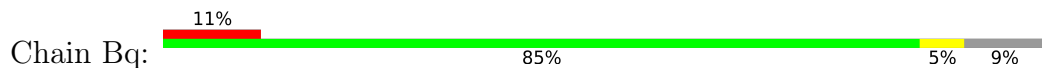




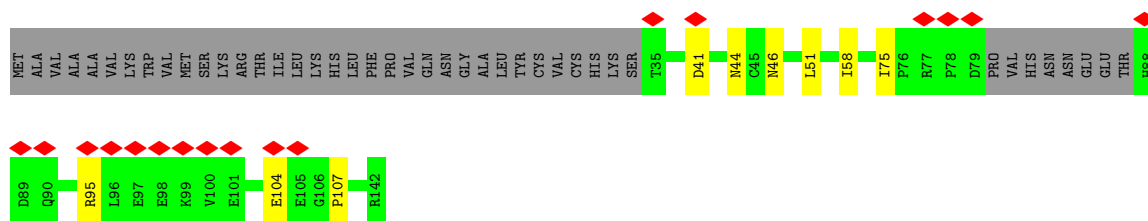
- Molecule 45: 39S ribosomal protein L40, mitochondrial



- Molecule 46: 39S ribosomal protein L41, mitochondrial



- Molecule 47: 39S ribosomal protein L42, mitochondrial



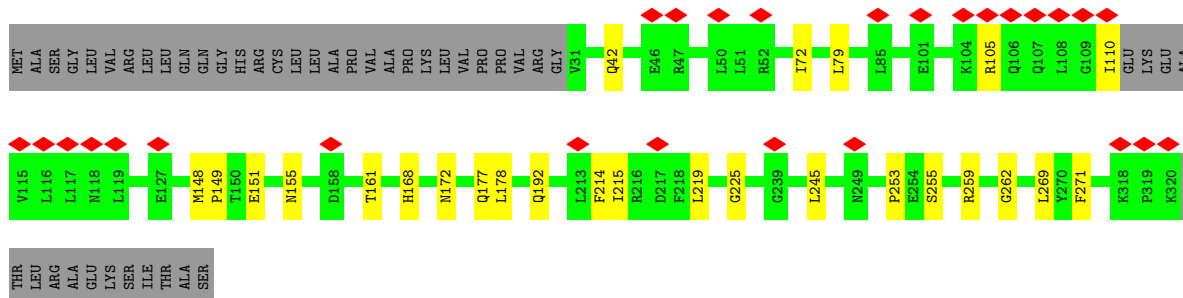
- Molecule 48: Large ribosomal subunit protein mL43



GLY LEU ARG SER LEU VAL ALA PRO ILE LEU LEU PRO GLN LEU LEU PRO GLY TRP PRO ASP PRO PRO ASP LEU THR VAL THR ASP PRO PRO ILE SER SER LEU THR ALA ALA PRO ALA MET LEU SER ALA VAL SER CYS LEU PRO ILE VAL PRO ALA LEU THR THR VAL CYS SER ALA

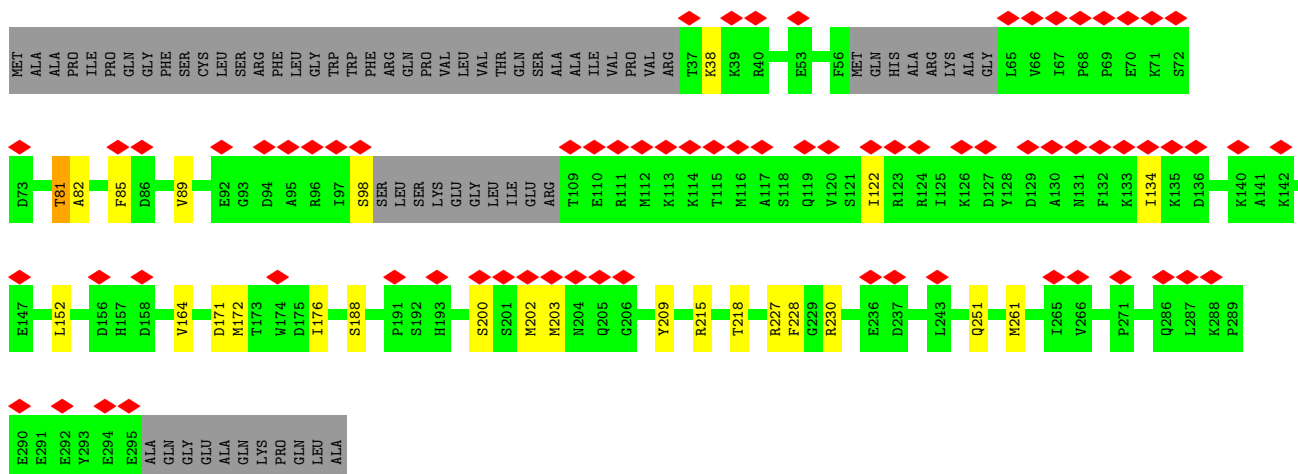
• Molecule 49: 39S ribosomal protein L44, mitochondrial

Chain Bt: 

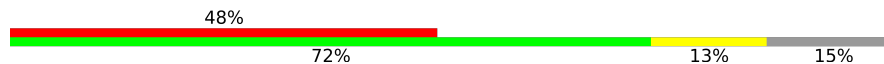


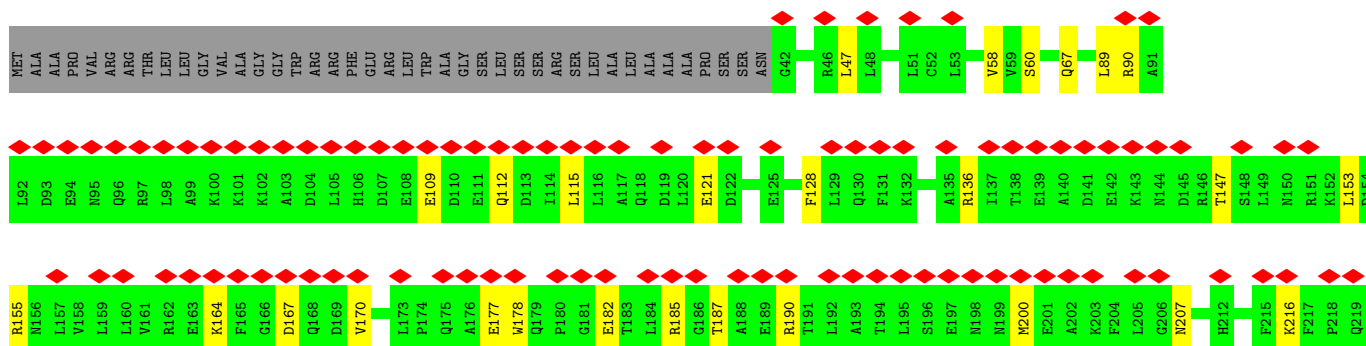
• Molecule 50: 39S ribosomal protein L45, mitochondrial

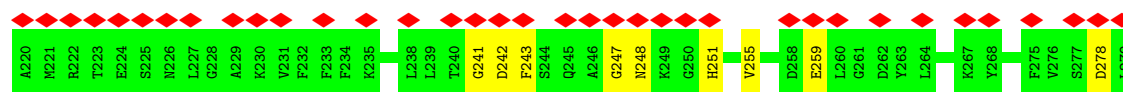
Chain Bu: 



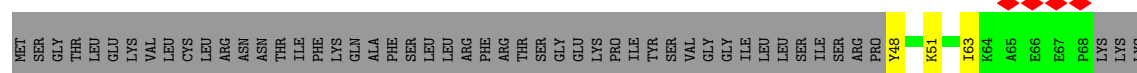
• Molecule 51: 39S ribosomal protein L46, mitochondrial

Chain Bv: 

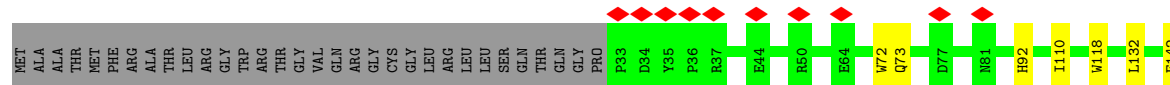
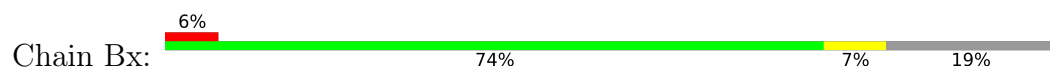




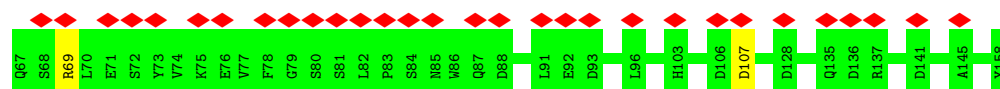
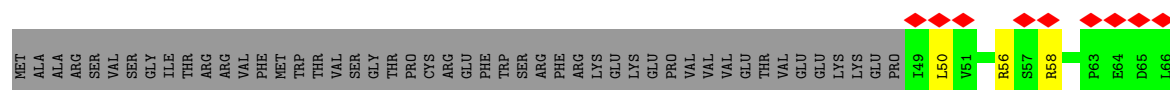
- Molecule 52: 39S ribosomal protein L48, mitochondrial



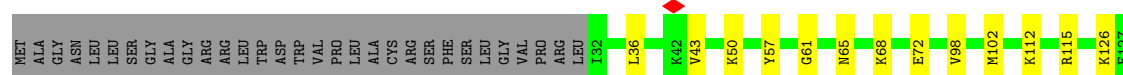
- Molecule 53: 39S ribosomal protein L49, mitochondrial



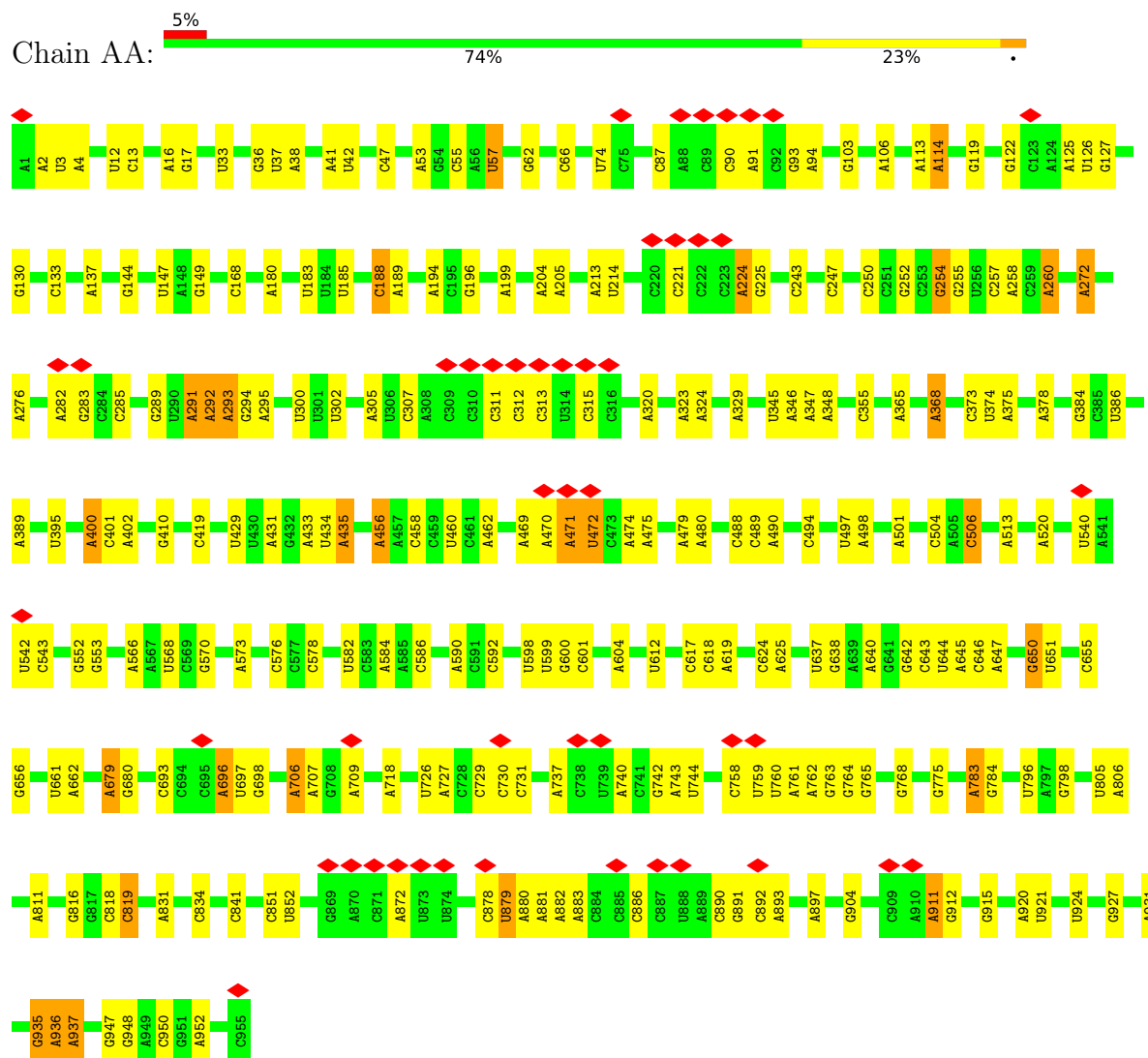
- Molecule 54: 39S ribosomal protein L50, mitochondrial



- Molecule 55: 39S ribosomal protein L51, mitochondrial

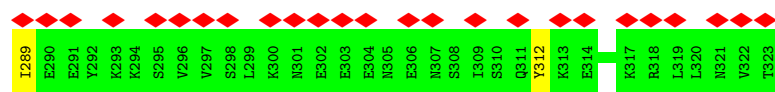


• Molecule 56: 12S rRNA

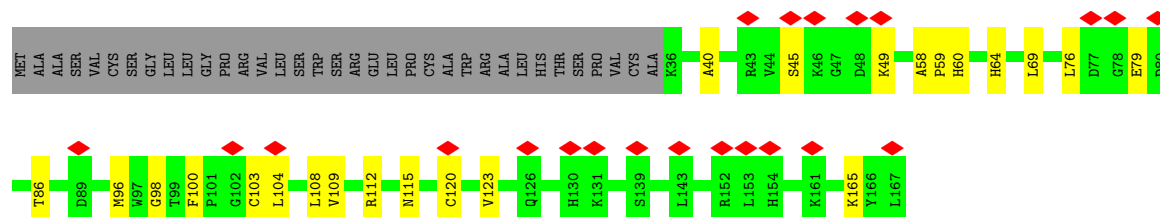


• Molecule 57: 28S ribosomal protein S35, mitochondrial

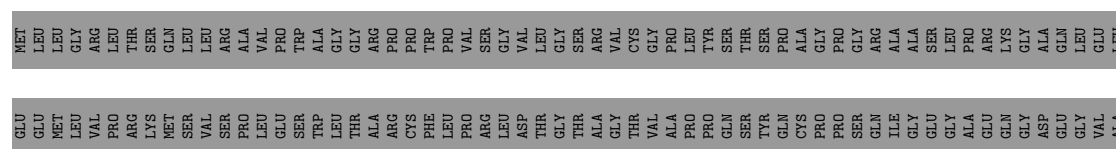




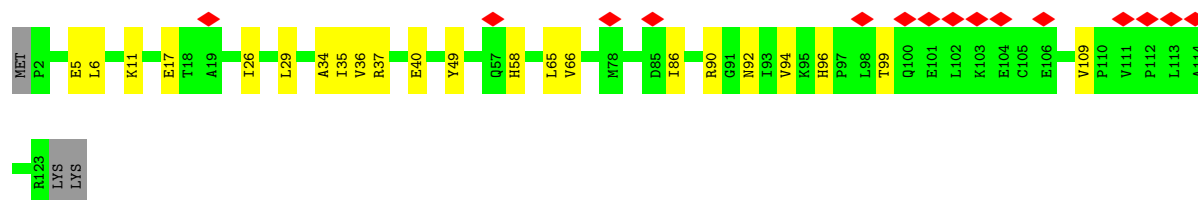
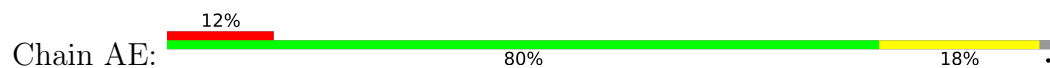
- Molecule 58: 28S ribosomal protein S24, mitochondrial



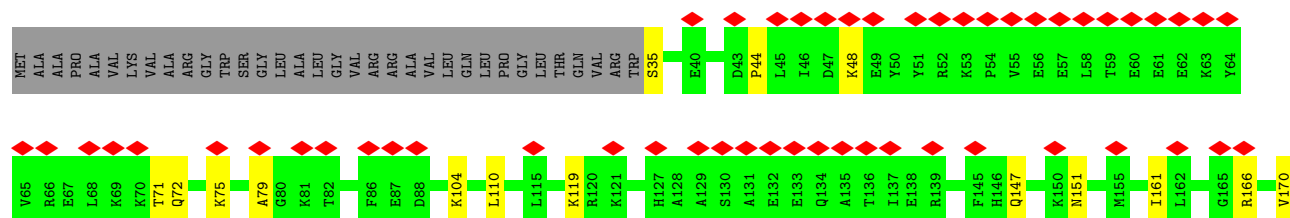
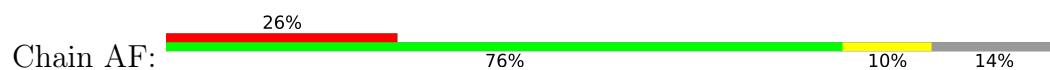
- Molecule 59: Aurora kinase A-interacting protein

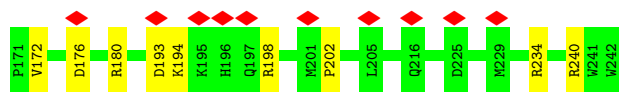


- Molecule 60: 28S ribosomal protein S6, mitochondrial



- Molecule 61: 28S ribosomal protein S7, mitochondrial

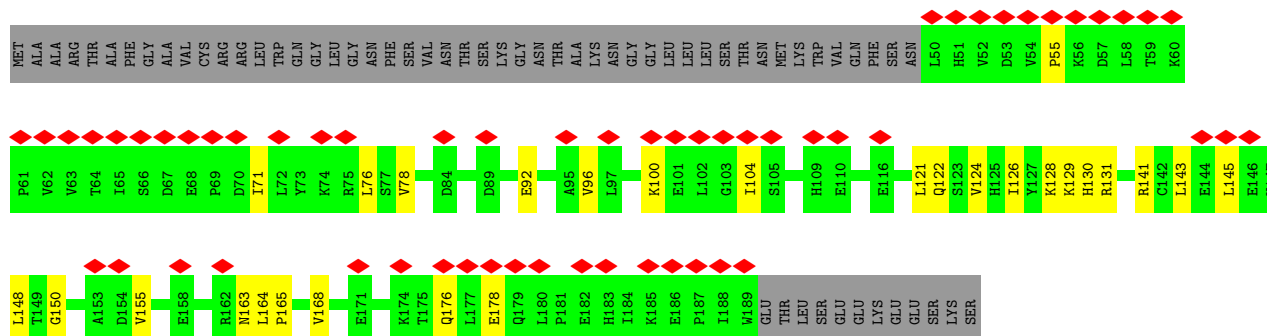




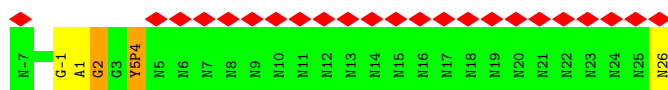
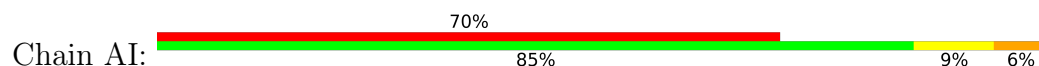
• Molecule 62: P-site Met-tRNA(Met)



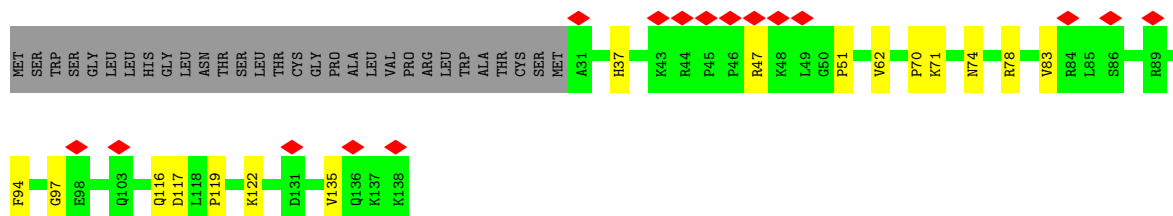
• Molecule 63: 28S ribosomal protein S10, mitochondrial



• Molecule 64: mRNA

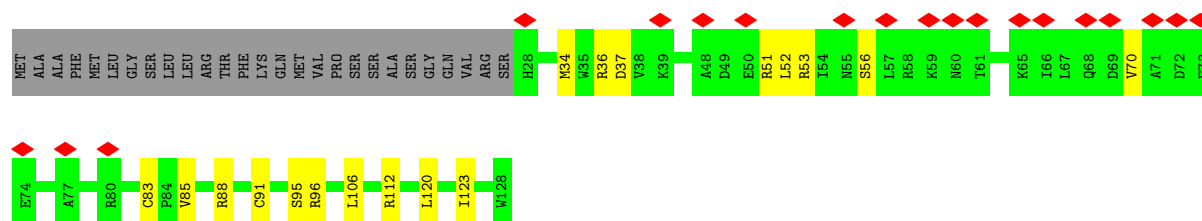


• Molecule 65: 28S ribosomal protein S12, mitochondrial

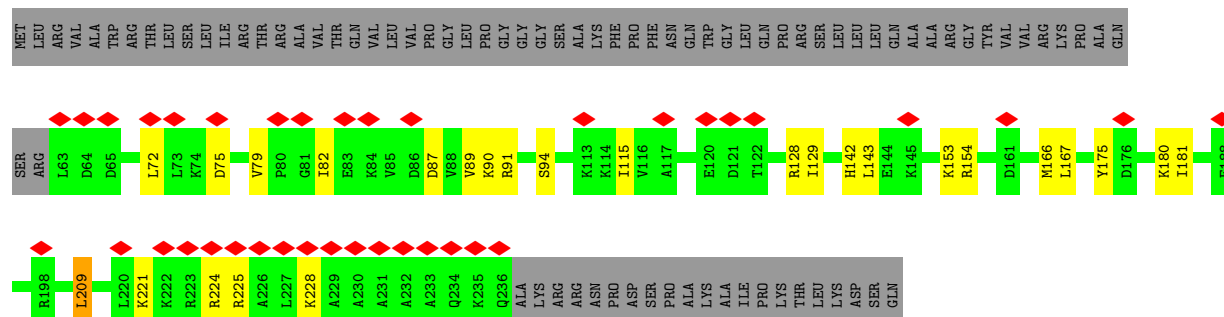


• Molecule 66: 28S ribosomal protein S14, mitochondrial

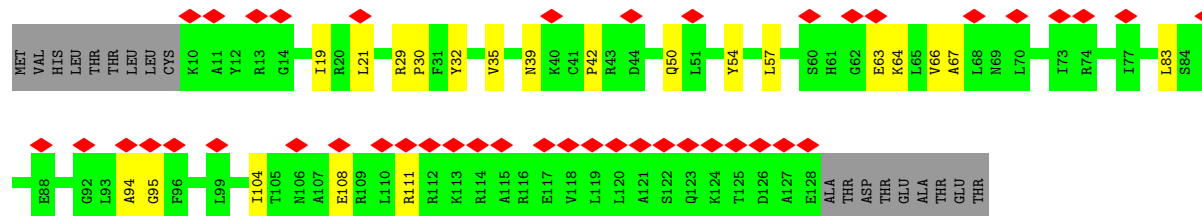
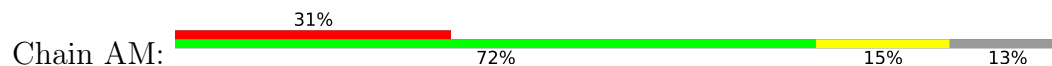




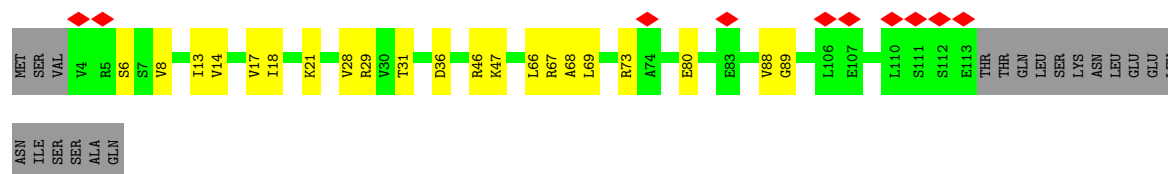
- Molecule 67: 28S ribosomal protein S15, mitochondrial



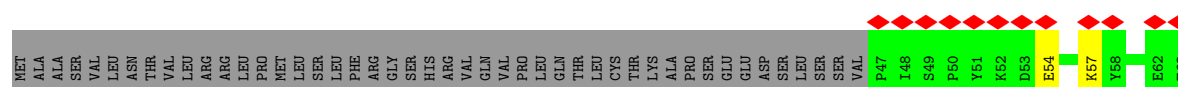
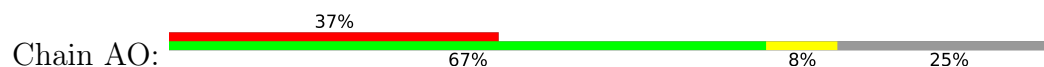
- Molecule 68: 28S ribosomal protein S16, mitochondrial

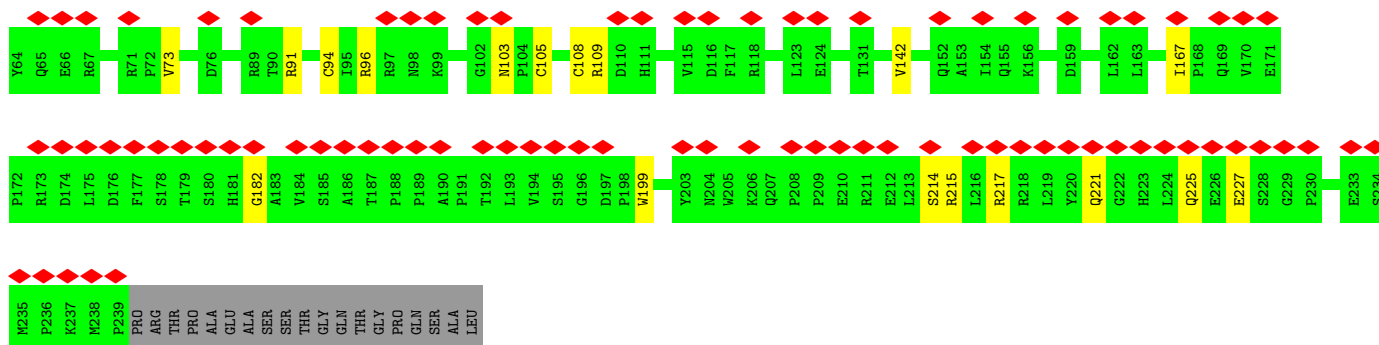


- Molecule 69: 28S ribosomal protein S17, mitochondrial

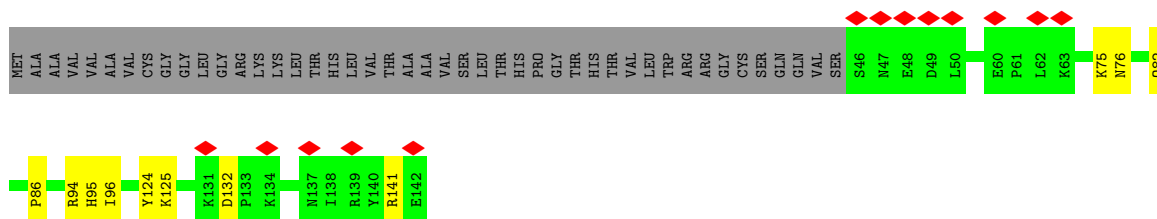


- Molecule 70: 28S ribosomal protein S18b, mitochondrial

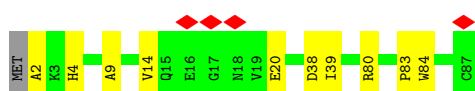
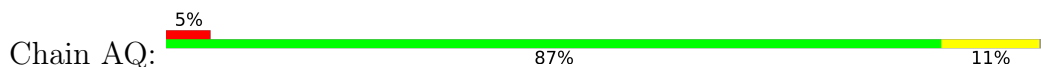




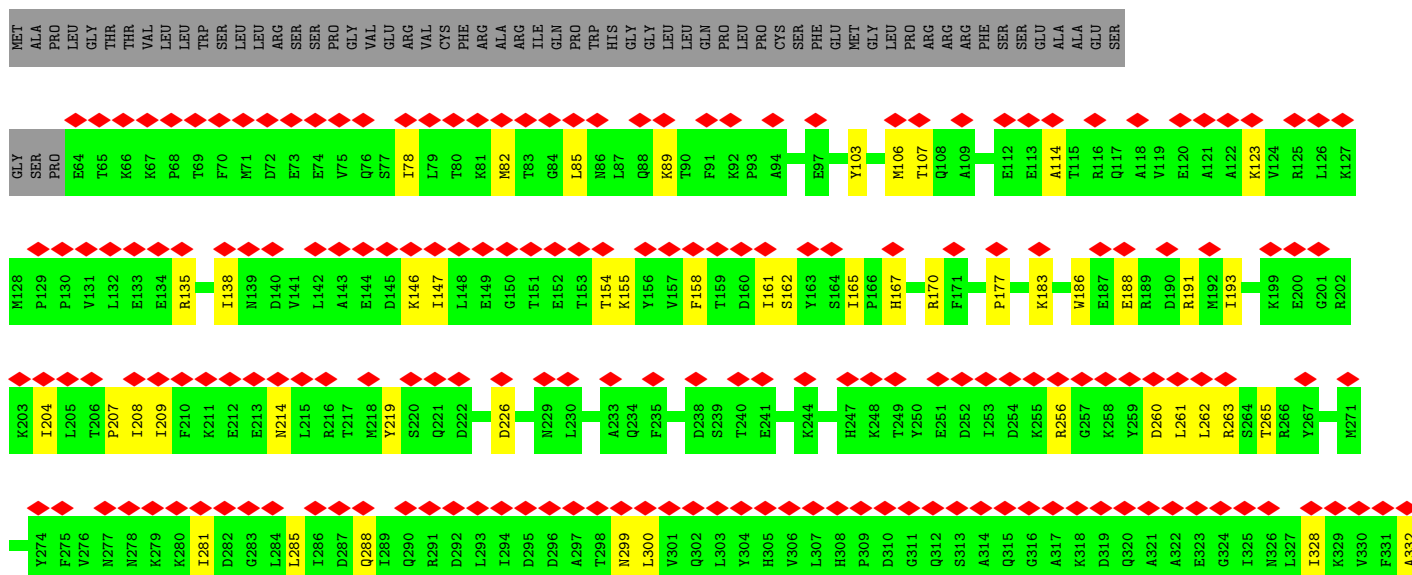
- Molecule 71: 28S ribosomal protein S18c, mitochondrial

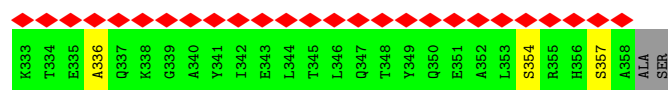


- Molecule 72: 28S ribosomal protein S21, mitochondrial

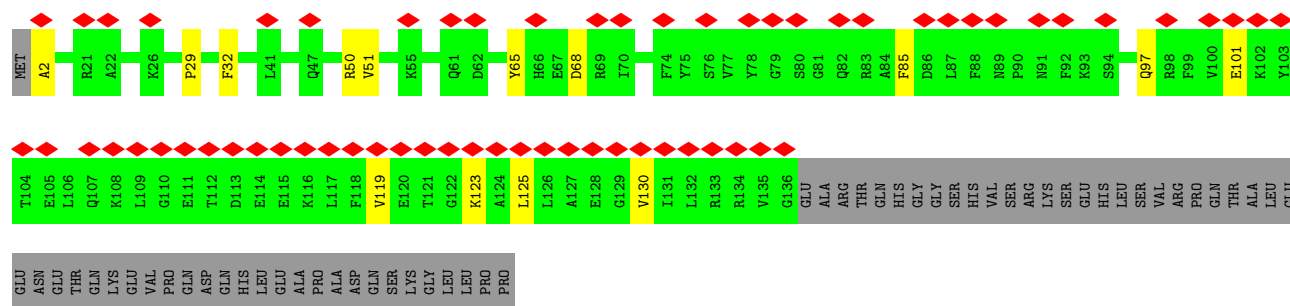


- Molecule 73: 28S ribosomal protein S22, mitochondrial

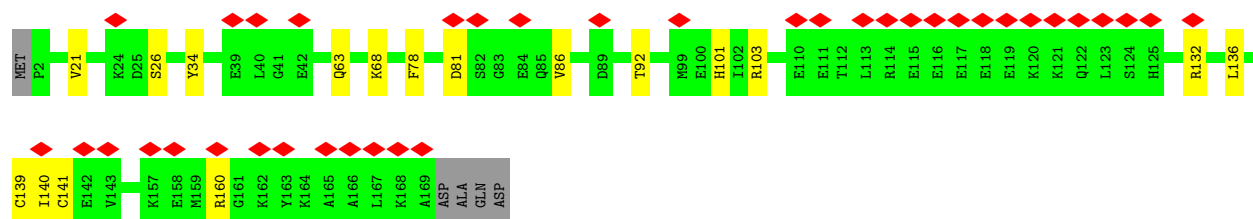
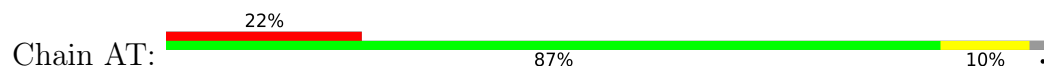




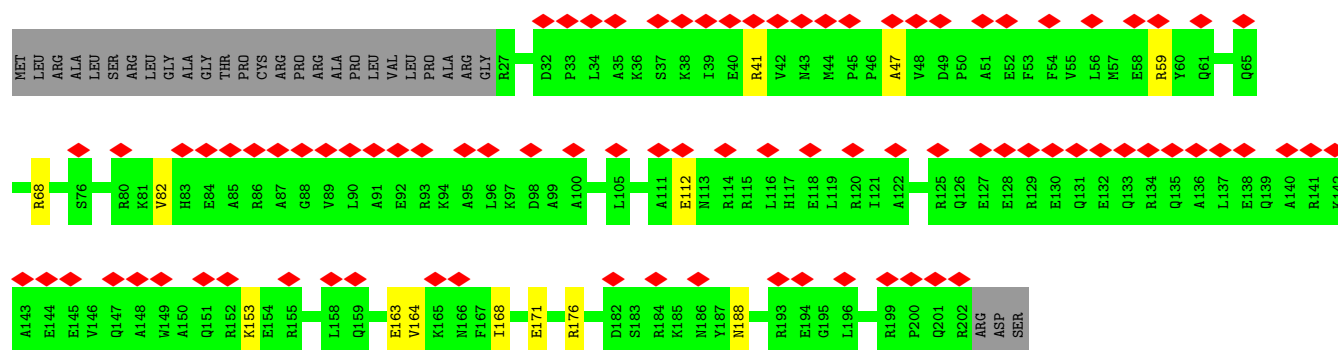
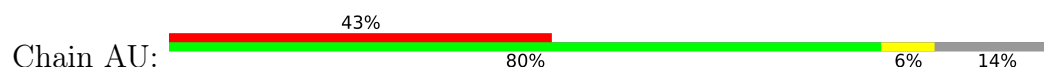
- Molecule 74: 28S ribosomal protein S23, mitochondrial



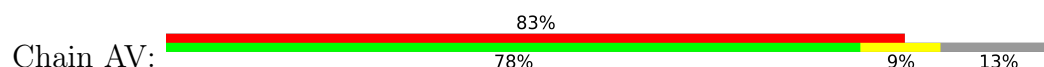
- Molecule 75: 28S ribosomal protein S25, mitochondrial

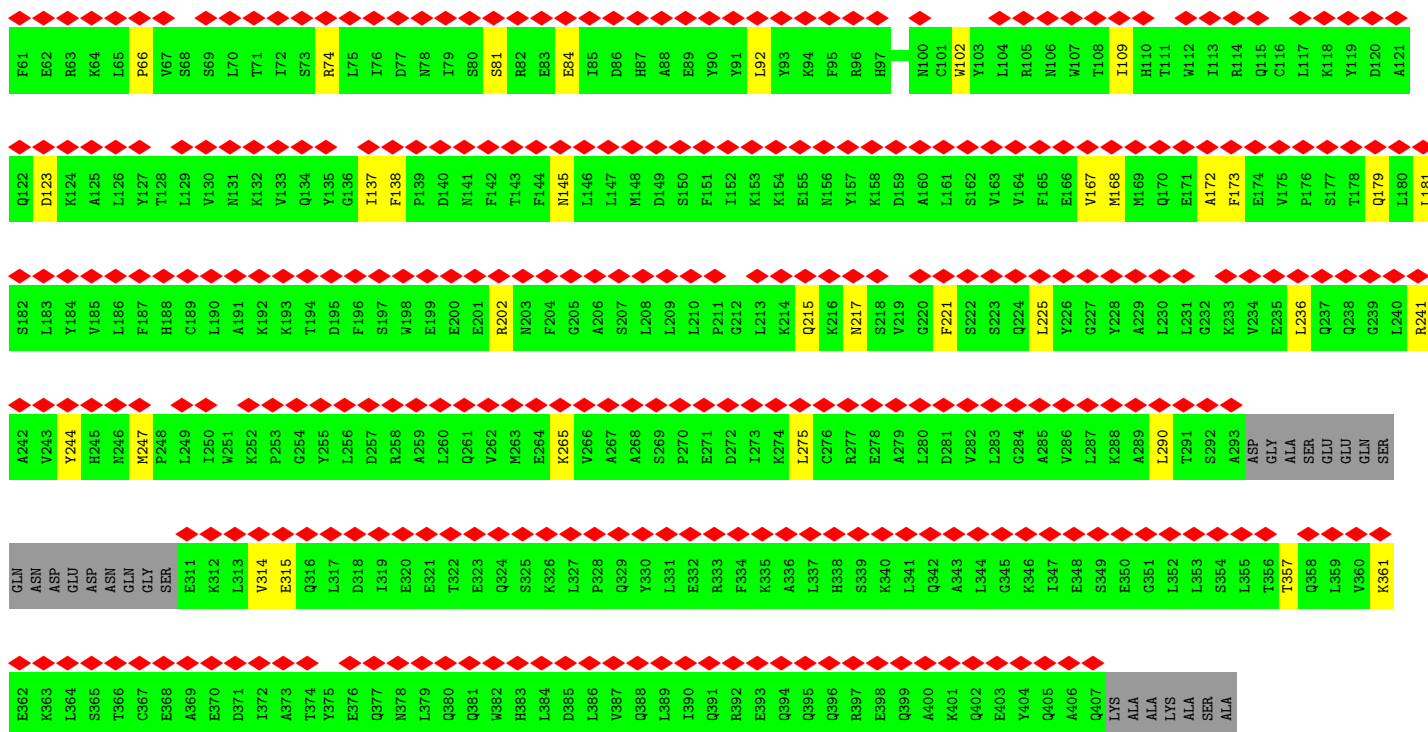


- Molecule 76: 28S ribosomal protein S26, mitochondrial

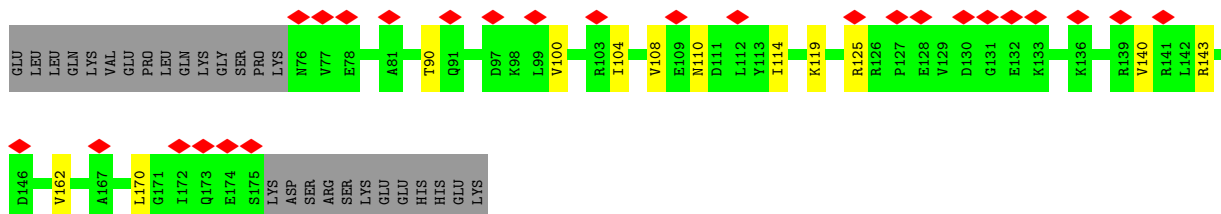
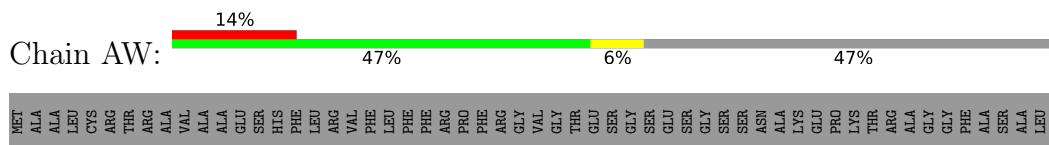


- Molecule 77: 28S ribosomal protein S27, mitochondrial

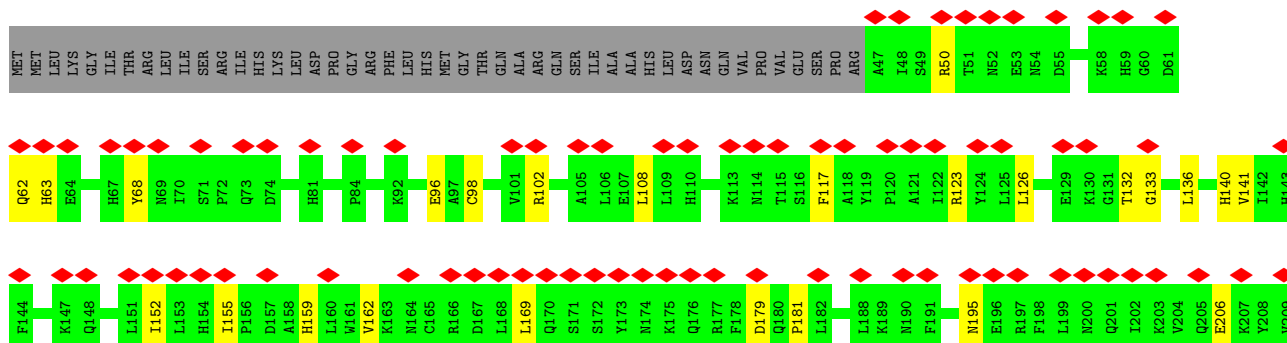
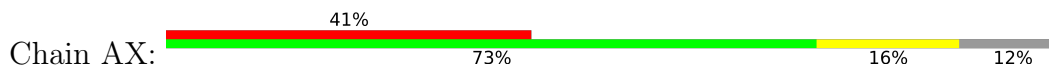


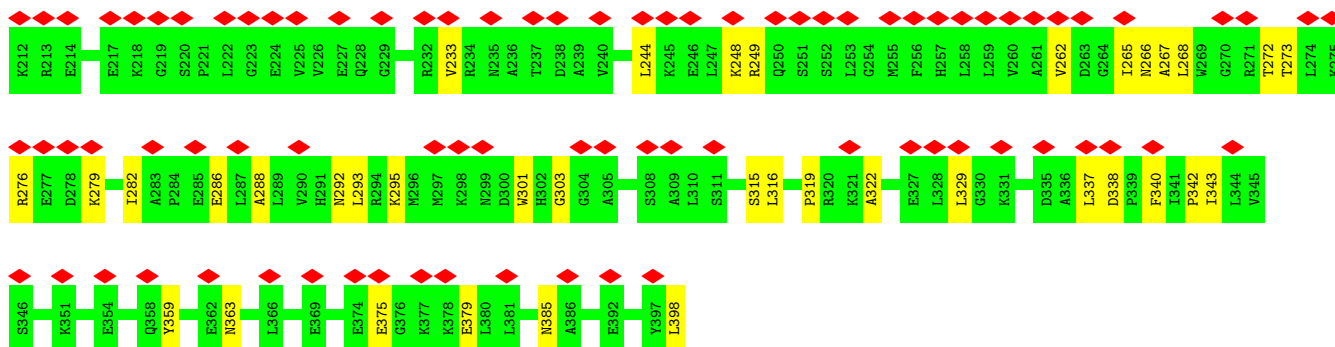


• Molecule 78: 28S ribosomal protein S28, mitochondrial

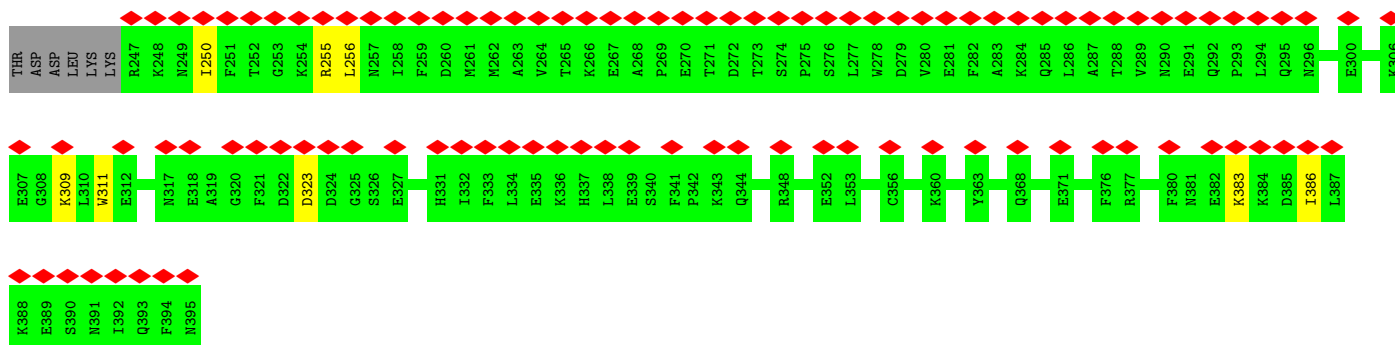
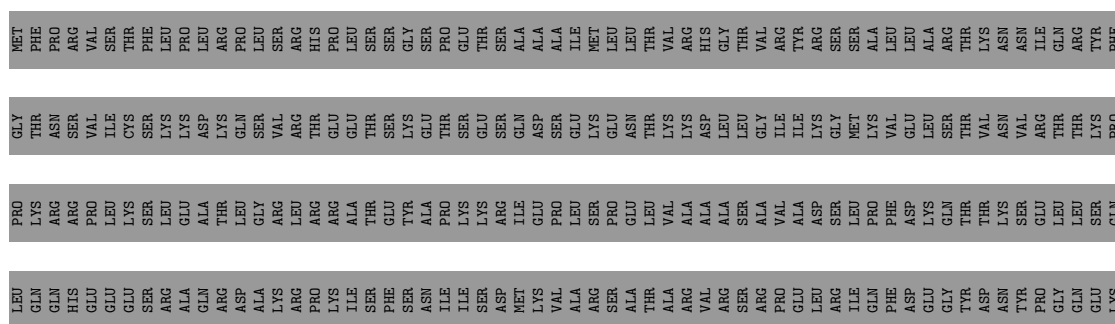


• Molecule 79: 28S ribosomal protein S29, mitochondrial

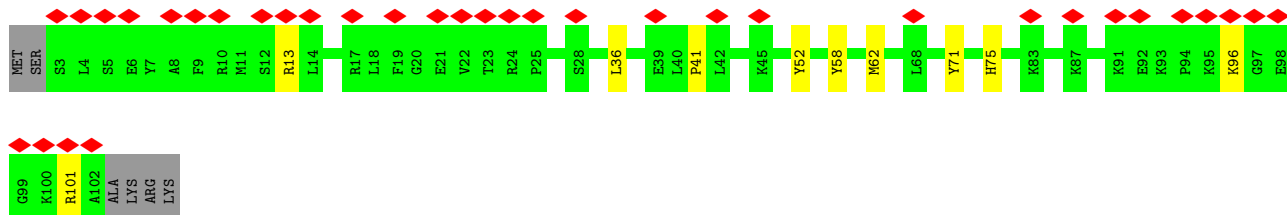
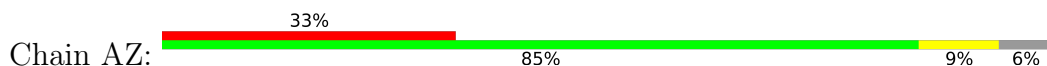




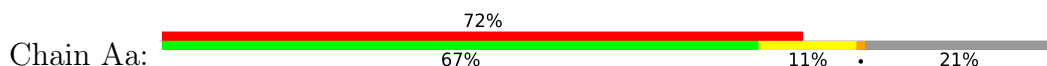
- Molecule 80: 28S ribosomal protein S31, mitochondrial

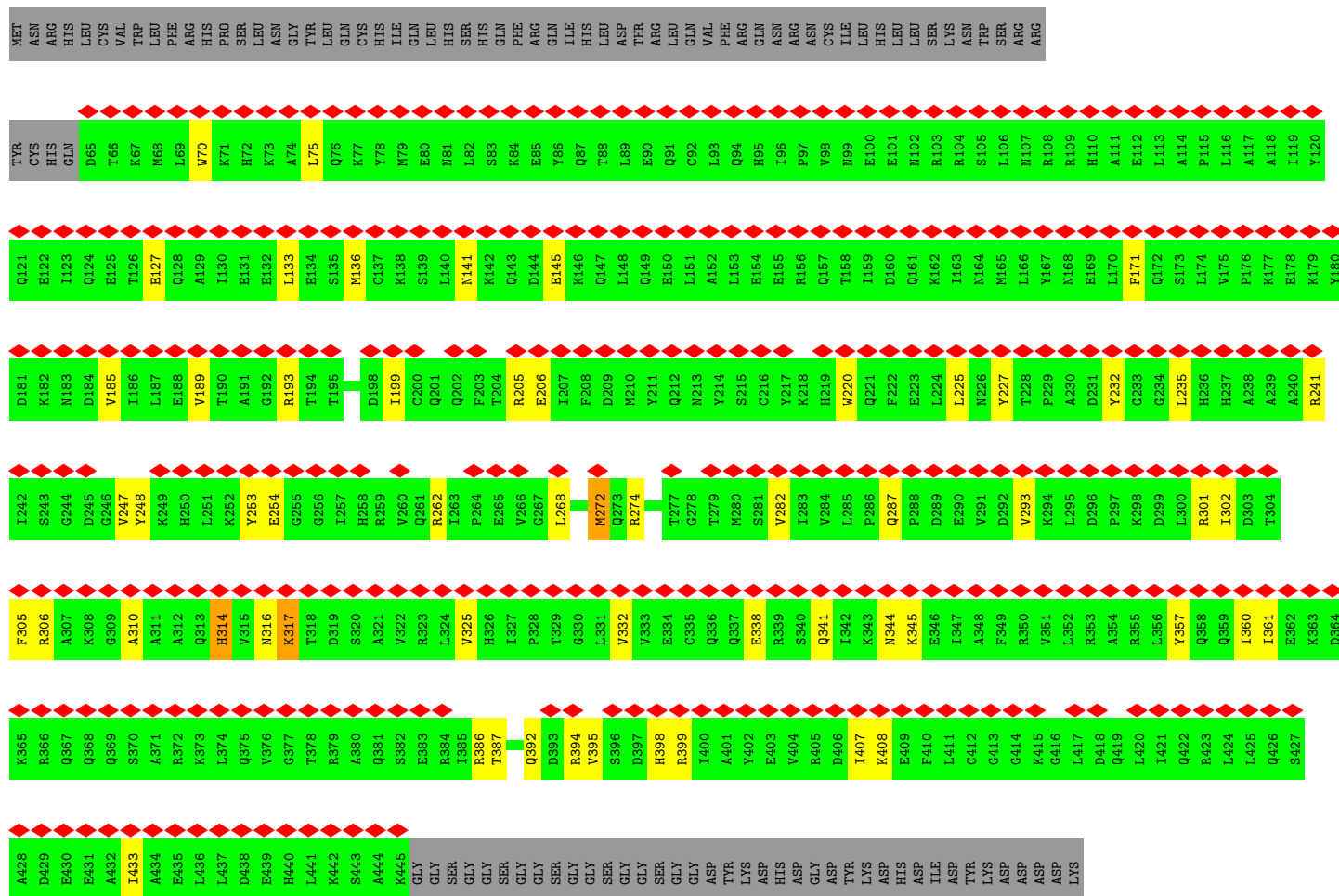


- Molecule 81: 28S ribosomal protein S33, mitochondrial

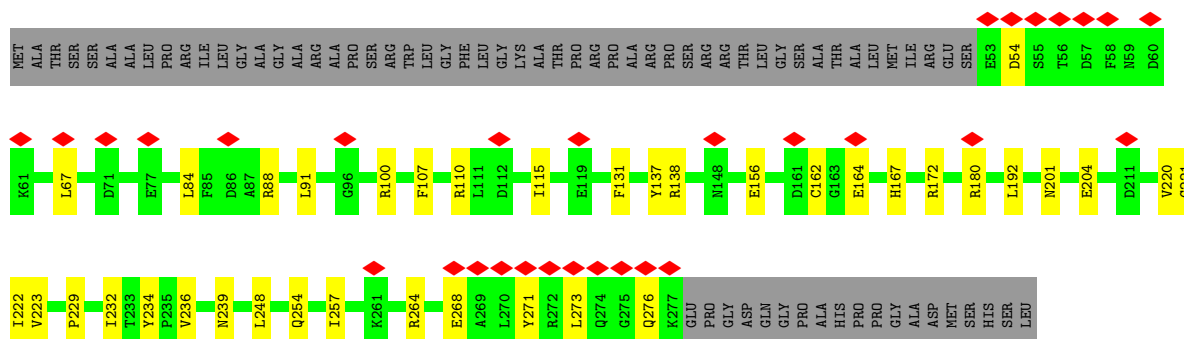


- Molecule 82: Peptide chain release factor 1, mitochondrial

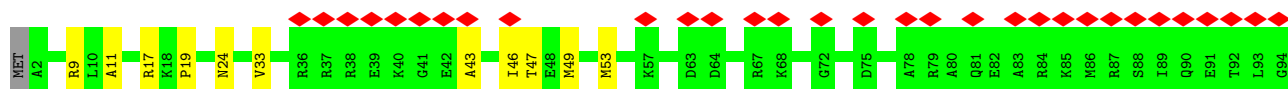
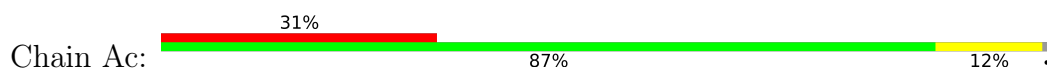


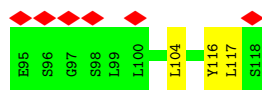


• Molecule 83: 28S ribosomal protein S2, mitochondrial

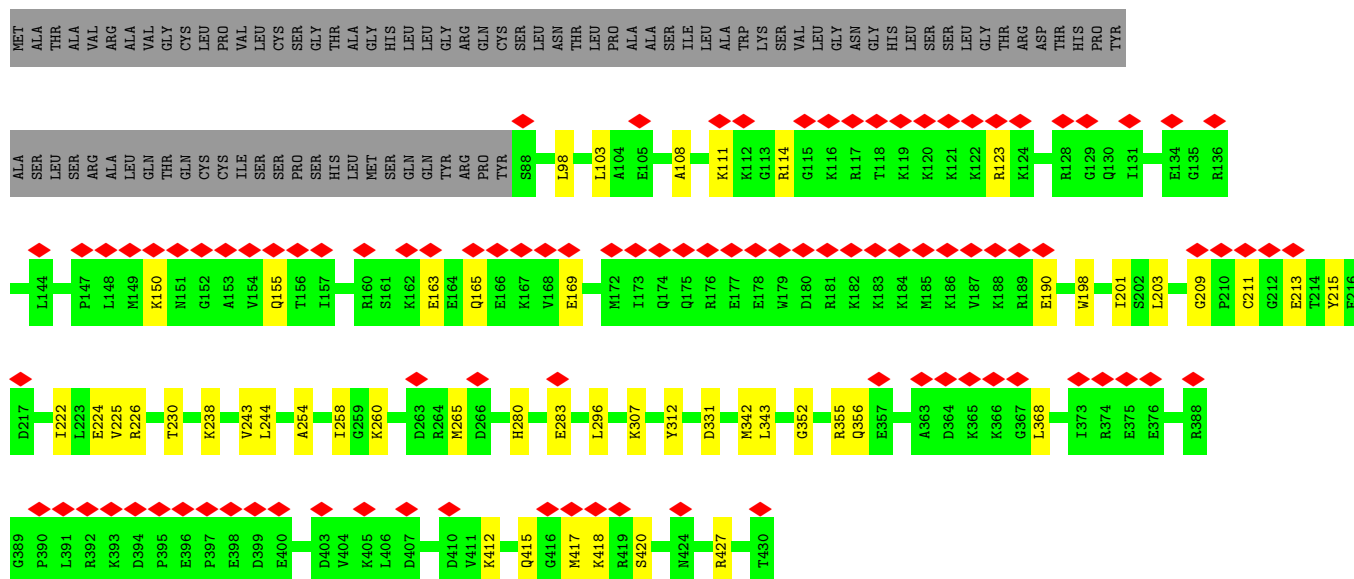


• Molecule 84: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

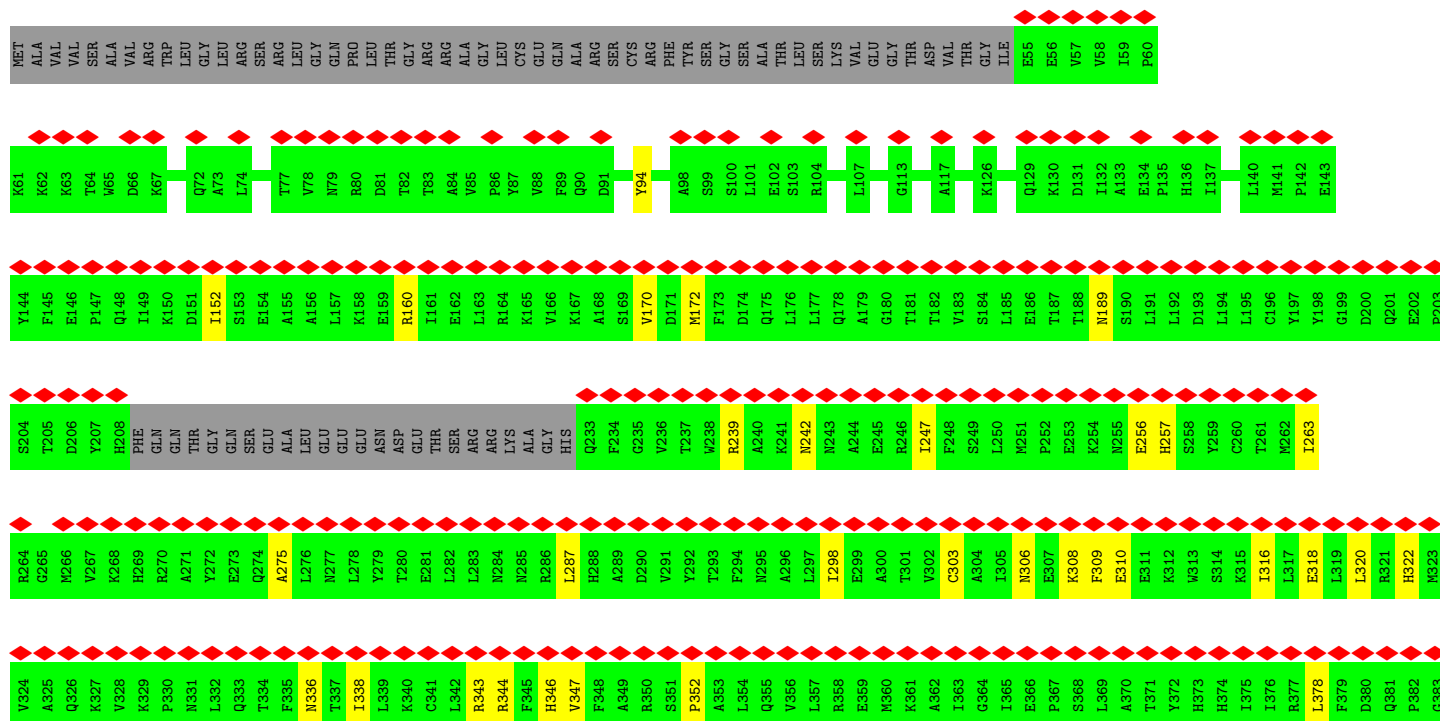
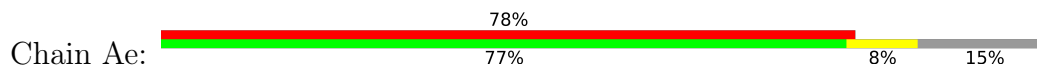




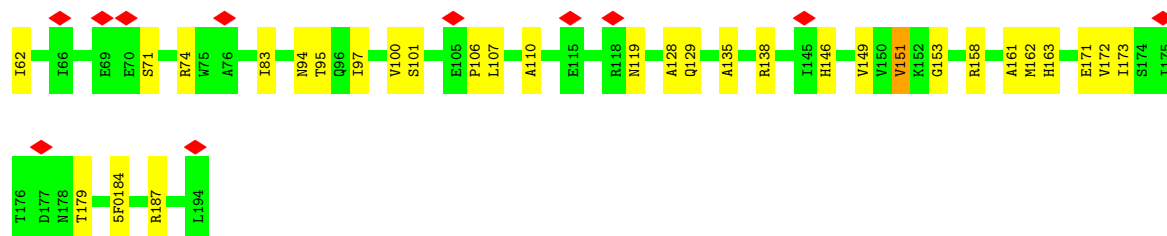
• Molecule 85: 28S ribosomal protein S5, mitochondrial



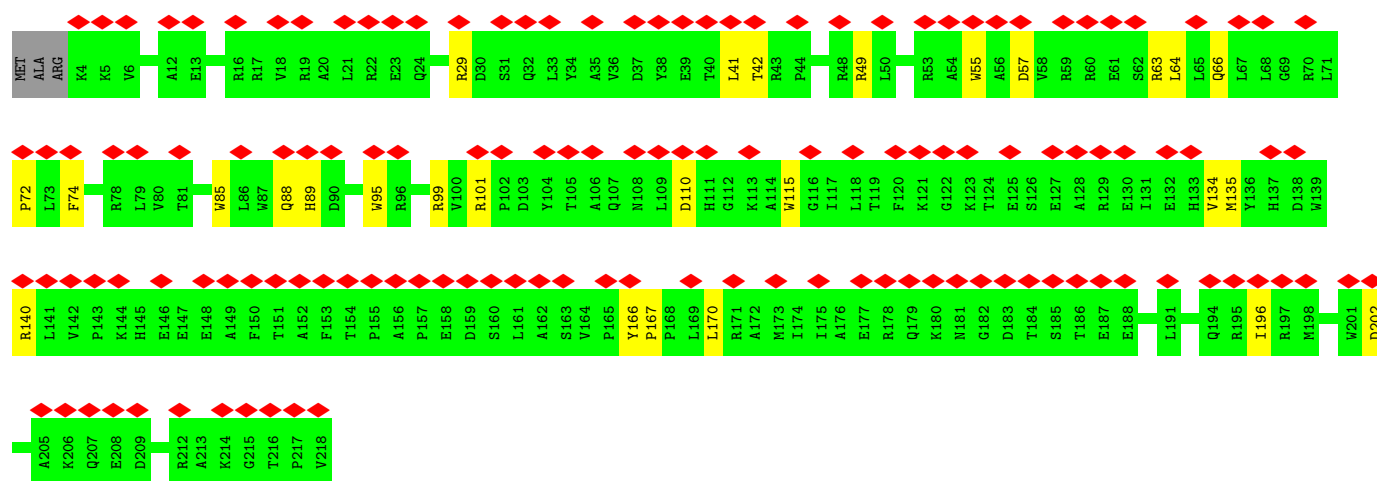
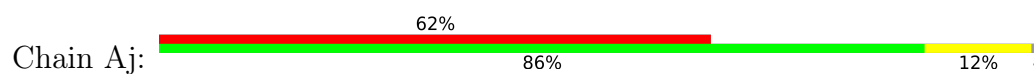
• Molecule 86: Pentatricopeptide repeat domain-containing protein 3, mitochondrial







- Molecule 89: 28S ribosomal protein S34, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.235	Depositor
Minimum map value	-1.433	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, B8T, PSU, OMU, 5F0, ACE, MG, 2MG, SAC, AYA, 5MC, RSQ, 5MU, ZN, MA6, 1MA, GDP, ATP, Y5P, FS2, K

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	B1	0.08	0/358	0.16	0/486
1	B2	0.09	0/259	0.19	0/350
1	B3	0.08	0/259	0.17	0/350
1	B4	0.06	0/246	0.14	0/331
1	B5	0.06	0/246	0.17	0/331
1	B6	0.06	0/246	0.16	0/331
2	B7	0.06	0/68	0.11	0/103
3	B8	0.10	0/36876	0.15	0/57402
4	B9	0.07	0/1627	0.13	0/2527
5	BA	0.09	0/1403	0.19	0/1886
6	BB	0.09	0/1274	0.20	0/1723
7	BC	0.08	0/1721	0.19	0/2333
8	BD	0.10	0/926	0.20	0/1244
9	BE	0.08	0/2099	0.18	0/2837
10	BF	0.08	0/1593	0.17	0/2136
11	BG	0.10	0/1021	0.22	0/1378
12	BH	0.08	0/913	0.18	0/1224
13	BI	0.09	0/469	0.20	0/621
14	BJ	0.10	0/383	0.20	0/507
15	BK	0.10	0/853	0.21	0/1136
16	BL	0.09	0/1896	0.20	0/2549
17	BM	0.09	0/2475	0.22	0/3355
18	BN	0.10	0/2090	0.21	0/2842
19	BO	0.09	0/1698	0.22	0/2292
20	BP	0.08	0/1731	0.20	0/2345
21	BQ	0.06	0/1348	0.17	0/1813
22	BR	0.10	0/1490	0.21	0/2021
23	BS	0.09	0/905	0.21	0/1218
24	BT	0.09	0/2381	0.21	0/3212
25	BU	0.08	0/1833	0.19	0/2468
26	BV	0.09	0/1283	0.20	0/1727

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	BW	0.09	0/1199	0.20	0/1623
28	BX	0.21	1/2027 (0.0%)	0.31	1/2734 (0.0%)
29	BY	0.10	0/1175	0.18	0/1572
30	BZ	0.10	0/1320	0.23	0/1789
31	Ba	0.08	0/760	0.17	0/1023
32	Bb	0.07	0/777	0.17	0/1048
33	Bc	0.06	0/707	0.17	0/960
34	Bd	0.64	1/805 (0.1%)	0.41	3/1081 (0.3%)
35	Be	0.09	0/819	0.20	0/1097
36	Bf	0.07	0/1223	0.17	0/1641
37	Bg	0.07	0/1384	0.17	0/1869
38	Bh	0.09	0/1362	0.22	0/1846
39	Bi	0.09	0/3239	0.20	0/4400
40	Bj	0.08	0/1354	0.22	0/1831
41	Bl	0.10	0/350	0.21	0/461
42	Bm	0.09	0/3305	0.20	0/4502
43	Bn	0.08	0/3043	0.20	0/4140
44	Bo	0.08	0/2447	0.19	0/3310
45	Bp	0.07	0/1269	0.16	0/1708
46	Bq	0.09	0/1025	0.20	0/1379
47	Br	0.09	0/866	0.24	0/1174
48	Bs	0.10	0/1219	0.22	0/1651
49	Bt	0.08	0/2347	0.19	0/3171
50	Bu	0.08	0/2039	0.20	0/2759
51	Bv	0.06	0/1970	0.17	0/2658
52	Bw	0.07	0/1273	0.18	0/1716
53	Bx	0.10	0/1151	0.21	0/1569
54	By	0.06	0/918	0.16	0/1249
55	Bz	0.10	0/850	0.21	0/1135
56	AA	0.10	0/22563	0.14	0/35124
57	AB	0.09	0/2313	0.20	0/3129
58	AC	0.11	0/1113	0.22	0/1505
59	AD	0.09	0/636	0.20	0/839
60	AE	0.10	0/989	0.21	0/1335
61	AF	0.08	0/1767	0.18	0/2373
62	AG	0.09	0/1588	0.16	0/2466
63	AH	0.10	0/1178	0.22	0/1598
64	AI	0.09	0/149	0.15	0/231
65	AJ	0.09	0/855	0.20	0/1148
66	AK	0.10	0/880	0.21	0/1182
67	AL	0.08	0/1477	0.18	0/1974
68	AM	0.10	0/963	0.21	0/1295
69	AN	0.10	0/886	0.22	0/1199

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
70	AO	0.09	0/1648	0.20	0/2243
71	AP	0.09	0/798	0.21	0/1070
72	AQ	0.09	0/748	0.18	0/994
73	AR	0.08	0/2456	0.18	0/3317
74	AS	0.08	0/1138	0.16	0/1533
75	AT	0.09	0/1402	0.20	0/1883
76	AU	0.08	0/1510	0.19	0/2025
77	AV	0.06	0/3030	0.16	0/4093
78	AW	0.09	0/801	0.19	0/1079
79	AX	0.08	0/2921	0.20	0/3954
80	AY	0.07	0/1280	0.18	0/1725
81	AZ	0.08	0/857	0.18	0/1141
82	Aa	0.18	1/3162 (0.0%)	0.25	0/4253
83	Ab	0.10	0/1871	0.21	0/2531
84	Ac	0.08	0/941	0.19	0/1257
85	Ad	0.10	0/2783	0.22	0/3724
86	Ae	0.07	0/4877	0.18	0/6598
87	Ag	0.08	0/2746	0.19	0/3681
88	Ai	0.09	0/1030	0.23	0/1386
89	Aj	0.09	0/1834	0.22	0/2484
All	All	0.10	3/189383 (0.0%)	0.18	4/268543 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
28	BX	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	Bd	99	GLN	C-N	18.10	1.58	1.33
28	BX	68	PRO	C-N	-8.62	1.23	1.33
82	Aa	361	ILE	C-N	-6.90	1.25	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BX	68	PRO	O-C-N	-12.01	106.42	122.64
34	Bd	99	GLN	O-C-N	8.05	131.33	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	Bd	99	GLN	CA-C-N	-6.10	114.20	122.86
34	Bd	99	GLN	C-N-CA	-6.10	114.20	122.86

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	BX	68	PRO	Mainchain

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	B1	354	0	377	3	0
1	B2	257	0	283	3	0
1	B3	257	0	283	1	0
1	B4	245	0	275	3	0
1	B5	245	0	275	1	0
1	B6	245	0	275	4	0
2	B7	62	0	34	0	0
3	B8	33070	0	16795	240	0
4	B9	1524	0	778	20	0
5	BA	1369	0	1410	11	0
6	BB	1251	0	1232	10	0
7	BC	1676	0	1687	14	0
8	BD	904	0	935	7	0
9	BE	2044	0	2060	14	0
10	BF	1556	0	1597	13	0
11	BG	996	0	1044	9	0
12	BH	898	0	916	5	0
13	BI	464	0	511	6	0
14	BJ	377	0	406	2	0
15	BK	832	0	883	12	0
16	BL	1859	0	1920	18	0
17	BM	2406	0	2415	21	0
18	BN	2031	0	2065	31	0
19	BO	1661	0	1734	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	BP	1695	0	1785	14	0
21	BQ	1330	0	1407	13	0
22	BR	1455	0	1452	15	0
23	BS	890	0	941	12	0
24	BT	2327	0	2395	20	0
25	BU	1786	0	1817	16	0
26	BV	1259	0	1294	18	0
27	BW	1173	0	1165	10	0
28	BX	1979	0	2022	23	0
29	BY	1154	0	1214	13	0
30	BZ	1293	0	1365	10	0
31	Ba	745	0	746	5	0
32	Bb	774	0	784	7	0
33	Bc	688	0	674	7	0
34	Bd	791	0	796	18	0
35	Be	798	0	804	15	0
36	Bf	1205	0	1223	13	0
37	Bg	1350	0	1327	10	0
38	Bh	1322	0	1348	8	0
39	Bi	3155	0	3139	26	0
40	Bj	1327	0	1353	44	0
41	Bl	342	0	361	1	0
42	Bm	3210	0	3206	35	0
43	Bn	2948	0	2841	37	0
44	Bo	2390	0	2397	26	0
45	Bp	1243	0	1265	12	0
46	Bq	997	0	987	6	0
47	Br	840	0	810	7	0
48	Bs	1196	0	1195	19	0
49	Bt	2299	0	2320	17	0
50	Bu	1985	0	1976	16	0
51	Bv	1931	0	1916	24	0
52	Bw	1252	0	1269	14	0
53	Bx	1113	0	1097	7	0
54	By	895	0	881	5	0
55	Bz	828	0	857	11	0
56	AA	20283	0	10300	124	0
57	AB	2265	0	2294	18	0
58	AC	1083	0	1088	16	0
59	AD	625	0	699	15	0
60	AE	972	0	1000	15	0
61	AF	1725	0	1769	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	AG	1504	0	764	25	0
63	AH	1152	0	1183	17	0
64	AI	463	0	286	3	0
65	AJ	839	0	887	12	0
66	AK	862	0	885	15	0
67	AL	1453	0	1540	20	0
68	AM	942	0	965	17	0
69	AN	868	0	928	15	0
70	AO	1592	0	1557	14	0
71	AP	781	0	806	11	0
72	AQ	744	0	758	10	0
73	AR	2409	0	2428	33	0
74	AS	1111	0	1115	10	0
75	AT	1371	0	1393	10	0
76	AU	1488	0	1499	13	0
77	AV	2969	0	2961	26	0
78	AW	789	0	802	9	0
79	AX	2849	0	2843	41	0
80	AY	1246	0	1197	7	0
81	AZ	839	0	858	9	0
82	Aa	3114	0	3115	42	0
83	Ab	1828	0	1815	25	0
84	Ac	935	0	971	11	0
85	Ad	2731	0	2804	35	0
86	Ae	4768	0	4764	33	0
87	Ag	2688	0	2687	26	0
88	Ai	1020	0	1053	20	0
89	Aj	1787	0	1796	23	0
90	AA	16	0	0	0	0
90	Ae	1	0	0	0	0
90	B8	30	0	0	0	0
90	BL	1	0	0	0	0
90	BT	1	0	0	0	0
90	Be	1	0	0	0	0
90	Bn	1	0	0	0	0
91	AA	120	0	0	0	0
91	AD	1	0	0	0	0
91	AG	2	0	0	0	0
91	AU	1	0	0	0	0
91	AX	1	0	0	0	0
91	Aa	1	0	0	0	0
91	Ab	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
91	Ad	1	0	0	0	0
91	B8	216	0	0	0	0
91	BD	1	0	0	0	0
91	BL	3	0	0	0	0
91	BN	1	0	0	0	0
91	BO	1	0	0	0	0
91	BR	1	0	0	0	0
91	BT	1	0	0	0	0
91	BV	1	0	0	0	0
91	Bx	1	0	0	0	0
92	B9	7	0	8	0	0
93	AO	1	0	0	0	0
93	BH	1	0	0	0	0
93	Bl	1	0	0	0	0
94	AP	4	0	0	0	0
94	AT	4	0	0	0	0
94	Bh	4	0	0	1	0
95	AG	8	0	8	0	0
96	AX	31	0	12	0	0
97	AX	28	0	12	2	0
98	AX	3	0	0	0	0
All	All	181140	0	154469	1351	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 1351 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)
3:B8:1401:U:H5''	82:Aa:310:ALA:HA	1.51	0.93
4:B9:6:U:H3	4:B9:63:G:H1	1.18	0.91
3:B8:926:G:H5'	59:AD:152:PHE:CE1	2.14	0.83
3:B8:1107:G:N3	19:BO:179:ASN:ND2	2.30	0.79
3:B8:969:C:H5''	59:AD:159:GLU:OE2	1.82	0.79

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	B1	44/198 (22%)	44 (100%)	0	0	100	100
1	B2	30/198 (15%)	30 (100%)	0	0	100	100
1	B3	30/198 (15%)	29 (97%)	1 (3%)	0	100	100
1	B4	29/198 (15%)	29 (100%)	0	0	100	100
1	B5	29/198 (15%)	29 (100%)	0	0	100	100
1	B6	29/198 (15%)	29 (100%)	0	0	100	100
5	BA	164/206 (80%)	162 (99%)	2 (1%)	0	100	100
6	BB	150/153 (98%)	148 (99%)	2 (1%)	0	100	100
7	BC	203/216 (94%)	201 (99%)	2 (1%)	0	100	100
8	BD	114/148 (77%)	113 (99%)	1 (1%)	0	100	100
9	BE	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
10	BF	179/250 (72%)	178 (99%)	1 (1%)	0	100	100
11	BG	120/161 (74%)	119 (99%)	1 (1%)	0	100	100
12	BH	108/188 (57%)	108 (100%)	0	0	100	100
13	BI	54/65 (83%)	53 (98%)	1 (2%)	0	100	100
14	BJ	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
15	BK	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
16	BL	236/305 (77%)	230 (98%)	6 (2%)	0	100	100
17	BM	303/348 (87%)	300 (99%)	3 (1%)	0	100	100
18	BN	250/311 (80%)	246 (98%)	4 (2%)	0	100	100
19	BO	200/267 (75%)	193 (96%)	7 (4%)	0	100	100
20	BP	210/261 (80%)	205 (98%)	5 (2%)	0	100	100
21	BQ	173/192 (90%)	172 (99%)	1 (1%)	0	100	100
22	BR	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
23	BS	113/145 (78%)	113 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	BT	289/296 (98%)	285 (99%)	4 (1%)	0	100	100
25	BU	220/251 (88%)	219 (100%)	1 (0%)	0	100	100
26	BV	152/175 (87%)	149 (98%)	3 (2%)	0	100	100
27	BW	142/180 (79%)	139 (98%)	3 (2%)	0	100	100
28	BX	236/292 (81%)	233 (99%)	3 (1%)	0	100	100
29	BY	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
30	BZ	159/205 (78%)	158 (99%)	1 (1%)	0	100	100
31	Ba	92/123 (75%)	91 (99%)	1 (1%)	0	100	100
32	Bb	99/112 (88%)	99 (100%)	0	0	100	100
33	Bc	80/138 (58%)	80 (100%)	0	0	100	100
34	Bd	90/128 (70%)	90 (100%)	0	0	100	100
35	Be	92/102 (90%)	92 (100%)	0	0	100	100
36	Bf	141/206 (68%)	140 (99%)	1 (1%)	0	100	100
37	Bg	159/222 (72%)	158 (99%)	1 (1%)	0	100	100
38	Bh	160/196 (82%)	158 (99%)	2 (1%)	0	100	100
39	Bi	382/439 (87%)	377 (99%)	5 (1%)	0	100	100
40	Bj	160/325 (49%)	156 (98%)	4 (2%)	0	100	100
41	Bl	36/103 (35%)	36 (100%)	0	0	100	100
42	Bm	392/423 (93%)	388 (99%)	4 (1%)	0	100	100
43	Bn	352/380 (93%)	343 (97%)	9 (3%)	0	100	100
44	Bo	292/338 (86%)	285 (98%)	7 (2%)	0	100	100
45	Bp	145/206 (70%)	145 (100%)	0	0	100	100
46	Bq	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
47	Br	96/142 (68%)	96 (100%)	0	0	100	100
48	Bs	149/215 (69%)	146 (98%)	3 (2%)	0	100	100
49	Bt	282/332 (85%)	278 (99%)	4 (1%)	0	100	100
50	Bu	235/306 (77%)	233 (99%)	2 (1%)	0	100	100
51	Bv	236/279 (85%)	230 (98%)	6 (2%)	0	100	100
52	Bw	153/212 (72%)	151 (99%)	2 (1%)	0	100	100
53	Bx	132/166 (80%)	129 (98%)	3 (2%)	0	100	100
54	By	108/158 (68%)	107 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	Bz	95/128 (74%)	95 (100%)	0	0	100	100
57	AB	277/323 (86%)	274 (99%)	3 (1%)	0	100	100
58	AC	130/167 (78%)	129 (99%)	1 (1%)	0	100	100
59	AD	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
60	AE	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
61	AF	206/242 (85%)	206 (100%)	0	0	100	100
63	AH	138/201 (69%)	136 (99%)	1 (1%)	1 (1%)	18	49
65	AJ	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
66	AK	99/128 (77%)	99 (100%)	0	0	100	100
67	AL	172/257 (67%)	171 (99%)	1 (1%)	0	100	100
68	AM	117/137 (85%)	115 (98%)	2 (2%)	0	100	100
69	AN	108/130 (83%)	107 (99%)	1 (1%)	0	100	100
70	AO	191/258 (74%)	190 (100%)	1 (0%)	0	100	100
71	AP	95/142 (67%)	95 (100%)	0	0	100	100
72	AQ	84/87 (97%)	84 (100%)	0	0	100	100
73	AR	293/360 (81%)	290 (99%)	3 (1%)	0	100	100
74	AS	133/190 (70%)	132 (99%)	1 (1%)	0	100	100
75	AT	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
76	AU	174/205 (85%)	174 (100%)	0	0	100	100
77	AV	358/414 (86%)	354 (99%)	4 (1%)	0	100	100
78	AW	98/187 (52%)	97 (99%)	1 (1%)	0	100	100
79	AX	350/398 (88%)	349 (100%)	1 (0%)	0	100	100
80	AY	147/395 (37%)	147 (100%)	0	0	100	100
81	AZ	98/106 (92%)	96 (98%)	2 (2%)	0	100	100
82	Aa	379/484 (78%)	376 (99%)	3 (1%)	0	100	100
83	Ab	223/296 (75%)	220 (99%)	3 (1%)	0	100	100
84	Ac	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
85	Ad	341/430 (79%)	335 (98%)	6 (2%)	0	100	100
86	Ae	584/689 (85%)	582 (100%)	2 (0%)	0	100	100
87	Ag	323/396 (82%)	318 (98%)	5 (2%)	0	100	100
88	Ai	134/194 (69%)	132 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
89	Aj	213/218 (98%)	212 (100%)	1 (0%)	0	100	100
All	All	14978/19969 (75%)	14810 (99%)	167 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
63	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	B1	40/158 (25%)	40 (100%)	0	100	100
1	B2	31/158 (20%)	31 (100%)	0	100	100
1	B3	31/158 (20%)	31 (100%)	0	100	100
1	B4	30/158 (19%)	30 (100%)	0	100	100
1	B5	30/158 (19%)	30 (100%)	0	100	100
1	B6	30/158 (19%)	30 (100%)	0	100	100
5	BA	146/176 (83%)	146 (100%)	0	100	100
6	BB	134/135 (99%)	132 (98%)	2 (2%)	57	75
7	BC	183/191 (96%)	183 (100%)	0	100	100
8	BD	94/119 (79%)	93 (99%)	1 (1%)	65	78
9	BE	220/229 (96%)	220 (100%)	0	100	100
10	BF	163/223 (73%)	162 (99%)	1 (1%)	78	83
11	BG	113/147 (77%)	113 (100%)	0	100	100
12	BH	99/164 (60%)	99 (100%)	0	100	100
13	BI	53/60 (88%)	53 (100%)	0	100	100
14	BJ	40/72 (56%)	40 (100%)	0	100	100
15	BK	88/166 (53%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	BL	192/245 (78%)	191 (100%)	1 (0%)	81	85
17	BM	260/290 (90%)	259 (100%)	1 (0%)	84	86
18	BN	219/262 (84%)	219 (100%)	0	100	100
19	BO	182/228 (80%)	181 (100%)	1 (0%)	81	85
20	BP	194/232 (84%)	194 (100%)	0	100	100
21	BQ	138/150 (92%)	138 (100%)	0	100	100
22	BR	154/155 (99%)	154 (100%)	0	100	100
23	BS	98/124 (79%)	98 (100%)	0	100	100
24	BT	246/249 (99%)	246 (100%)	0	100	100
25	BU	189/211 (90%)	188 (100%)	1 (0%)	81	85
26	BV	134/150 (89%)	134 (100%)	0	100	100
27	BW	126/155 (81%)	126 (100%)	0	100	100
28	BX	220/256 (86%)	220 (100%)	0	100	100
29	BY	118/126 (94%)	118 (100%)	0	100	100
30	BZ	146/180 (81%)	146 (100%)	0	100	100
31	Ba	74/97 (76%)	74 (100%)	0	100	100
32	Bb	83/90 (92%)	83 (100%)	0	100	100
33	Bc	76/116 (66%)	76 (100%)	0	100	100
34	Bd	85/113 (75%)	85 (100%)	0	100	100
35	Be	80/87 (92%)	80 (100%)	0	100	100
36	Bf	135/181 (75%)	135 (100%)	0	100	100
37	Bg	138/178 (78%)	138 (100%)	0	100	100
38	Bh	147/169 (87%)	146 (99%)	1 (1%)	76	82
39	Bi	340/381 (89%)	339 (100%)	1 (0%)	86	87
40	Bj	150/287 (52%)	150 (100%)	0	100	100
41	Bl	37/89 (42%)	37 (100%)	0	100	100
42	Bm	353/368 (96%)	352 (100%)	1 (0%)	86	87
43	Bn	313/332 (94%)	313 (100%)	0	100	100
44	Bo	270/303 (89%)	269 (100%)	1 (0%)	84	86
45	Bp	136/190 (72%)	136 (100%)	0	100	100
46	Bq	104/112 (93%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	Br	96/133 (72%)	96 (100%)	0	100	100
48	Bs	132/185 (71%)	130 (98%)	2 (2%)	57	75
49	Bt	251/288 (87%)	251 (100%)	0	100	100
50	Bu	223/274 (81%)	221 (99%)	2 (1%)	70	80
51	Bv	207/236 (88%)	207 (100%)	0	100	100
52	Bw	139/188 (74%)	139 (100%)	0	100	100
53	Bx	124/148 (84%)	124 (100%)	0	100	100
54	By	104/148 (70%)	104 (100%)	0	100	100
55	Bz	86/110 (78%)	85 (99%)	1 (1%)	63	78
57	AB	257/291 (88%)	257 (100%)	0	100	100
58	AC	115/143 (80%)	115 (100%)	0	100	100
59	AD	65/166 (39%)	64 (98%)	1 (2%)	57	75
60	AE	104/107 (97%)	103 (99%)	1 (1%)	68	79
61	AF	185/209 (88%)	185 (100%)	0	100	100
63	AH	130/180 (72%)	129 (99%)	1 (1%)	73	81
65	AJ	93/118 (79%)	93 (100%)	0	100	100
66	AK	91/113 (80%)	91 (100%)	0	100	100
67	AL	158/226 (70%)	157 (99%)	1 (1%)	78	83
68	AM	97/113 (86%)	97 (100%)	0	100	100
69	AN	96/115 (84%)	95 (99%)	1 (1%)	68	79
70	AO	174/230 (76%)	174 (100%)	0	100	100
71	AP	88/123 (72%)	88 (100%)	0	100	100
72	AQ	78/79 (99%)	78 (100%)	0	100	100
73	AR	264/318 (83%)	264 (100%)	0	100	100
74	AS	116/164 (71%)	116 (100%)	0	100	100
75	AT	153/157 (98%)	152 (99%)	1 (1%)	76	82
76	AU	152/174 (87%)	152 (100%)	0	100	100
77	AV	325/364 (89%)	324 (100%)	1 (0%)	86	87
78	AW	87/158 (55%)	86 (99%)	1 (1%)	65	78
79	AX	311/351 (89%)	311 (100%)	0	100	100
80	AY	137/357 (38%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
81	AZ	90/95 (95%)	90 (100%)	0	100	100
82	Aa	338/427 (79%)	334 (99%)	4 (1%)	63	78
83	Ab	198/249 (80%)	198 (100%)	0	100	100
84	Ac	100/101 (99%)	100 (100%)	0	100	100
85	Ad	286/357 (80%)	285 (100%)	1 (0%)	86	87
86	Ae	526/609 (86%)	525 (100%)	1 (0%)	87	89
87	Ag	285/342 (83%)	284 (100%)	1 (0%)	84	86
88	Ai	104/146 (71%)	103 (99%)	1 (1%)	68	79
89	Aj	188/190 (99%)	188 (100%)	0	100	100
All	All	13415/17218 (78%)	13382 (100%)	33 (0%)	84	89

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
82	Aa	317	LYS
85	Ad	163	GLU
88	Ai	151	VAL
48	Bs	75	VAL
44	Bo	143	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
68	AM	50	GLN
82	Aa	368	GLN
73	AR	288	GLN
79	AX	180	GLN
86	Ae	306	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B7	2/3 (66%)	1 (50%)	0
3	B8	1556/1561 (99%)	236 (15%)	1 (0%)
4	B9	71/72 (98%)	11 (15%)	0
56	AA	954/955 (99%)	122 (12%)	1 (0%)
62	AG	70/71 (98%)	11 (15%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
64	AI	6/33 (18%)	2 (33%)	0
All	All	2659/2695 (98%)	383 (14%)	2 (0%)

5 of 383 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B7	76	A
3	B8	2	C
3	B8	11	G
3	B8	19	C
3	B8	22	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	B8	575	A
56	AA	400	A

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

24 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	$\# Z > 2$
3	OMU	B8	1369	3,90	19,22,23	1.21	3 (15%)	25,31,34	1.79	5 (20%)
4	2MG	B9	10	4	23,26,27	0.45	0	33,38,41	0.52	0
64	Y5P	AI	4	64	14,19,20	2.24	1 (7%)	18,26,29	0.50	0
88	5F0	Ai	184	88	8,8,9	1.44	2 (25%)	8,9,11	1.60	1 (12%)
3	OMG	B8	1370	3	23,26,27	1.17	3 (13%)	32,38,41	1.93	6 (18%)
4	PSU	B9	37	4	18,21,22	1.36	2 (11%)	21,30,33	1.97	3 (14%)
62	PSU	AG	51	62	18,21,22	1.38	2 (11%)	21,30,33	1.94	3 (14%)
4	1MA	B9	9	4	21,25,26	0.47	0	30,37,40	0.77	1 (3%)
84	AYA	Ac	2	84	6,7,8	0.76	0	6,8,10	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
72	AYA	AQ	2	72	6,7,8	0.78	0	6,8,10	0.61	0
3	OMG	B8	1145	3,90,62	23,26,27	1.17	3 (13%)	32,38,41	1.92	6 (18%)
56	5MC	AA	841	56	19,22,23	1.56	3 (15%)	26,32,35	1.09	2 (7%)
56	MA6	AA	936	56	23,26,27	2.36	5 (21%)	33,38,41	3.77	13 (39%)
56	5MU	AA	429	56	19,22,23	1.38	6 (31%)	27,32,35	2.06	6 (22%)
3	PSU	B8	1397	3	18,21,22	1.40	2 (11%)	21,30,33	2.00	3 (14%)
62	RSQ	AG	31	64,62	19,23,24	0.36	0	25,33,36	0.46	0
3	1MA	B8	947	3	21,25,26	0.43	0	30,37,40	0.73	1 (3%)
6	AYA	BB	2	6	6,7,8	0.81	0	6,8,10	0.62	0
62	PSU	AG	46	62	18,21,22	1.38	2 (11%)	21,30,33	1.96	3 (14%)
22	SAC	BR	2	22	7,8,9	0.57	0	7,9,11	1.03	1 (14%)
32	AYA	Bb	2	32	6,7,8	0.69	0	6,8,10	0.70	0
56	B8T	AA	839	90,56	19,22,23	0.37	0	25,31,34	0.35	0
56	MA6	AA	937	56	23,26,27	2.37	5 (21%)	33,38,41	3.78	13 (39%)
62	PSU	AG	24	62	18,21,22	1.35	2 (11%)	21,30,33	2.06	4 (19%)

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
3	OMU	B8	1369	3,90	-	0/9/27/28	0/2/2/2
4	2MG	B9	10	4	-	0/9/27/28	0/3/3/3
64	Y5P	AI	4	64	-	5/7/33/34	0/2/2/2
88	5F0	Ai	184	88	-	4/9/9/10	-
3	OMG	B8	1370	3	-	0/9/27/28	0/3/3/3
4	PSU	B9	37	4	-	0/7/25/26	0/2/2/2
62	PSU	AG	51	62	-	3/7/25/26	0/2/2/2
4	1MA	B9	9	4	-	0/7/25/26	0/3/3/3
84	AYA	Ac	2	84	-	2/5/6/8	-
72	AYA	AQ	2	72	-	0/5/6/8	-
3	OMG	B8	1145	3,90,62	-	0/9/27/28	0/3/3/3
56	5MC	AA	841	56	-	0/7/25/26	0/2/2/2
56	MA6	AA	936	56	-	0/11/29/30	0/3/3/3
56	5MU	AA	429	56	-	0/7/25/26	0/2/2/2
3	PSU	B8	1397	3	-	0/7/25/26	0/2/2/2
62	RSQ	AG	31	64,62	-	1/9/27/28	0/2/2/2
3	1MA	B8	947	3	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AYA	BB	2	6	-	1/5/6/8	-
62	PSU	AG	46	62	-	0/7/25/26	0/2/2/2
22	SAC	BR	2	22	-	0/7/8/10	-
32	AYA	Bb	2	32	-	3/5/6/8	-
56	B8T	AA	839	90,56	-	0/7/27/28	0/2/2/2
56	MA6	AA	937	56	-	2/11/29/30	0/3/3/3
62	PSU	AG	24	62	-	0/7/25/26	0/2/2/2

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	AI	4	Y5P	C2-N3	8.27	1.33	1.27
56	AA	936	MA6	C5-N7	6.97	1.51	1.39
56	AA	937	MA6	C5-N7	6.96	1.51	1.39
56	AA	937	MA6	C8-N9	-5.80	1.27	1.37
56	AA	936	MA6	C8-N9	-5.75	1.27	1.37

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	AA	937	MA6	C4-N9-C8	15.14	121.63	105.74
56	AA	936	MA6	C4-N9-C8	14.95	121.43	105.74
62	AG	24	PSU	N1-C2-N3	6.41	121.93	115.17
56	AA	936	MA6	N3-C4-N9	6.37	138.00	127.17
56	AA	936	MA6	C4-C5-N7	-6.34	103.34	110.58

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	AG	51	PSU	O4'-C1'-C5-C4
62	AG	51	PSU	O4'-C1'-C5-C6
32	Bb	2	AYA	OT-CT-N-CA
32	Bb	2	AYA	CM-CT-N-CA
88	Ai	184	5F0	CA-C1-OD1-CXT

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	AG	51	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	AQ	2	AYA	1	0
56	AA	936	MA6	1	0
62	AG	31	RSQ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 415 ligands modelled in this entry, 408 are monoatomic - leaving 7 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	$\# Z > 2$
94	FS2	AT	201	68,75	0,5,14	-	-	-		
97	GDP	AX	503	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
94	FS2	AP	201	60,71	0,5,14	-	-	-		
94	FS2	Bh	201	20,38	0,5,14	-	-	-		
92	VAL	B9	101	4	4,6,7	0.54	0	6,7,9	0.87	0
95	MET	AG	101	62	6,7,8	0.47	0	2,7,9	0.14	0
96	ATP	AX	501	91	32,33,33	0.29	0	48,52,52	0.30	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
94	FS2	AT	201	68,75	-	-	0/2/2/6
97	GDP	AX	503	-	-	4/16/32/32	0/3/3/3
94	FS2	AP	201	60,71	-	-	0/2/2/6
94	FS2	Bh	201	20,38	-	-	0/2/2/6
92	VAL	B9	101	4	-	3/5/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
95	MET	AG	101	62	-	1/5/6/8	-
96	ATP	AX	501	91	-	1/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
97	AX	503	GDP	C5-C4	3.16	1.47	1.38
97	AX	503	GDP	C6-N1	-2.44	1.34	1.38
97	AX	503	GDP	C5-N7	-2.04	1.35	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
97	AX	503	GDP	C5-C4-N3	-6.19	118.53	128.39
97	AX	503	GDP	C2-N3-C4	5.01	120.93	112.30
97	AX	503	GDP	N9-C4-N3	4.60	135.14	125.95
97	AX	503	GDP	C6-C5-N7	3.14	136.01	130.29
97	AX	503	GDP	C4-C5-N7	-2.57	106.60	110.67

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	B9	101	VAL	N-CA-CB-CG2
92	B9	101	VAL	C-CA-CB-CG1
92	B9	101	VAL	C-CA-CB-CG2
95	AG	101	MET	O-C-CA-CB
97	AX	503	GDP	C5'-O5'-PA-O3A

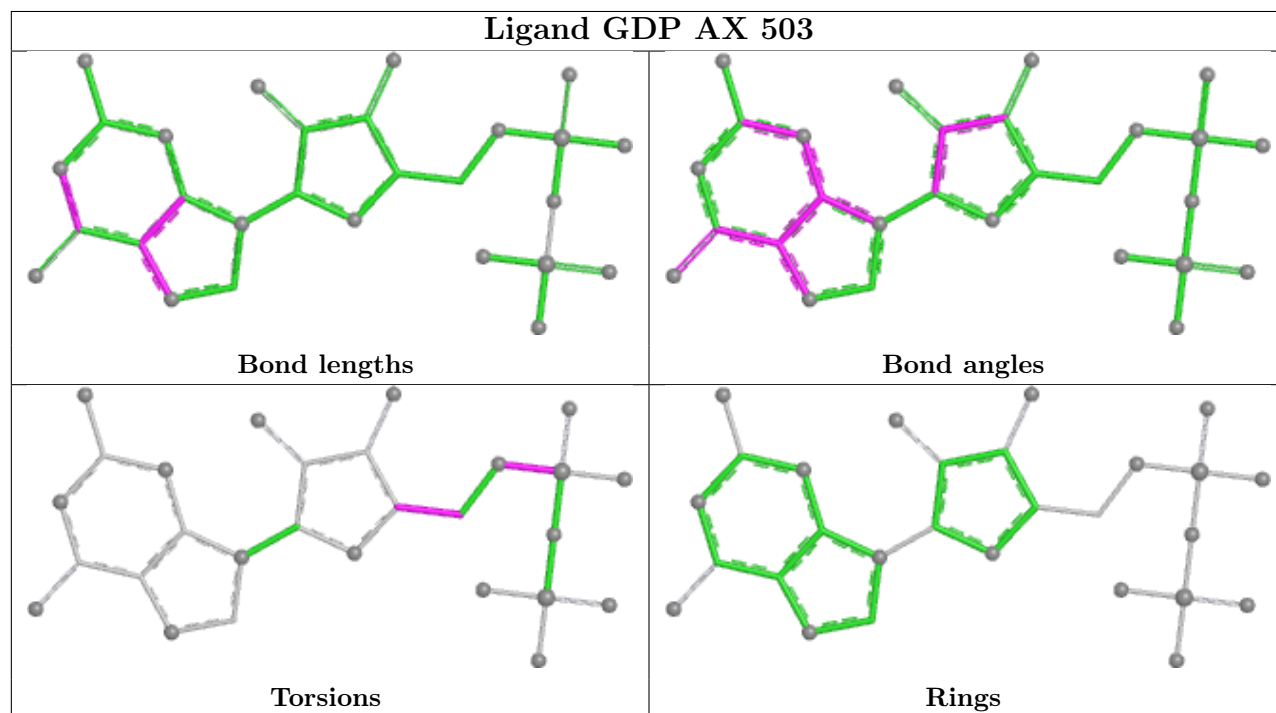
There are no ring outliers.

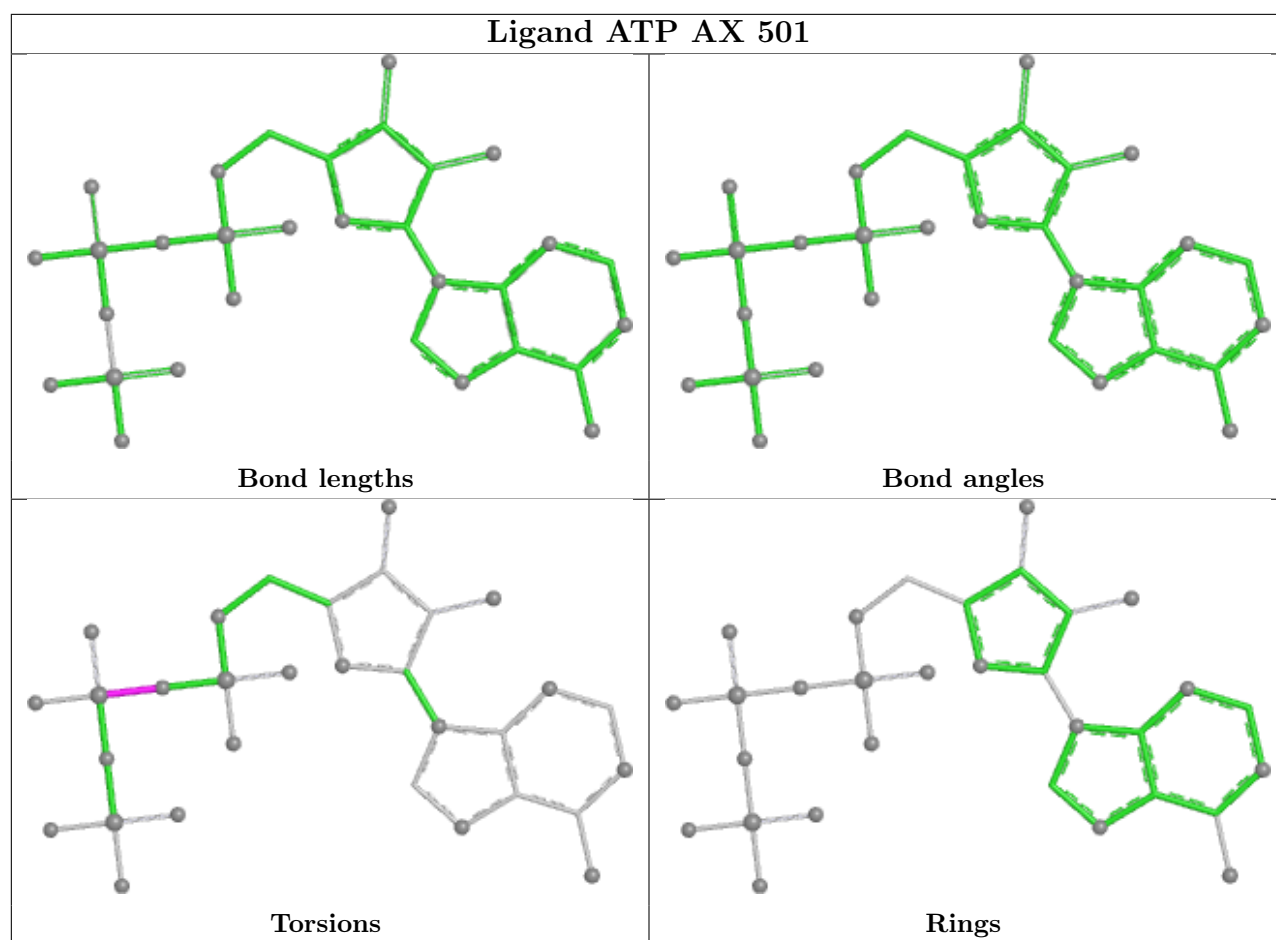
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
97	AX	503	GDP	2	0
94	Bh	201	FS2	1	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](#)

There are no chain breaks in this entry.

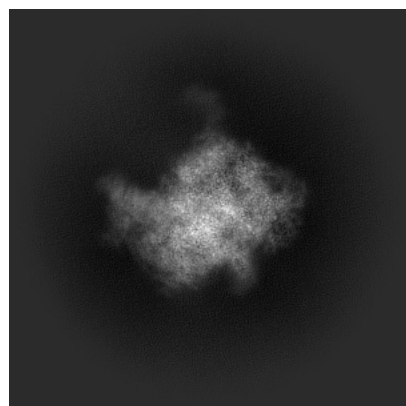
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16897. These allow visual inspection of the internal detail of the map and identification of artifacts.

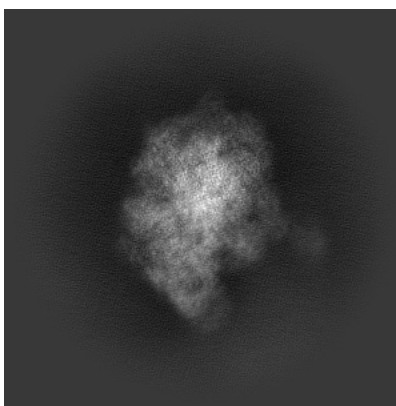
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

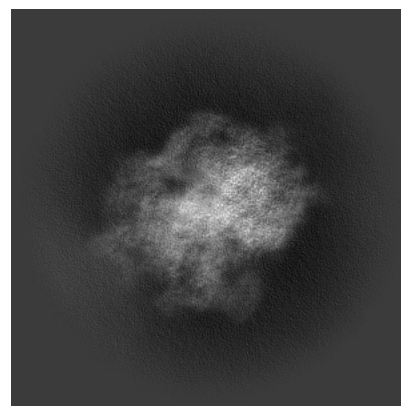
6.1.1 Primary map



X

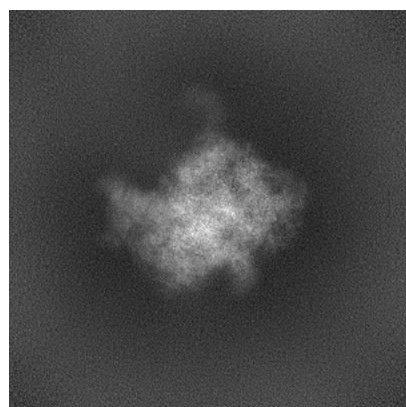


Y

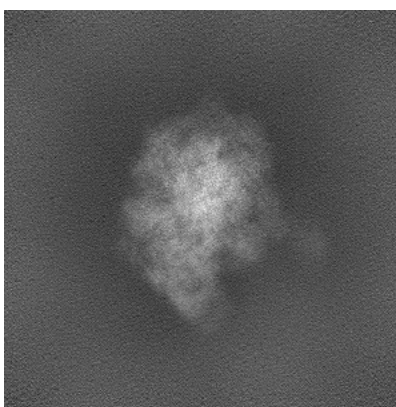


Z

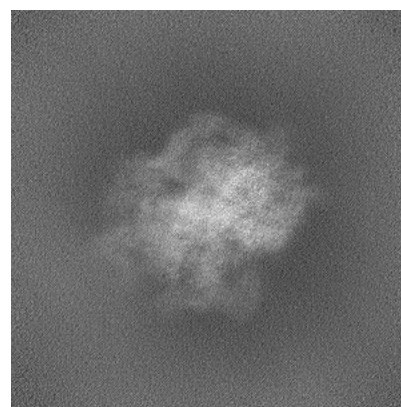
6.1.2 Raw map



X



Y

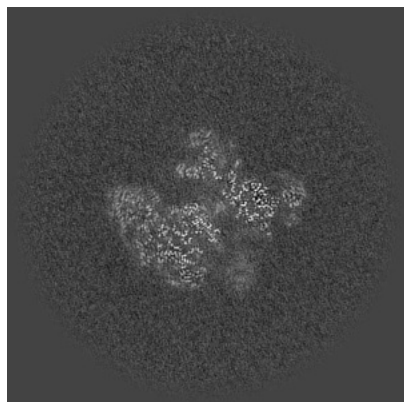


Z

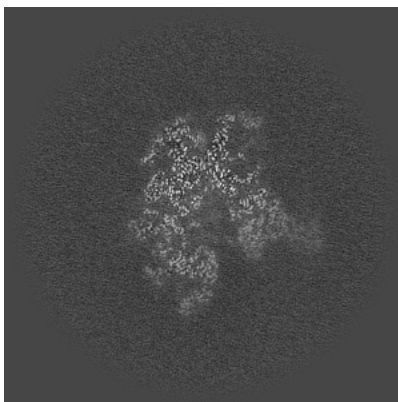
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

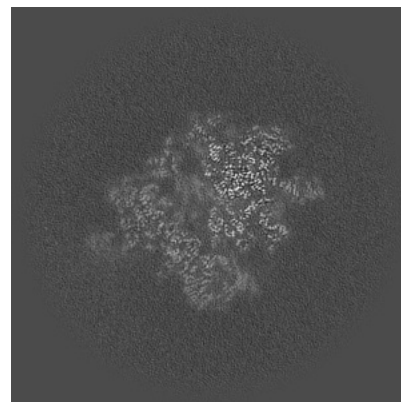
6.2.1 Primary map



X Index: 256

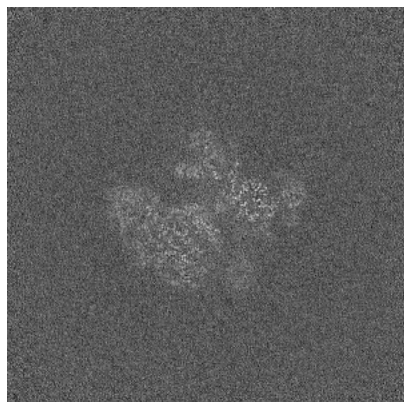


Y Index: 256

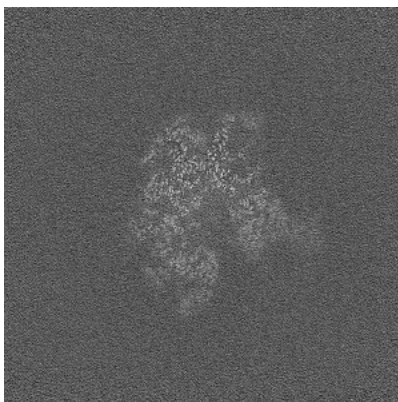


Z Index: 256

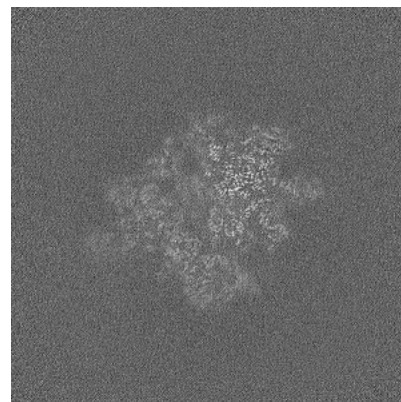
6.2.2 Raw map



X Index: 256



Y Index: 256

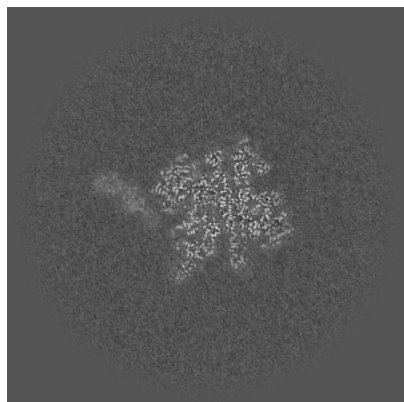


Z Index: 256

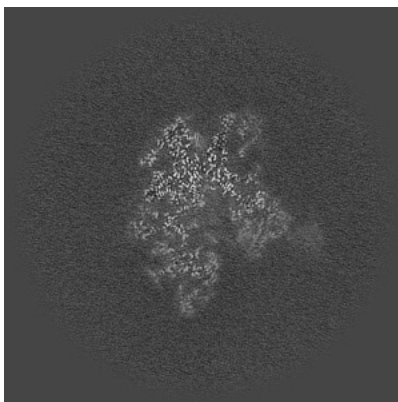
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

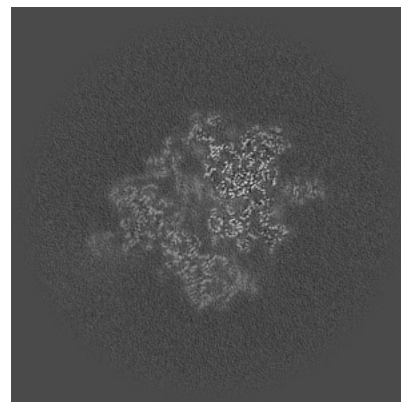
6.3.1 Primary map



X Index: 297

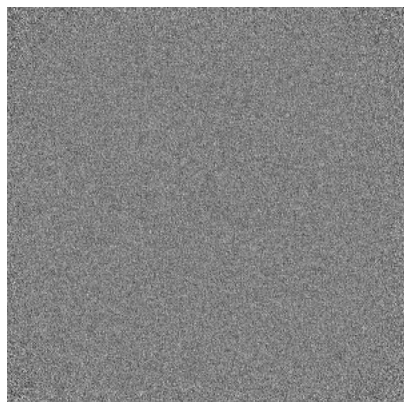


Y Index: 254

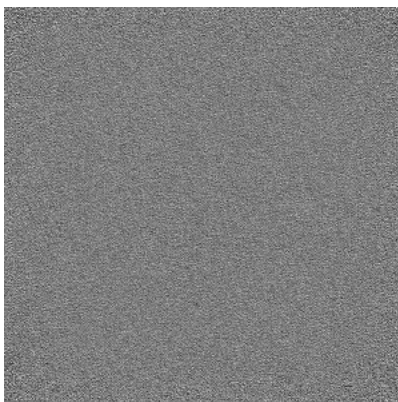


Z Index: 257

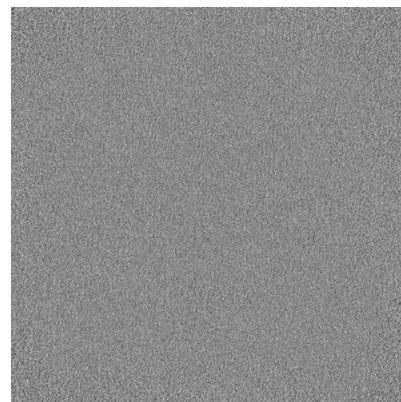
6.3.2 Raw map



X Index: 0



Y Index: 0

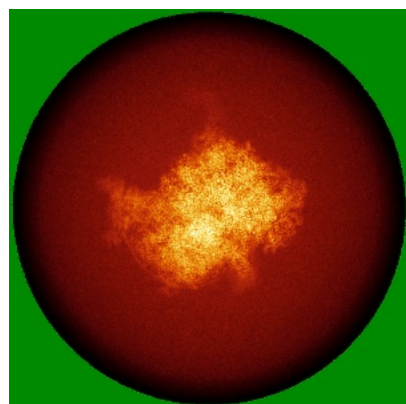


Z Index: 0

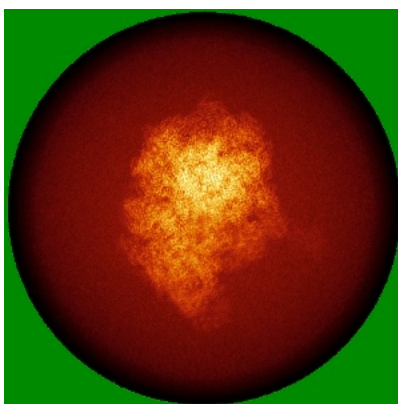
The images above show the largest variance slices of the map in three orthogonal directions.

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

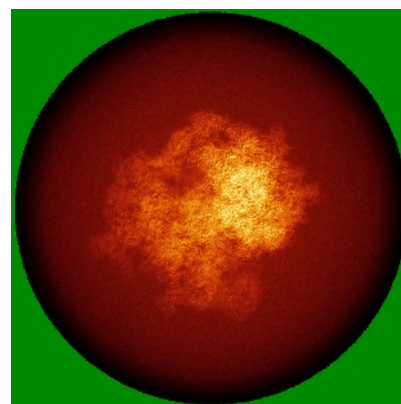
6.4.1 Primary map



X

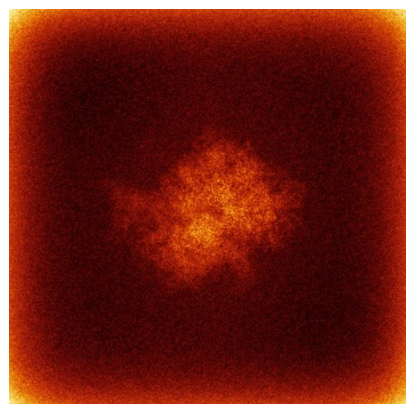


Y

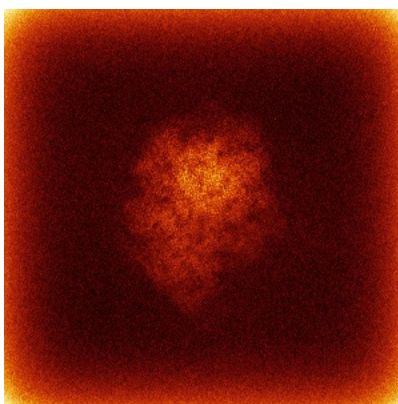


Z

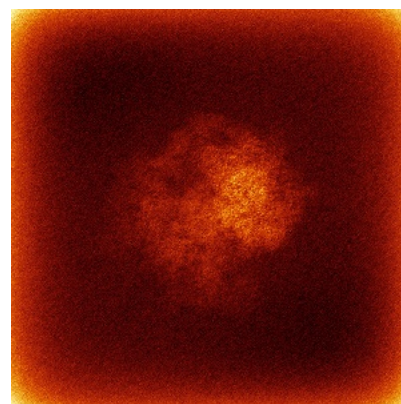
6.4.2 Raw map



X



Y

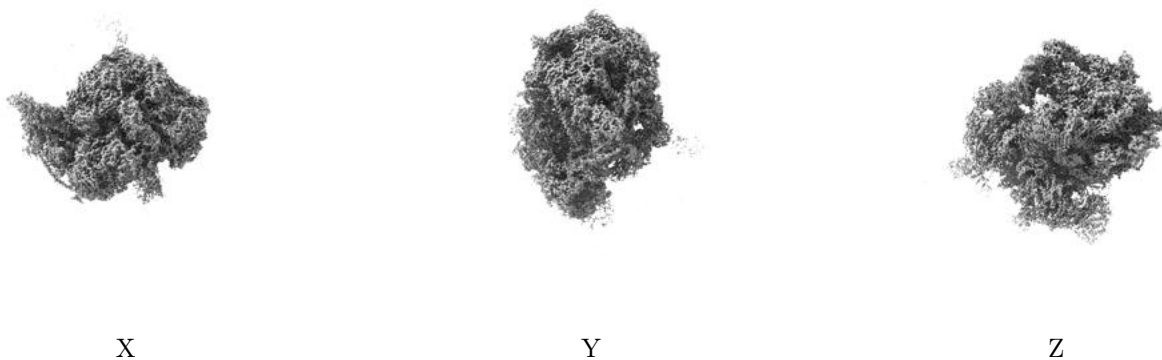


Z

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.

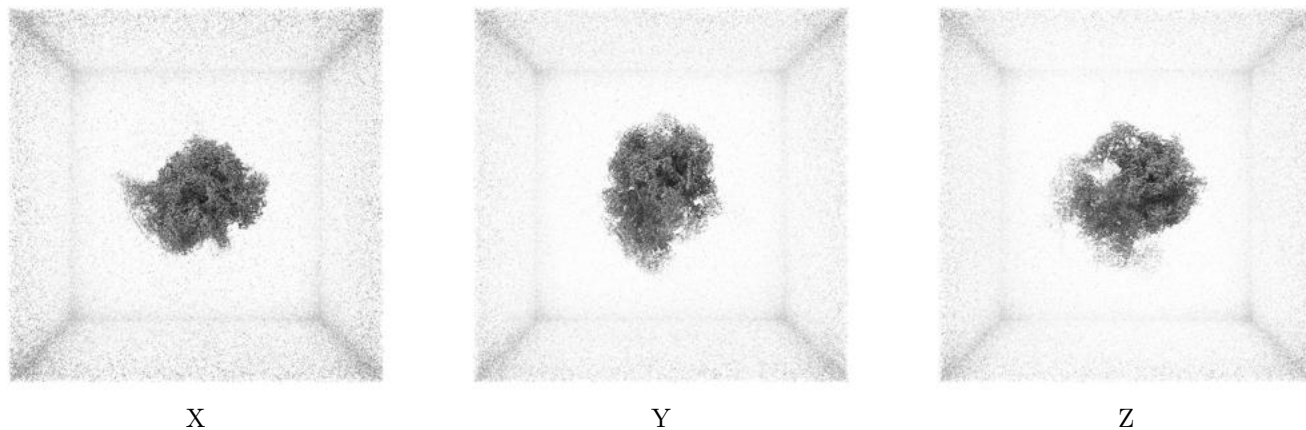
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

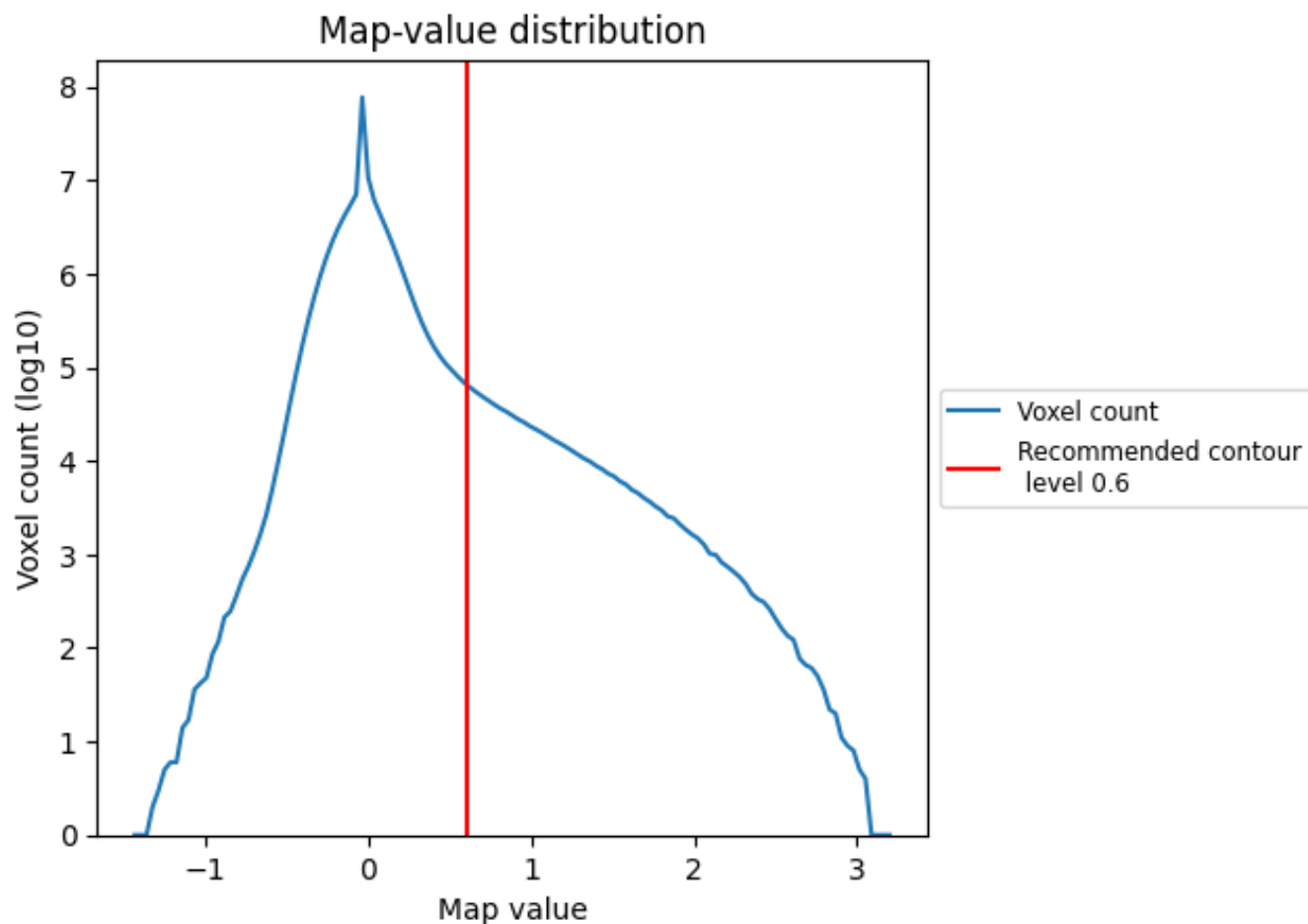
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

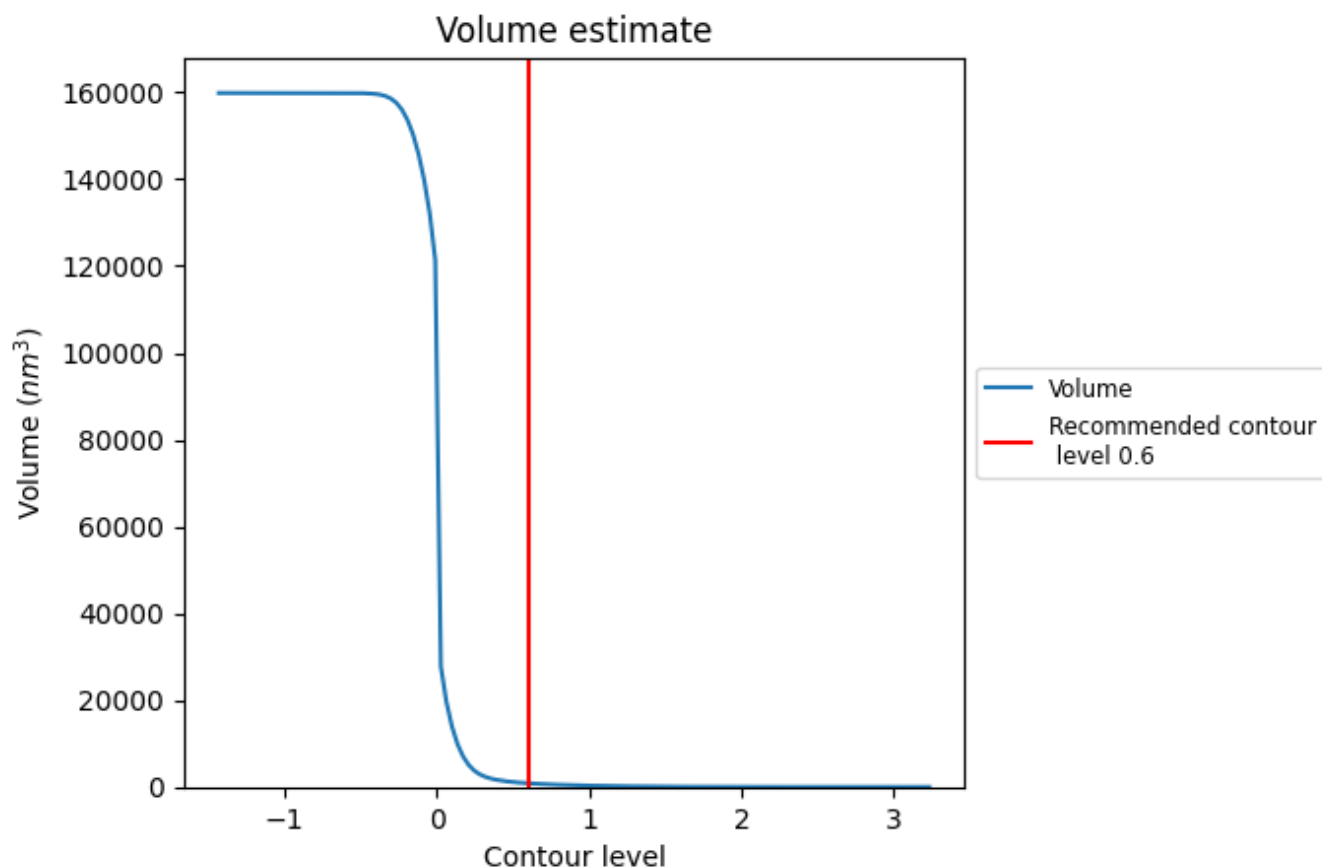
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

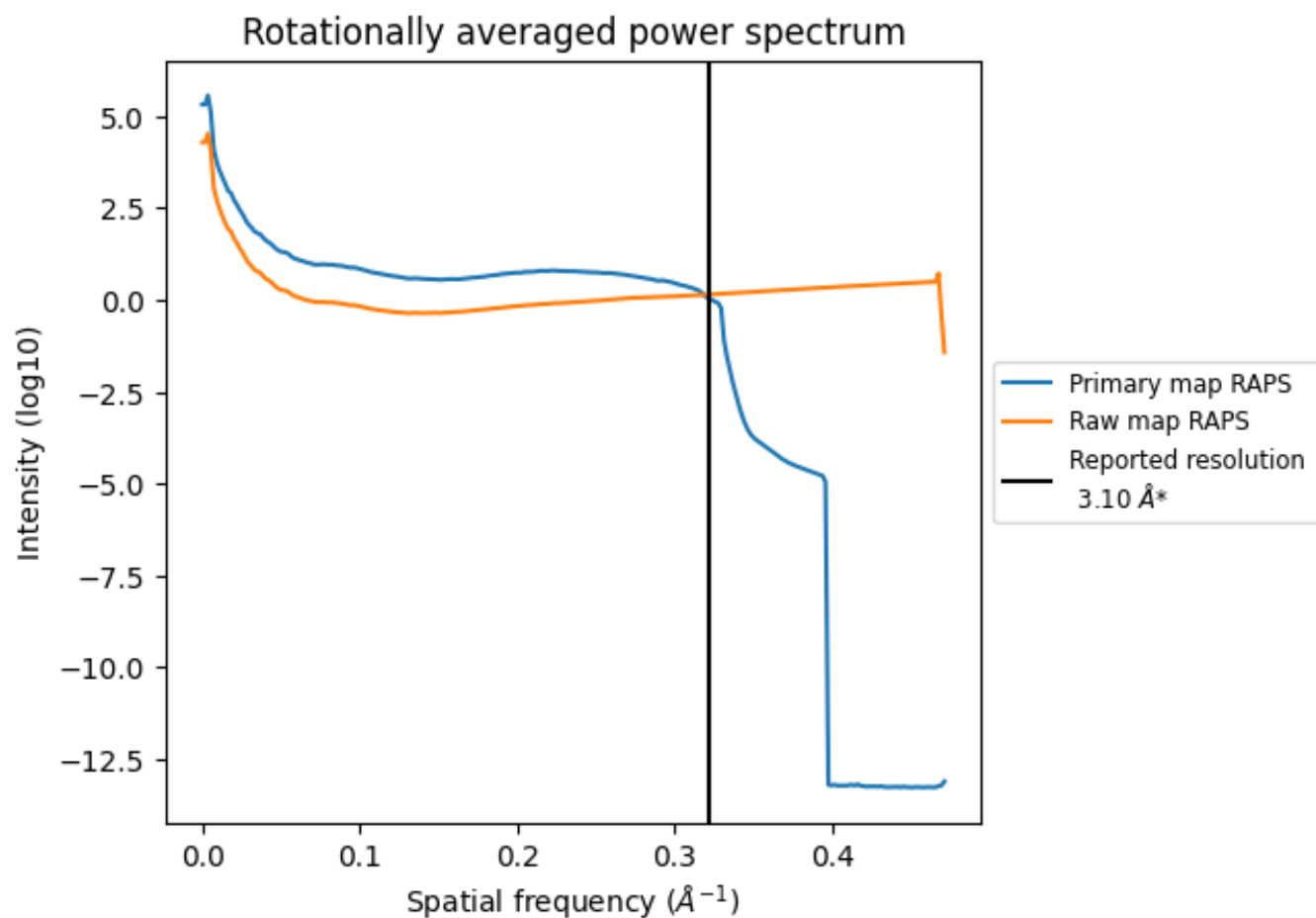
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 850 nm³; this corresponds to an approximate mass of 768 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

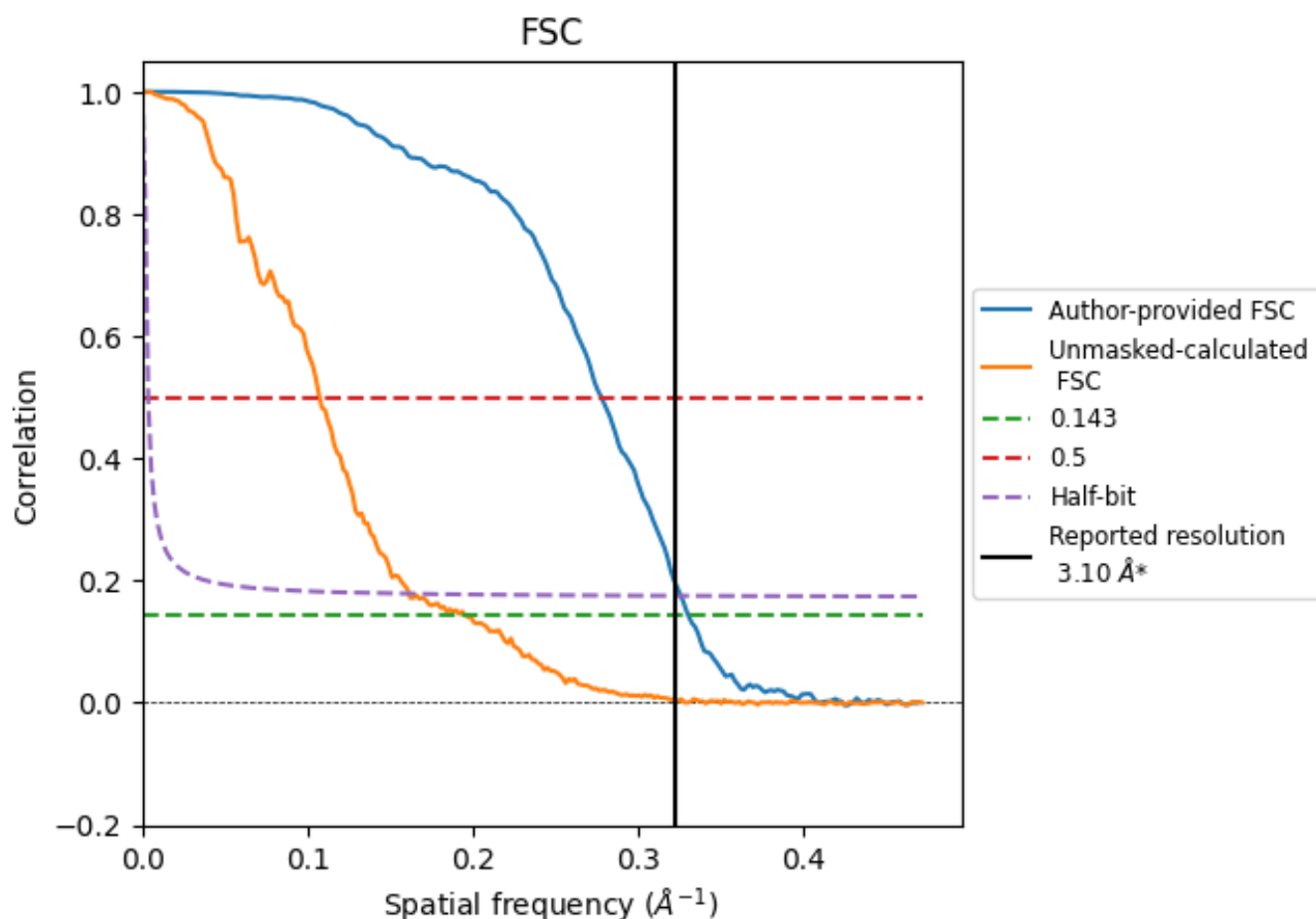


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

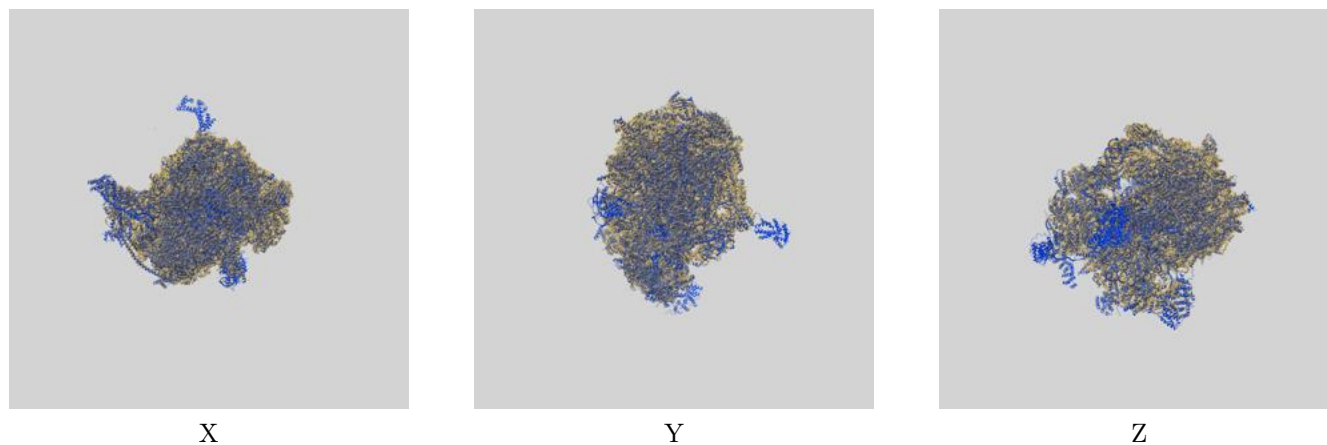
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.03	3.60	3.07
Unmasked-calculated*	5.12	9.33	6.20

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

9 Map-model fit [i](#)

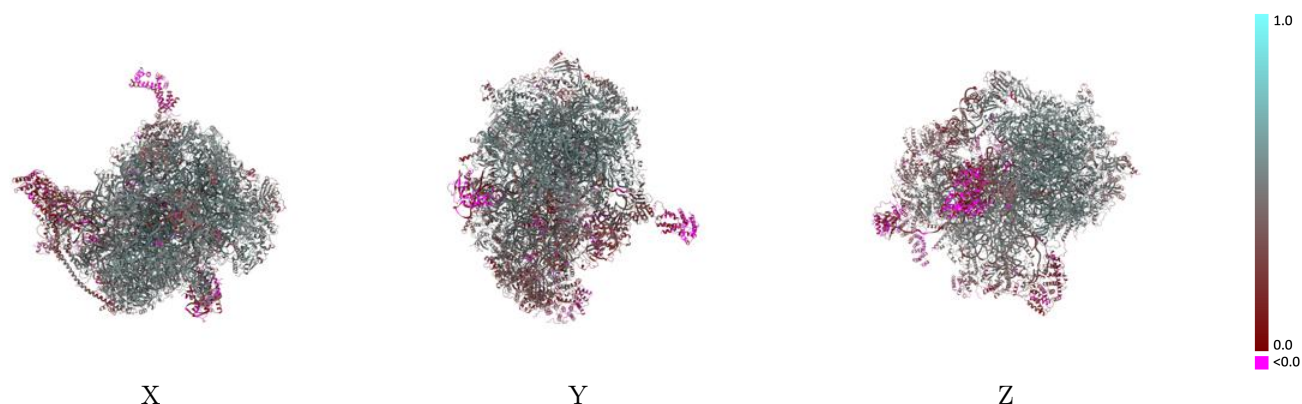
This section contains information regarding the fit between EMDB map EMD-16897 and PDB model 8OIR. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



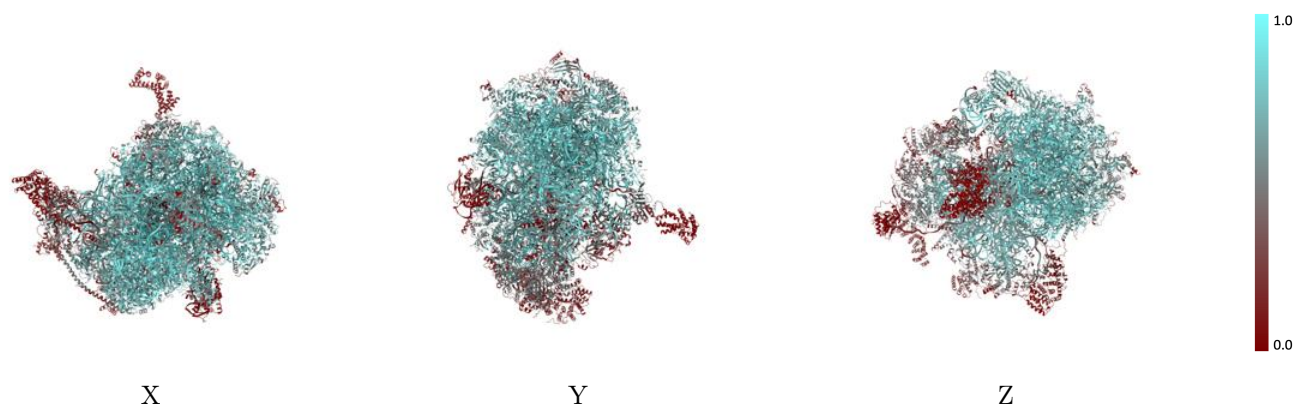
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



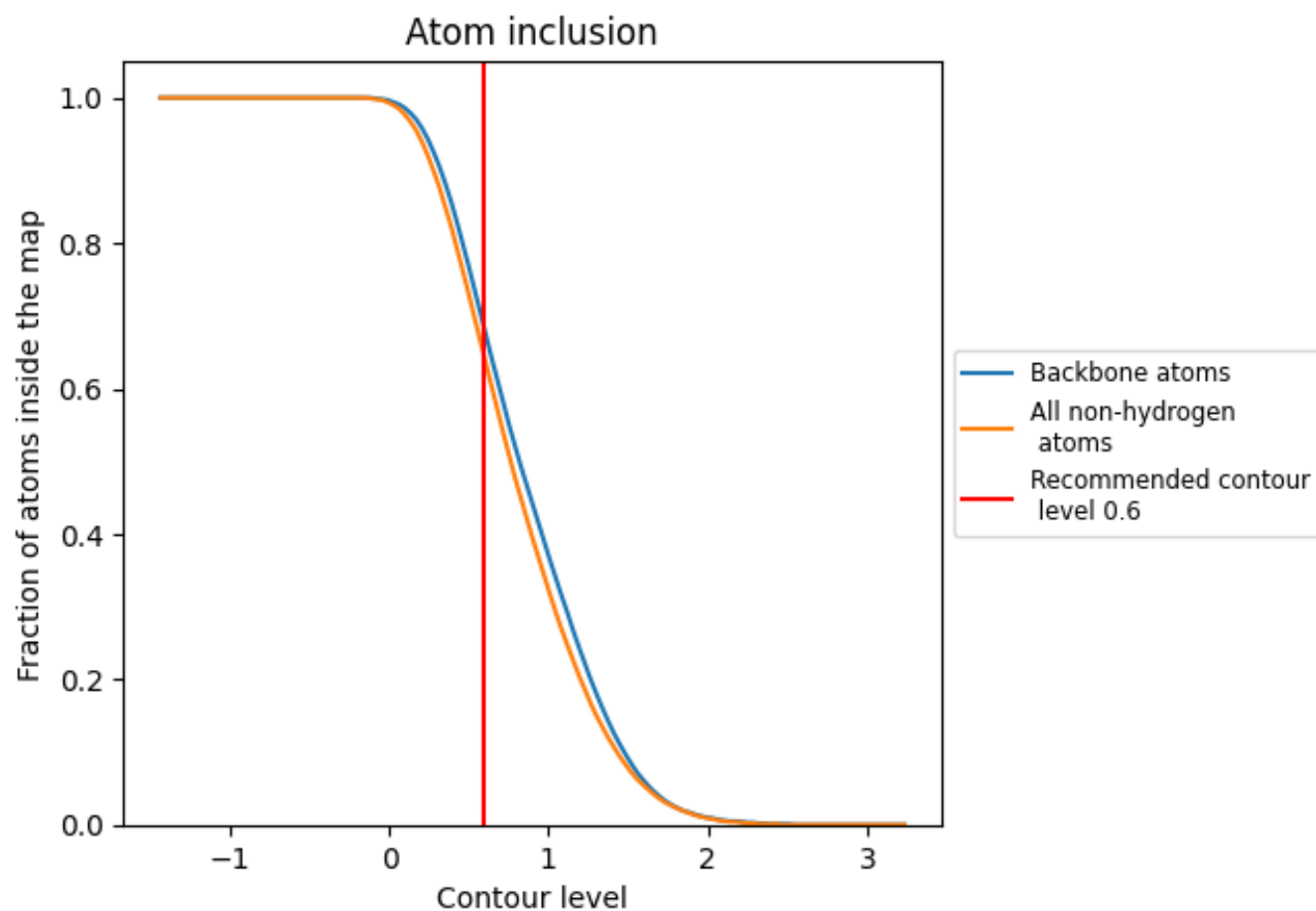
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 64% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6420	 0.4340
AA	 0.8150	 0.4790
AB	 0.3570	 0.3290
AC	 0.5900	 0.4550
AD	 0.7380	 0.4870
AE	 0.6540	 0.4620
AF	 0.5200	 0.3960
AG	 0.5960	 0.3520
AH	 0.4660	 0.3820
AI	 0.2980	 0.2680
AJ	 0.6150	 0.4720
AK	 0.6460	 0.4420
AL	 0.5800	 0.4160
AM	 0.4750	 0.3660
AN	 0.6290	 0.4660
AO	 0.4210	 0.3620
AP	 0.6890	 0.4560
AQ	 0.7250	 0.4960
AR	 0.2830	 0.3010
AS	 0.4320	 0.3820
AT	 0.5770	 0.4360
AU	 0.4320	 0.3210
AV	 0.1230	 0.1670
AW	 0.5510	 0.4450
AX	 0.4170	 0.3270
AY	 0.2770	 0.2700
AZ	 0.4770	 0.3850
Aa	 0.1040	 0.1450
Ab	 0.6440	 0.4560
Ac	 0.5410	 0.4080
Ad	 0.5540	 0.4430
Ae	 0.0870	 0.1490
Ag	 0.4860	 0.3980
Ai	 0.6660	 0.4600
Aj	 0.3440	 0.2900



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Chain	Atom inclusion	Q-score
B1	0.0250	0.0860
B2	0.0120	0.0790
B3	0.0000	0.0200
B4	0.0000	-0.0130
B5	0.0000	-0.0520
B6	0.0000	-0.0490
B7	0.1940	0.3470
B8	0.8840	0.5250
B9	0.6940	0.3640
BA	0.7960	0.5460
BB	0.6990	0.4820
BC	0.5560	0.4450
BD	0.8260	0.5500
BE	0.7320	0.5060
BF	0.7670	0.5230
BG	0.7950	0.5420
BH	0.7290	0.5250
BI	0.6870	0.4900
BJ	0.8970	0.5870
BK	0.8660	0.5720
BL	0.8430	0.5530
BM	0.7980	0.5260
BN	0.7950	0.5390
BO	0.3140	0.2410
BP	0.3560	0.2890
BQ	0.2080	0.2080
BR	0.8320	0.5450
BS	0.7970	0.5290
BT	0.7920	0.5350
BU	0.7690	0.5050
BV	0.7910	0.5360
BW	0.7820	0.5100
BX	0.7020	0.4810
BY	0.8200	0.5480
BZ	0.7750	0.5280
Ba	0.6910	0.4730
Bb	0.4760	0.3690
Bc	0.3090	0.2860
Bd	0.3770	0.2790
Be	0.8470	0.5590
Bf	0.5530	0.4140
Bg	0.4910	0.3460

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Chain	Atom inclusion	Q-score
Bh	 0.7670	 0.5090
Bi	 0.7620	 0.5130
Bj	 0.0160	 0.0330
Bl	 0.8440	 0.5380
Bm	 0.7600	 0.5120
Bn	 0.7000	 0.4620
Bo	 0.6140	 0.4520
Bp	 0.3970	 0.3110
Bq	 0.6910	 0.4910
Br	 0.6560	 0.4670
Bs	 0.7900	 0.5450
Bt	 0.6770	 0.4880
Bu	 0.5010	 0.4150
Bv	 0.3390	 0.2660
Bw	 0.4740	 0.3670
Bx	 0.7450	 0.5160
By	 0.5060	 0.4300
Bz	 0.8460	 0.5650