



wwPDB EM Validation Summary Report ⓘ

Jun 17, 2026 – 03:30 pm BST

PDB ID : 6GAW / pdb_00006gaw
EMDB ID : EMD-4368
Title : Unique features of mammalian mitochondrial translation initiation revealed by cryo-EM. This file contains the complete 55S ribosome.
Authors : Kummer, E.; Leibundgut, M.; Boehringer, D.; Ban, N.
Deposited on : 2018-04-13
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
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

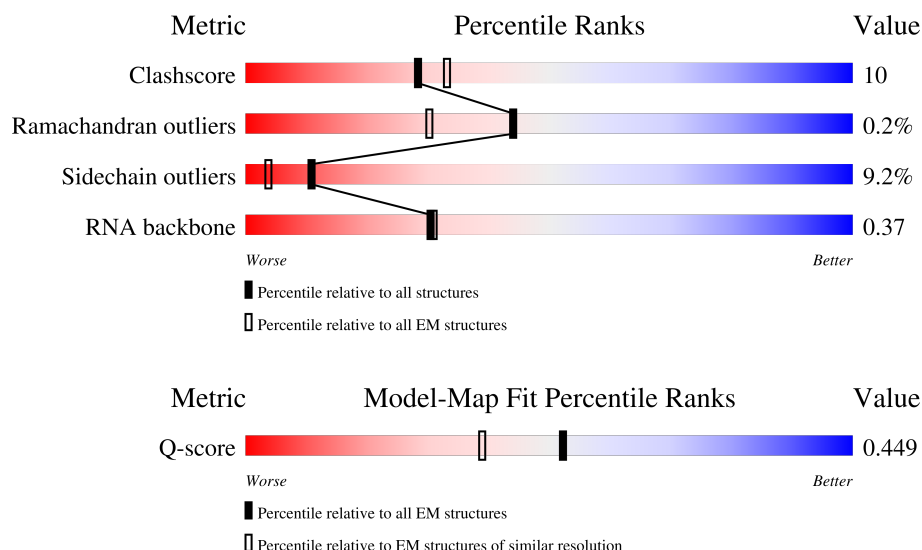
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	BL	198	35% 30% 5% • 65%
1	CL	198	21% 14% 8% • 77%
1	DL	198	14% 8% 5% • 86%

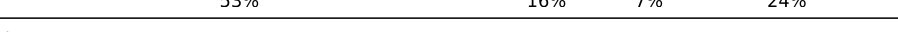
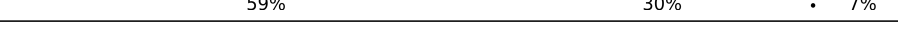
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Mol	Chain	Length	Quality of chain
1	EL	198	
1	FL	198	
1	GL	198	
1	HL	198	
2	B0	148	
3	B1	256	
4	B2	252	
5	B3	161	
6	B4	126	
7	B5	188	
8	B6	65	
9	B7	95	
10	B8	188	
11	B9	100	
12	BA	1571	
13	BB	73	
14	BC	650	
15	BD	306	
16	BE	348	
17	BF	294	
18	BI	268	
19	BJ	262	
20	BK	192	
21	BN	178	
22	BO	145	

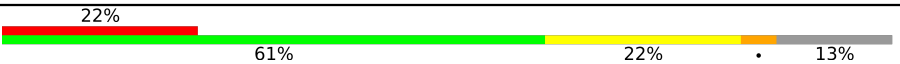
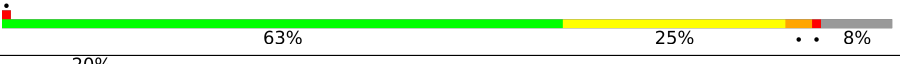
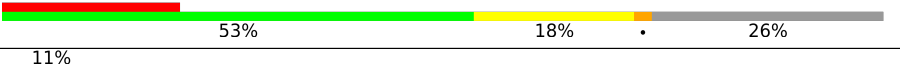
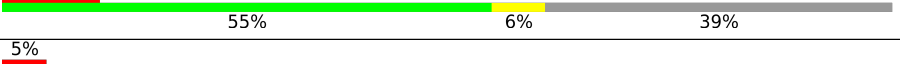
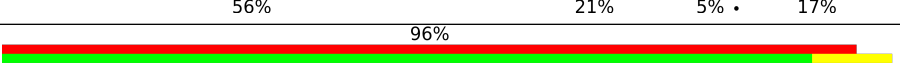
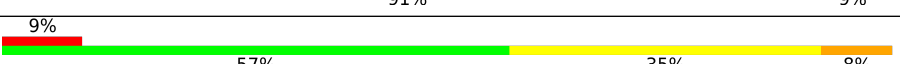
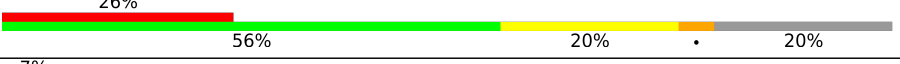
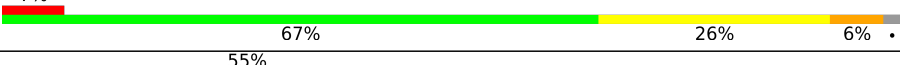
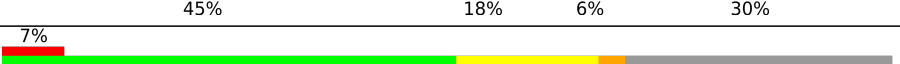
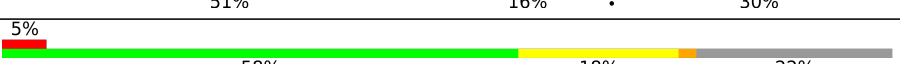
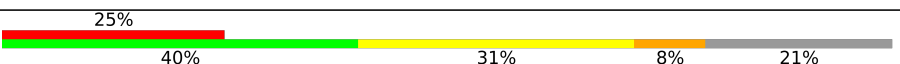
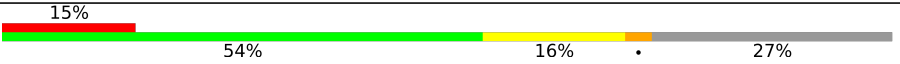
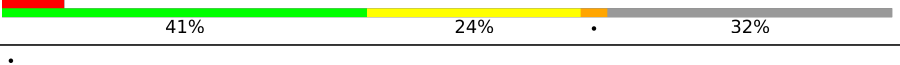
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Mol	Chain	Length	Quality of chain
23	BP	296	
24	BQ	251	
25	BR	169	
26	BS	180	
27	BT	292	
28	BU	149	
29	BV	209	
30	BW	210	
31	BX	150	
32	BY	216	
33	Ba	423	
34	Bb	380	
35	Bc	334	
36	Bd	206	
37	Be	135	
38	Bf	142	
39	Bg	159	
40	Bh	332	
41	Bi	306	
42	Bj	279	
43	Bk	212	
44	Bl	166	
45	Bm	159	
46	Bn	128	
47	Bo	124	

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Mol	Chain	Length	Quality of chain
48	Bp	112	
49	Bq	138	
50	Bt	102	
51	Bu	205	
52	Bv	222	
53	Bw	433	
54	Bx	196	
55	Bz	82	
56	AA	962	
57	AB	289	
58	AC	167	
59	AE	430	
60	AF	124	
61	AG	242	
62	AI	397	
63	AJ	201	
64	AK	196	
65	AL	139	
66	AN	128	
67	AO	239	
68	AP	135	
69	AQ	130	
70	AR	143	
71	AU	87	
72	AV	71	

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Mol	Chain	Length	Quality of chain
73	AX	201	
74	AZ	18	
75	Aa	382	
76	Ab	190	
77	Ac	173	
78	Ad	205	
79	Ae	455	
80	Af	188	
81	Ag	397	
82	Ah	387	
83	Ai	106	
84	Aj	218	
85	Ak	325	
86	Am	118	
87	An	199	
88	Ao	692	
89	Ap	258	

2 Entry composition

There are 98 unique types of molecules in this entry. The entry contains 178372 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 Mitochondrial ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	CL	45	Total	C	N	O	0	0
			317	203	52	62		
1	DL	27	Total	C	N	O	0	0
			213	137	33	43		
1	EL	28	Total	C	N	O	0	0
			222	143	35	44		
1	FL	27	Total	C	N	O	0	0
			213	137	33	43		
1	GL	27	Total	C	N	O	0	0
			213	137	33	43		
1	HL	26	Total	C	N	O	0	0
			205	131	32	42		
1	BL	70	Total	C	N	O	0	0
			537	346	93	98		

- Molecule 2 is a protein called Mitochondrial ribosomal protein L27.

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

- Molecule 3 is a protein called Mitochondrial ribosomal protein L28.

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

- Molecule 4 is a protein called Mitochondrial ribosomal protein L47.

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

- Molecule 5 is a protein called uL30m.

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

- Molecule 6 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B4	45	Total	C	N	O	S	0	0
			381	239	77	62	3		

- Molecule 7 is a protein called bL32m.

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

- Molecule 8 is a protein called bL33m.

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

- Molecule 9 is a protein called Mitochondrial ribosomal protein L34.

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

- Molecule 10 is a protein called Mitochondrial ribosomal protein L35.

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

- Molecule 11 is a protein called Ribosomal protein.

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

- Molecule 12 is a RNA chain called 16S ribosomal RNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BA	1549	Total	C	N	O	P	0	0
			32950	14798	5993	10610	1549		

- Molecule 13 is a RNA chain called tRNA-Phe, mitochondrial.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	71	C	-	insertion	GB 76262549
BB	72	C	-	insertion	GB 76262549
BB	73	A	-	insertion	GB 76262549

- Molecule 14 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BC	571	Total	C	N	O	S	0	0
			4364	2743	765	839	17		

- Molecule 15 is a protein called 39S ribosomal protein L2, mitochondrial.

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

- Molecule 16 is a protein called ICT1.

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

- Molecule 17 is a protein called Mitochondrial ribosomal protein L4.

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

- Molecule 18 is a protein called Mitochondrial ribosomal protein L9.

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

- Molecule 19 is a protein called Mitochondrial ribosomal protein L10.

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

- Molecule 20 is a protein called Mitochondrial ribosomal protein L11.

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

- Molecule 21 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 22 is a protein called uL14m.

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

- Molecule 23 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L16, mitochondrial.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	237	HIS	TYR	conflict	UNP F1RI89

- Molecule 25 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 26 is a protein called Mitochondrial ribosomal protein L18.

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

- Molecule 27 is a protein called Mitochondrial ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BT	240	Total	C	N	O	S	0	0
			1954	1253	338	354	9		

- Molecule 28 is a protein called Mitochondrial ribosomal protein L20.

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

- Molecule 29 is a protein called Mitochondrial ribosomal protein L21.

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

- Molecule 30 is a protein called uL22m.

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

- Molecule 31 is a protein called uL23m.

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

- Molecule 32 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 33 is a protein called Mitochondrial ribosomal protein L37.

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

- Molecule 34 is a protein called Mitochondrial ribosomal protein L38.

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

- Molecule 35 is a protein called Mitochondrial ribosomal protein L39.

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

- Molecule 36 is a protein called 39S ribosomal protein L40, mitochondrial isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bd	99	Total	C	N	O	S	0	0
			832	528	148	155	1		

- Molecule 37 is a protein called Mitochondrial ribosomal protein L41.

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

- Molecule 38 is a protein called mL42.

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

- Molecule 39 is a protein called mL43.

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

- Molecule 40 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 41 is a protein called mL45.

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

- Molecule 42 is a protein called Mitochondrial ribosomal protein L46.

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

- Molecule 43 is a protein called Mitochondrial ribosomal protein L48.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bk	136	Total	C	N	O	S	0	0
			1087	692	185	205	5		

- Molecule 44 is a protein called 39S ribosomal protein L49, mitochondrial.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	59	ARG	LYS	conflict	UNP A0A0R4J8D6

- Molecule 45 is a protein called mL50.

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

- Molecule 46 is a protein called Mitochondrial ribosomal protein L51.

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

- Molecule 47 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 48 is a protein called mL53.

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

- Molecule 49 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bq	68	Total	C	N	O	S	0	0
			542	344	102	95	1		

- Molecule 50 is a protein called Mitochondrial ribosomal protein L57.

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

- Molecule 51 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 52 is a protein called mL64.

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

- Molecule 53 is a protein called mL65.

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

- Molecule 54 is a protein called Mitochondrial ribosomal protein S18A.

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

- Molecule 55 is a protein called unassigned secondary structure elements.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	Bz	82	Total	C	N	O	0	0
			410	246	82	82		

- Molecule 56 is a RNA chain called 12S ribosomal RNA, mitochondrial.

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

- Molecule 57 is a protein called Mitochondrial ribosomal protein S2.

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

- Molecule 58 is a protein called Mitochondrial ribosomal protein S24.

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

- Molecule 59 is a protein called Mitochondrial ribosomal protein S5.

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

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

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

- Molecule 61 is a protein called Mitochondrial ribosomal protein S7.

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

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

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

- Molecule 63 is a protein called Mitochondrial ribosomal protein S10.

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

- Molecule 64 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 65 is a protein called Mitochondrial ribosomal protein S12.

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

- Molecule 66 is a protein called Mitochondrial ribosomal protein S14.

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

- Molecule 67 is a protein called Uncharacterized protein.

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

- Molecule 68 is a protein called bS16m.

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

- Molecule 69 is a protein called uS17m.

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

- Molecule 70 is a protein called Mitochondrial ribosomal protein S18C.

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

- Molecule 71 is a protein called bS21m.

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

- Molecule 72 is a RNA chain called P-site fMet-tRNA^{Met}, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AV	71	Total	C	N	O	P	0	0
			1498	673	264	491	70		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	69	C	-	insertion	GB 1390216722
AV	70	C	-	insertion	GB 1390216722
AV	71	A	-	insertion	GB 1390216722

- Molecule 73 is a RNA chain called MT-CO3 mRNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AX	17	Total	C	N	O	P	0	0
			354	161	65	112	16		

- Molecule 74 is a protein called unassigned secondary structure elements.

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

- Molecule 75 is a protein called Mitochondrial ribosomal protein S22.

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

- Molecule 76 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 77 is a protein called Mitochondrial ribosomal protein S25.

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

- Molecule 78 is a protein called Mitochondrial ribosomal protein S26.

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

- Molecule 79 is a protein called mS27.

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

- Molecule 80 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 81 is a protein called Death associated protein 3.

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

- Molecule 82 is a protein called mS31.

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

- Molecule 83 is a protein called mS33.

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

- Molecule 84 is a protein called 28S ribosomal protein S34, mitochondrial.

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

- Molecule 85 is a protein called 28S ribosomal protein S35, mitochondrial.

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

- Molecule 86 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

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

- Molecule 87 is a protein called Aurora kinase A interacting protein 1.

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

- Molecule 88 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Ao	572	Total	C	N	O	S	0	0
			4526	2898	770	834	24		

- Molecule 89 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 90 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
90	B3	1	Total	Mg	0
			1	1	
90	BA	202	Total	Mg	0
			202	202	
90	BB	1	Total	Mg	0
			1	1	
90	BC	2	Total	Mg	0
			2	2	
90	BD	3	Total	Mg	0
			3	3	

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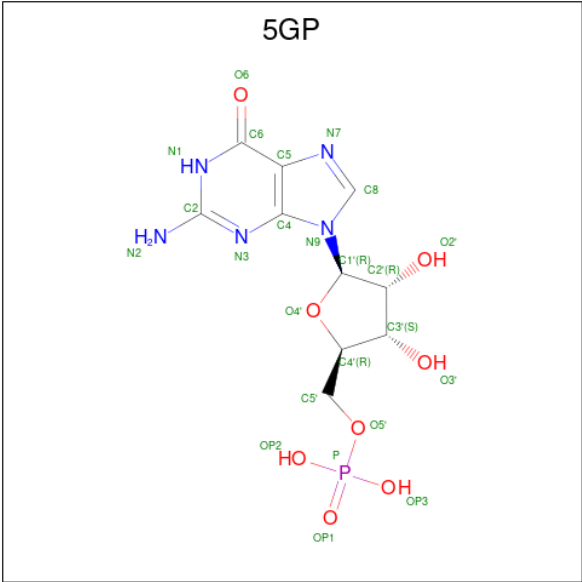
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Mol	Chain	Residues	Atoms		AltConf
90	BE	1	Total 1	Mg 1	0
90	BJ	1	Total 1	Mg 1	0
90	BP	2	Total 2	Mg 2	0
90	Be	1	Total 1	Mg 1	0
90	Bl	1	Total 1	Mg 1	0
90	Bt	2	Total 2	Mg 2	0
90	AA	105	Total 105	Mg 105	0
90	AB	1	Total 1	Mg 1	0
90	AX	1	Total 1	Mg 1	0
90	Ag	1	Total 1	Mg 1	0
90	An	1	Total 1	Mg 1	0

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

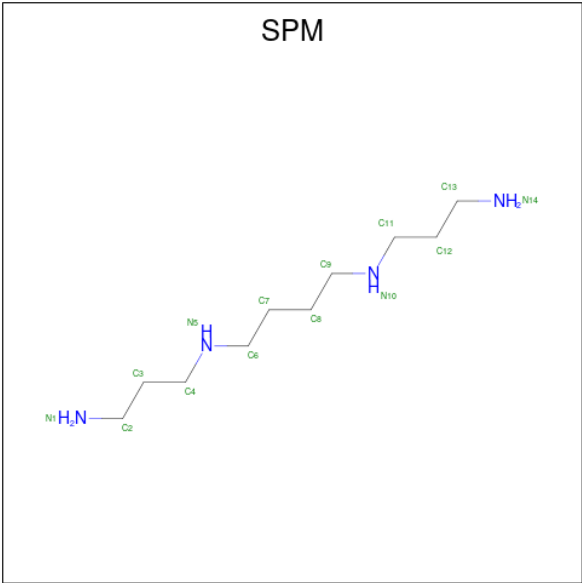
Mol	Chain	Residues	Atoms		AltConf
91	B5	1	Total 1	Zn 1	0
91	B9	1	Total 1	Zn 1	0
91	Bx	1	Total 1	Zn 1	0
91	AR	1	Total 1	Zn 1	0
91	Ac	1	Total 1	Zn 1	0
91	Ap	1	Total 1	Zn 1	0

- Molecule 92 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P).



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

- Molecule 93 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



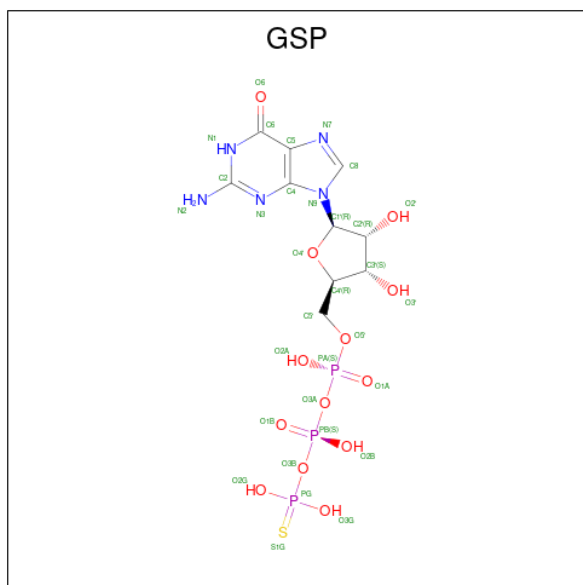
Mol	Chain	Residues	Atoms			AltConf
93	BA	1	Total	C	N	0
			14	10	4	
93	BR	1	Total	C	N	0
			14	10	4	

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

- Molecule 94 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).

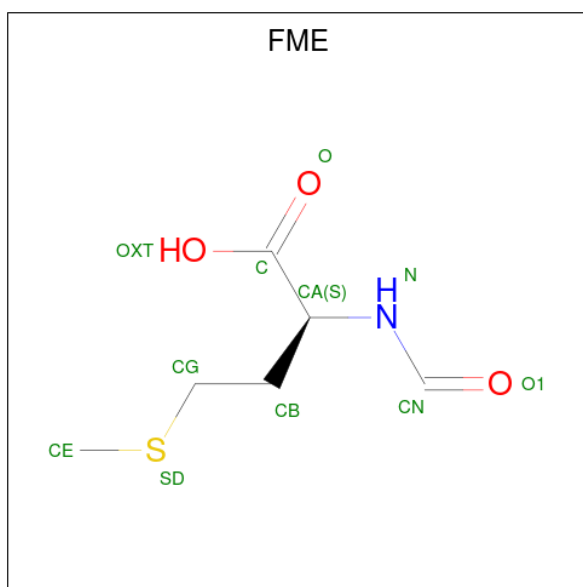


Mol	Chain	Residues	Atoms						AltConf
94	BC	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	

- Molecule 95 is SODIUM ION (CCD ID: NA) (formula: Na).

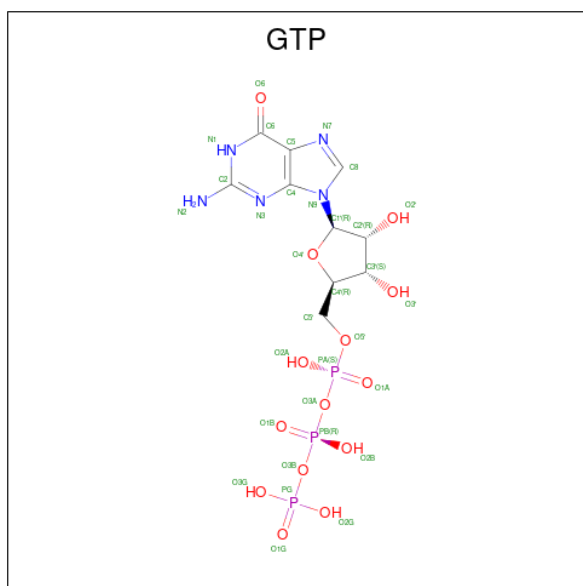
Mol	Chain	Residues	Atoms		AltConf
95	BC	1	Total	Na	0
			1	1	

- Molecule 96 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
96	AV	1	10	6	1	2	1	0

- Molecule 97 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

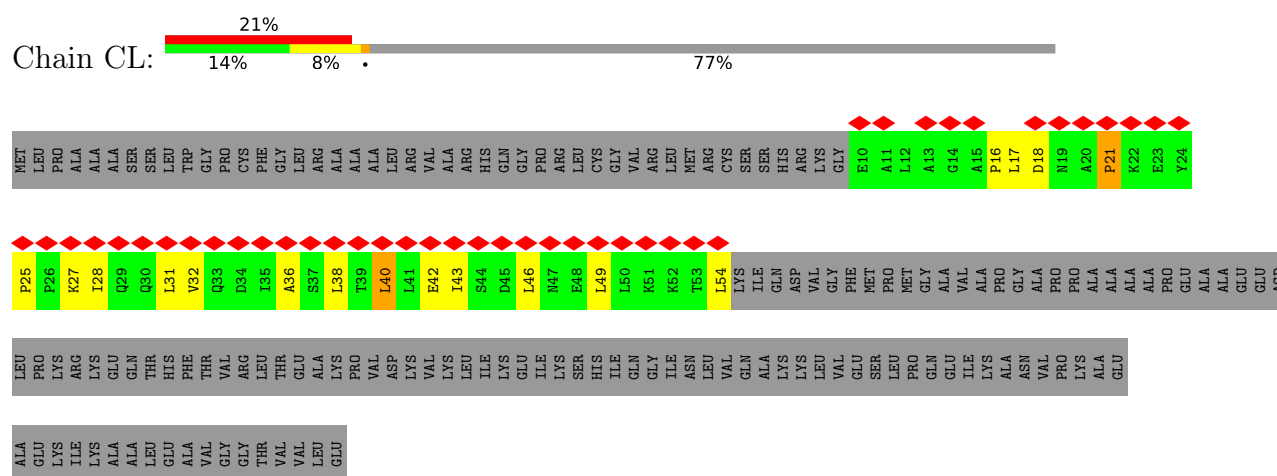


Mol	Chain	Residues	Atoms		AltConf
98	BC	2	Total 2	O 2	0
98	Ag	3	Total 3	O 3	0

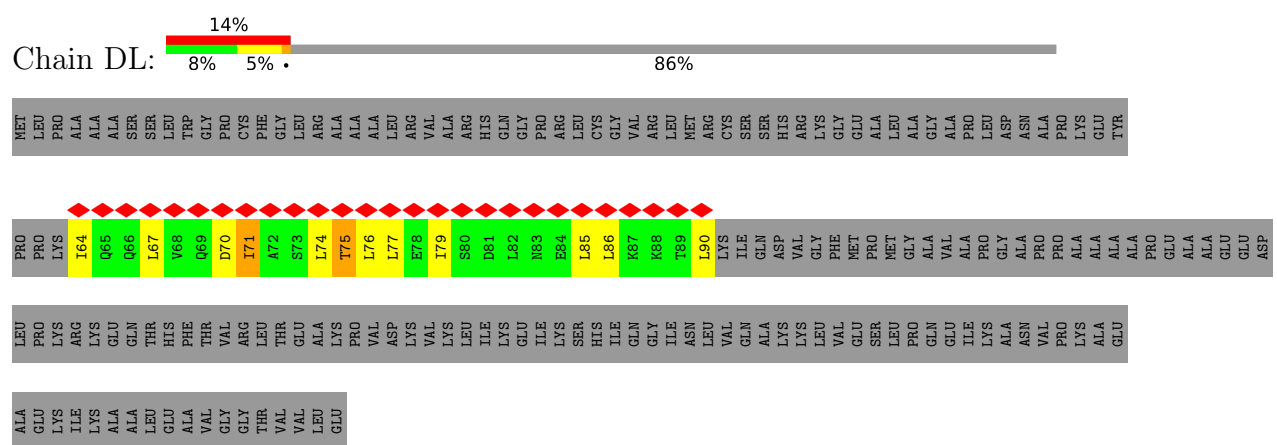
3 Residue-property plots

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.

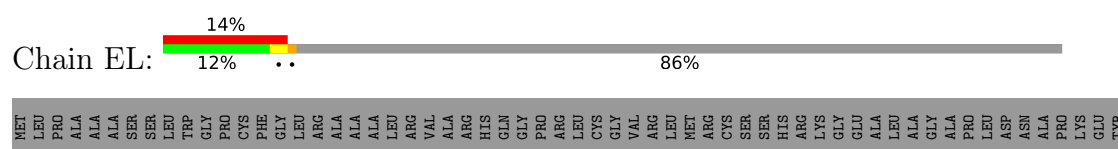
• Molecule 1: Mitochondrial ribosomal protein L12

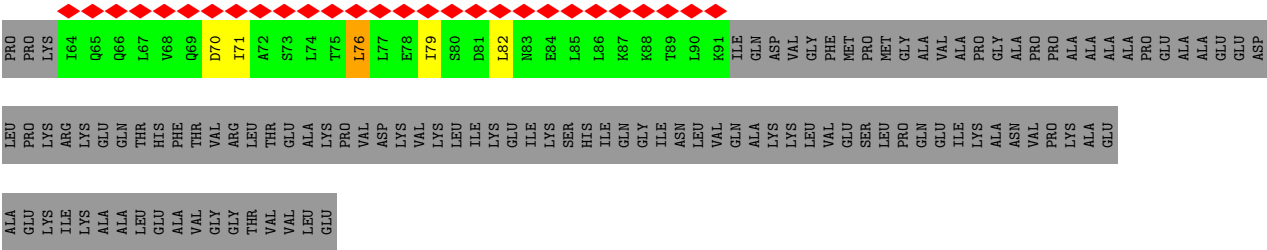


• Molecule 1: Mitochondrial ribosomal protein L12

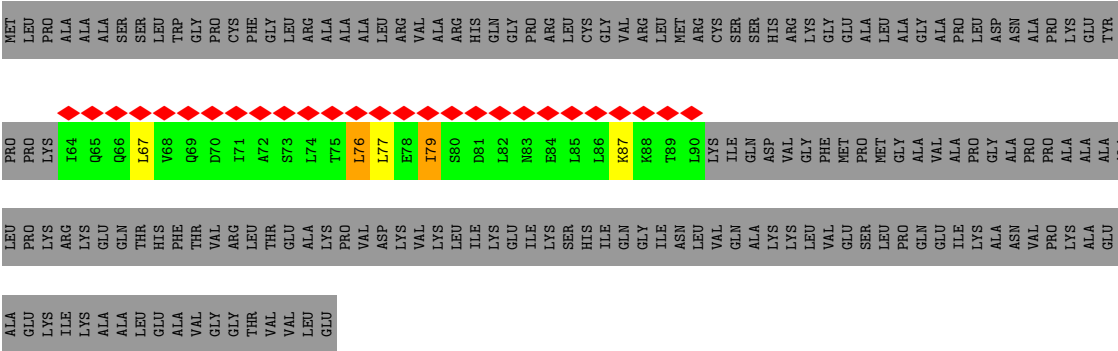


• Molecule 1: Mitochondrial ribosomal protein L12

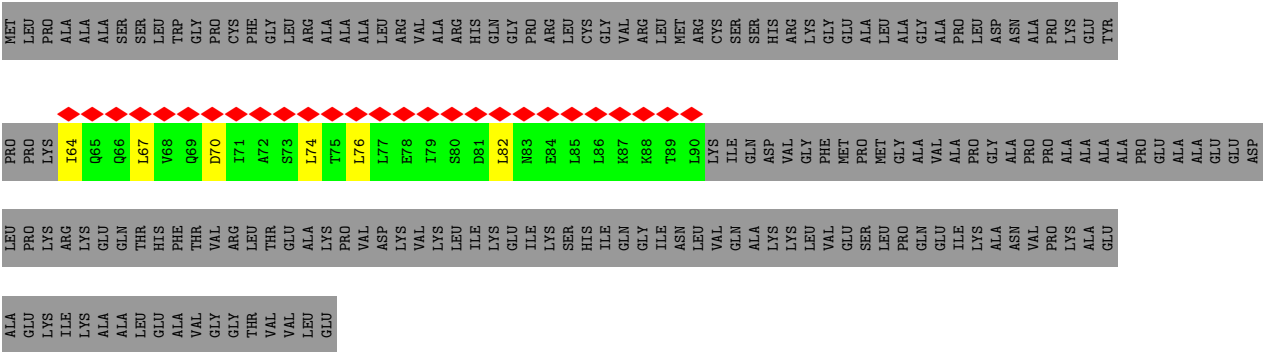




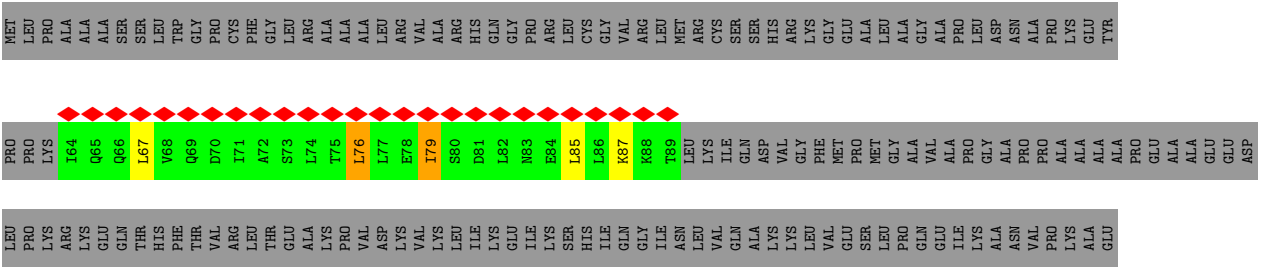
• Molecule 1: Mitochondrial ribosomal protein L12



• Molecule 1: Mitochondrial ribosomal protein L12



• Molecule 1: Mitochondrial ribosomal protein L12



ALA
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LEU
GLU
ALA
VAL
GLY
GLY
THR
VAL
VAL
LEU
GLU

• Molecule 1: Mitochondrial ribosomal protein L12



MET
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LEU
PRO
LYS
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ILE
ALA
LYS
GLN
LEU
SER
SER
LEU
GLN
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VAL
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CYS
PHE
GLY
LEU
ARG
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P139
V140
D141
K142
V143
K144
L145
I146
K147
E148
I149
K150
S151
H152
I153
Q154
G155
I156
N157
L158
V159
Q160
A161
K162
K163
L164
V165
E166
S167
L168
P169
Q170
E171
I172
K173
A174
N175
V176
P177
K178
A179
E180

• Molecule 2: Mitochondrial ribosomal protein L27



MET
ALA
LEU
ALA
VAL
LEU
ALA
LEU
ARG
THR
ARG
ALA
ALA
VAL
THR
ALA
LEU
SER
SER
PRO
PRO
GLN
ALA
ALA
ALA
LEU
ALA
VAL
VAL
ARG
TYR
SER
SER
LYS
LYS
THR
GLY
SER
S39
K40
K45
K49
R50
I53
K54
K55
M56
E57
G58
H59
H62
N65
T69

R74
W75
H76
T100
V117
T118
A119
L120
A124
V125
L126
Y127
K128
V131
S131
V132
V133
V134
P135
T141
L148

• Molecule 3: Mitochondrial ribosomal protein L28



MET
P72
K5
V6
R15
L16
W17
P25
R26
H27
Y28
L29
R30
S31
L32
E33
E34
A35
R36
P40
V41
H42
Y43
H46
R61
D64
P67
P68
V69
P72
S76
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W86
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K96
R100
V101
R102
K103
V104

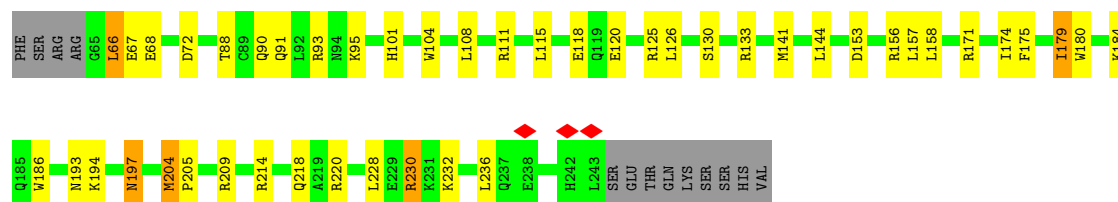
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L161
K162
R163
G164
M165
L166
I167
R168
Q172
D173
D173
P174
G175
L176
H177
P178
D179
R184
D189
R190
Y191
K192
T196
P197
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A201
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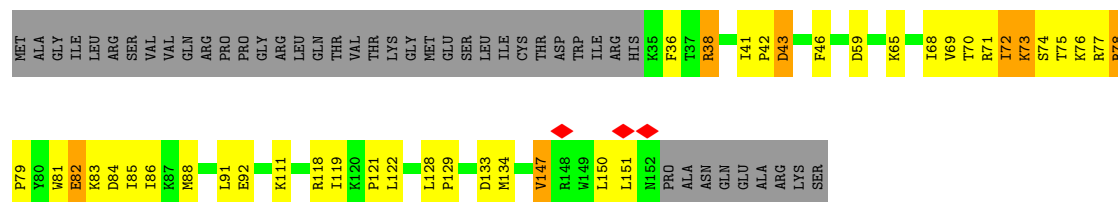
• Molecule 4: Mitochondrial ribosomal protein L47



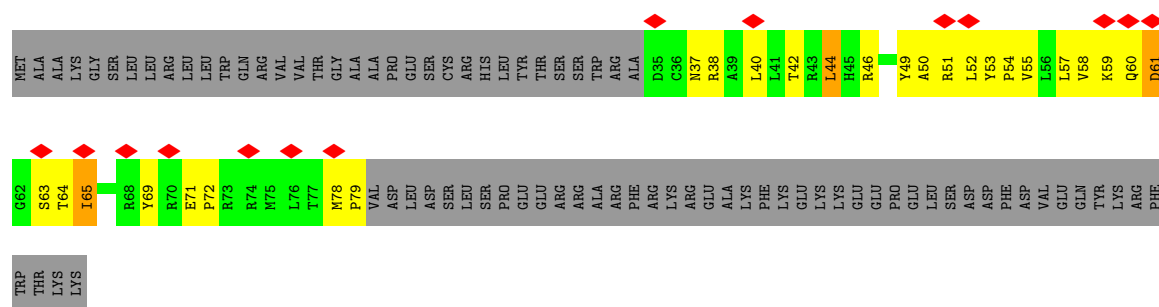
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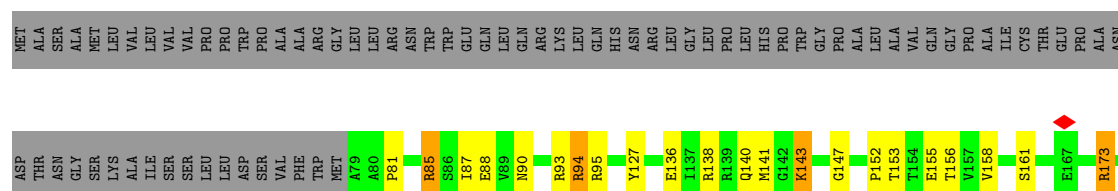
- Molecule 5: uL30m



- Molecule 6: 39S ribosomal protein L55, mitochondrial

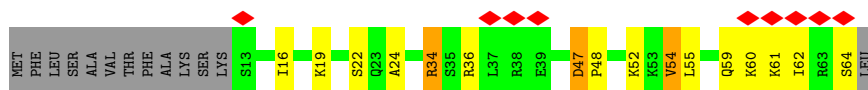


- Molecule 7: bL32m

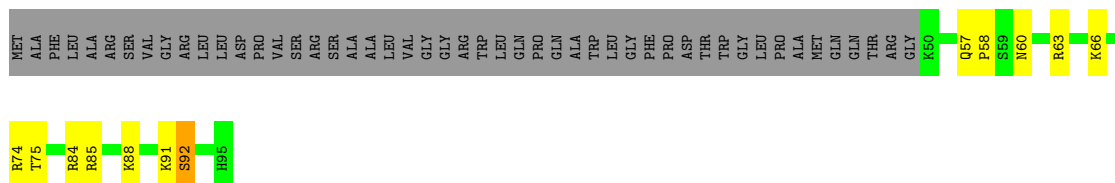
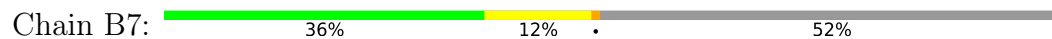


- Molecule 8: bL33m

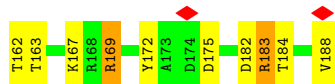
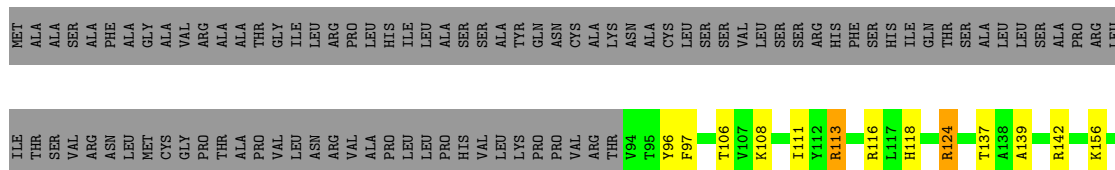




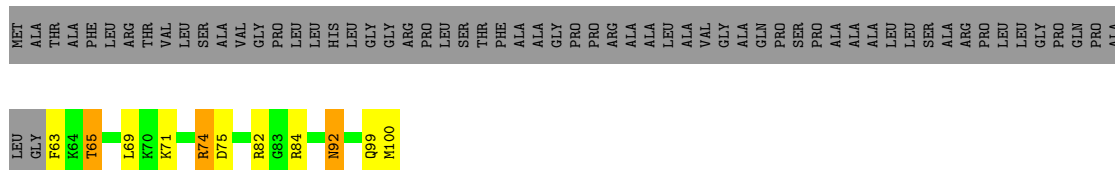
• Molecule 9: Mitochondrial ribosomal protein L34



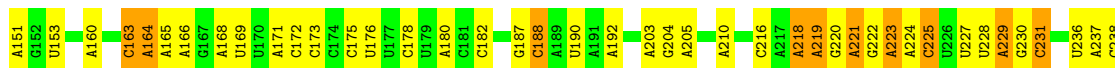
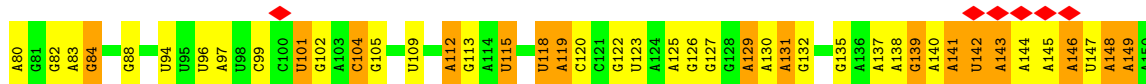
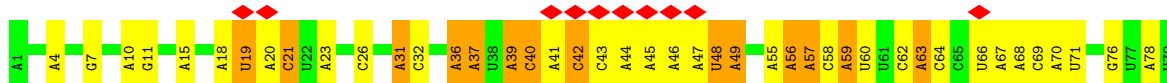
• Molecule 10: Mitochondrial ribosomal protein L35

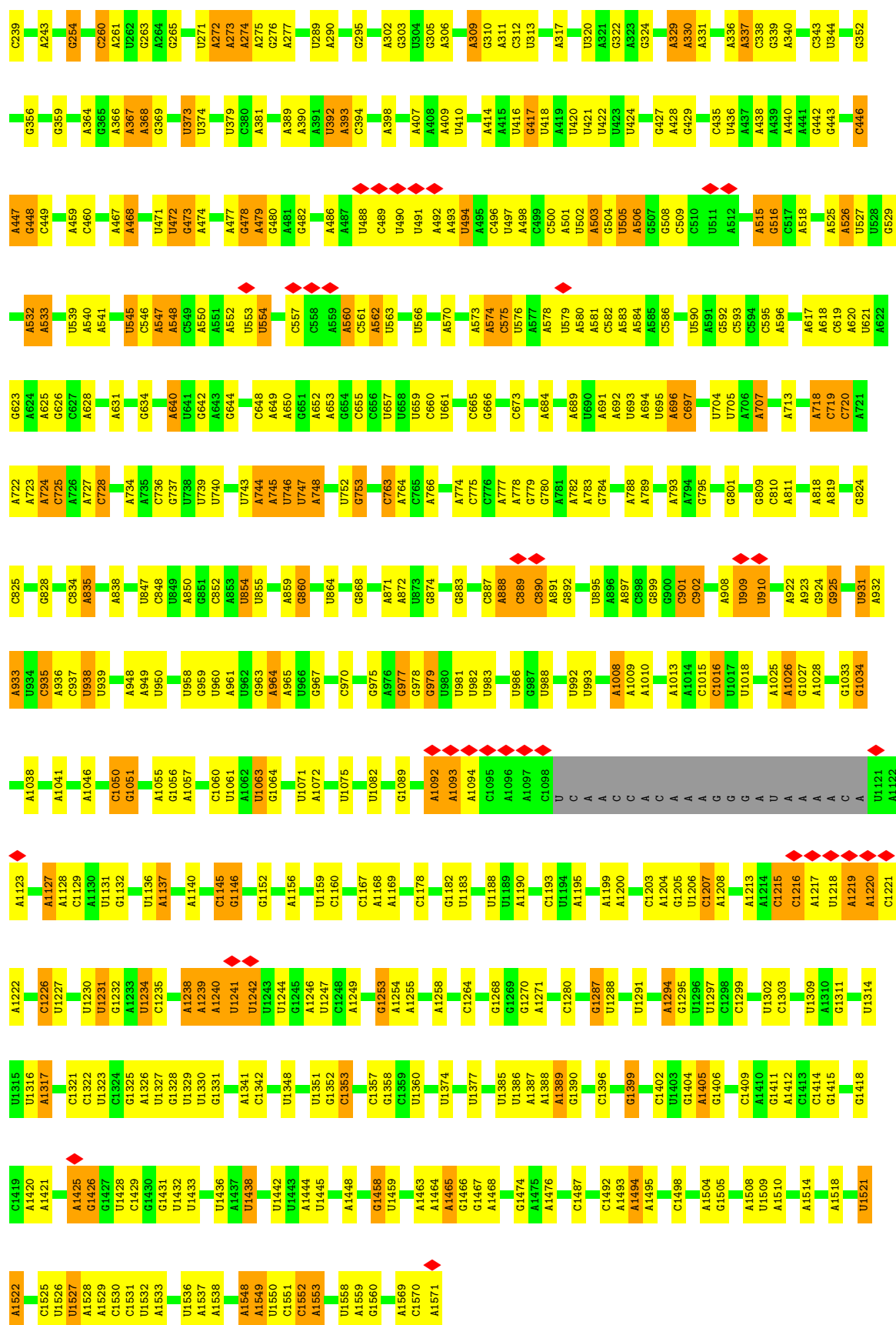


• Molecule 11: Ribosomal protein

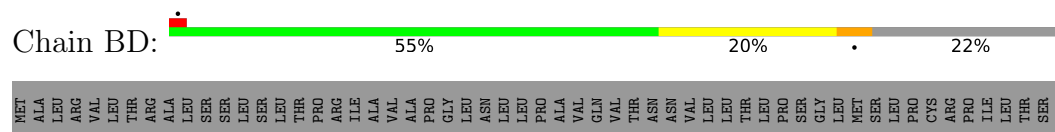


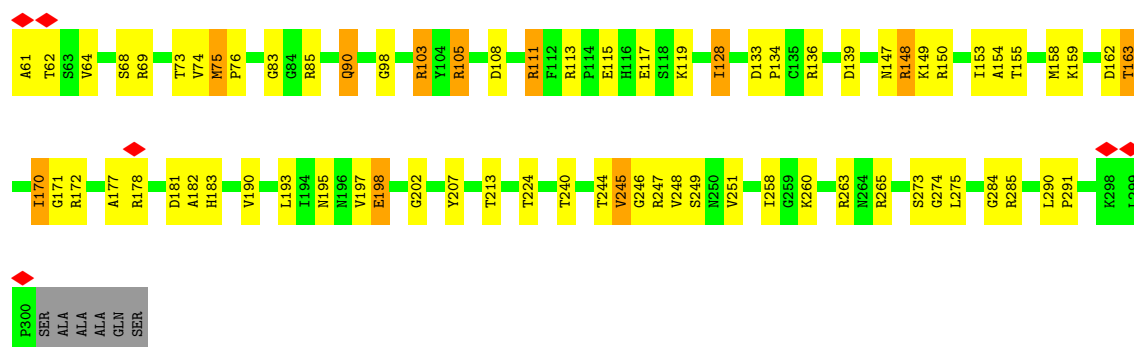
• Molecule 12: 16S ribosomal RNA, mitochondrial



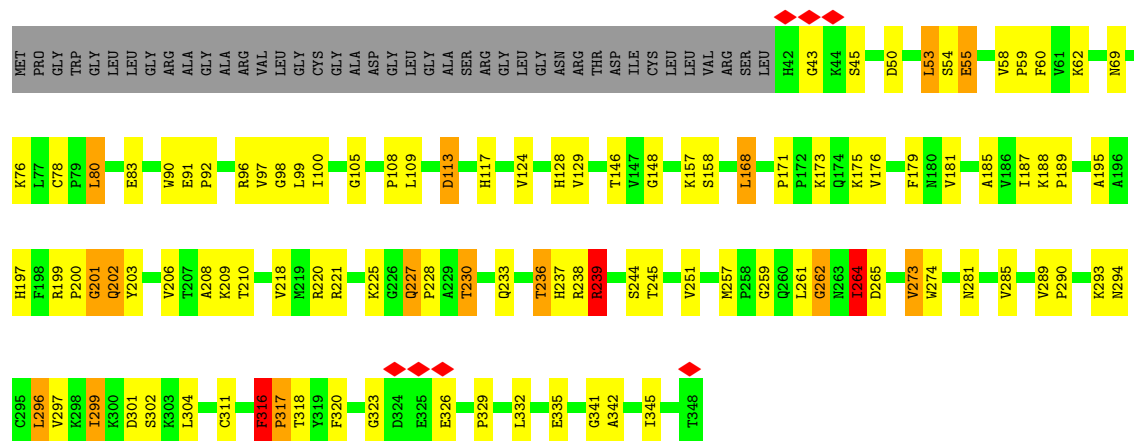


- Molecule 13: tRNA-Phe, mitochondrial

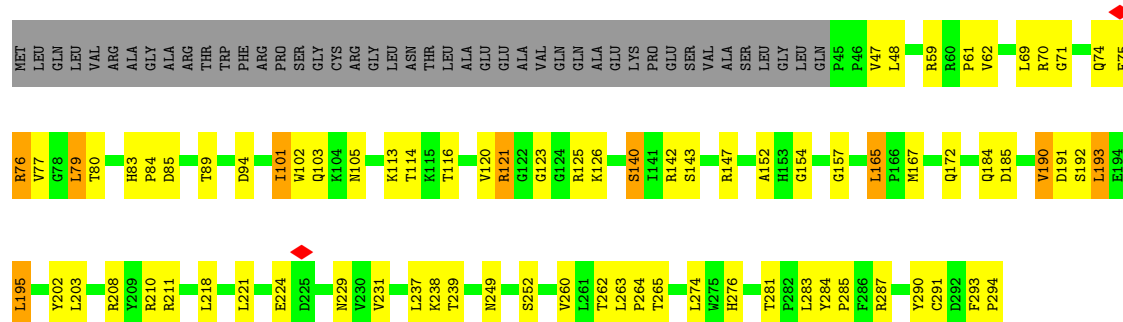




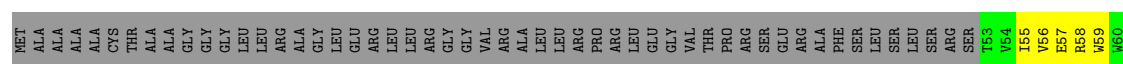
• Molecule 16: ICT1

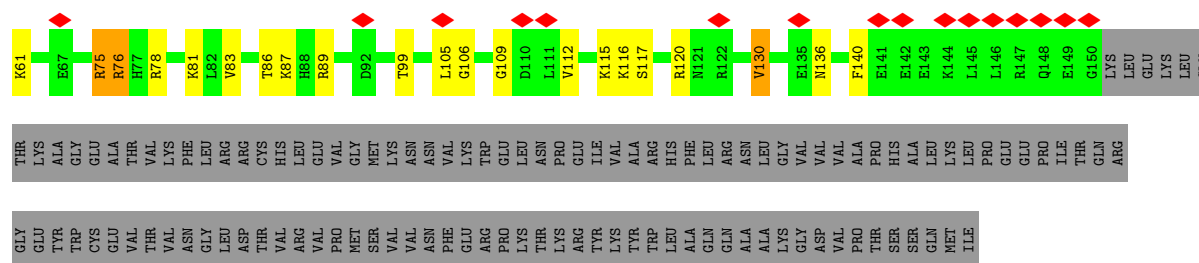


• Molecule 17: Mitochondrial ribosomal protein L4

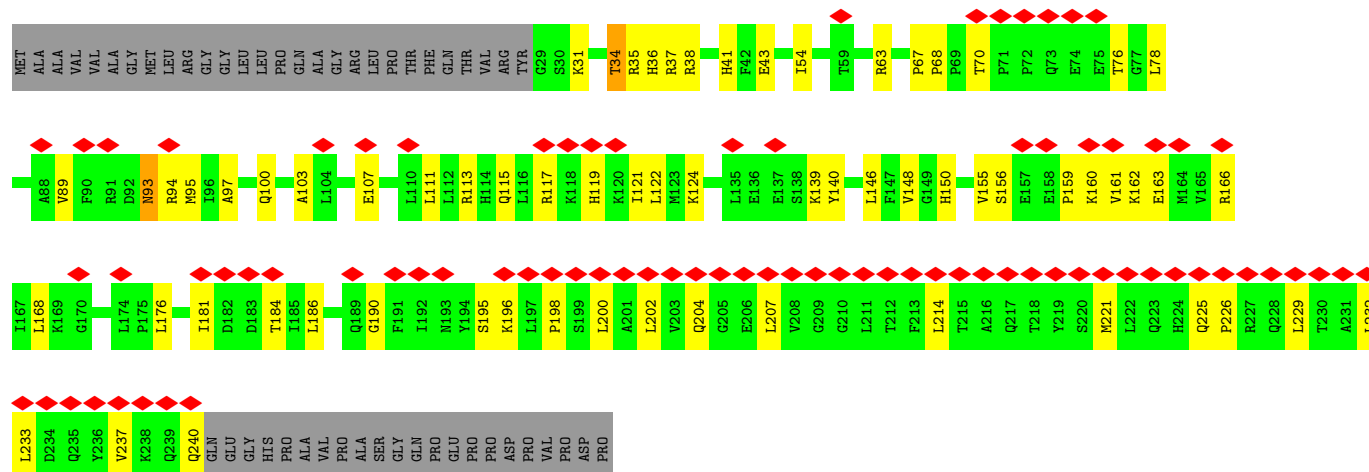


• Molecule 18: Mitochondrial ribosomal protein L9

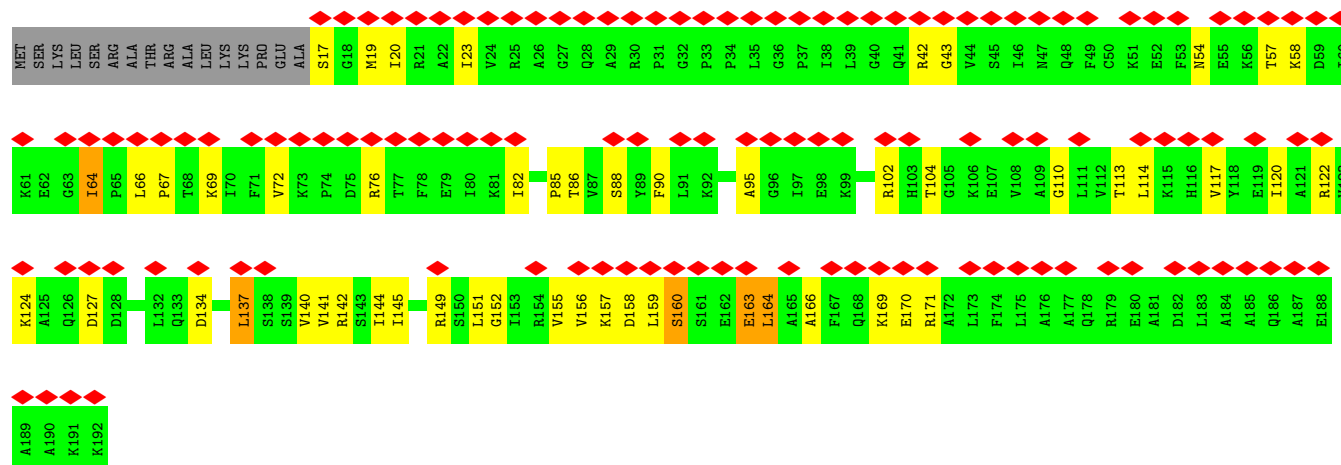




• Molecule 19: Mitochondrial ribosomal protein L10

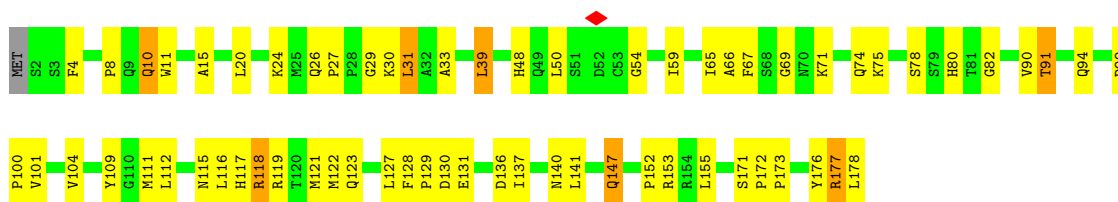


• Molecule 20: Mitochondrial ribosomal protein L11

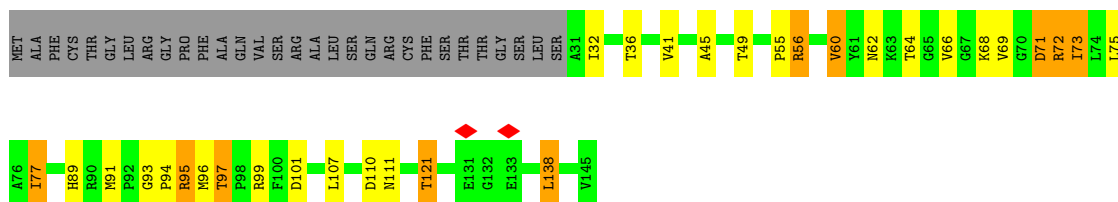


• Molecule 21: 39S ribosomal protein L13, mitochondrial

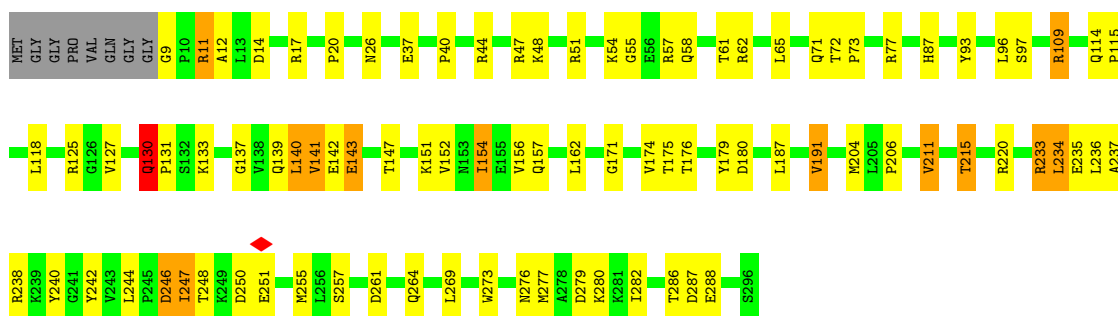




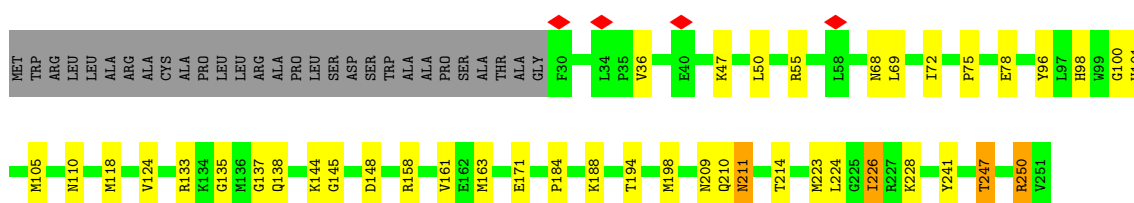
• Molecule 22: uL14m



• Molecule 23: 39S ribosomal protein L15, mitochondrial

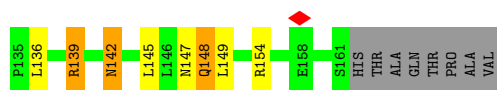


• Molecule 24: 39S ribosomal protein L16, mitochondrial

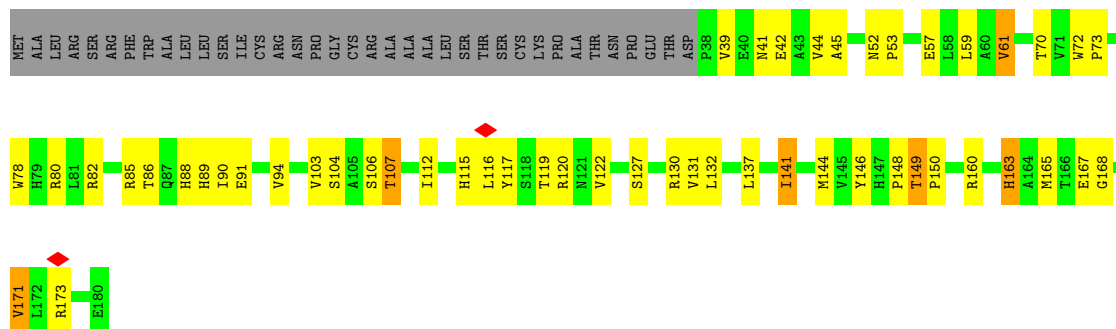


• Molecule 25: 39S ribosomal protein L17, mitochondrial

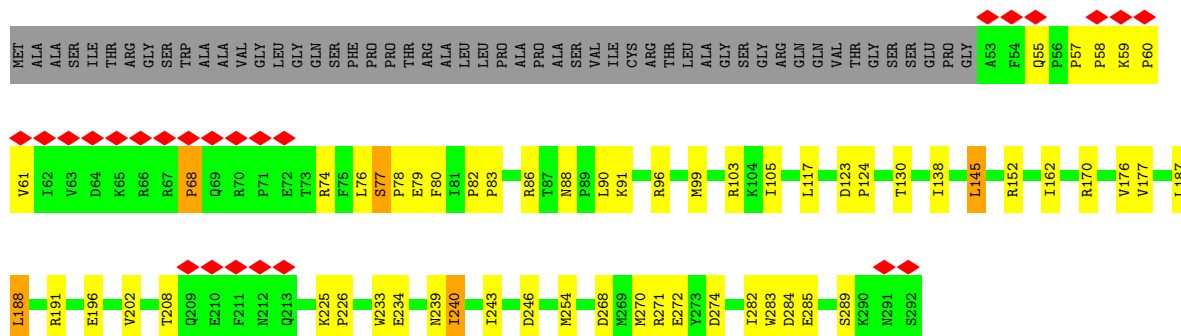




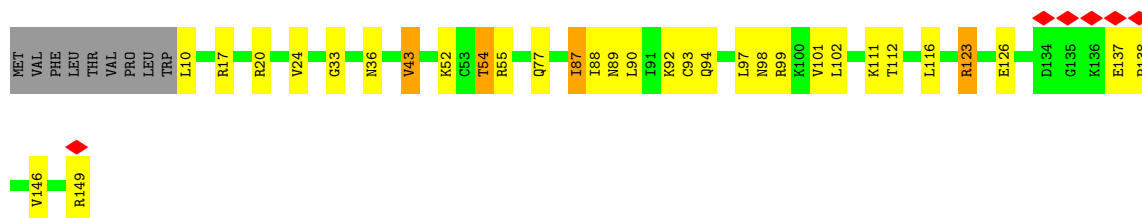
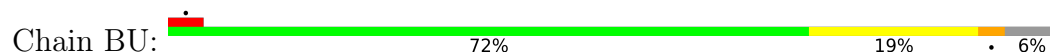
- Molecule 26: Mitochondrial ribosomal protein L18



- Molecule 27: Mitochondrial ribosomal protein L19

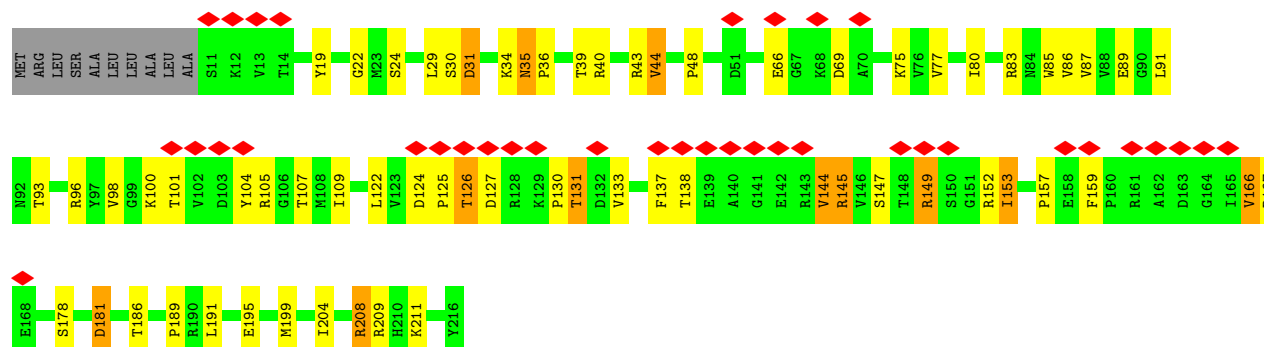
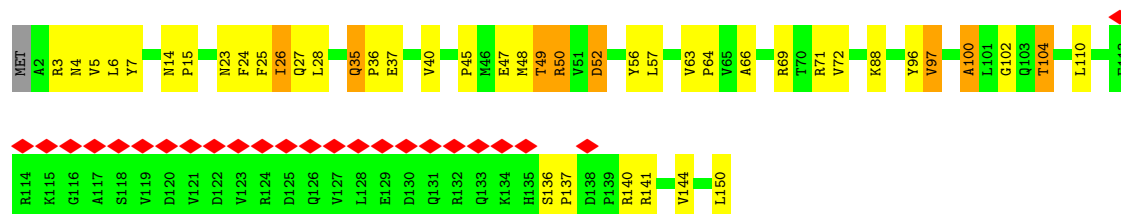
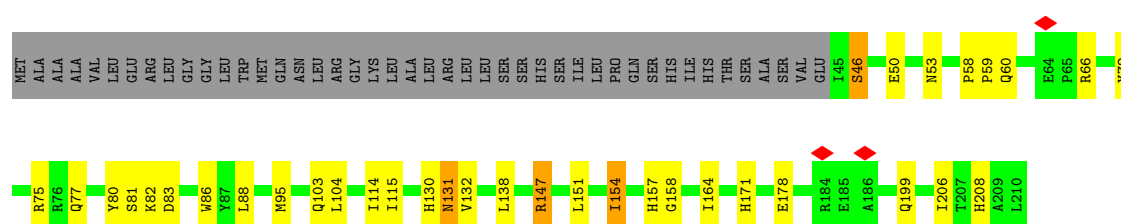
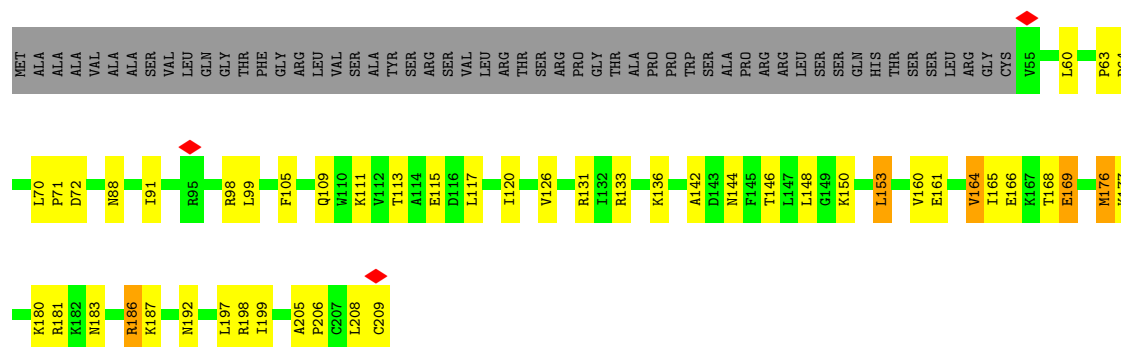


- Molecule 28: Mitochondrial ribosomal protein L20



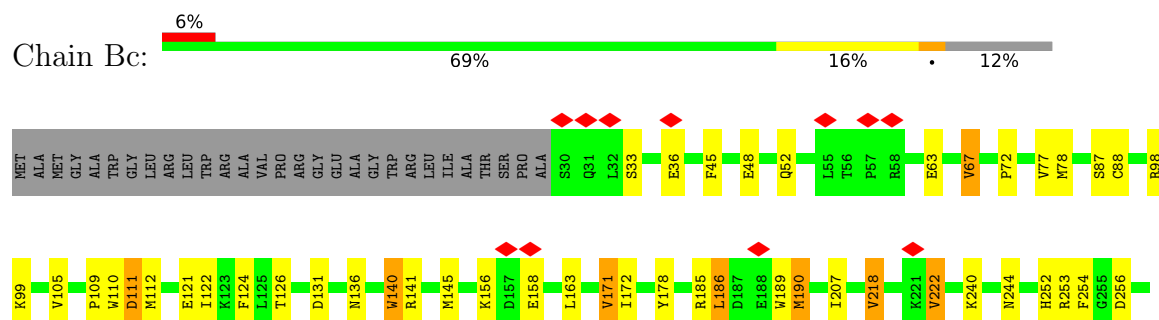
- Molecule 29: Mitochondrial ribosomal protein L21





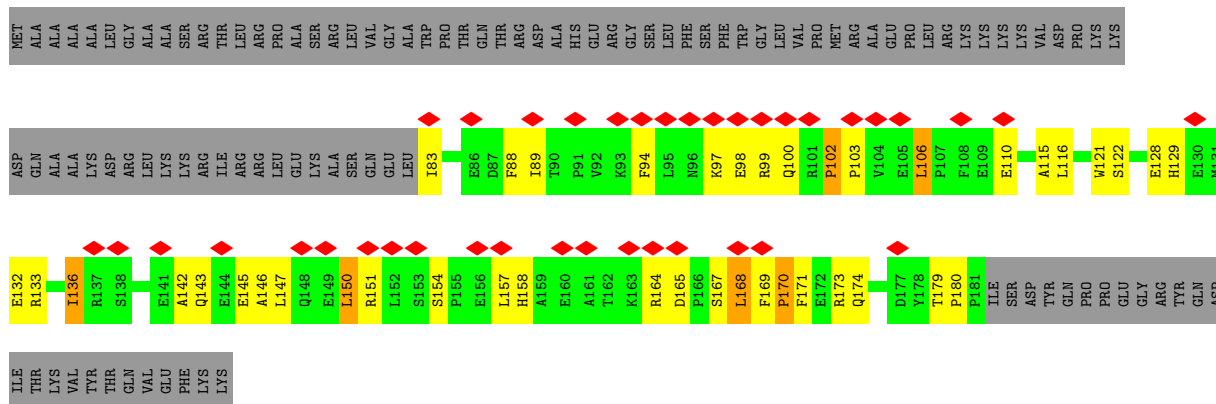
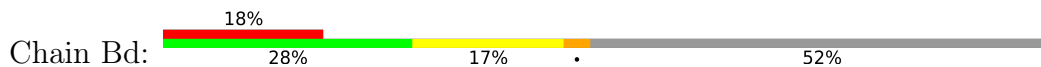
- Molecule 34: Mitochondrial ribosomal protein L38

- Molecule 35: Mitochondrial ribosomal protein L39

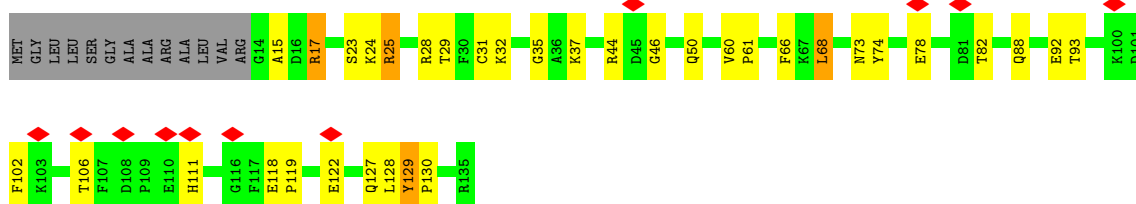




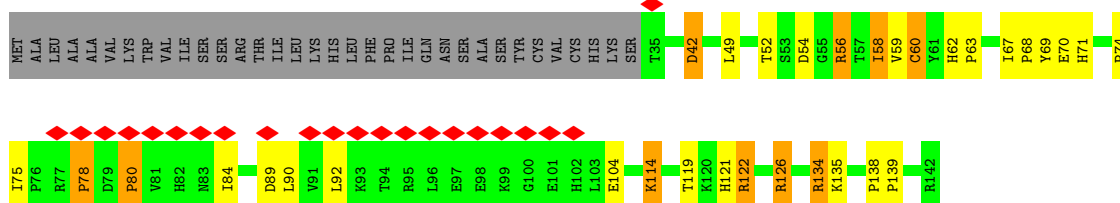
- Molecule 36: 39S ribosomal protein L40, mitochondrial isoform 1



- Molecule 37: Mitochondrial ribosomal protein L41



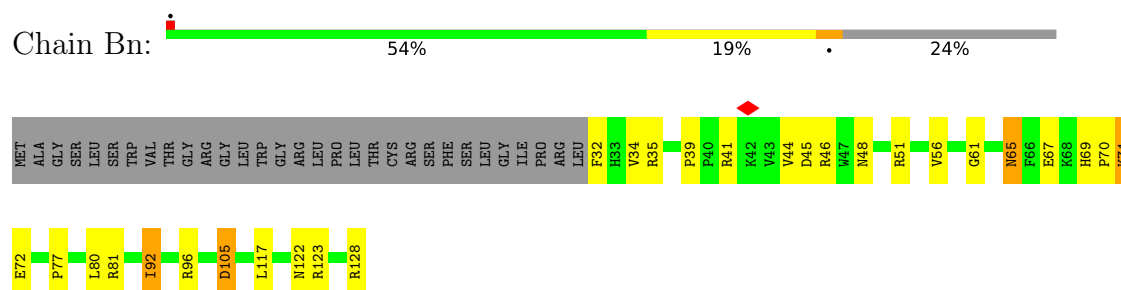
- Molecule 38: mL42



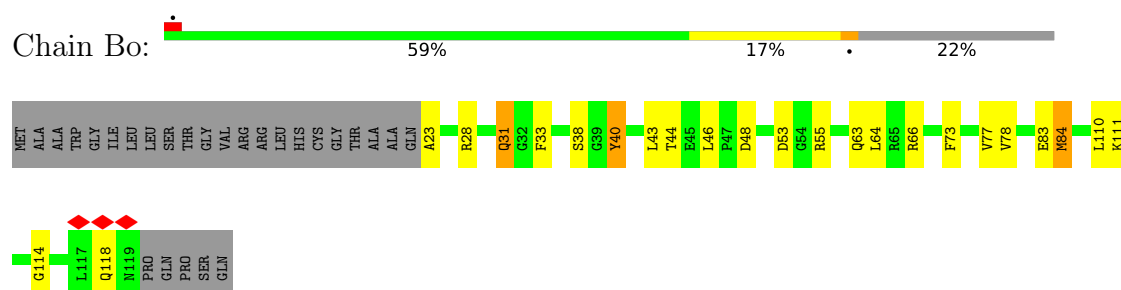
- Molecule 39: mL43



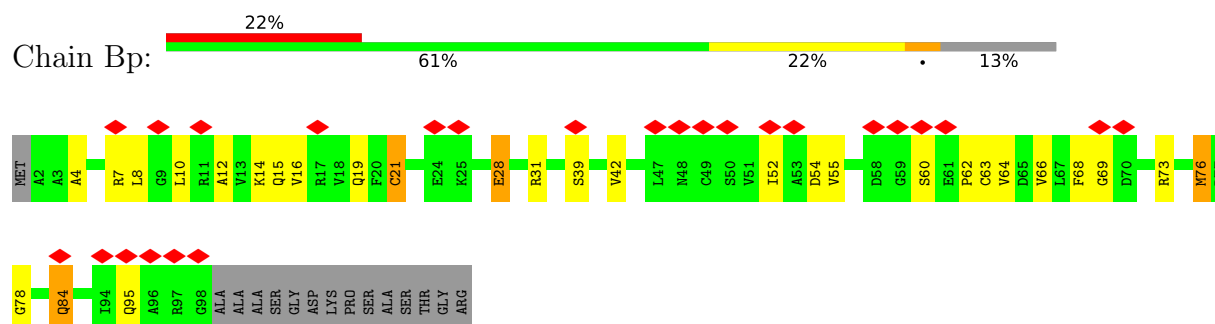
- Molecule 46: Mitochondrial ribosomal protein L51



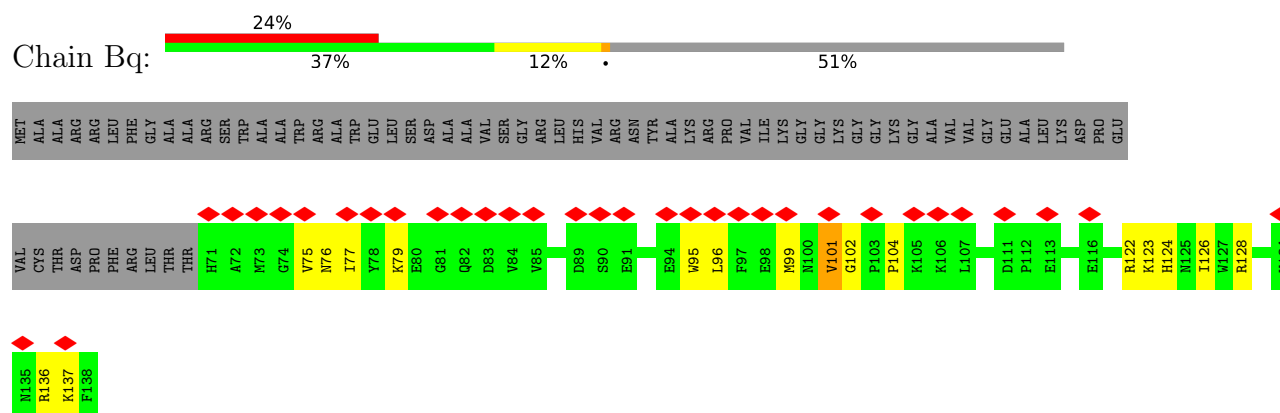
- Molecule 47: 39S ribosomal protein L52, mitochondrial



- Molecule 48: mL53

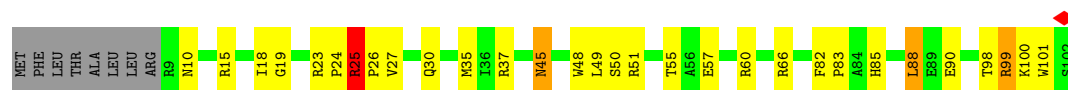


- Molecule 49: mL54

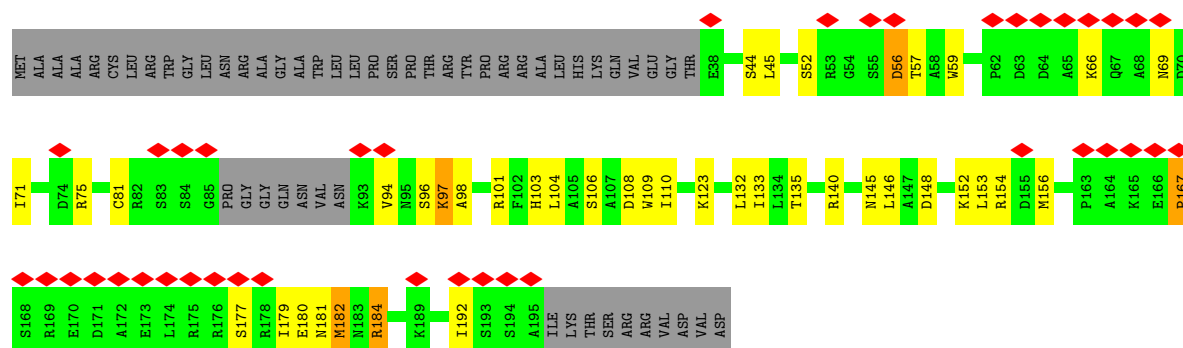


- Molecule 50: Mitochondrial ribosomal protein L57

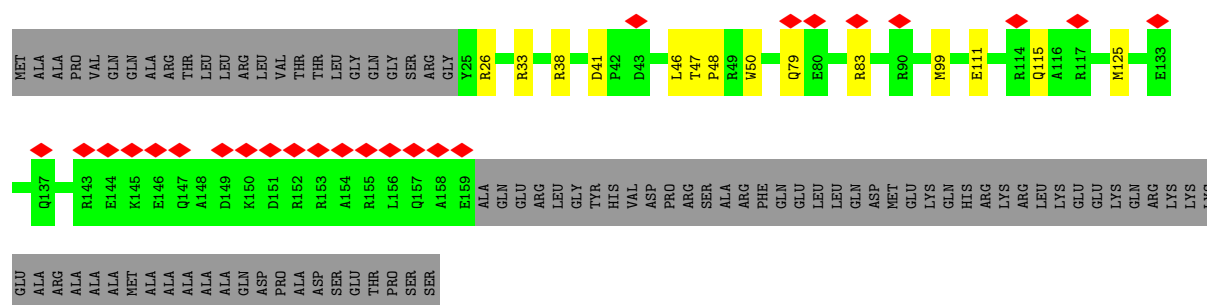




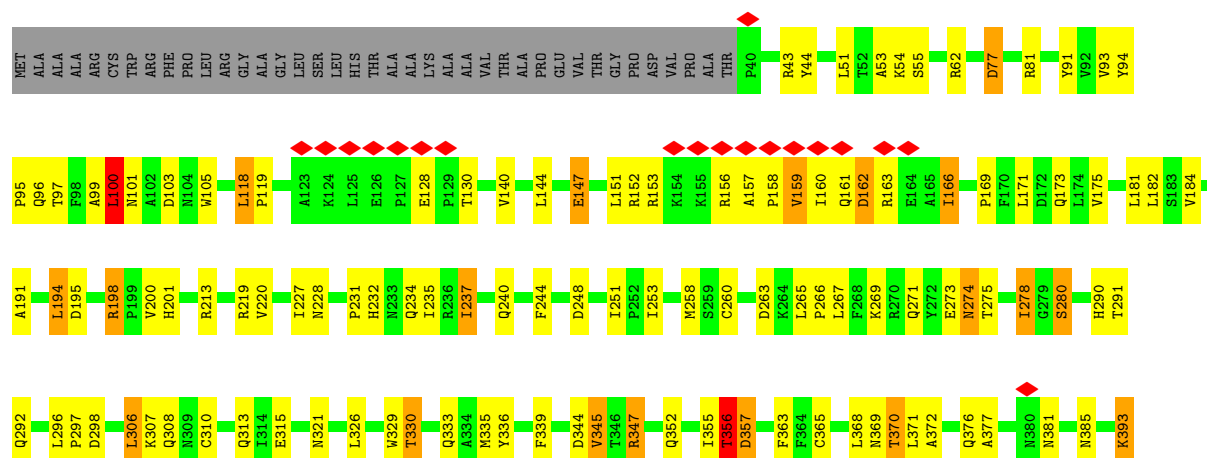
- Molecule 51: Peptidyl-tRNA hydrolase ICT1, mitochondrial



- Molecule 52: mL64

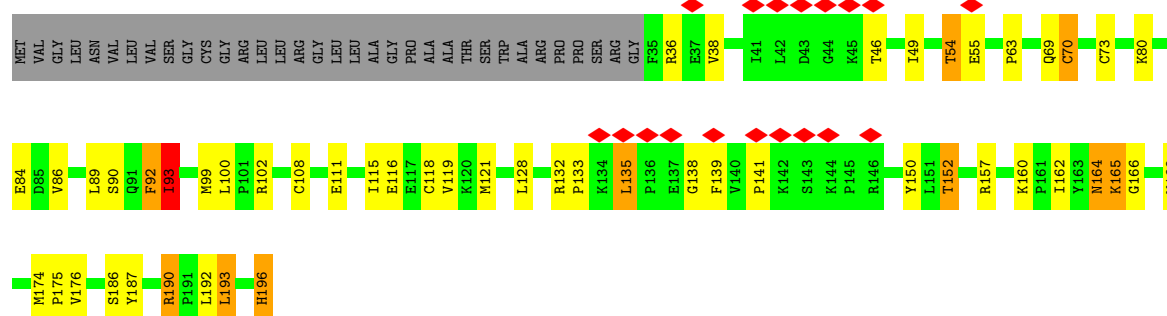


- Molecule 53: mL65

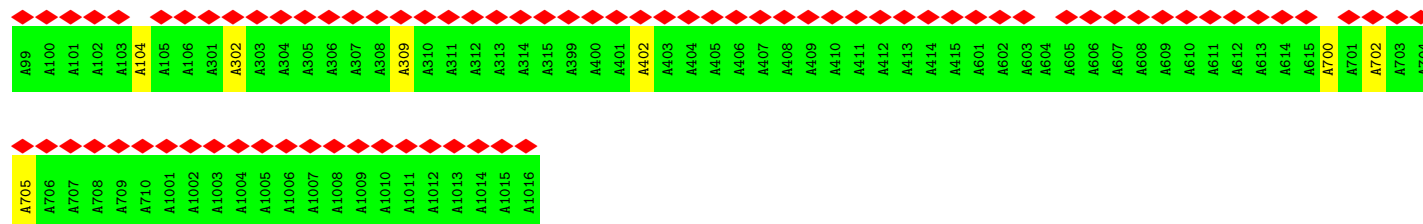
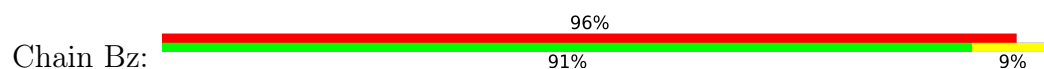




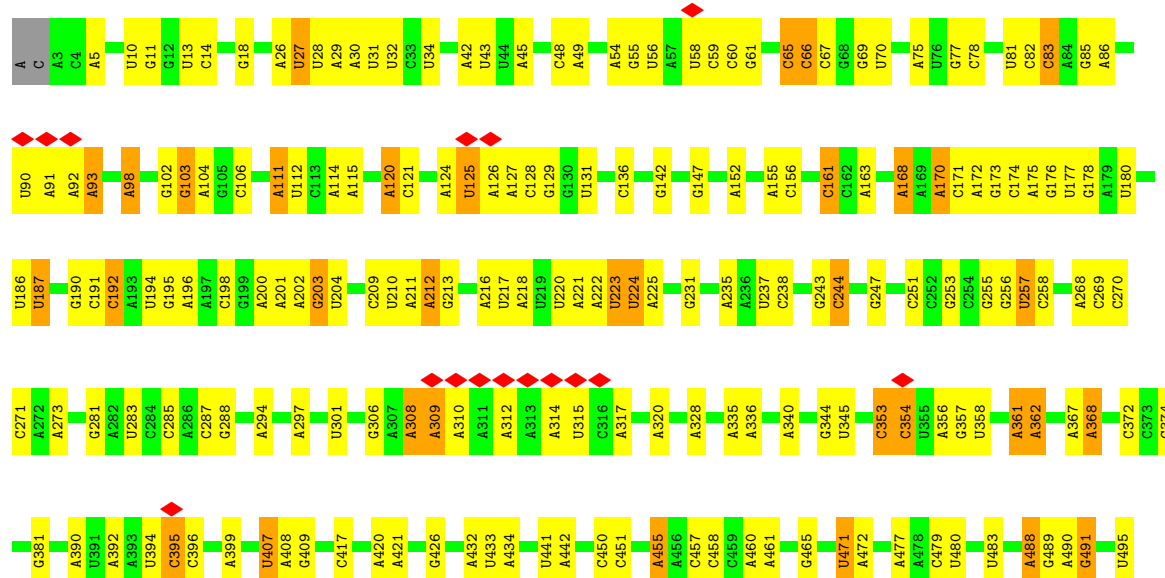
• Molecule 54: Mitochondrial ribosomal protein S18A

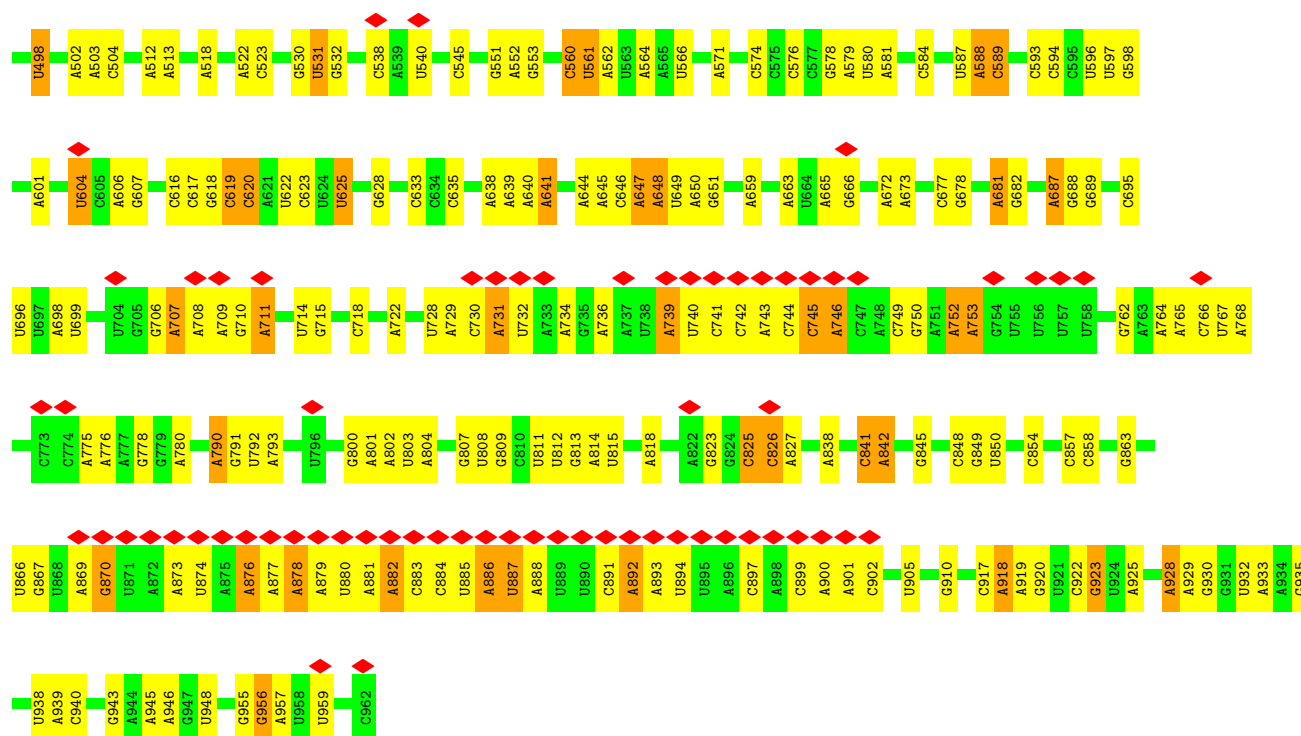


• Molecule 55: unassigned secondary structure elements

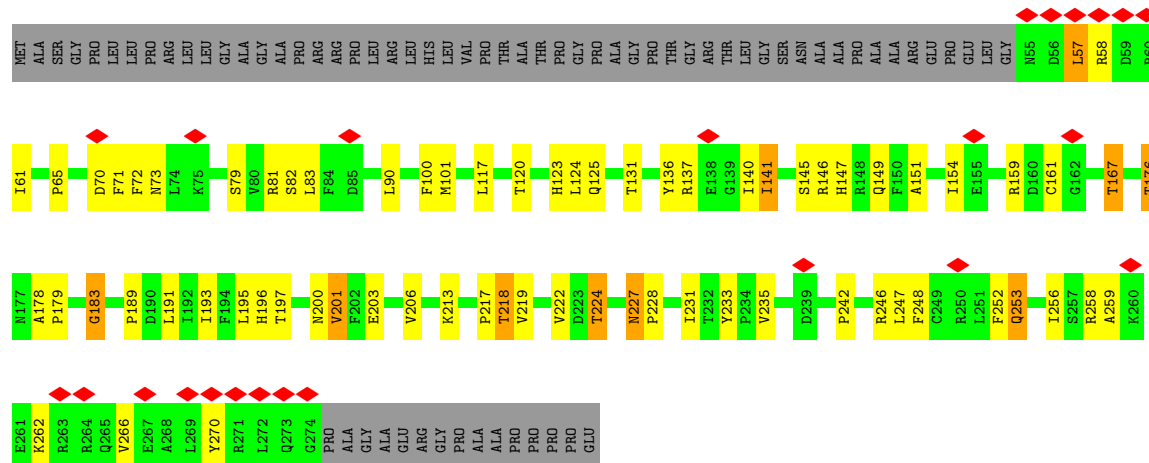


• Molecule 56: 12S ribosomal RNA, mitochondrial

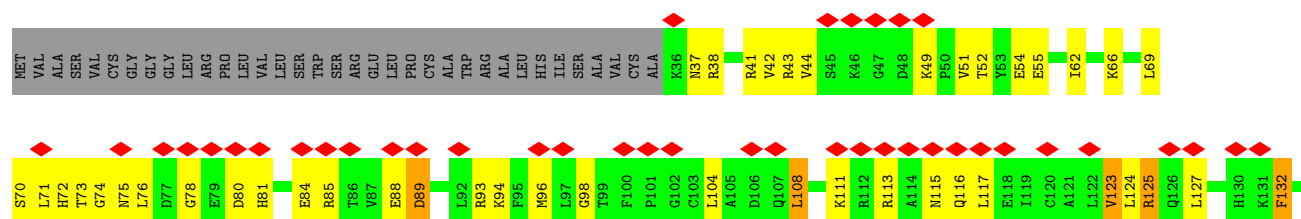


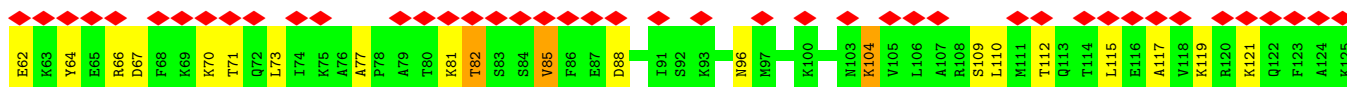


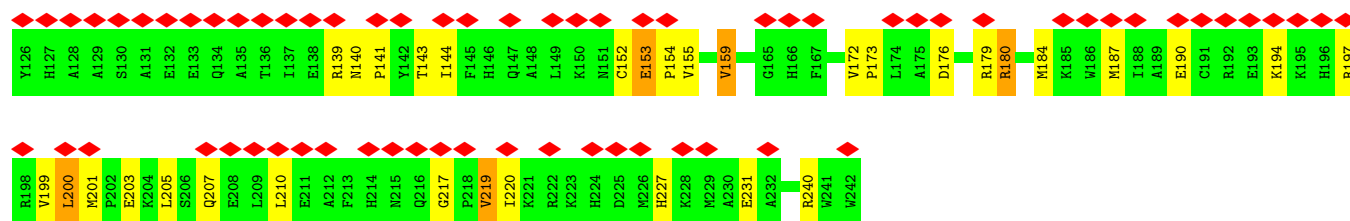
• Molecule 57: Mitochondrial ribosomal protein S2



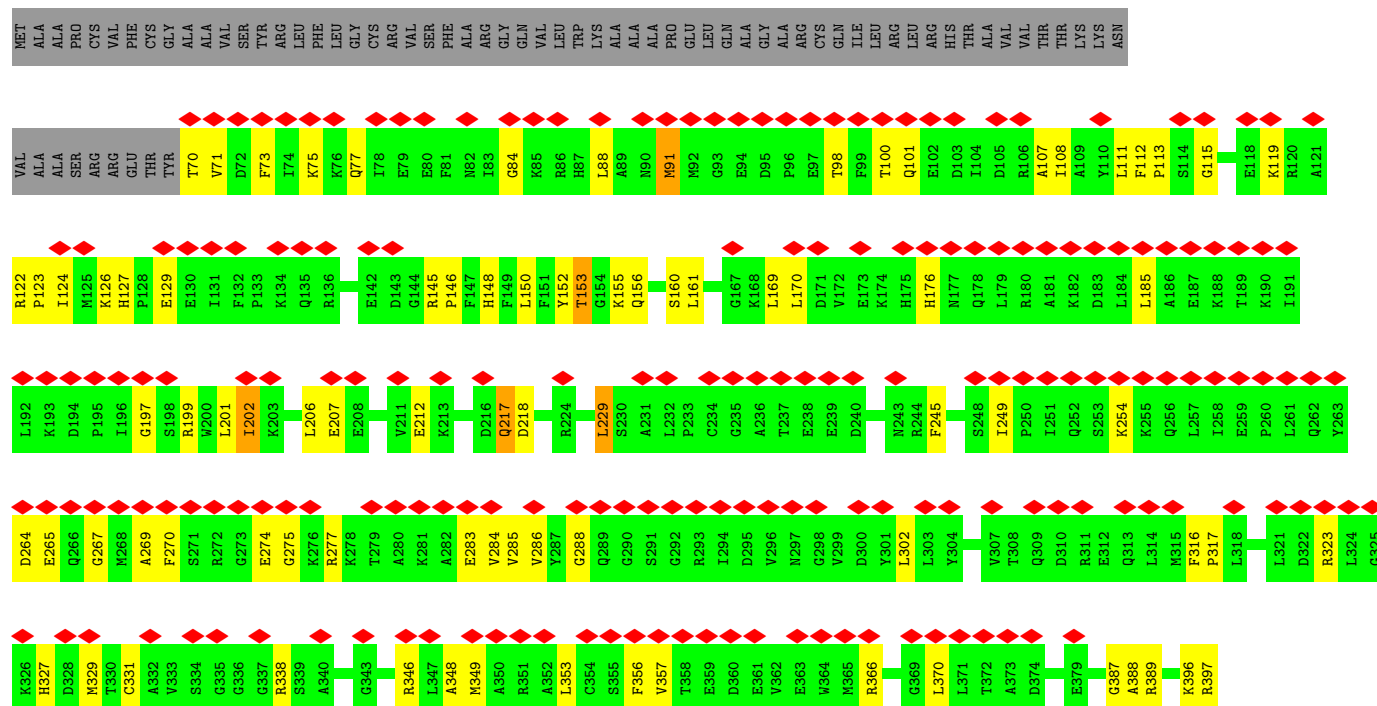
• Molecule 58: Mitochondrial ribosomal protein S24







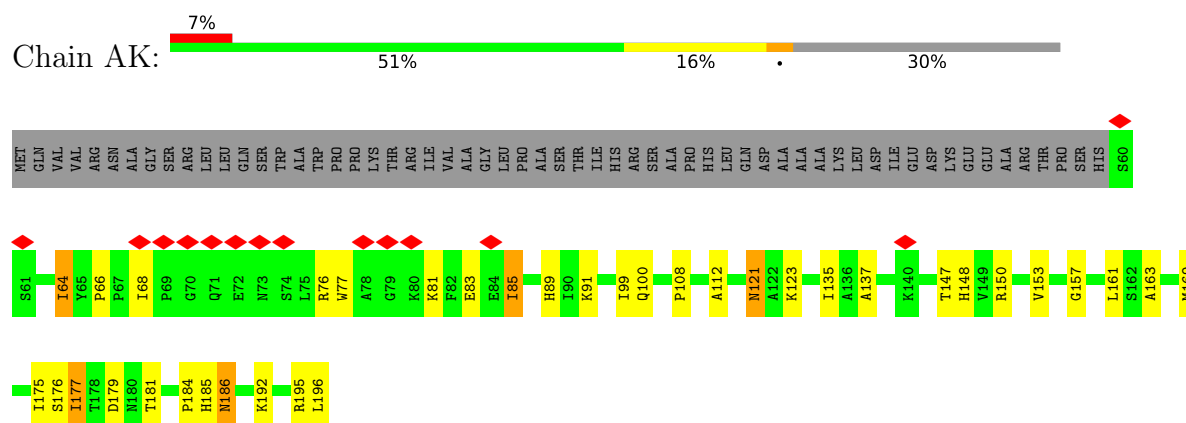
- Molecule 62: 28S ribosomal protein S9, mitochondrial



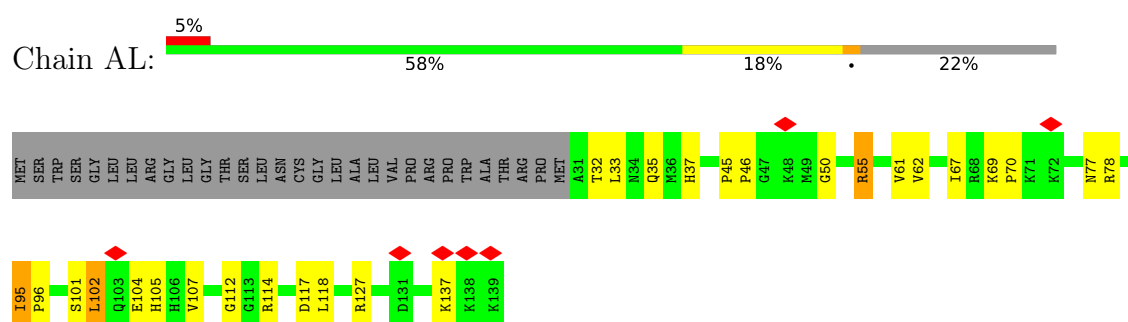
- Molecule 63: Mitochondrial ribosomal protein S10



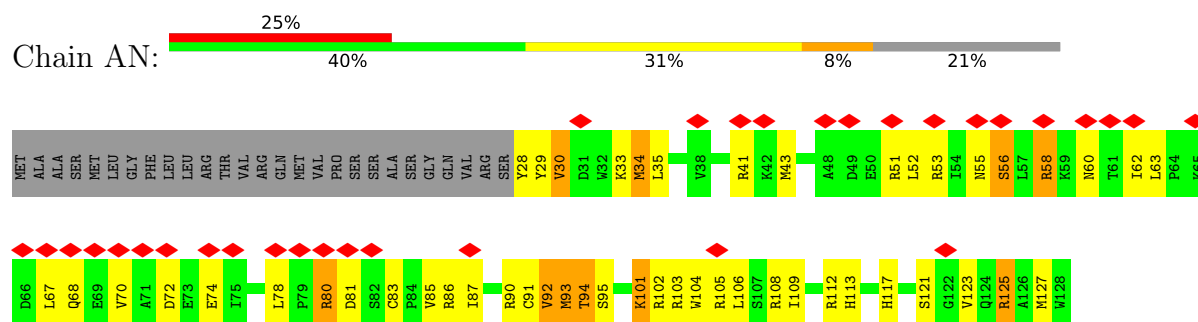
- Molecule 64: 28S ribosomal protein S11, mitochondrial



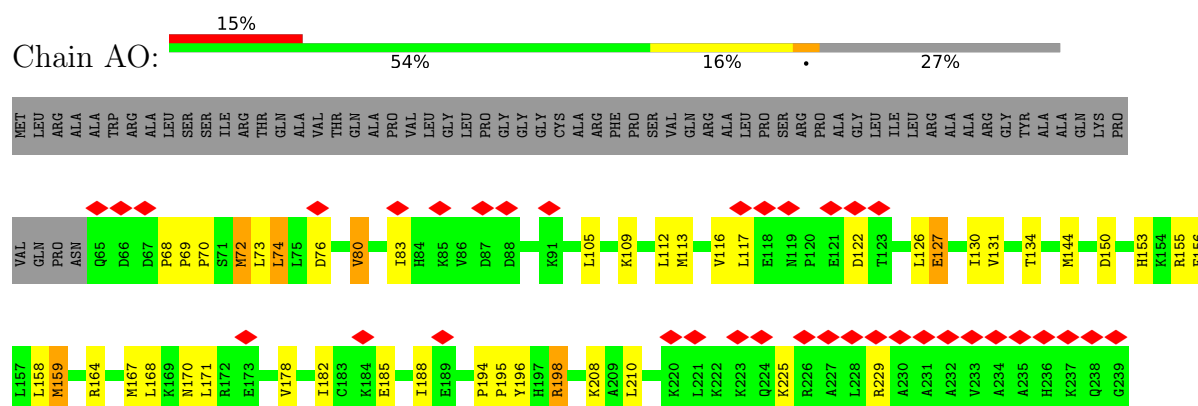
- Molecule 65: Mitochondrial ribosomal protein S12



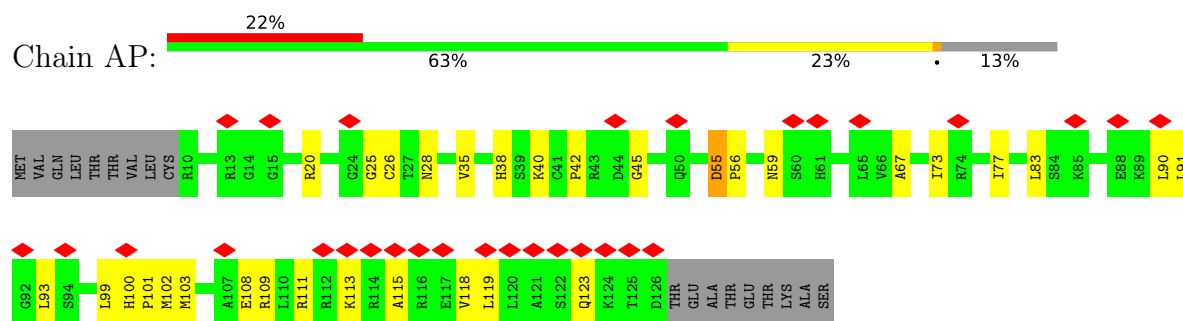
- Molecule 66: Mitochondrial ribosomal protein S14



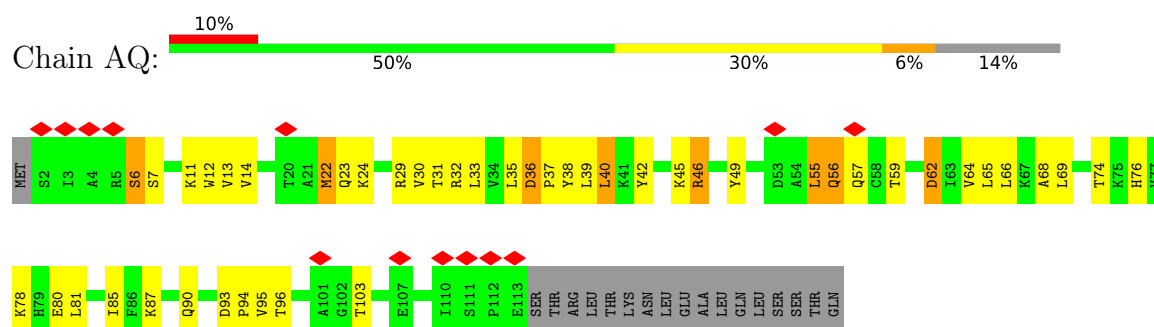
- Molecule 67: Uncharacterized protein



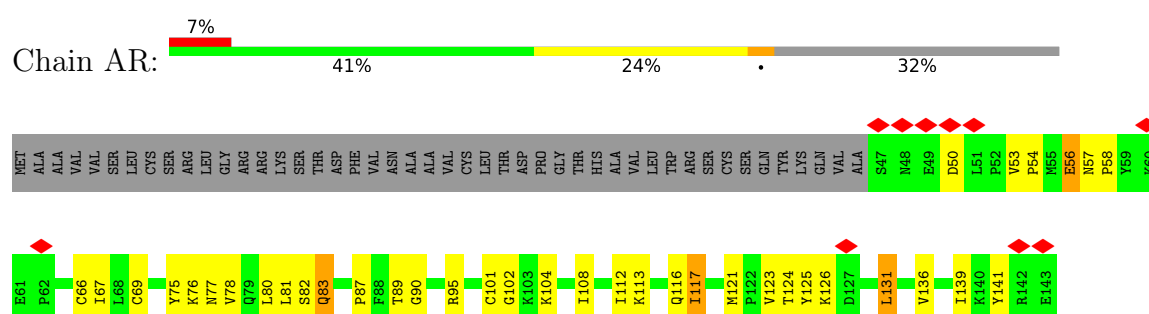
- Molecule 68: bS16m



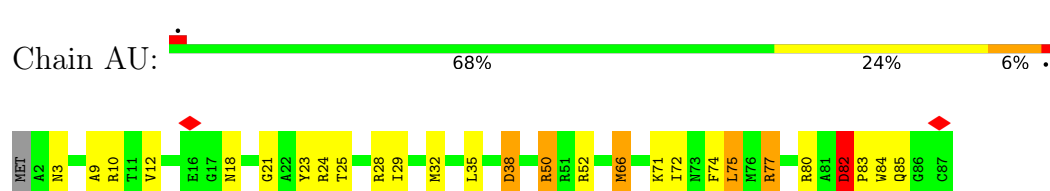
- Molecule 69: uS17m



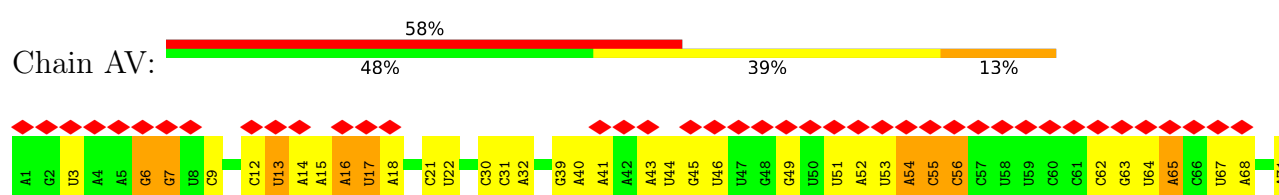
- Molecule 70: Mitochondrial ribosomal protein S18C



- Molecule 71: bS21m

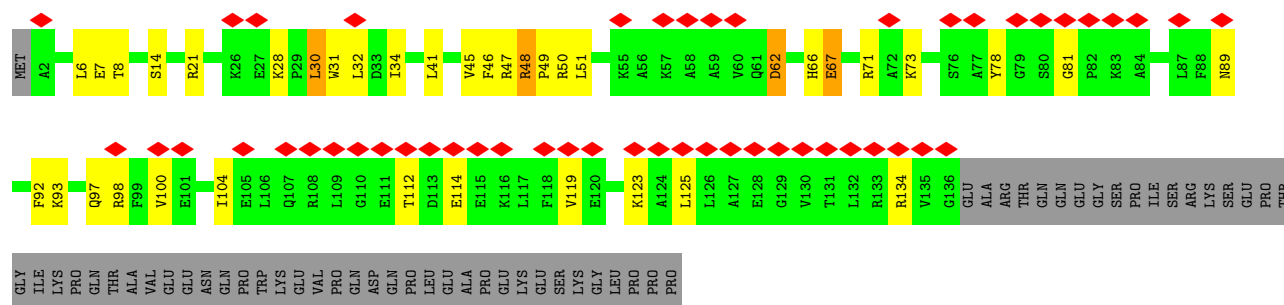


- Molecule 72: P-site fMet-tRNA^{Met}, mitochondrial

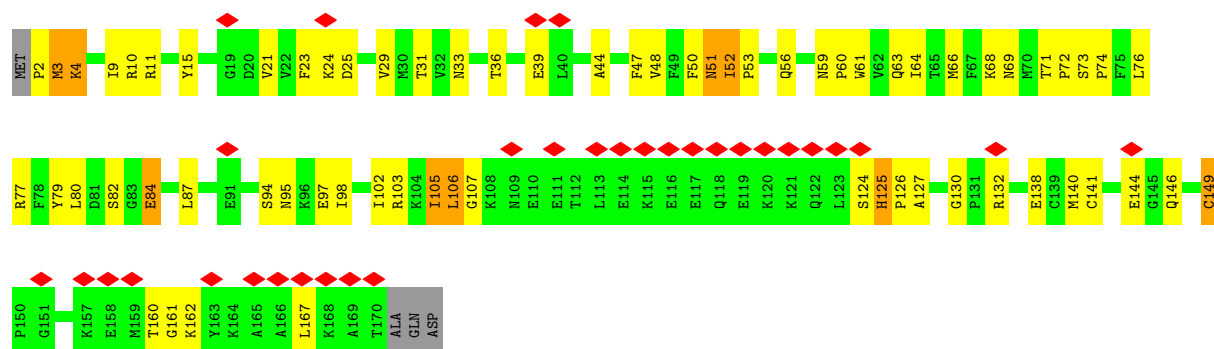


- Molecule 73: MT-CO3 mRNA, mitochondrial

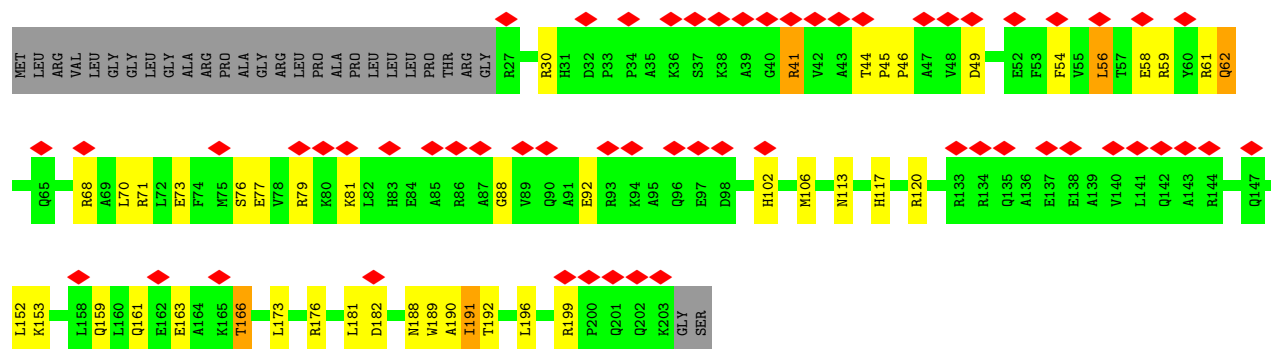




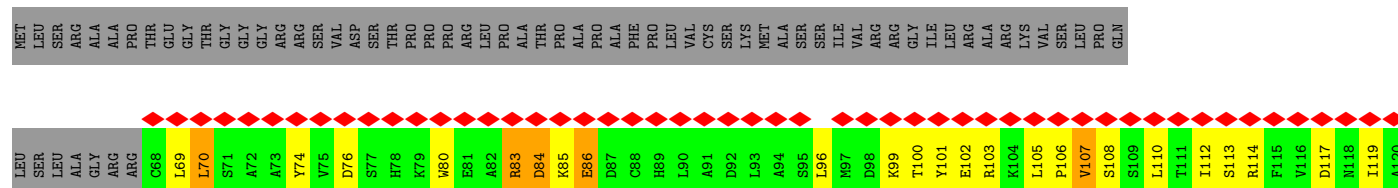
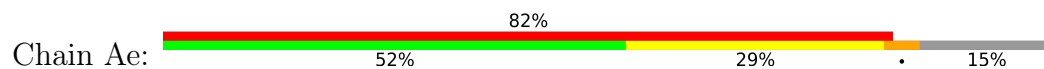
• Molecule 77: Mitochondrial ribosomal protein S25

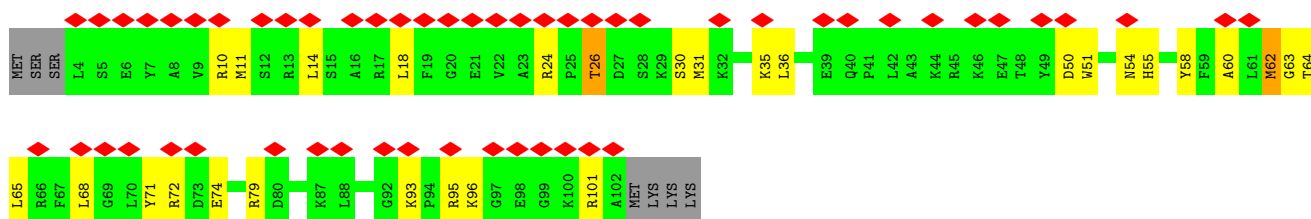


• Molecule 78: Mitochondrial ribosomal protein S26

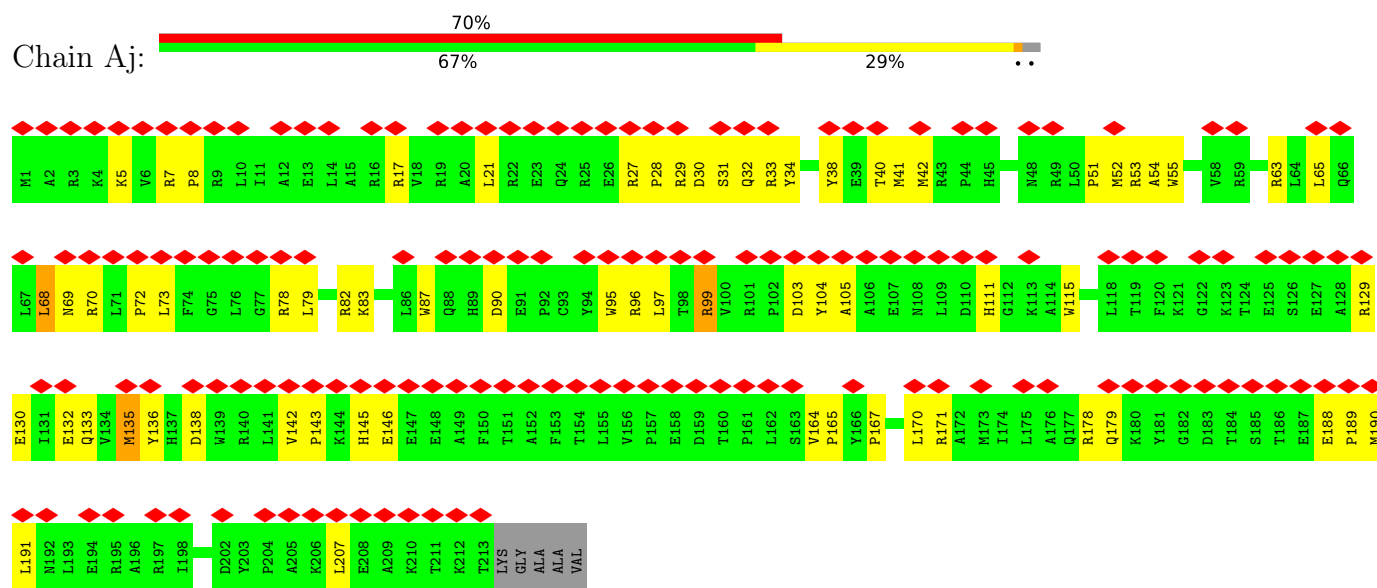


• Molecule 79: mS27

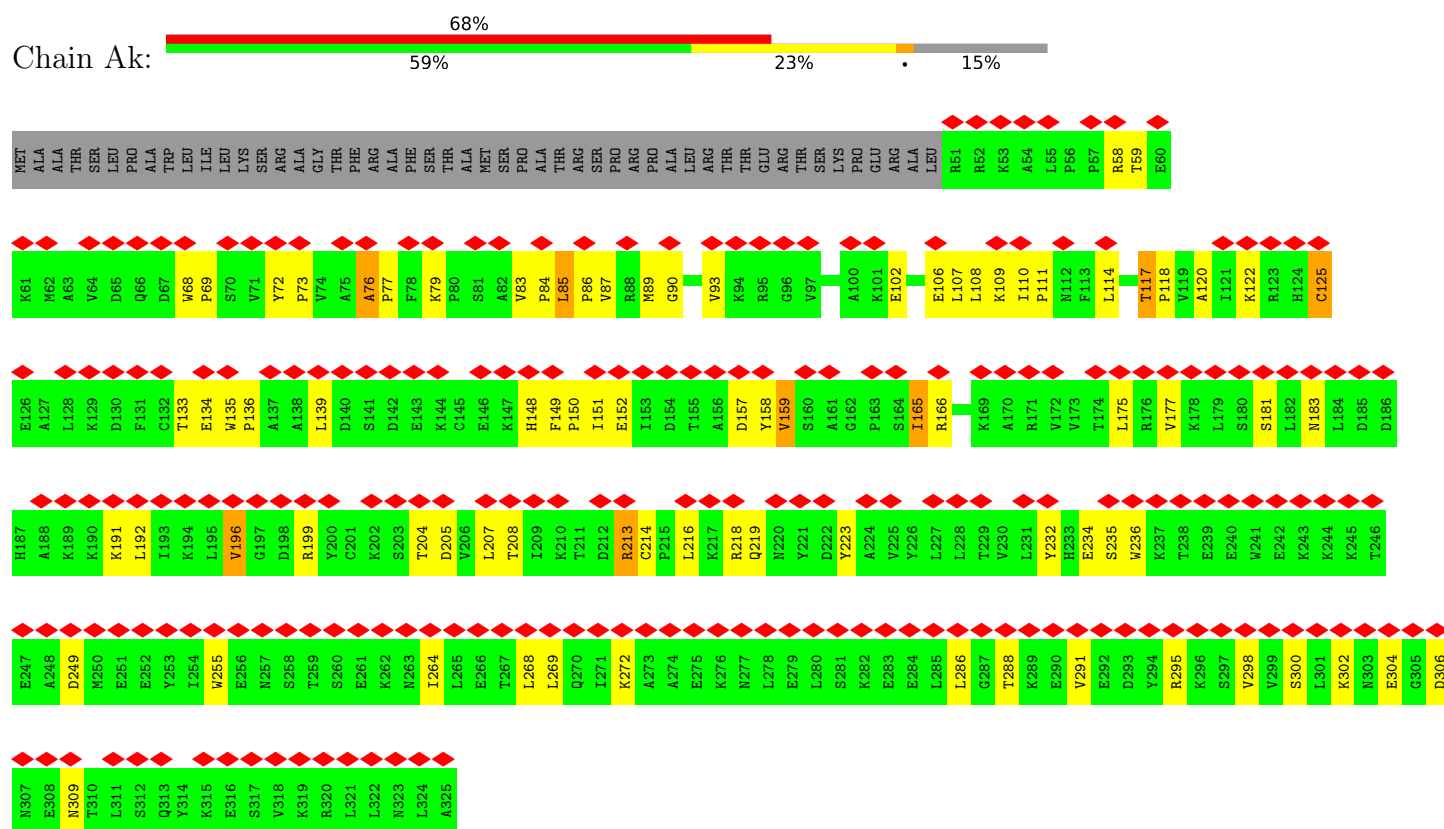




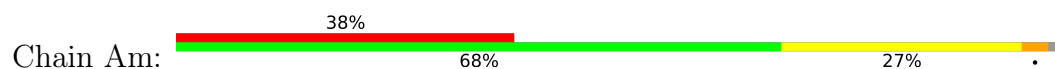
- Molecule 84: 28S ribosomal protein S34, mitochondrial

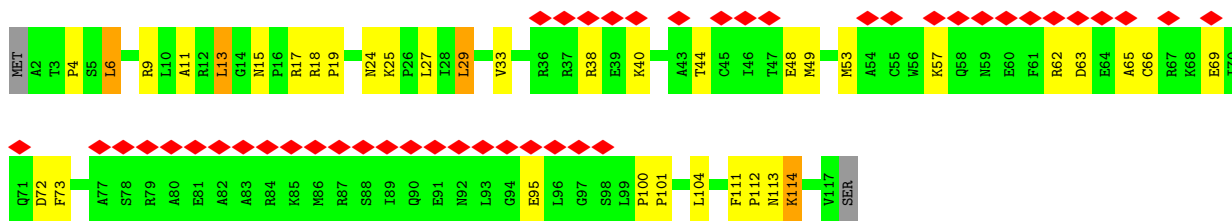


- Molecule 85: 28S ribosomal protein S35, mitochondrial



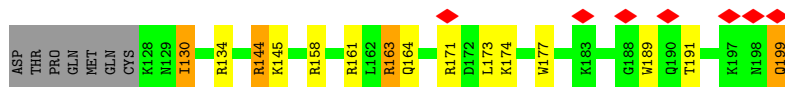
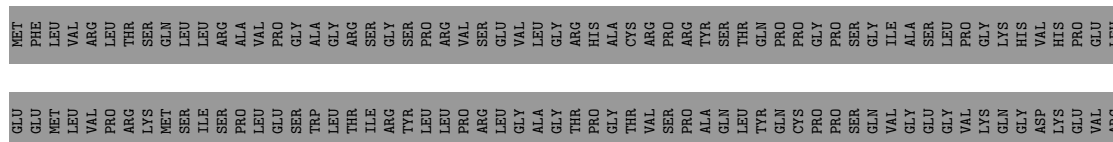
- Molecule 86: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1





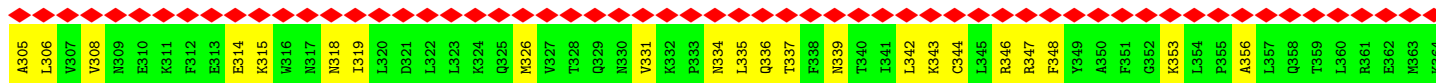
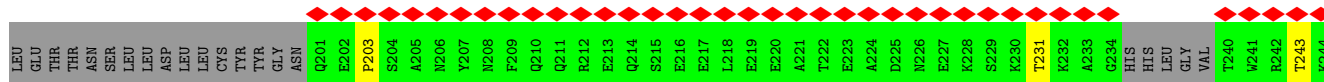
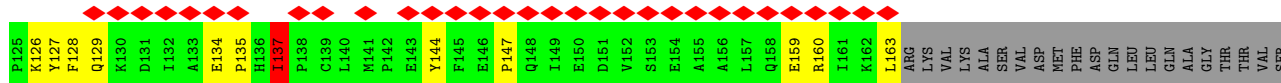
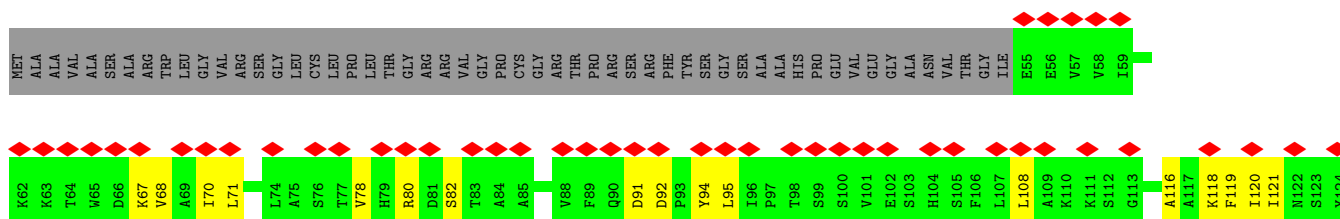
- Molecule 87: Aurora kinase A interacting protein 1

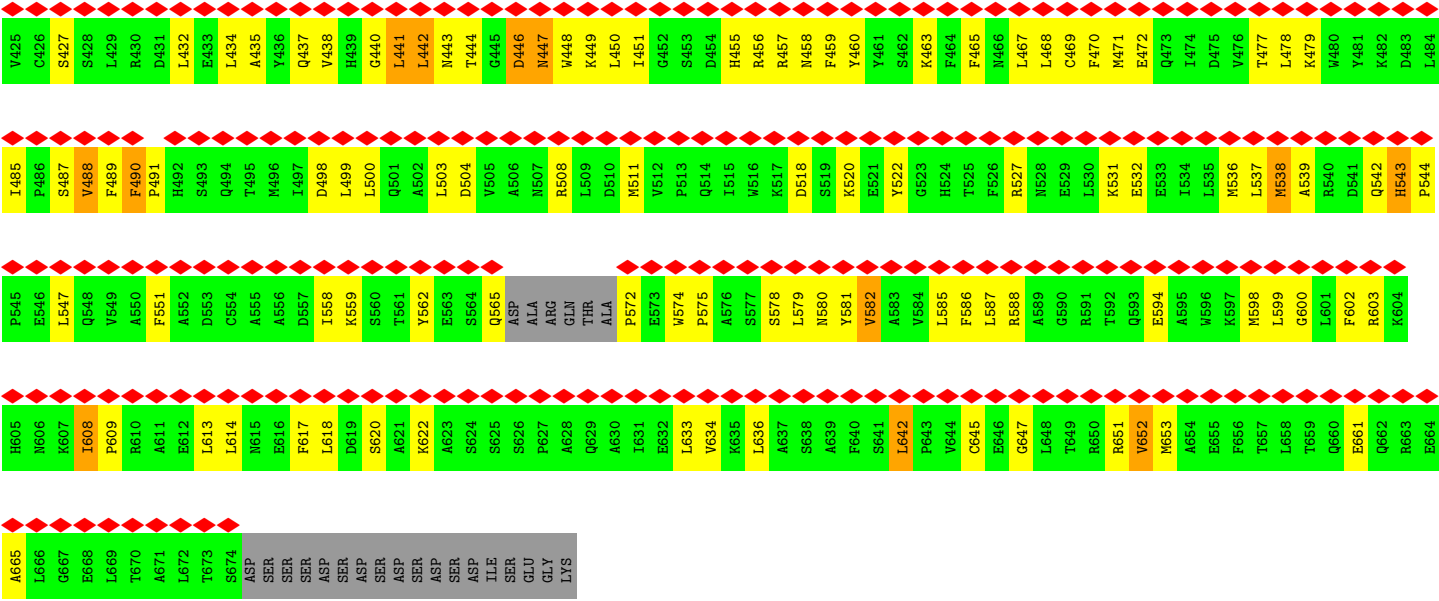
Chain An: 29% 6% 64%



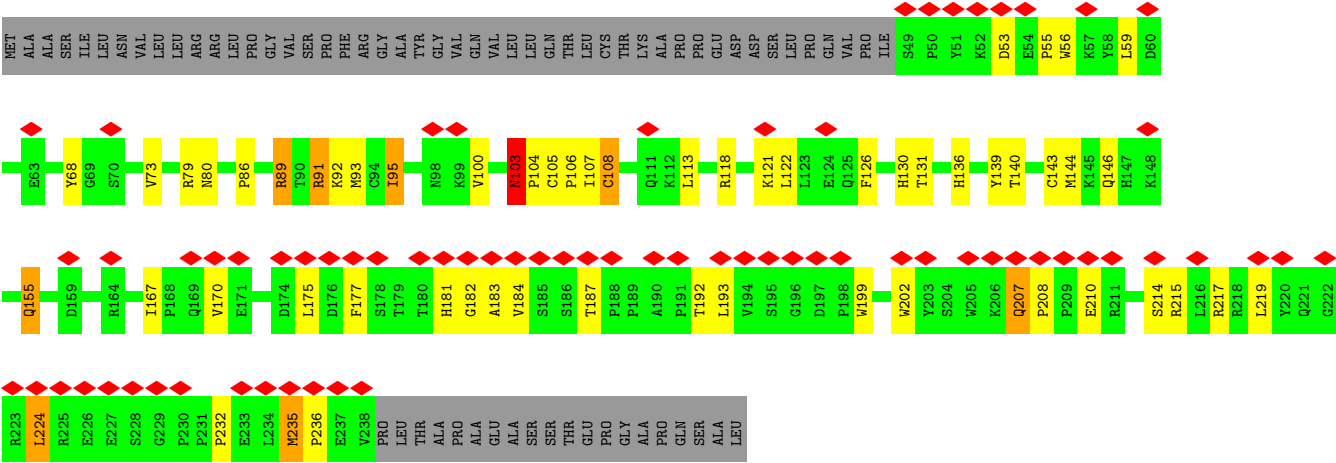
- Molecule 88: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain Ao: 53% 28% 17%





• Molecule 89: 28S ribosomal protein S18b, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	139206	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.453	Depositor
Minimum map value	-0.743	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	390.59, 390.59, 390.59	wwPDB
Map dimensions	281, 281, 281	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, GSP, GTP, MG, SPM, NA, ZN, 5GP

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	BL	0.52	0/542	0.81	0/729
1	CL	0.58	0/319	1.10	4/435 (0.9%)
1	DL	0.47	0/212	0.62	0/286
1	EL	0.56	0/221	0.67	0/297
1	FL	0.56	0/212	0.64	0/286
1	GL	0.59	0/212	0.62	0/286
1	HL	0.57	0/204	0.65	0/275
2	B0	0.63	0/880	0.88	1/1189 (0.1%)
3	B1	0.43	0/2093	0.82	0/2835
4	B2	0.51	0/1586	0.82	0/2123
5	B3	0.56	0/993	0.95	2/1341 (0.1%)
6	B4	0.32	0/388	0.96	2/523 (0.4%)
7	B5	0.52	0/917	0.90	4/1227 (0.3%)
8	B6	0.34	0/430	0.89	2/570 (0.4%)
9	B7	0.74	0/395	0.85	0/524
10	B8	0.62	0/853	0.89	0/1136
11	B9	0.53	0/342	0.78	0/450
12	BA	0.39	0/36903	0.44	0/57455
13	BB	0.19	0/1595	0.30	0/2475
14	BC	0.41	0/4432	0.81	4/5989 (0.1%)
15	BD	0.57	0/1898	0.94	5/2555 (0.2%)
16	BE	0.59	0/2493	1.02	14/3387 (0.4%)
17	BF	0.63	0/2069	0.93	5/2816 (0.2%)
18	BI	0.42	0/819	0.86	1/1101 (0.1%)
19	BJ	0.44	0/1742	0.83	2/2358 (0.1%)
20	BK	0.42	0/1323	0.85	1/1785 (0.1%)
21	BN	0.59	0/1487	0.88	5/2017 (0.2%)
22	BO	0.55	0/912	0.89	0/1231
23	BP	0.57	0/2368	0.92	5/3198 (0.2%)
24	BQ	0.50	0/1850	0.84	3/2491 (0.1%)
25	BR	0.59	0/1262	0.83	0/1700
26	BS	0.47	0/1197	0.89	0/1624

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	BT	0.53	0/2002	0.93	7/2708 (0.3%)
28	BU	0.68	0/1179	0.86	0/1578
29	BV	0.60	0/1256	0.96	2/1706 (0.1%)
30	BW	0.60	0/1407	0.88	3/1891 (0.2%)
31	BX	0.53	0/1211	0.94	2/1646 (0.1%)
32	BY	0.38	0/1719	0.90	4/2329 (0.2%)
33	Ba	0.48	0/3267	0.87	1/4455 (0.0%)
34	Bb	0.45	0/3047	0.91	5/4139 (0.1%)
35	Bc	0.41	0/2464	0.85	6/3330 (0.2%)
36	Bd	0.42	0/853	0.94	5/1153 (0.4%)
37	Be	0.47	0/1000	0.97	4/1345 (0.3%)
38	Bf	0.48	0/851	0.92	3/1159 (0.3%)
39	Bg	0.57	0/1191	0.95	4/1614 (0.2%)
40	Bh	0.47	0/2372	0.92	8/3211 (0.2%)
41	Bi	0.41	0/2199	0.89	7/2980 (0.2%)
42	Bj	0.37	0/1811	0.82	0/2436
43	Bk	0.37	0/1108	0.83	0/1499
44	Bl	0.51	0/1135	0.86	0/1549
45	Bm	0.38	0/917	0.78	1/1248 (0.1%)
46	Bn	0.66	0/860	0.91	1/1150 (0.1%)
47	Bo	0.47	0/787	0.84	3/1056 (0.3%)
48	Bp	0.40	0/752	0.86	2/1013 (0.2%)
49	Bq	0.42	0/558	0.83	1/756 (0.1%)
50	Bt	0.60	0/798	1.08	4/1073 (0.4%)
51	Bu	0.36	0/1214	0.78	1/1630 (0.1%)
52	Bv	0.37	0/1157	0.72	0/1560
53	Bw	0.55	0/3206	0.92	7/4354 (0.2%)
54	Bx	0.53	0/1364	0.98	5/1849 (0.3%)
55	Bz	0.44	0/404	0.67	0/556
56	AA	0.27	0/22852	0.37	0/35580
57	AB	0.54	0/1804	0.93	7/2445 (0.3%)
58	AC	0.50	0/1105	0.83	0/1496
59	AE	0.42	0/2785	0.81	4/3735 (0.1%)
60	AF	0.44	0/999	0.90	3/1347 (0.2%)
61	AG	0.53	0/1763	0.87	2/2368 (0.1%)
62	AI	0.48	0/2707	0.79	0/3636
63	AJ	0.55	0/1181	0.89	3/1597 (0.2%)
64	AK	0.46	0/1027	1.02	7/1389 (0.5%)
65	AL	0.38	0/858	0.93	5/1152 (0.4%)
66	AN	0.61	0/874	0.90	2/1171 (0.2%)
67	AO	0.46	0/1473	0.95	7/1970 (0.4%)
68	AP	0.59	0/954	0.94	3/1284 (0.2%)
69	AQ	0.51	0/894	0.93	2/1213 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
70	AR	0.52	0/802	0.92	1/1079 (0.1%)
71	AU	0.46	0/745	0.90	2/993 (0.2%)
72	AV	0.20	0/1673	0.33	0/2602
73	AX	0.24	0/395	0.44	0/612
74	AZ	0.49	0/89	0.79	0/123
75	Aa	0.58	0/2428	0.87	3/3279 (0.1%)
76	Ab	0.49	0/1126	0.90	2/1514 (0.1%)
77	Ac	0.52	1/1399 (0.1%)	0.96	5/1881 (0.3%)
78	Ad	0.54	0/1490	0.88	4/2005 (0.2%)
79	Ae	0.47	0/3171	0.86	7/4292 (0.2%)
80	Af	0.47	0/790	0.83	1/1064 (0.1%)
81	Ag	0.48	0/2945	0.81	2/3984 (0.1%)
82	Ah	0.50	0/1045	0.84	2/1409 (0.1%)
83	Ai	0.46	0/841	0.84	0/1121
84	Aj	0.49	1/1835 (0.1%)	0.85	3/2484 (0.1%)
85	Ak	0.52	0/2268	0.88	8/3069 (0.3%)
86	Am	0.44	0/947	0.90	6/1268 (0.5%)
87	An	0.44	0/650	0.85	0/858
88	Ao	0.47	0/4626	0.84	14/6269 (0.2%)
89	Ap	0.51	0/1616	0.96	6/2195 (0.3%)
All	All	0.45	2/187395 (0.0%)	0.74	257/266151 (0.1%)

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
6	B4	0	1
16	BE	0	1
34	Bb	0	1
46	Bn	0	1
53	Bw	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	Aj	167	PRO	CA-C	5.23	1.54	1.51
77	Ac	52	ILE	CA-CB	5.22	1.56	1.54

The worst 5 of 257 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Bh	284	GLY	CA-C-N	12.87	132.92	120.31
40	Bh	284	GLY	C-N-CA	12.87	132.92	120.31
50	Bt	23	ARG	CA-C-N	11.56	131.15	119.82
50	Bt	23	ARG	C-N-CA	11.56	131.15	119.82
27	BT	68	PRO	N-CA-CB	9.95	113.70	103.25

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B4	61	ASP	Peptide
16	BE	316	PHE	Peptide
34	Bb	210	GLU	Peptide
46	Bn	65	ASN	Peptide
53	Bw	356	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BL	537	0	591	8	0
1	CL	317	0	309	16	0
1	DL	213	0	234	12	0
1	EL	222	0	247	6	0
1	FL	213	0	234	6	0
1	GL	213	0	234	4	0
1	HL	205	0	223	9	0
2	B0	857	0	878	16	0
3	B1	2036	0	2058	41	0
4	B2	1548	0	1583	27	0
5	B3	968	0	1018	32	0
6	B4	381	0	400	18	0
7	B5	902	0	916	22	0
8	B6	425	0	471	11	0
9	B7	387	0	413	10	0
10	B8	833	0	883	20	0
11	B9	335	0	359	11	0
12	BA	32950	0	16673	326	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	BB	1427	0	726	17	0
14	BC	4364	0	4371	78	0
15	BD	1860	0	1923	43	0
16	BE	2420	0	2418	71	0
17	BF	2011	0	2049	61	0
18	BI	805	0	845	19	0
19	BJ	1705	0	1804	49	0
20	BK	1303	0	1343	41	0
21	BN	1444	0	1437	51	0
22	BO	896	0	946	29	0
23	BP	2312	0	2373	63	0
24	BQ	1803	0	1841	28	0
25	BR	1240	0	1260	27	0
26	BS	1168	0	1159	43	0
27	BT	1954	0	1943	33	0
28	BU	1159	0	1228	27	0
29	BV	1231	0	1278	36	0
30	BW	1374	0	1405	23	0
31	BX	1181	0	1139	29	0
32	BY	1678	0	1683	41	0
33	Ba	3173	0	3153	75	0
34	Bb	2952	0	2840	87	0
35	Bc	2408	0	2415	40	0
36	Bd	832	0	828	44	0
37	Be	972	0	971	23	0
38	Bf	827	0	736	32	0
39	Bg	1167	0	1173	38	0
40	Bh	2319	0	2332	58	0
41	Bi	2138	0	2139	60	0
42	Bj	1775	0	1797	75	0
43	Bk	1087	0	1080	32	0
44	Bl	1097	0	1080	15	0
45	Bm	893	0	878	23	0
46	Bn	837	0	860	23	0
47	Bo	772	0	773	19	0
48	Bp	742	0	749	20	0
49	Bq	542	0	485	19	0
50	Bt	780	0	792	27	0
51	Bu	1198	0	1192	27	0
52	Bv	1131	0	1093	10	0
53	Bw	3126	0	3153	93	0
54	Bx	1325	0	1354	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	Bz	410	0	404	6	0
56	AA	20411	0	10345	208	0
57	AB	1762	0	1774	45	0
58	AC	1075	0	1087	33	0
59	AE	2732	0	2774	71	0
60	AF	981	0	1012	26	0
61	AG	1721	0	1747	39	0
62	AI	2650	0	2613	65	0
63	AJ	1155	0	1193	42	0
64	AK	1007	0	1042	26	0
65	AL	840	0	890	22	0
66	AN	858	0	883	44	0
67	AO	1448	0	1536	28	0
68	AP	932	0	951	24	0
69	AQ	875	0	931	40	0
70	AR	784	0	813	32	0
71	AU	734	0	745	25	0
72	AV	1498	0	765	14	0
73	AX	354	0	187	7	0
74	AZ	90	0	89	4	0
75	Aa	2378	0	2392	56	0
76	Ab	1101	0	1118	27	0
77	Ac	1367	0	1385	48	0
78	Ad	1467	0	1466	34	0
79	Ae	3109	0	3029	102	0
80	Af	778	0	791	18	0
81	Ag	2875	0	2886	81	0
82	Ah	1015	0	969	34	0
83	Ai	824	0	842	25	0
84	Aj	1788	0	1799	46	0
85	Ak	2222	0	2270	64	0
86	Am	930	0	959	25	0
87	An	639	0	709	12	0
88	Ao	4526	0	4434	154	0
89	Ap	1564	0	1531	35	0
90	AA	105	0	0	0	0
90	AB	1	0	0	0	0
90	AX	1	0	0	0	0
90	Ag	1	0	0	0	0
90	An	1	0	0	0	0
90	B3	1	0	0	0	0
90	BA	202	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	BB	1	0	0	0	0
90	BC	2	0	0	0	0
90	BD	3	0	0	0	0
90	BE	1	0	0	0	0
90	BJ	1	0	0	0	0
90	BP	2	0	0	0	0
90	Be	1	0	0	0	0
90	Bl	1	0	0	0	0
90	Bt	2	0	0	0	0
91	AR	1	0	0	0	0
91	Ac	1	0	0	0	0
91	Ap	1	0	0	0	0
91	B5	1	0	0	0	0
91	B9	1	0	0	0	0
91	Bx	1	0	0	0	0
92	BA	48	0	24	0	0
93	AA	14	0	26	0	0
93	BA	14	0	26	1	0
93	BR	14	0	26	0	0
94	BC	32	0	12	1	0
95	BC	1	0	0	0	0
96	AV	10	0	10	0	0
97	Ag	32	0	12	2	0
98	Ag	3	0	0	0	0
98	BC	2	0	0	0	0
All	All	178372	0	151265	3127	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 10.

The worst 5 of 3127 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)
37:Be:25:ARG:HG2	37:Be:25:ARG:HH11	1.04	1.17
62:Al:254:LYS:HB3	62:Al:366:ARG:HH12	1.19	1.07
26:BS:85:ARG:HB3	26:BS:120:ARG:HH12	1.20	1.05
87:An:144:ARG:HG3	87:An:144:ARG:HH11	1.23	1.02
17:BF:287:ARG:HD2	52:Bv:33:ARG:HH12	1.25	1.00

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	BL	68/198 (34%)	65 (96%)	3 (4%)	0	100	100
1	CL	43/198 (22%)	41 (95%)	1 (2%)	1 (2%)	5	29
1	DL	25/198 (13%)	25 (100%)	0	0	100	100
1	EL	26/198 (13%)	25 (96%)	1 (4%)	0	100	100
1	FL	25/198 (13%)	25 (100%)	0	0	100	100
1	GL	25/198 (13%)	25 (100%)	0	0	100	100
1	HL	24/198 (12%)	24 (100%)	0	0	100	100
2	B0	108/148 (73%)	104 (96%)	4 (4%)	0	100	100
3	B1	242/256 (94%)	237 (98%)	5 (2%)	0	100	100
4	B2	177/252 (70%)	172 (97%)	5 (3%)	0	100	100
5	B3	116/161 (72%)	114 (98%)	2 (2%)	0	100	100
6	B4	43/126 (34%)	40 (93%)	3 (7%)	0	100	100
7	B5	108/188 (57%)	106 (98%)	2 (2%)	0	100	100
8	B6	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
9	B7	44/95 (46%)	43 (98%)	1 (2%)	0	100	100
10	B8	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
11	B9	36/100 (36%)	36 (100%)	0	0	100	100
14	BC	569/650 (88%)	548 (96%)	20 (4%)	1 (0%)	43	73
15	BD	238/306 (78%)	226 (95%)	12 (5%)	0	100	100
16	BE	305/348 (88%)	284 (93%)	18 (6%)	3 (1%)	12	45
17	BF	248/294 (84%)	237 (96%)	11 (4%)	0	100	100
18	BI	96/268 (36%)	91 (95%)	5 (5%)	0	100	100
19	BJ	210/262 (80%)	202 (96%)	8 (4%)	0	100	100
20	BK	174/192 (91%)	166 (95%)	7 (4%)	1 (1%)	21	56
21	BN	175/178 (98%)	172 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	BO	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
23	BP	286/296 (97%)	276 (96%)	10 (4%)	0	100	100
24	BQ	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
25	BR	151/169 (89%)	146 (97%)	5 (3%)	0	100	100
26	BS	141/180 (78%)	131 (93%)	9 (6%)	1 (1%)	18	52
27	BT	238/292 (82%)	229 (96%)	8 (3%)	1 (0%)	30	62
28	BU	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
29	BV	153/209 (73%)	147 (96%)	6 (4%)	0	100	100
30	BW	164/210 (78%)	159 (97%)	5 (3%)	0	100	100
31	BX	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
32	BY	204/216 (94%)	193 (95%)	11 (5%)	0	100	100
33	Ba	391/423 (92%)	377 (96%)	14 (4%)	0	100	100
34	Bb	352/380 (93%)	329 (94%)	23 (6%)	0	100	100
35	Bc	293/334 (88%)	281 (96%)	12 (4%)	0	100	100
36	Bd	97/206 (47%)	89 (92%)	7 (7%)	1 (1%)	12	45
37	Be	120/135 (89%)	115 (96%)	5 (4%)	0	100	100
38	Bf	106/142 (75%)	102 (96%)	2 (2%)	2 (2%)	6	33
39	Bg	146/159 (92%)	137 (94%)	9 (6%)	0	100	100
40	Bh	287/332 (86%)	276 (96%)	11 (4%)	0	100	100
41	Bi	258/306 (84%)	248 (96%)	10 (4%)	0	100	100
42	Bj	211/279 (76%)	199 (94%)	12 (6%)	0	100	100
43	Bk	132/212 (62%)	126 (96%)	6 (4%)	0	100	100
44	Bl	131/166 (79%)	128 (98%)	3 (2%)	0	100	100
45	Bm	107/159 (67%)	104 (97%)	3 (3%)	0	100	100
46	Bn	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
47	Bo	95/124 (77%)	91 (96%)	4 (4%)	0	100	100
48	Bp	95/112 (85%)	90 (95%)	5 (5%)	0	100	100
49	Bq	66/138 (48%)	64 (97%)	1 (2%)	1 (2%)	8	37
50	Bt	92/102 (90%)	87 (95%)	5 (5%)	0	100	100
51	Bu	147/205 (72%)	136 (92%)	10 (7%)	1 (1%)	18	52
52	Bv	133/222 (60%)	132 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	Bw	385/433 (89%)	365 (95%)	18 (5%)	2 (0%)	24	59
54	Bx	160/196 (82%)	156 (98%)	3 (2%)	1 (1%)	21	56
55	Bz	70/82 (85%)	70 (100%)	0	0	100	100
57	AB	218/289 (75%)	213 (98%)	5 (2%)	0	100	100
58	AC	130/167 (78%)	122 (94%)	8 (6%)	0	100	100
59	AE	341/430 (79%)	327 (96%)	14 (4%)	0	100	100
60	AF	120/124 (97%)	117 (98%)	3 (2%)	0	100	100
61	AG	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
62	AI	326/397 (82%)	313 (96%)	13 (4%)	0	100	100
63	AJ	138/201 (69%)	129 (94%)	7 (5%)	2 (1%)	9	39
64	AK	135/196 (69%)	129 (96%)	5 (4%)	1 (1%)	18	52
65	AL	107/139 (77%)	105 (98%)	2 (2%)	0	100	100
66	AN	99/128 (77%)	99 (100%)	0	0	100	100
67	AO	173/239 (72%)	167 (96%)	6 (4%)	0	100	100
68	AP	115/135 (85%)	113 (98%)	2 (2%)	0	100	100
69	AQ	110/130 (85%)	106 (96%)	4 (4%)	0	100	100
70	AR	95/143 (66%)	93 (98%)	2 (2%)	0	100	100
71	AU	84/87 (97%)	84 (100%)	0	0	100	100
74	AZ	16/18 (89%)	15 (94%)	1 (6%)	0	100	100
75	Aa	290/382 (76%)	284 (98%)	6 (2%)	0	100	100
76	Ab	133/190 (70%)	129 (97%)	4 (3%)	0	100	100
77	Ac	167/173 (96%)	157 (94%)	9 (5%)	1 (1%)	21	56
78	Ad	175/205 (85%)	170 (97%)	5 (3%)	0	100	100
79	Ae	386/455 (85%)	350 (91%)	32 (8%)	4 (1%)	12	45
80	Af	97/188 (52%)	92 (95%)	5 (5%)	0	100	100
81	Ag	351/397 (88%)	338 (96%)	13 (4%)	0	100	100
82	Ah	118/387 (30%)	116 (98%)	2 (2%)	0	100	100
83	Ai	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
84	Aj	211/218 (97%)	207 (98%)	4 (2%)	0	100	100
85	Ak	273/325 (84%)	265 (97%)	8 (3%)	0	100	100
86	Am	114/118 (97%)	109 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
87	An	70/199 (35%)	68 (97%)	2 (3%)	0	100	100
88	Ao	564/692 (82%)	532 (94%)	32 (6%)	0	100	100
89	Ap	188/258 (73%)	182 (97%)	6 (3%)	0	100	100
All	All	14839/20063 (74%)	14258 (96%)	557 (4%)	24 (0%)	44	73

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CL	21	PRO
14	BC	502	PRO
27	BT	68	PRO
38	Bf	78	PRO
38	Bf	80	PRO

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	BL	59/157 (38%)	58 (98%)	1 (2%)	53	75
1	CL	30/157 (19%)	29 (97%)	1 (3%)	33	65
1	DL	26/157 (17%)	23 (88%)	3 (12%)	5	24
1	EL	27/157 (17%)	25 (93%)	2 (7%)	13	43
1	FL	26/157 (17%)	24 (92%)	2 (8%)	12	41
1	GL	26/157 (17%)	25 (96%)	1 (4%)	29	62
1	HL	25/157 (16%)	23 (92%)	2 (8%)	11	40
2	B0	90/115 (78%)	80 (89%)	10 (11%)	6	25
3	B1	219/229 (96%)	192 (88%)	27 (12%)	4	22
4	B2	164/228 (72%)	146 (89%)	18 (11%)	6	26
5	B3	110/147 (75%)	99 (90%)	11 (10%)	7	30
6	B4	42/114 (37%)	35 (83%)	7 (17%)	2	11
7	B5	99/163 (61%)	89 (90%)	10 (10%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	B6	49/60 (82%)	46 (94%)	3 (6%)	17	49
9	B7	41/78 (53%)	39 (95%)	2 (5%)	22	55
10	B8	87/162 (54%)	77 (88%)	10 (12%)	5	24
11	B9	36/77 (47%)	31 (86%)	5 (14%)	3	17
14	BC	464/553 (84%)	447 (96%)	17 (4%)	30	63
15	BD	193/248 (78%)	168 (87%)	25 (13%)	4	20
16	BE	263/290 (91%)	237 (90%)	26 (10%)	7	31
17	BF	217/251 (86%)	193 (89%)	24 (11%)	6	25
18	BI	88/228 (39%)	83 (94%)	5 (6%)	18	51
19	BJ	192/230 (84%)	184 (96%)	8 (4%)	26	60
20	BK	129/151 (85%)	120 (93%)	9 (7%)	14	45
21	BN	156/157 (99%)	140 (90%)	16 (10%)	7	28
22	BO	99/123 (80%)	85 (86%)	14 (14%)	3	17
23	BP	245/249 (98%)	217 (89%)	28 (11%)	5	24
24	BQ	190/210 (90%)	180 (95%)	10 (5%)	20	53
25	BR	132/143 (92%)	118 (89%)	14 (11%)	6	27
26	BS	123/153 (80%)	114 (93%)	9 (7%)	13	43
27	BT	212/258 (82%)	190 (90%)	22 (10%)	7	28
28	BU	118/127 (93%)	110 (93%)	8 (7%)	14	46
29	BV	136/178 (76%)	124 (91%)	12 (9%)	9	35
30	BW	144/180 (80%)	131 (91%)	13 (9%)	9	34
31	BX	116/134 (87%)	103 (89%)	13 (11%)	6	25
32	BY	185/192 (96%)	163 (88%)	22 (12%)	5	23
33	Ba	348/365 (95%)	310 (89%)	38 (11%)	6	26
34	Bb	310/328 (94%)	273 (88%)	37 (12%)	5	23
35	Bc	271/299 (91%)	255 (94%)	16 (6%)	18	50
36	Bd	92/181 (51%)	85 (92%)	7 (8%)	12	42
37	Be	100/108 (93%)	85 (85%)	15 (15%)	3	15
38	Bf	80/133 (60%)	68 (85%)	12 (15%)	3	15
39	Bg	128/136 (94%)	110 (86%)	18 (14%)	3	17
40	Bh	251/284 (88%)	223 (89%)	28 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	Bi	236/275 (86%)	220 (93%)	16 (7%)	14	46
42	Bj	190/242 (78%)	173 (91%)	17 (9%)	9	34
43	Bk	119/181 (66%)	112 (94%)	7 (6%)	18	50
44	Bl	122/147 (83%)	106 (87%)	16 (13%)	4	19
45	Bm	103/145 (71%)	95 (92%)	8 (8%)	11	41
46	Bn	88/113 (78%)	79 (90%)	9 (10%)	7	29
47	Bo	77/97 (79%)	69 (90%)	8 (10%)	7	28
48	Bp	79/88 (90%)	75 (95%)	4 (5%)	21	54
49	Bq	50/114 (44%)	48 (96%)	2 (4%)	28	61
50	Bt	75/82 (92%)	60 (80%)	15 (20%)	1	7
51	Bu	126/177 (71%)	112 (89%)	14 (11%)	6	25
52	Bv	115/183 (63%)	112 (97%)	3 (3%)	40	69
53	Bw	340/373 (91%)	299 (88%)	41 (12%)	5	22
54	Bx	149/173 (86%)	133 (89%)	16 (11%)	6	27
57	AB	187/233 (80%)	171 (91%)	16 (9%)	10	36
58	AC	115/142 (81%)	97 (84%)	18 (16%)	2	13
59	AE	282/351 (80%)	252 (89%)	30 (11%)	6	27
60	AF	107/109 (98%)	94 (88%)	13 (12%)	5	22
61	AG	181/205 (88%)	165 (91%)	16 (9%)	9	35
62	AI	273/333 (82%)	260 (95%)	13 (5%)	23	56
63	AJ	130/181 (72%)	114 (88%)	16 (12%)	4	22
64	AK	103/151 (68%)	94 (91%)	9 (9%)	9	36
65	AL	92/116 (79%)	87 (95%)	5 (5%)	20	53
66	AN	92/114 (81%)	77 (84%)	15 (16%)	2	12
67	AO	159/205 (78%)	146 (92%)	13 (8%)	10	39
68	AP	97/113 (86%)	93 (96%)	4 (4%)	27	60
69	AQ	97/114 (85%)	83 (86%)	14 (14%)	3	16
70	AR	89/127 (70%)	83 (93%)	6 (7%)	15	47
71	AU	77/78 (99%)	66 (86%)	11 (14%)	3	16
75	Aa	258/330 (78%)	230 (89%)	28 (11%)	6	26
76	Ab	113/162 (70%)	104 (92%)	9 (8%)	11	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	Ac	152/155 (98%)	140 (92%)	12 (8%)	11	40
78	Ad	149/168 (89%)	139 (93%)	10 (7%)	15	47
79	Ae	325/393 (83%)	296 (91%)	29 (9%)	9	34
80	Af	86/160 (54%)	76 (88%)	10 (12%)	5	24
81	Ag	312/350 (89%)	290 (93%)	22 (7%)	13	44
82	Ah	109/346 (32%)	102 (94%)	7 (6%)	16	48
83	Ai	86/93 (92%)	79 (92%)	7 (8%)	11	39
84	Aj	188/190 (99%)	178 (95%)	10 (5%)	20	53
85	Ak	249/289 (86%)	225 (90%)	24 (10%)	8	32
86	Am	100/102 (98%)	88 (88%)	12 (12%)	5	23
87	An	66/174 (38%)	59 (89%)	7 (11%)	6	27
88	Ao	478/604 (79%)	455 (95%)	23 (5%)	23	56
89	Ap	170/225 (76%)	150 (88%)	20 (12%)	5	23
All	All	12929/17064 (76%)	11743 (91%)	1186 (9%)	11	33

5 of 1186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
69	AQ	22	MET
88	Ao	256	GLU
71	AU	80	ARG
69	AQ	6	SER
79	Ae	322	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 312 such sidechains are listed below:

Mol	Chain	Res	Type
69	AQ	57	GLN
84	Aj	32	GLN
75	Aa	243	GLN
79	Ae	257	ASN
88	Ao	318	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	BA	1547/1571 (98%)	471 (30%)	7 (0%)
13	BB	64/73 (87%)	24 (37%)	0
56	AA	959/962 (99%)	237 (24%)	3 (0%)
72	AV	70/71 (98%)	25 (35%)	0
73	AX	16/201 (7%)	10 (62%)	1 (6%)
All	All	2656/2878 (92%)	767 (28%)	11 (0%)

5 of 767 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	BA	4	A
12	BA	7	G
12	BA	11	G
12	BA	15	A
12	BA	19	U

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
56	AA	395	C
56	AA	743	A
73	AX	12	A
56	AA	882	A
12	BA	1220	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 341 ligands modelled in this entry, 333 are monoatomic - leaving 8 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	$\# Z > 2$
96	FME	AV	101	72	8,9,10	0.97	0	7,9,11	0.80	0
92	5GP	BA	3204	-	26,26,26	0.90	1 (3%)	40,40,40	1.84	9 (22%)
93	SPM	AA	3001	-	13,13,13	0.43	0	12,12,12	0.77	0
92	5GP	BA	3203	-	26,26,26	0.99	1 (3%)	40,40,40	2.20	10 (25%)
93	SPM	BR	201	-	13,13,13	0.39	0	12,12,12	0.80	0
97	GTP	Ag	500	90	30,34,34	0.77	1 (3%)	46,54,54	1.69	12 (26%)
94	GSP	BC	901	90	30,34,34	1.90	2 (6%)	41,54,54	1.78	9 (21%)
93	SPM	BA	3205	-	13,13,13	0.23	0	12,12,12	1.02	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
96	FME	AV	101	72	-	4/7/9/11	-
92	5GP	BA	3204	-	-	5/10/26/26	0/3/3/3
93	SPM	AA	3001	-	-	7/11/11/11	-
92	5GP	BA	3203	-	-	5/10/26/26	0/3/3/3
93	SPM	BR	201	-	-	8/11/11/11	-
97	GTP	Ag	500	90	-	6/22/38/38	0/3/3/3
94	GSP	BC	901	90	-	0/21/38/38	0/3/3/3
93	SPM	BA	3205	-	-	4/11/11/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
94	BC	901	GSP	PG-S1G	-9.31	1.70	1.90
92	BA	3203	5GP	C6-N1	-2.70	1.33	1.38
94	BC	901	GSP	C2-N3	2.40	1.38	1.33
92	BA	3204	5GP	C6-N1	-2.35	1.34	1.38
97	Ag	500	GTP	C2-N3	2.25	1.38	1.33

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	BA	3203	5GP	C5-C4-N3	-7.88	115.68	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	BA	3204	5GP	C5-C4-N3	-6.47	117.96	128.46
92	BA	3203	5GP	C2-N3-C4	5.63	122.34	112.30
94	BC	901	GSP	C5-C4-N3	-5.36	119.76	128.46
92	BA	3203	5GP	N9-C4-N3	5.17	136.32	125.94

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
92	BA	3203	5GP	C5'-O5'-P-OP3
92	BA	3203	5GP	C5'-O5'-P-OP2
92	BA	3204	5GP	C5'-O5'-P-OP1
92	BA	3204	5GP	C5'-O5'-P-OP2
96	AV	101	FME	C-CA-CB-CG

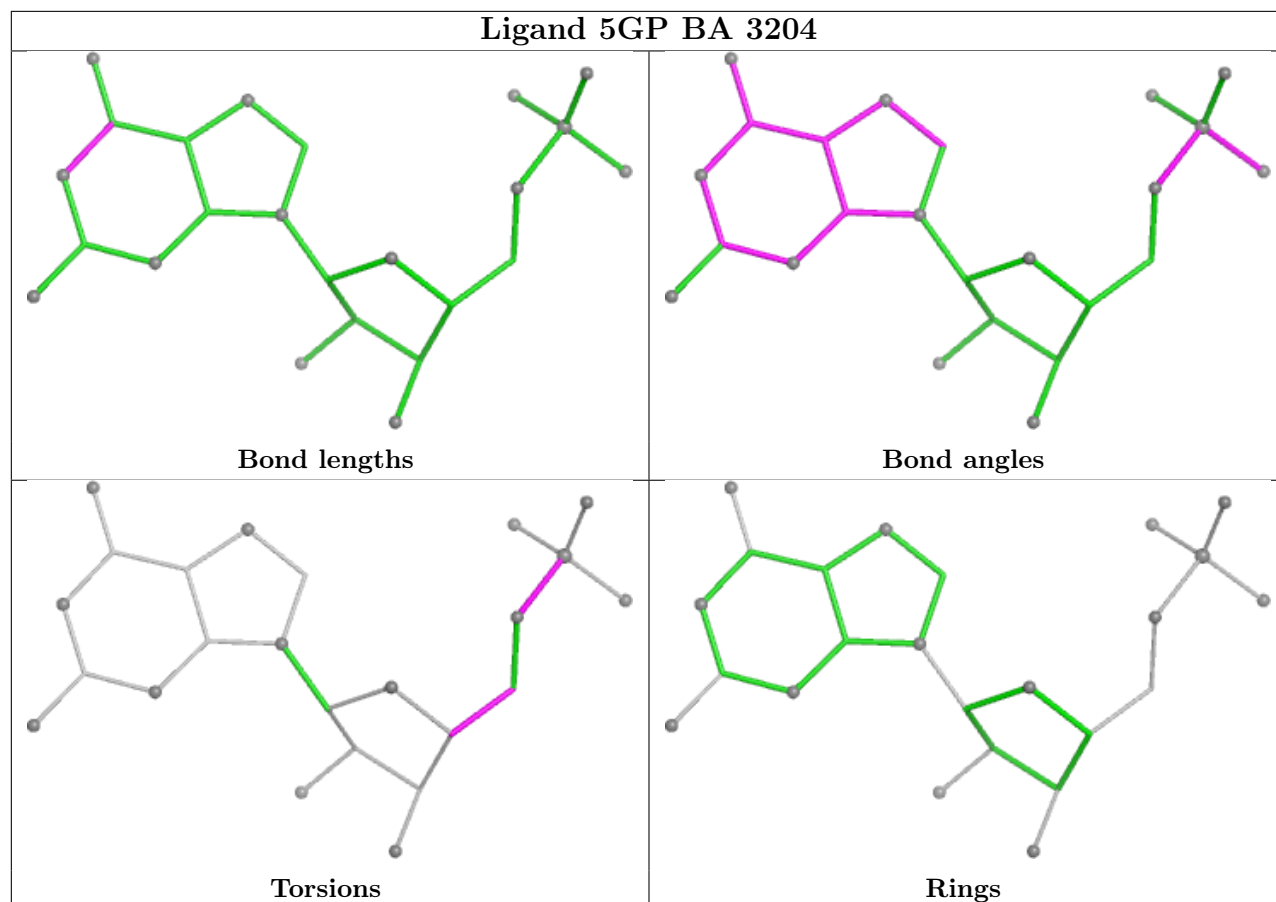
There are no ring outliers.

3 monomers are involved in 4 short contacts:

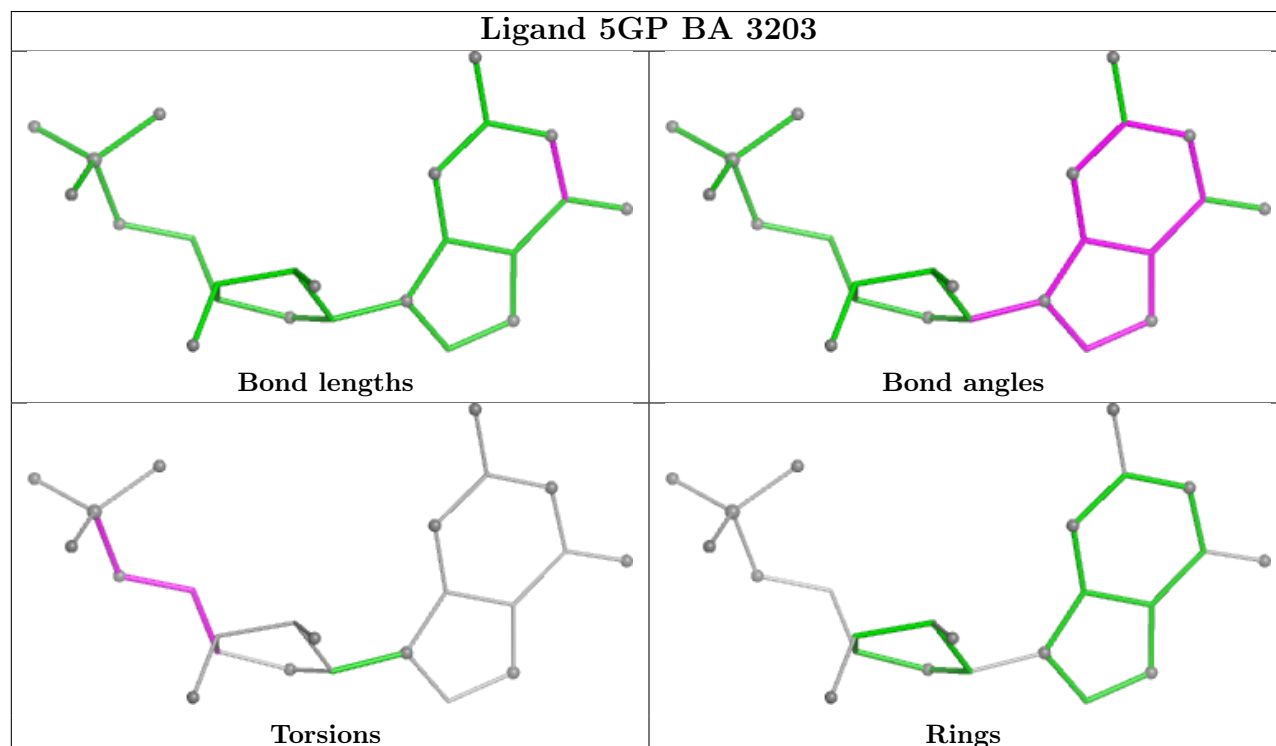
Mol	Chain	Res	Type	Clashes	Symm-Clashes
97	Ag	500	GTP	2	0
94	BC	901	GSP	1	0
93	BA	3205	SPM	1	0

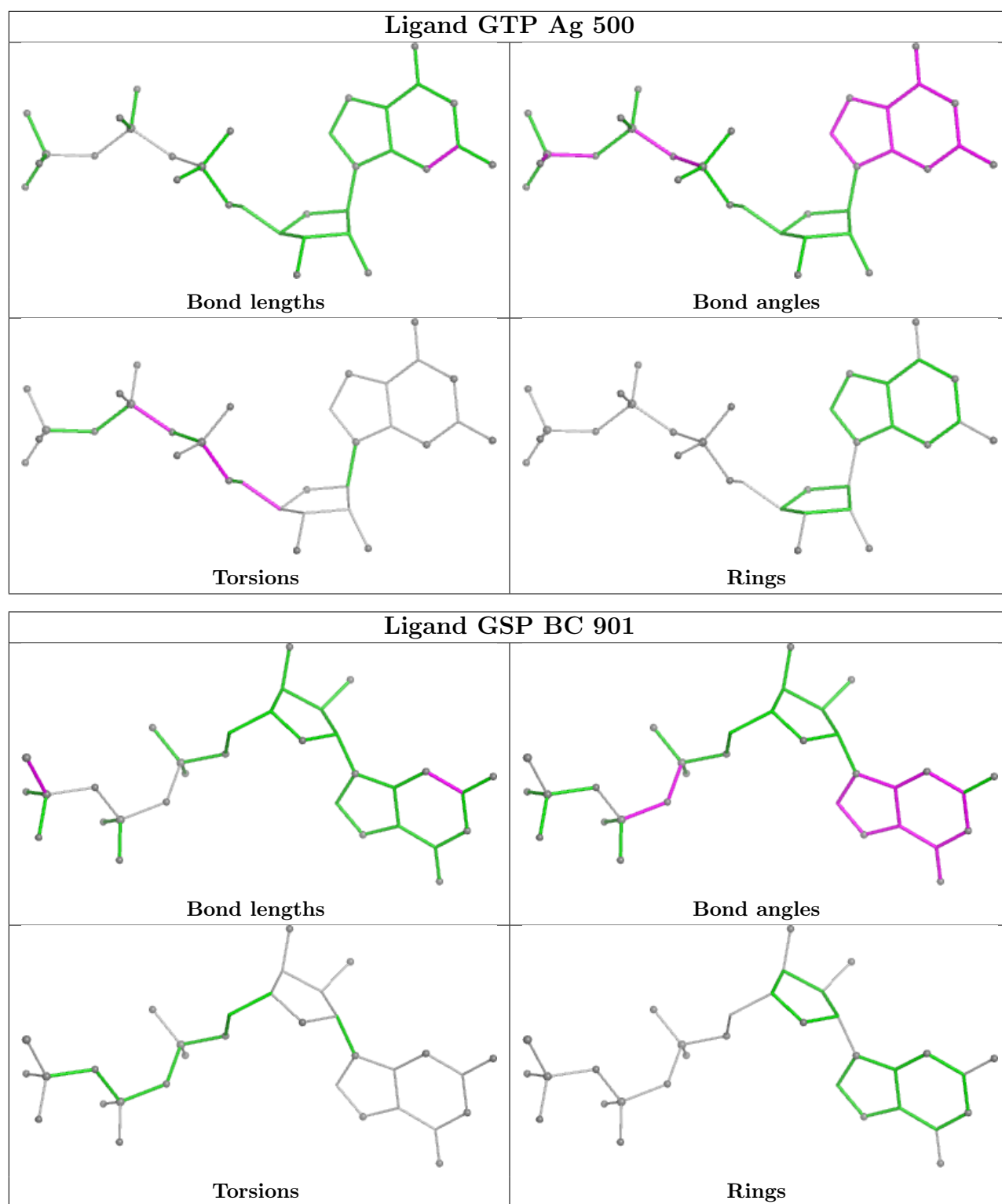
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 5GP BA 3204



Ligand 5GP BA 3203





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	Bz	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bz	710:ALA	C	1001:ALA	N	59.86
1	Bz	415:ALA	C	601:ALA	N	51.54
1	Bz	106:ALA	C	301:ALA	N	30.13
1	Bz	615:ALA	C	700:ALA	N	17.90
1	Bz	315:ALA	C	399:ALA	N	16.24

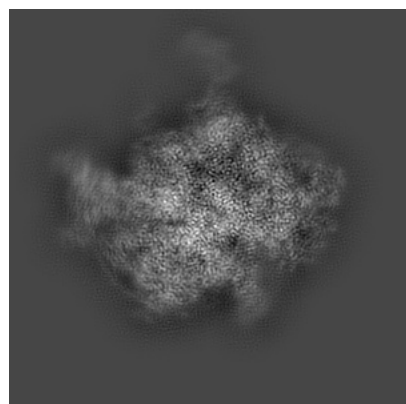
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4368. These allow visual inspection of the internal detail of the map and identification of artifacts.

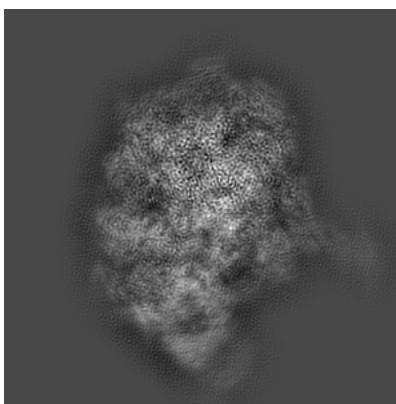
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

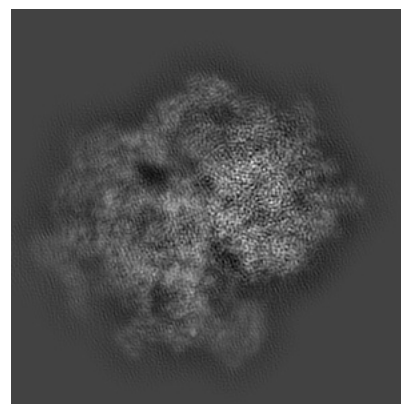
6.1.1 Primary map



X

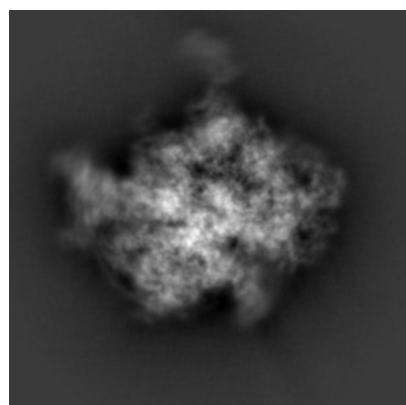


Y

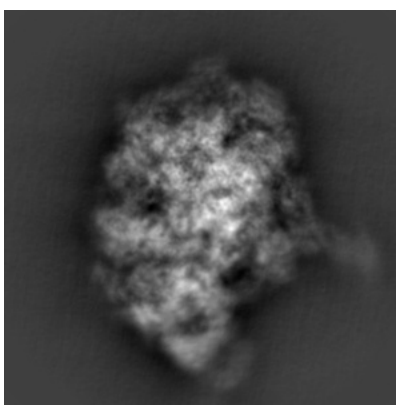


Z

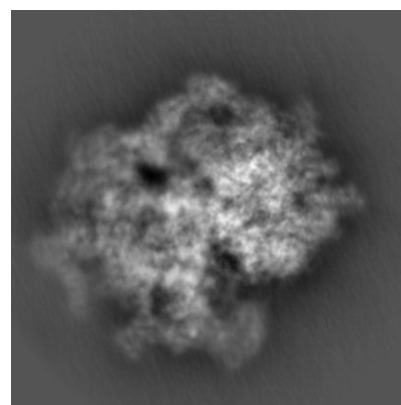
6.1.2 Raw map



X



Y

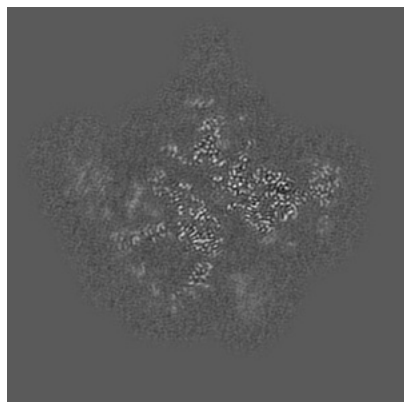


Z

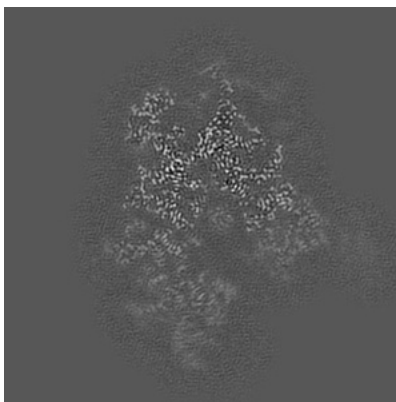
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

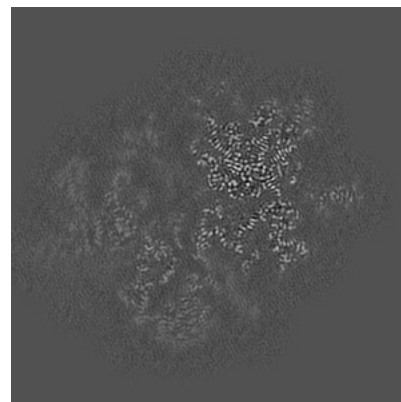
6.2.1 Primary map



X Index: 140

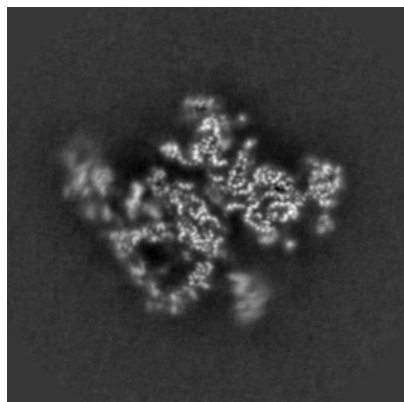


Y Index: 140

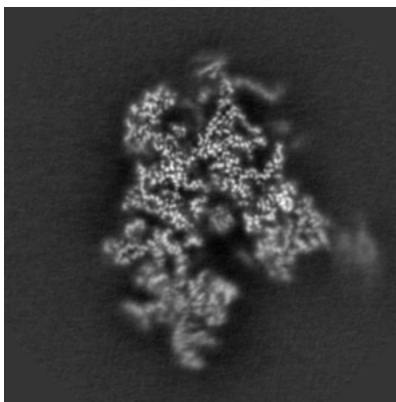


Z Index: 140

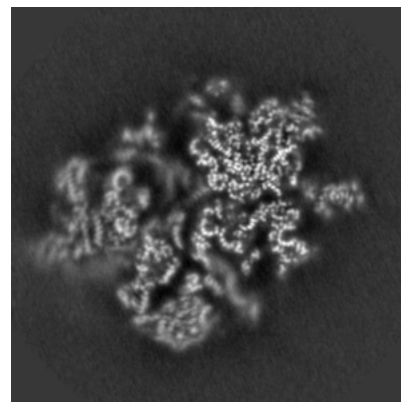
6.2.2 Raw map



X Index: 140



Y Index: 140

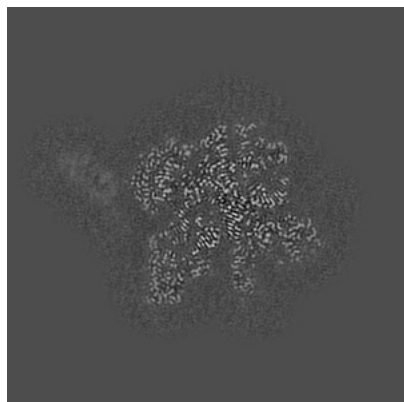


Z Index: 140

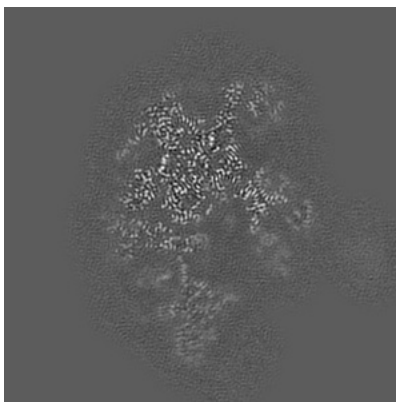
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

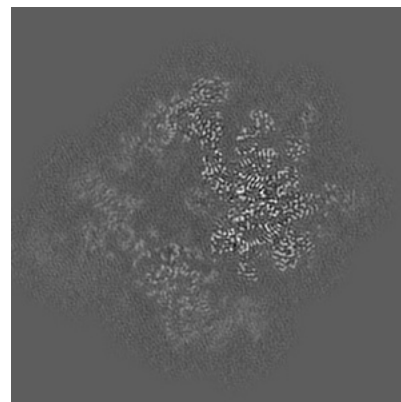
6.3.1 Primary map



X Index: 166

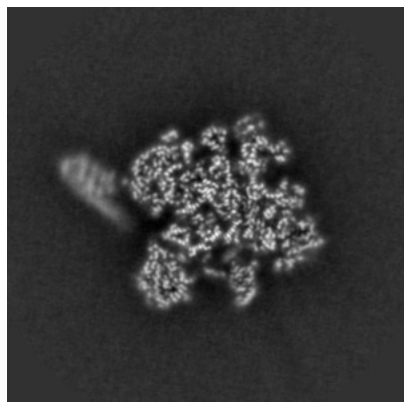


Y Index: 133

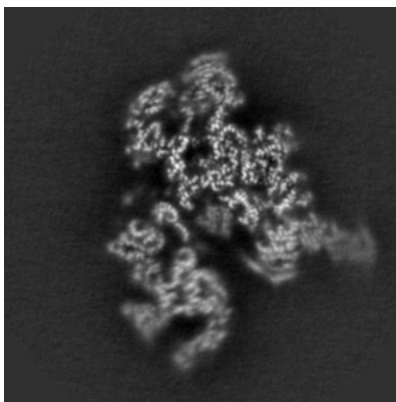


Z Index: 151

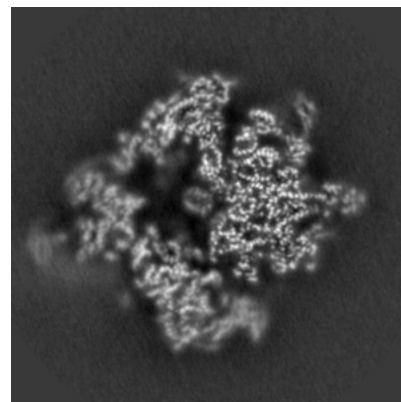
6.3.2 Raw map



X Index: 169



Y Index: 147

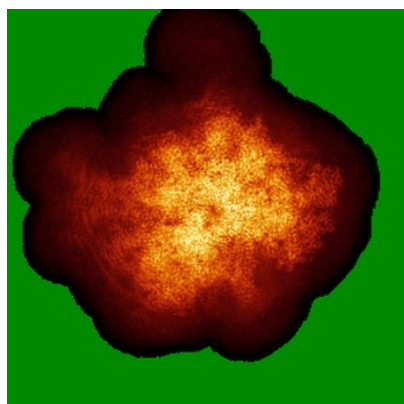


Z Index: 150

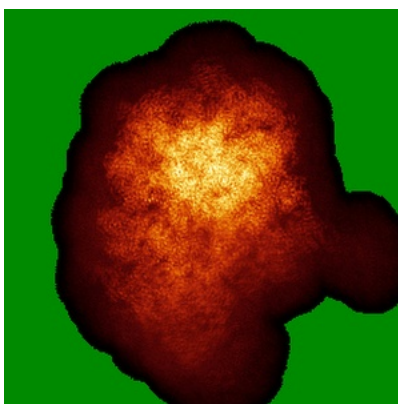
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

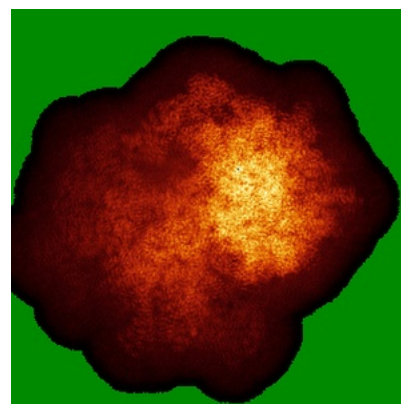
6.4.1 Primary map



X



Y

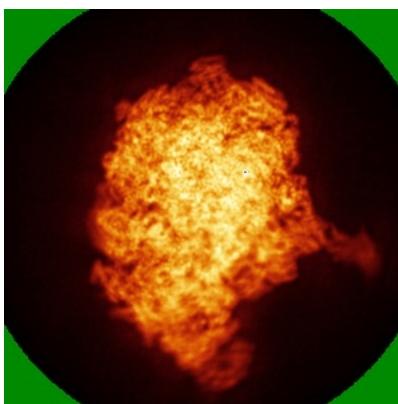


Z

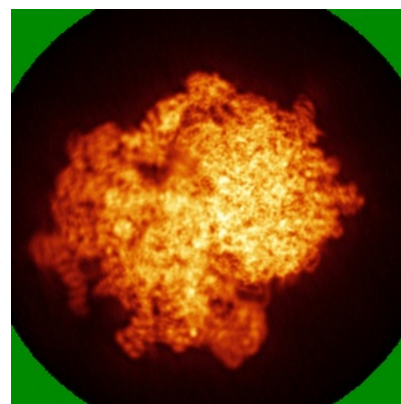
6.4.2 Raw map



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 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

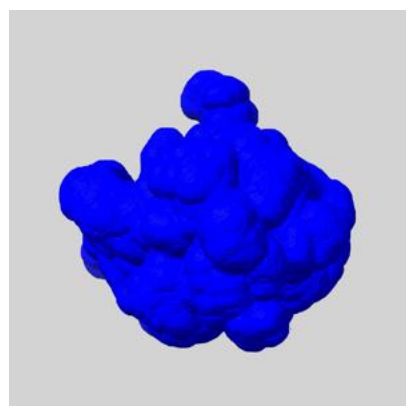
6.6 Mask visualisation [i](#)

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

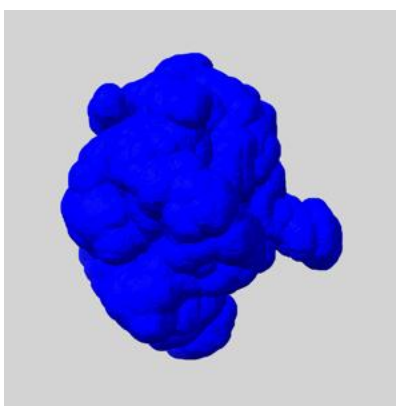
A mask typically either:

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

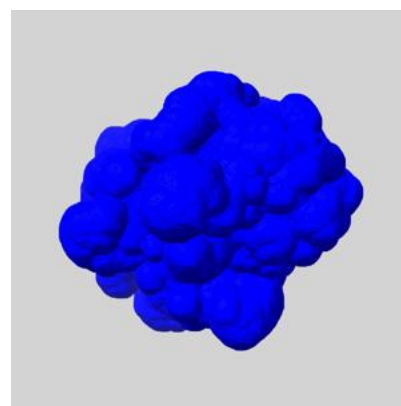
6.6.1 emd_4368_msk_1.map [i](#)



X



Y

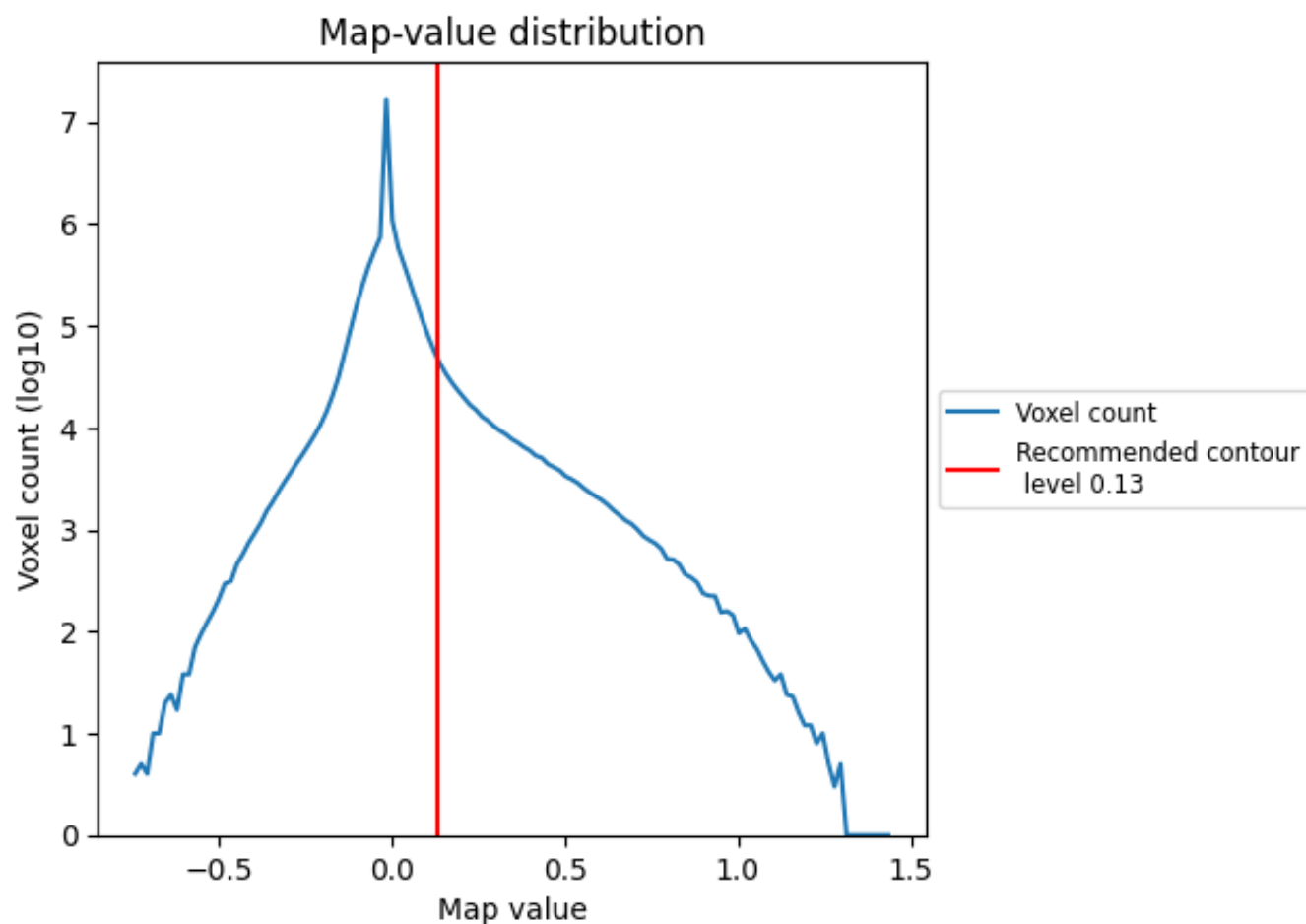


Z

7 Map analysis [i](#)

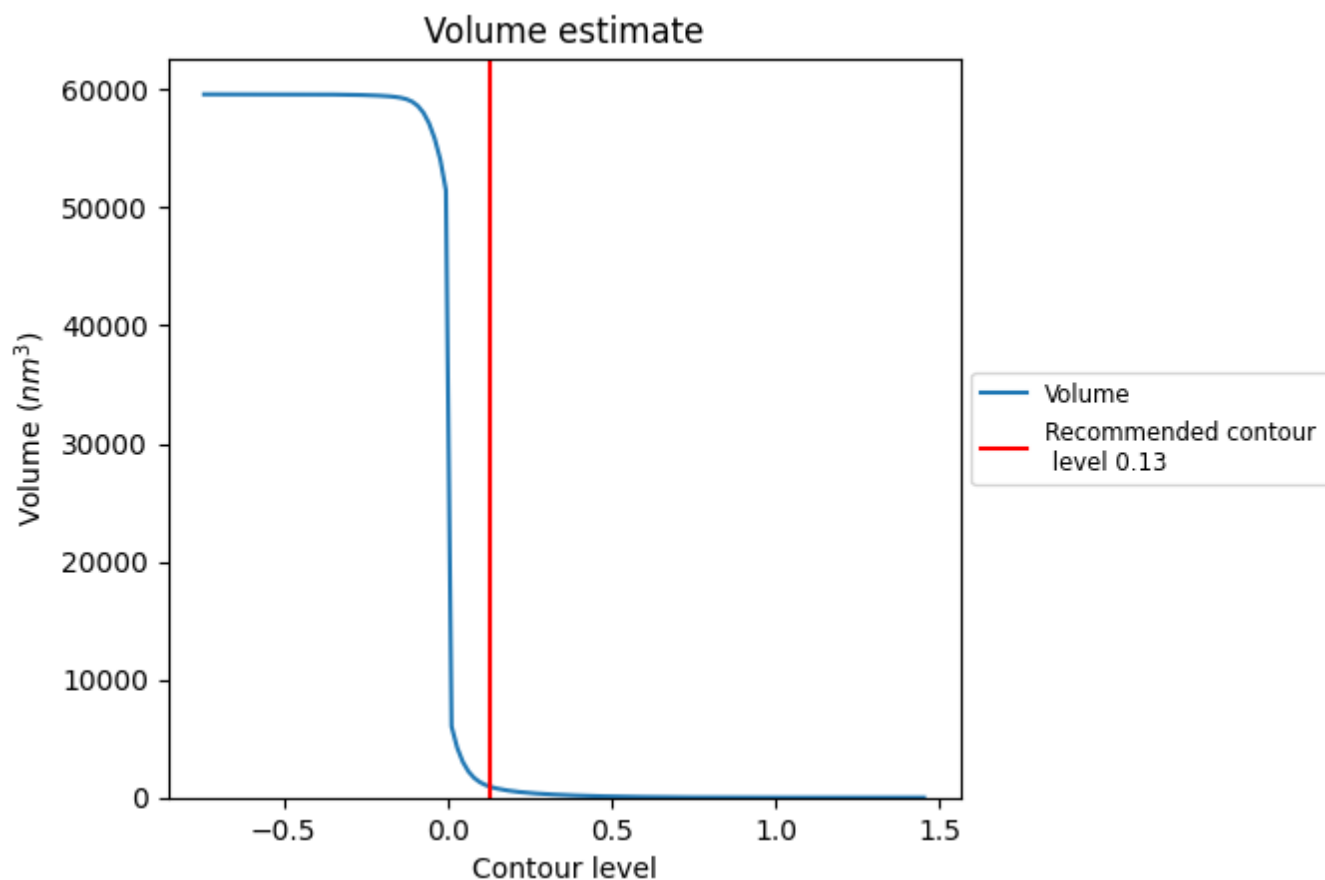
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

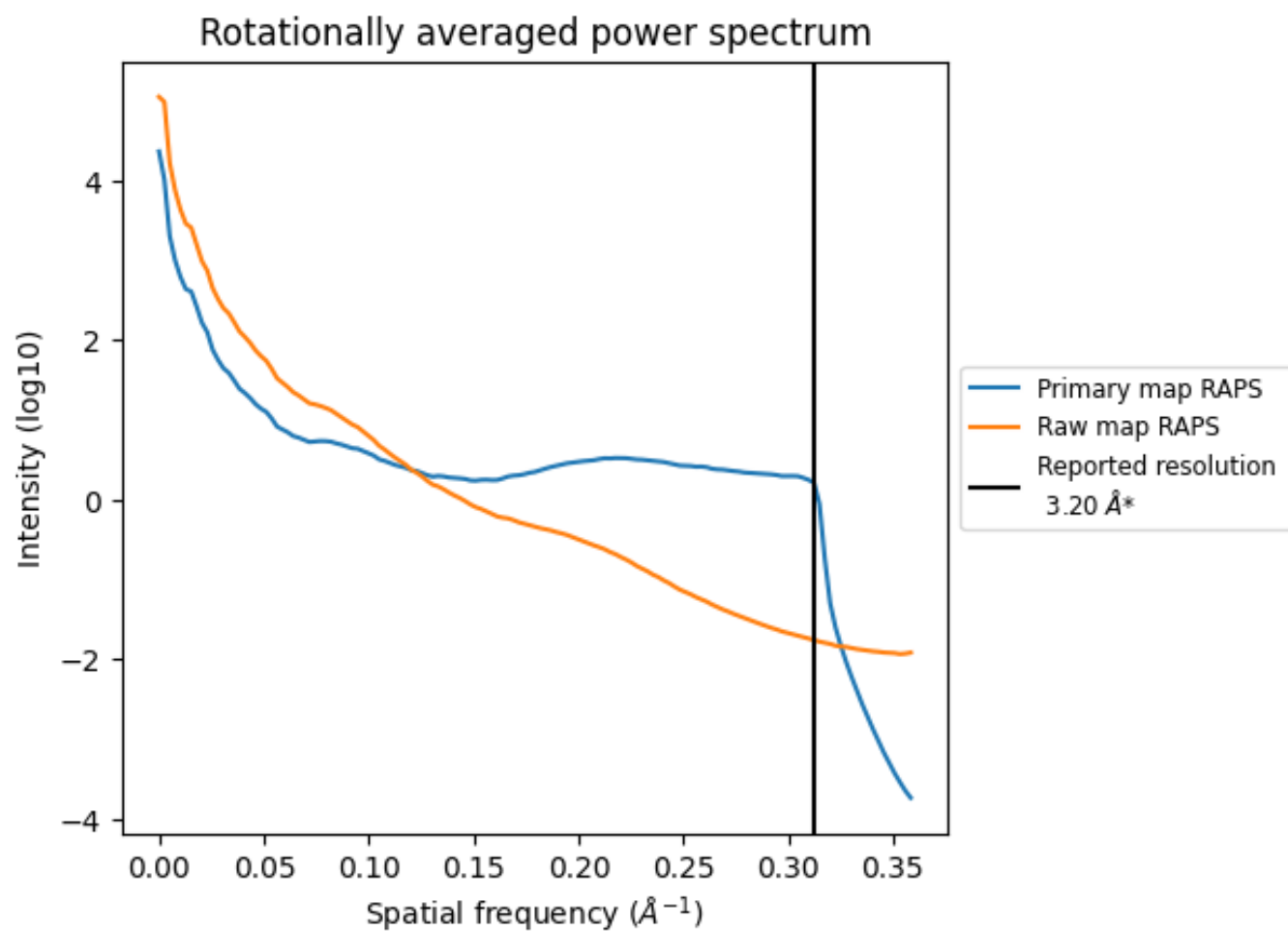
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 920 nm³; this corresponds to an approximate mass of 831 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 ⓘ

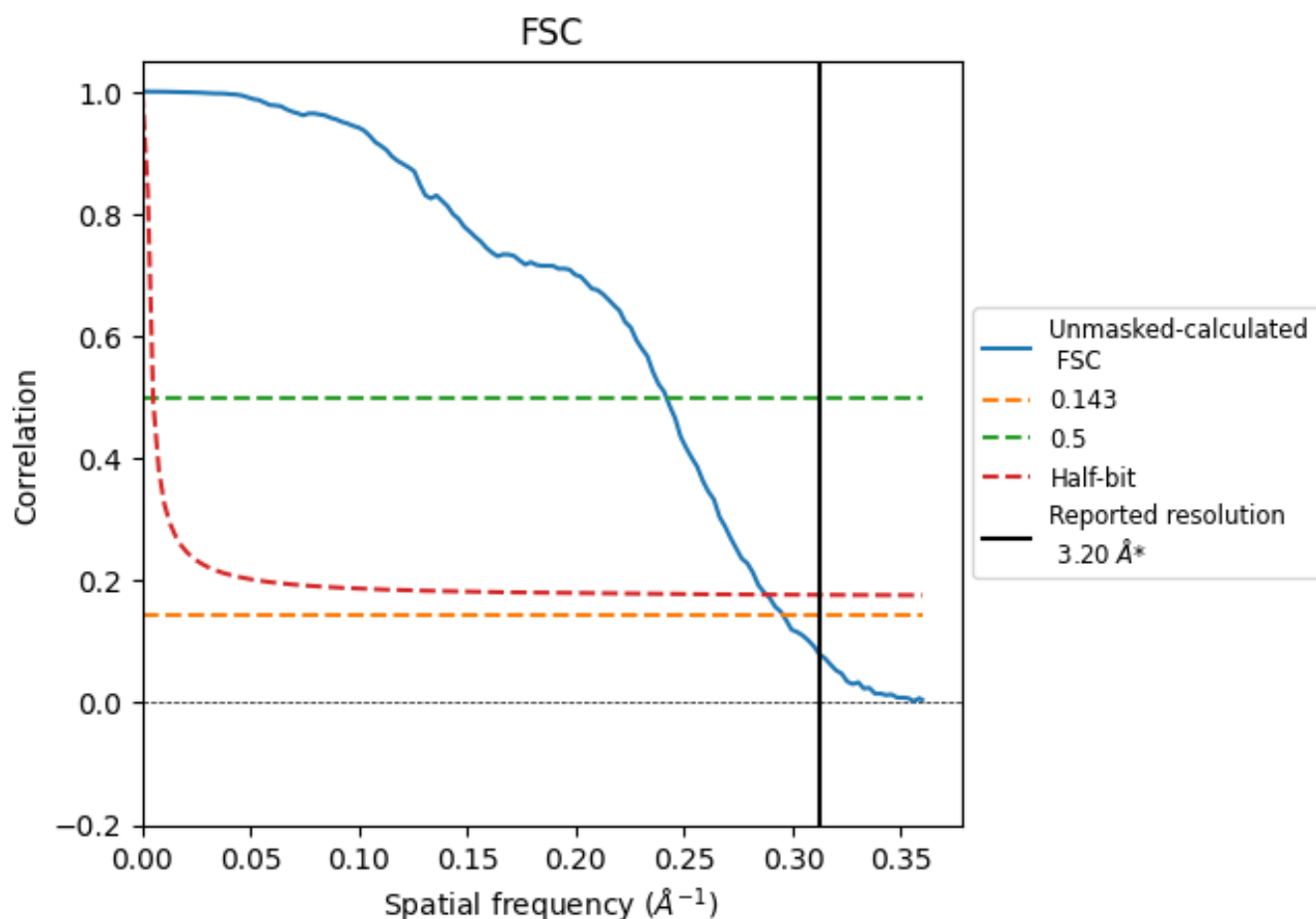


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

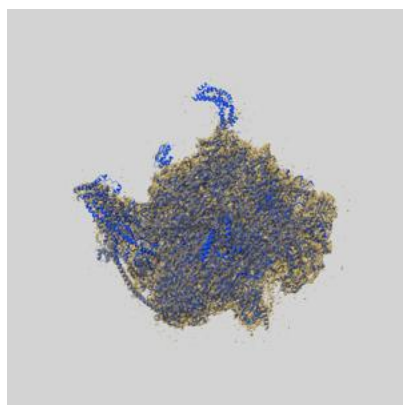
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	4.14	3.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

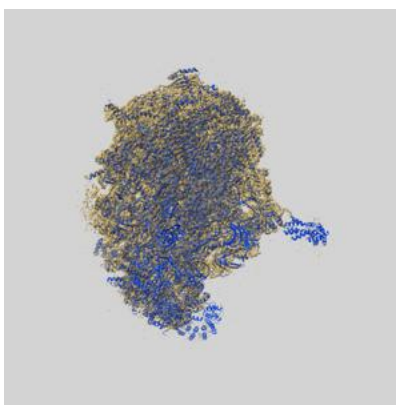
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4368 and PDB model 6GAW. Per-residue inclusion information can be found in section [3](#) on page [26](#).

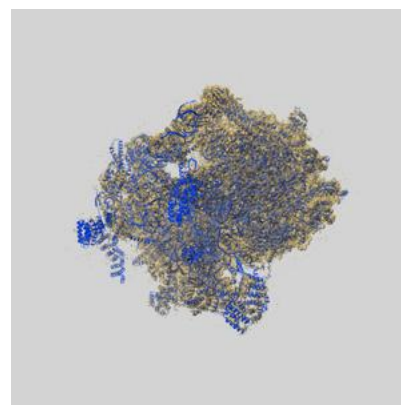
9.1 Map-model overlay [i](#)



X



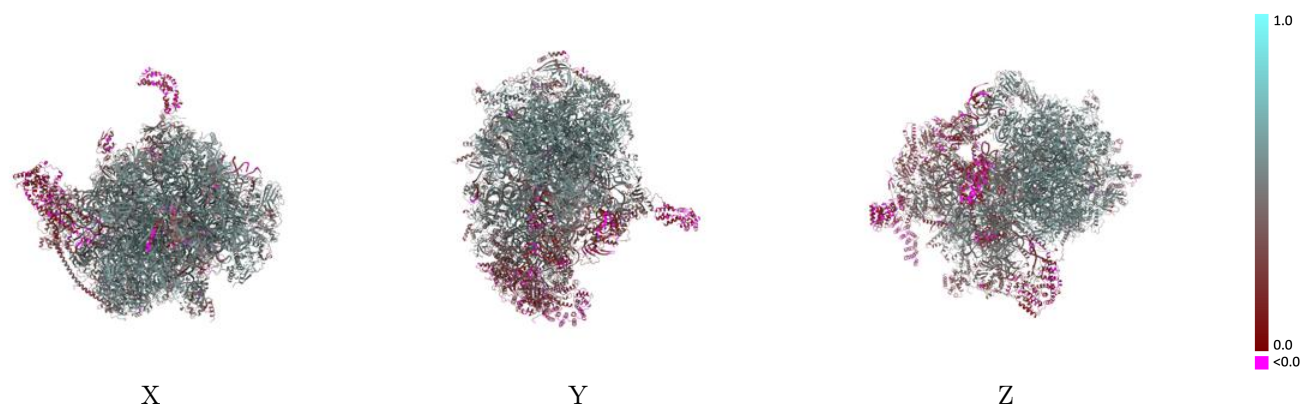
Y



Z

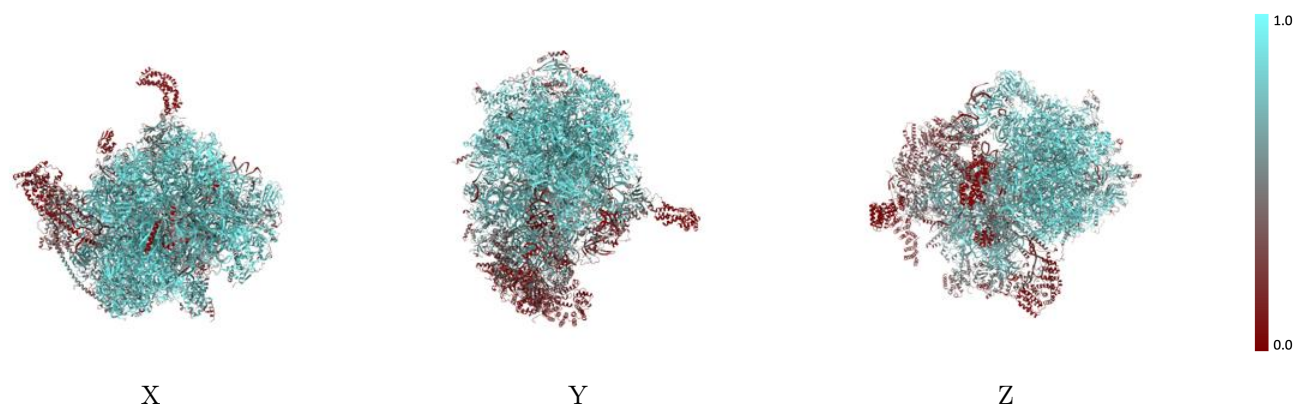
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



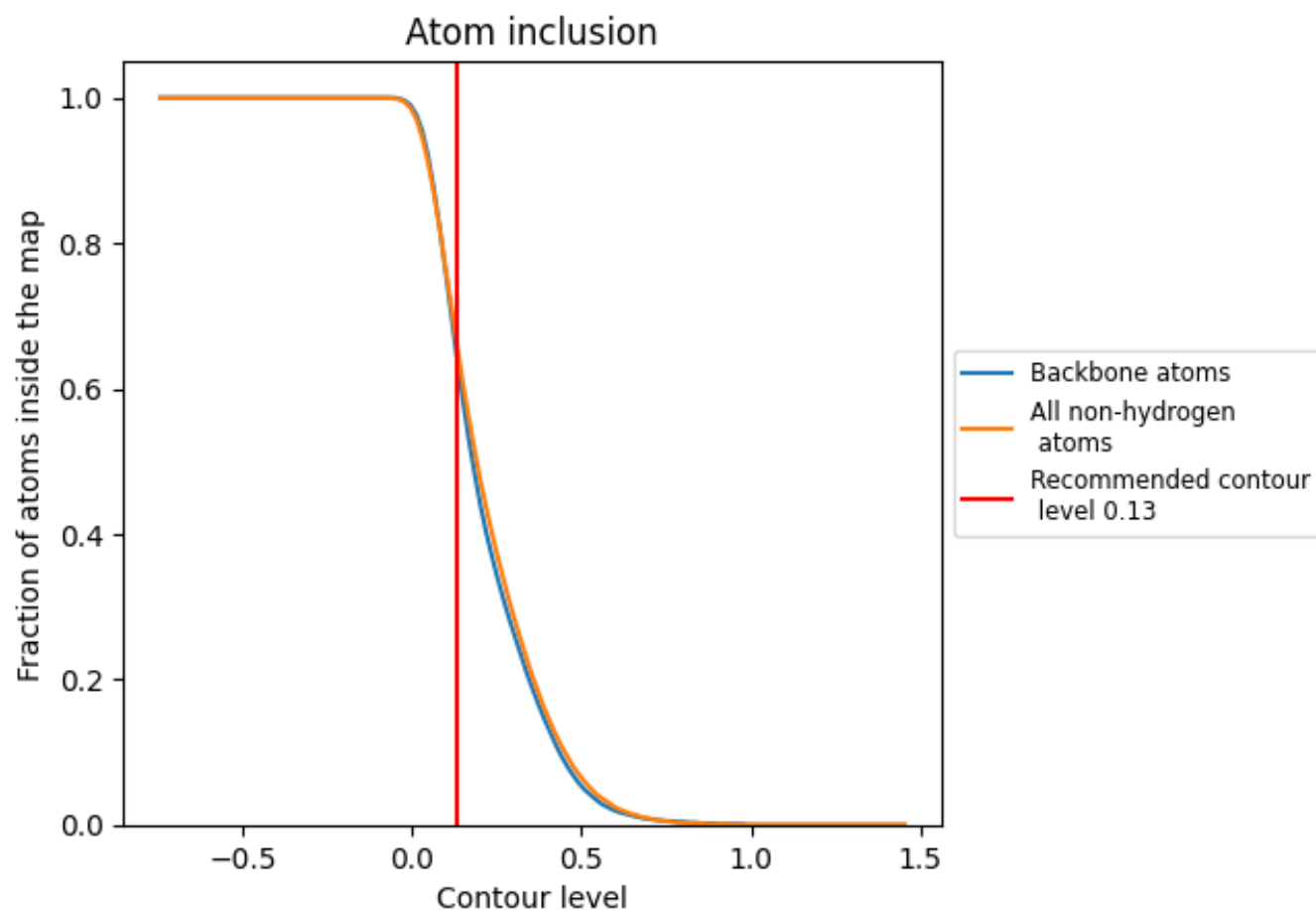
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 67% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.4490
AA	 0.7870	 0.4730
AB	 0.6540	 0.4630
AC	 0.4770	 0.4340
AE	 0.5570	 0.4420
AF	 0.7110	 0.5020
AG	 0.3320	 0.3290
AI	 0.3990	 0.3330
AJ	 0.3240	 0.3080
AK	 0.6590	 0.4780
AL	 0.7300	 0.5200
AN	 0.5280	 0.4060
AO	 0.6030	 0.4290
AP	 0.5490	 0.3920
AQ	 0.6390	 0.4540
AR	 0.7050	 0.4800
AU	 0.7460	 0.5060
AV	 0.4010	 0.3030
AX	 0.1800	 0.1870
AZ	 0.2440	 0.2290
Aa	 0.3800	 0.3060
Ab	 0.5330	 0.4040
Ac	 0.6080	 0.4360
Ad	 0.5070	 0.3310
Ae	 0.1270	 0.1240
Af	 0.5810	 0.4450
Ag	 0.2040	 0.2230
Ah	 0.2320	 0.2310
Ai	 0.3800	 0.3240
Aj	 0.2890	 0.2510
Ak	 0.2460	 0.2530
Am	 0.4920	 0.3980
An	 0.6950	 0.5050
Ao	 0.0670	 0.1060
Ap	 0.5180	 0.3850



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Chain	Atom inclusion	Q-score
B0	 0.8910	 0.5710
B1	 0.7650	 0.4980
B2	 0.8300	 0.5390
B3	 0.8500	 0.5500
B4	 0.5550	 0.3310
B5	 0.8400	 0.5470
B6	 0.6390	 0.4760
B7	 0.9270	 0.6030
B8	 0.9030	 0.5850
B9	 0.8940	 0.5710
BA	 0.9150	 0.5630
BB	 0.5430	 0.2790
BC	 0.4340	 0.3750
BD	 0.8540	 0.5590
BE	 0.8520	 0.5520
BF	 0.8700	 0.5600
BI	 0.6740	 0.4570
BJ	 0.4640	 0.3340
BK	 0.2670	 0.2110
BL	 0.0240	 0.1230
BN	 0.8940	 0.5730
BO	 0.8230	 0.5420
BP	 0.8570	 0.5520
BQ	 0.8270	 0.5420
BR	 0.8690	 0.5640
BS	 0.8160	 0.5240
BT	 0.7610	 0.5120
BU	 0.8770	 0.5630
BV	 0.8390	 0.5520
BW	 0.8640	 0.5650
BX	 0.7950	 0.5120
BY	 0.6430	 0.4670
Ba	 0.8290	 0.5310
Bb	 0.7840	 0.4880
Bc	 0.7520	 0.4910
Bd	 0.4750	 0.2810
Be	 0.7600	 0.4980
Bf	 0.7460	 0.4730
Bg	 0.8780	 0.5640
Bh	 0.7960	 0.5070
Bi	 0.5650	 0.4090
Bj	 0.3400	 0.2220

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Chain	Atom inclusion	Q-score
Bk	 0.5230	 0.3700
Bl	 0.8450	 0.5460
Bm	 0.4910	 0.4160
Bn	 0.8980	 0.5730
Bo	 0.7870	 0.5200
Bp	 0.5690	 0.3840
Bq	 0.4930	 0.3500
Bt	 0.8730	 0.5670
Bu	 0.6080	 0.4020
Bv	 0.6450	 0.4400
Bw	 0.8210	 0.5270
Bx	 0.7890	 0.5160
Bz	 0.0780	 0.0740
CL	 0.0950	 0.1430
DL	 0.0380	 0.0930
EL	 0.0000	 0.0630
FL	 0.0050	 -0.0030
GL	 0.0000	 0.0290
HL	 0.0000	 0.0450