Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 02:01 pm GMT

PDB ID	:	6YDW
EMDB ID	:	EMD-10779
Title	:	55S mammalian mitochondrial ribosome with mtEFG1 and two tRNAMet (TI-POST)
Authors	:	Kummer, E.; Ban, N.
Deposited on	:	2020-03-21
Resolution	:	4.20 Å(reported)

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

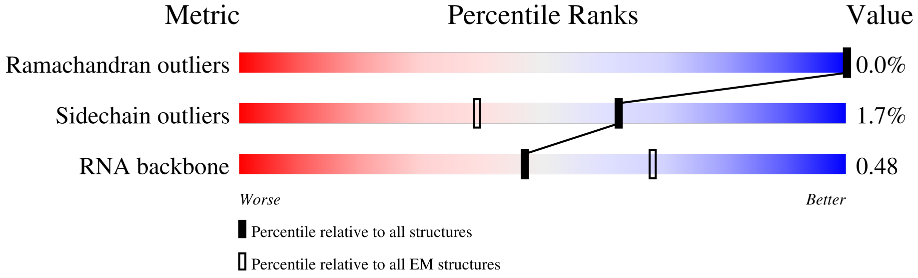
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance ⓘ

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

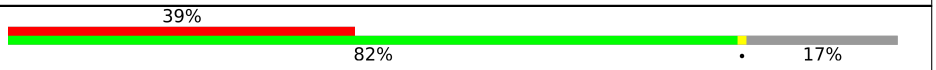
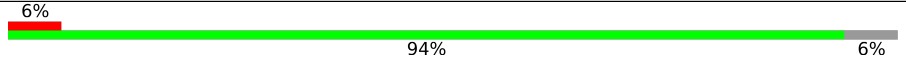
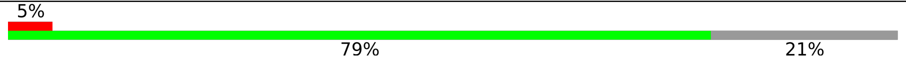
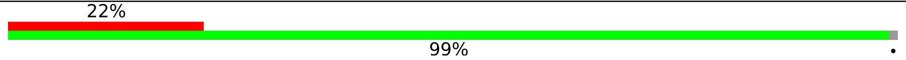
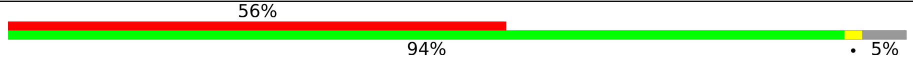
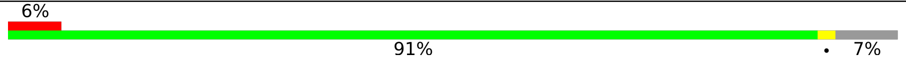
The reported resolution of this entry is 4.20 Å.

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	AI	397	
2	BT	292	
3	BU	149	
4	BV	209	
5	BW	210	
6	BX	150	
7	BY	216	
8	Ba	423	

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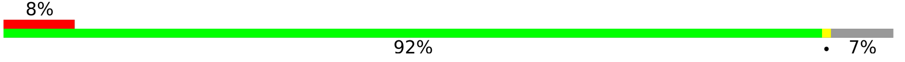
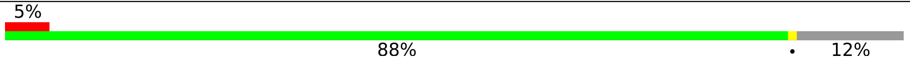
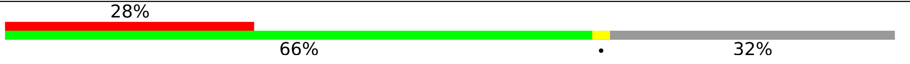
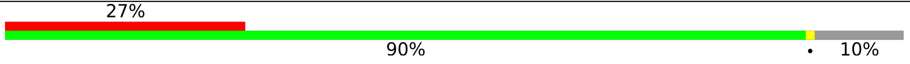
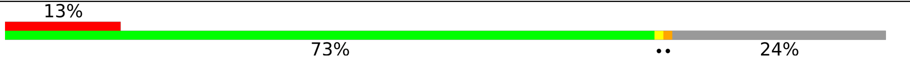
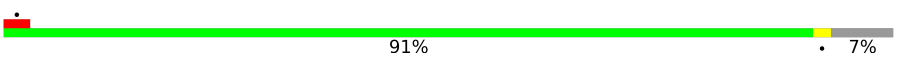
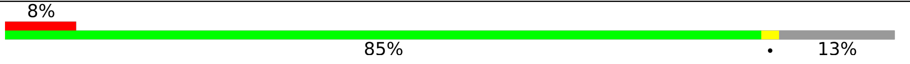
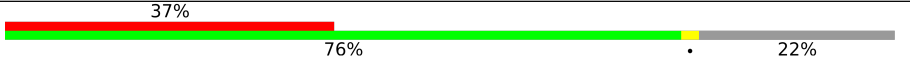
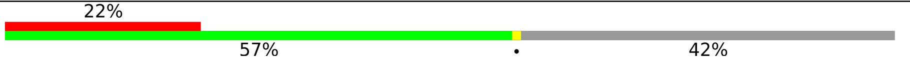
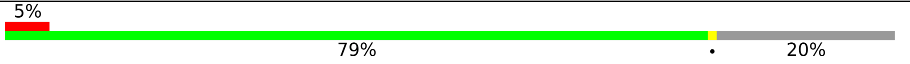
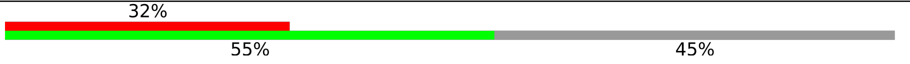
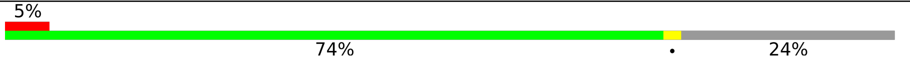
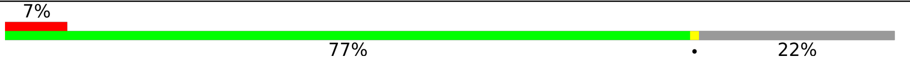
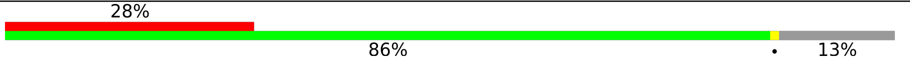
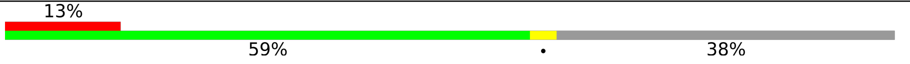
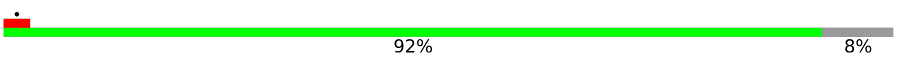
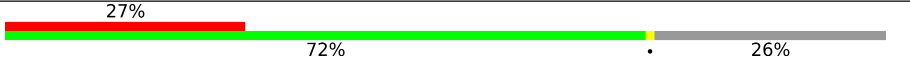
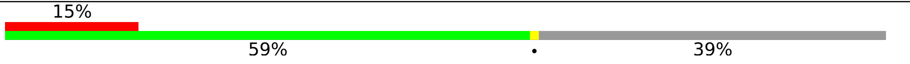
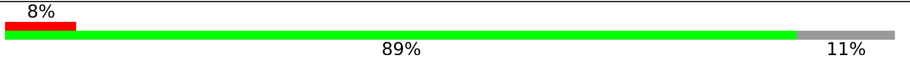
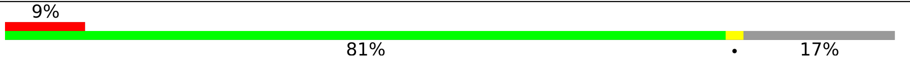
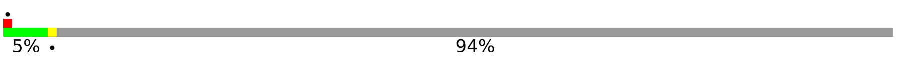
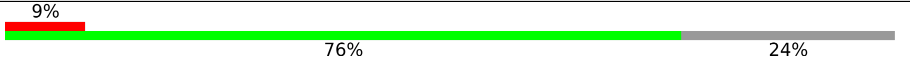
Mol	Chain	Length	Quality of chain
9	Bb	380	
10	Bc	334	
11	Bd	206	
12	Be	135	
13	Bf	142	
14	Bg	159	
15	Bh	332	
16	Bi	306	
17	Bj	279	
18	Bk	269	
19	Bl	166	
20	Bm	198	
21	Bn	128	
22	Bo	124	
23	Bp	112	
24	Bq	138	
25	Bt	102	
26	Bu	205	
27	Bv	222	
28	B0	148	
29	Bw	433	
30	Bx	196	
31	AA	16770	
31	BA	16770	
32	AB	289	

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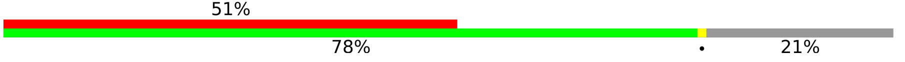
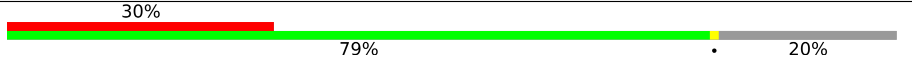
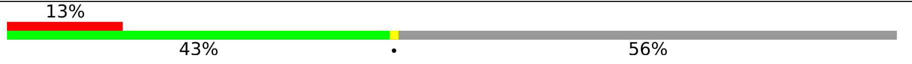
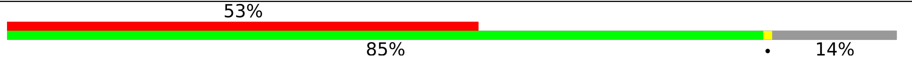
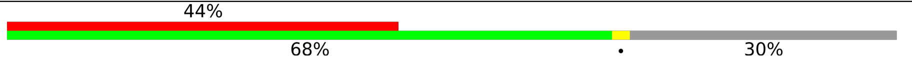
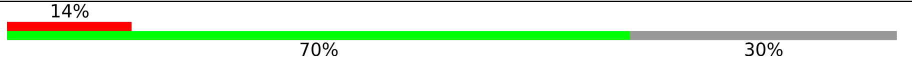
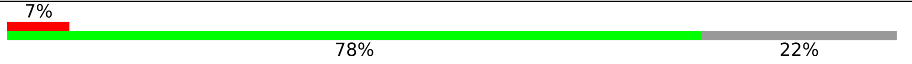
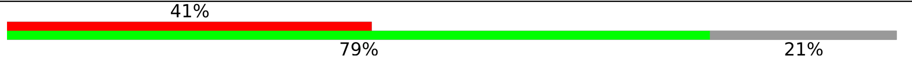
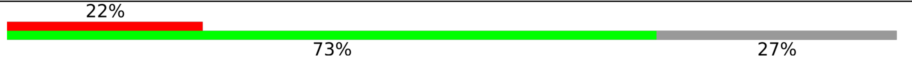
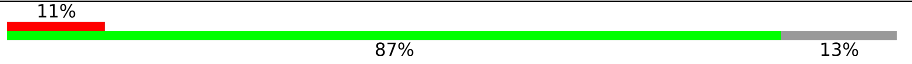
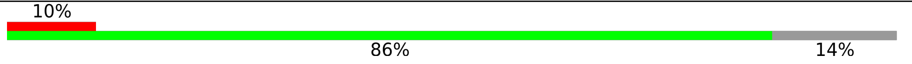
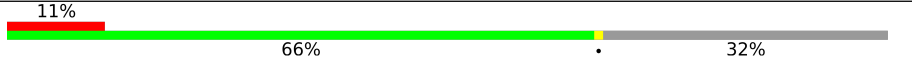
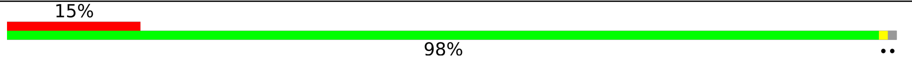
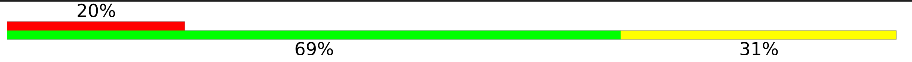
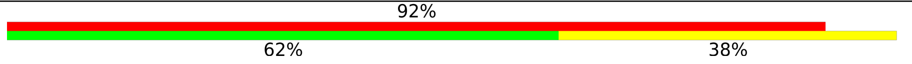
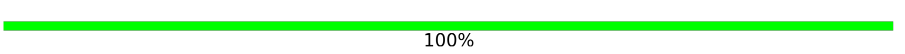
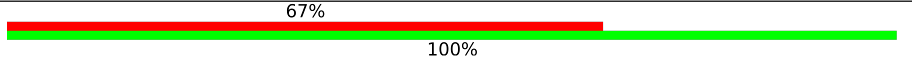
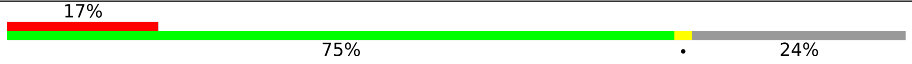
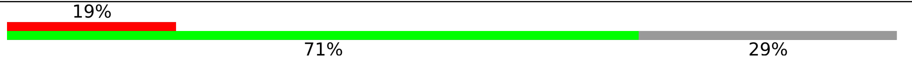
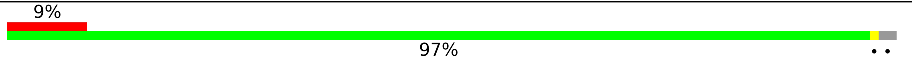
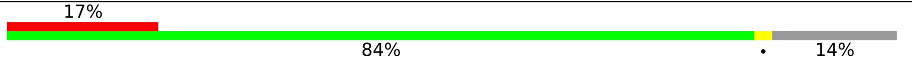
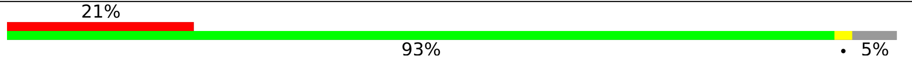
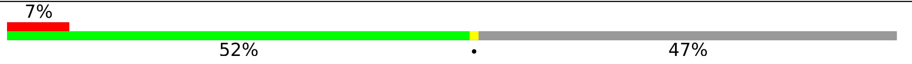
Mol	Chain	Length	Quality of chain
33	AC	167	
34	AE	430	
35	AF	276	
36	AG	242	
37	AJ	200	
38	AK	196	
39	AL	139	
40	AN	128	
41	AO	239	
42	AP	135	
43	AQ	130	
44	AR	143	
45	AU	87	
46	AV	71	
46	AY	71	
47	AX	6	
48	AZ	18	
49	Aa	382	
50	Ab	190	
51	Ac	173	
52	Ad	205	
53	Ae	455	
54	B1	256	
55	Af	188	
56	Ag	410	

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Mol	Chain	Length	Quality of chain
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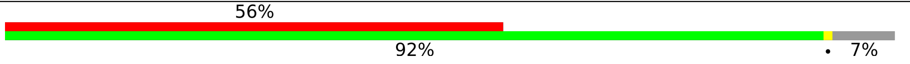
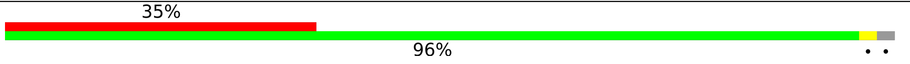
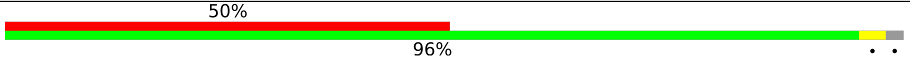
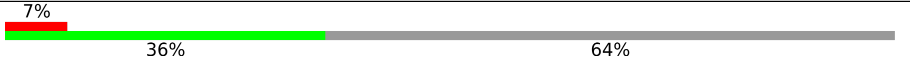
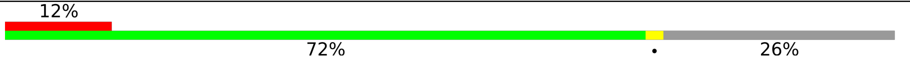
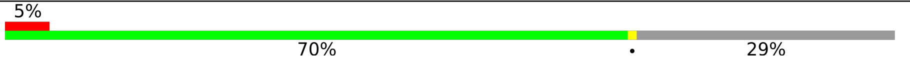
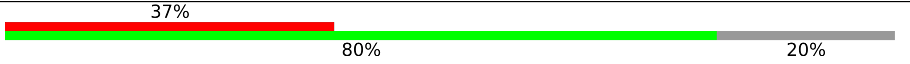
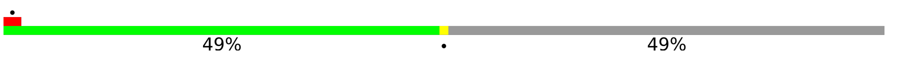
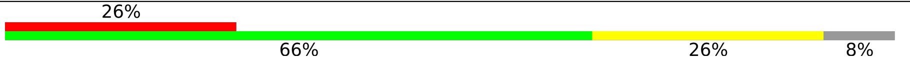
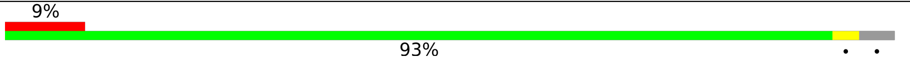
58	Ai	106	
59	Aj	218	
60	Ak	325	
61	Am	118	
62	An	199	
63	Ao	692	
64	Ap	258	
65	CL	198	
65	DL	198	
65	EL	198	
65	FL	198	
65	GL	198	
65	HL	198	
65	LL	198	
66	B2	252	
67	B3	161	
68	B4	126	
69	B5	188	
70	B6	65	
71	B7	95	
72	B8	188	
73	B9	100	
74	BB	73	
75	BC	721	

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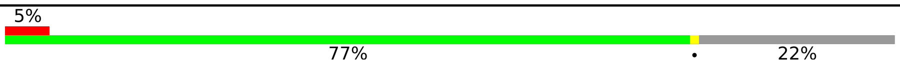
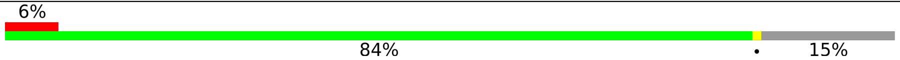
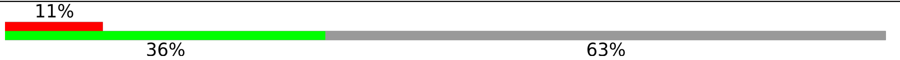
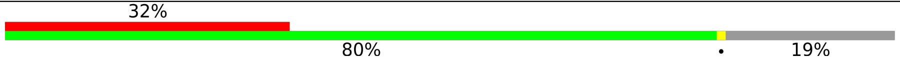
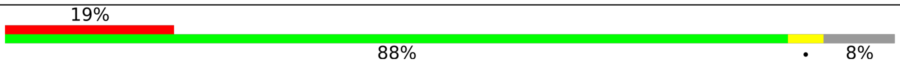
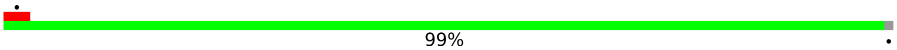
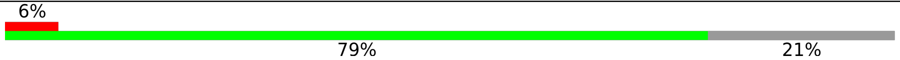
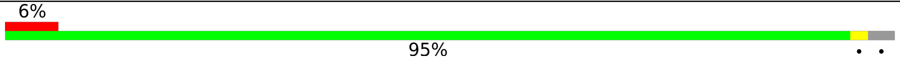
Mol	Chain	Length	Quality of chain
76	BD	306	
77	BE	348	
78	BF	294	
79	BI	268	
80	BJ	262	
81	BK	192	
82	BN	178	
83	BO	145	
84	BP	296	
85	BQ	251	
86	BR	169	
87	BS	180	

2 Entry composition (i)

There are 95 unique types of molecules in this entry. The entry contains 180836 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 Uncharacterized protein.

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

- Molecule 2 is a protein called Mitochondrial ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BT	222	1840	1178	318	335	9	0	0

- Molecule 3 is a protein called Mitochondrial ribosomal protein L20.

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

- Molecule 4 is a protein called Mitochondrial ribosomal protein L21.

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

- Molecule 5 is a protein called Uncharacterized protein.

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

- Molecule 6 is a protein called Uncharacterized protein.

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

- Molecule 7 is a protein called Uncharacterized protein.

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

- Molecule 8 is a protein called Mitochondrial ribosomal protein L37.

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

- Molecule 9 is a protein called Mitochondrial ribosomal protein L38.

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

- Molecule 10 is a protein called Mitochondrial ribosomal protein L39.

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

- Molecule 11 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Bd	140	1177	742	213	221	1	0	0

- Molecule 12 is a protein called Mitochondrial ribosomal protein L41.

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

- Molecule 13 is a protein called Uncharacterized protein.

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

- Molecule 14 is a protein called Mitochondrial ribosomal protein L43.

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

- Molecule 15 is a protein called Uncharacterized protein.

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

- Molecule 16 is a protein called Mitochondrial ribosomal protein L45.

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

- Molecule 17 is a protein called Mitochondrial ribosomal protein L46.

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

- Molecule 18 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 19 is a protein called Mrpl34.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 20 is a protein called Mitochondrial ribosomal protein L50.

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

- Molecule 21 is a protein called Mitochondrial ribosomal protein L51.

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

- Molecule 22 is a protein called Uncharacterized protein.

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

- Molecule 23 is a protein called mL53.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bp	12	ALA	SER	conflict	UNP A0A341D604
Bp	107	SER	GLY	conflict	UNP A0A341D604

- Molecule 24 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Bq	85	697	446	128	121	2	0	0

- Molecule 25 is a protein called Mitochondrial ribosomal protein L57.

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

- Molecule 26 is a protein called Uncharacterized protein.

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

- Molecule 27 is a protein called Uncharacterized protein.

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

- Molecule 28 is a protein called Mitochondrial ribosomal protein L27.

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

- Molecule 29 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 30 is a protein called Mitochondrial ribosomal protein S18A.

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

- Molecule 31 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	AA	960	20411	9162	3708	6581	960	0	0
			Total	C	N	O	P		
31	BA	1544	32844	14750	5972	10578	1544	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	2316	G	A	conflict	GB 347448639
AA	2973	C	U	conflict	GB 347448639
AA	11929	C	U	conflict	GB 347448639
AA	12670	C	U	conflict	GB 347448639

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Chain	Residue	Modelled	Actual	Comment	Reference
AA	13439	A	G	conflict	GB 347448639
AA	14686	A	C	conflict	GB 347448639
AA	15015	G	A	conflict	GB 347448639
AA	15689	U	C	conflict	GB 347448639
AA	15828	G	C	conflict	GB 347448639
AA	16058	G	A	conflict	GB 347448639
BA	1287	G	A	conflict	GB 347448639
BA	1944	C	U	conflict	GB 347448639
BA	10900	C	U	conflict	GB 347448639
BA	11641	C	U	conflict	GB 347448639
BA	12410	A	G	conflict	GB 347448639
BA	13657	A	C	conflict	GB 347448639
BA	13986	G	A	conflict	GB 347448639
BA	14660	U	C	conflict	GB 347448639
BA	14799	G	C	conflict	GB 347448639
BA	15029	G	A	conflict	GB 347448639

- Molecule 32 is a protein called Mitochondrial ribosomal protein S2.

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

- Molecule 33 is a protein called Mitochondrial ribosomal protein S24.

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

- Molecule 34 is a protein called Mitochondrial ribosomal protein S5.

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

- Molecule 35 is a protein called Uncharacterized protein.

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

- Molecule 36 is a protein called Mitochondrial ribosomal protein S7.

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

- Molecule 37 is a protein called Mitochondrial ribosomal protein S10.

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

- Molecule 38 is a protein called uS11m.

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

- Molecule 39 is a protein called Mitochondrial ribosomal protein S12.

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

- Molecule 40 is a protein called Mitochondrial ribosomal protein S14.

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

- Molecule 41 is a protein called uS15m.

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

- Molecule 42 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 43 is a protein called uS17m.

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

- Molecule 44 is a protein called Mitochondrial ribosomal protein S18C.

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

- Molecule 45 is a protein called bS21m.

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

- Molecule 46 is a RNA chain called tRNAMet.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	69	C	-	insertion	GB 1208989970
AV	70	C	-	insertion	GB 1208989970
AV	71	A	-	insertion	GB 1208989970
AY	69	C	-	insertion	GB 1208989970
AY	70	C	-	insertion	GB 1208989970
AY	71	A	-	insertion	GB 1208989970

- Molecule 47 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
47	AX	6	128	57	22	43	6	0	0

- Molecule 48 is a protein called unknown peptide.

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

- Molecule 49 is a protein called Mitochondrial ribosomal protein S22.

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

- Molecule 50 is a protein called mS23.

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

- Molecule 51 is a protein called Mitochondrial ribosomal protein S25.

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

- Molecule 52 is a protein called Mitochondrial ribosomal protein S26.

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

- Molecule 53 is a protein called Mitochondrial ribosomal protein S27.

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

- Molecule 54 is a protein called Mitochondrial ribosomal protein L28.

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

- Molecule 55 is a protein called Mitoribosomal protein ms28, mrps28.

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

- Molecule 56 is a protein called Death associated protein 3.

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

- Molecule 57 is a protein called Mitochondrial ribosomal protein S31.

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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	180	UNK	-	insertion	UNP F1RME2
Ah	181	GLN	-	insertion	UNP F1RME2
Ah	182	LYS	-	insertion	UNP F1RME2
Ah	184	GLY	-	insertion	UNP F1RME2
Ah	185	GLU	LYS	conflict	UNP F1RME2
Ah	187	PRO	LYS	conflict	UNP F1RME2
Ah	189	ILE	LEU	conflict	UNP F1RME2
Ah	190	SER	ILE	conflict	UNP F1RME2
Ah	237	SER	-	insertion	UNP F1RME2
Ah	238	PHE	-	insertion	UNP F1RME2

- Molecule 58 is a protein called mS33.

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

- Molecule 59 is a protein called mS34.

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

- Molecule 60 is a protein called Mitochondrial ribosomal protein S35.

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

- Molecule 61 is a protein called mS37.

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

- Molecule 62 is a protein called Aurora kinase A interacting protein 1.

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

- Molecule 63 is a protein called mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Ao	572	Total	C	N	O	S	0	0
			4525	2897	770	834	24		

- Molecule 64 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 65 is a protein called Mitochondrial ribosomal protein L12.

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

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
65	LL	70	537	346	93	98	0	0

- Molecule 66 is a protein called Mitochondrial ribosomal protein L47.

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

- Molecule 67 is a protein called Uncharacterized protein.

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

- Molecule 68 is a protein called Uncharacterized protein.

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

- Molecule 69 is a protein called Uncharacterized protein.

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

- Molecule 70 is a protein called Uncharacterized protein.

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

- Molecule 71 is a protein called Mitochondrial ribosomal protein L34.

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

- Molecule 72 is a protein called Mitochondrial ribosomal protein L35.

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

- Molecule 73 is a protein called Ribosomal protein.

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

- Molecule 74 is a RNA chain called CP tRNA-Phe.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 75 is a protein called Elongation factor G, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	BC	694	5425	3422	935	1035	33	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	31	GLY	-	expression tag	UNP Q96RP9
BC	32	GLY	-	expression tag	UNP Q96RP9
BC	33	SER	-	expression tag	UNP Q96RP9
BC	34	GLY	-	expression tag	UNP Q96RP9
BC	35	SER	-	expression tag	UNP Q96RP9
BC	36	GLY	-	expression tag	UNP Q96RP9

- Molecule 76 is a protein called Uncharacterized protein.

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

- Molecule 77 is a protein called ICT1.

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

- Molecule 78 is a protein called Mitochondrial ribosomal protein L4.

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

- Molecule 79 is a protein called Mitochondrial ribosomal protein L9.

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

- Molecule 80 is a protein called Mitochondrial ribosomal protein L10.

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

- Molecule 81 is a protein called Mitochondrial ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	BK	176	Total	C	N	O	S	0	0
			1339	851	243	243	2		

- Molecule 82 is a protein called Uncharacterized protein.

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

- Molecule 83 is a protein called Uncharacterized protein.

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

- Molecule 84 is a protein called Uncharacterized protein.

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

- Molecule 85 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	BQ	222	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 86 is a protein called Uncharacterized protein.

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

- Molecule 87 is a protein called Mitochondrial ribosomal protein L18.

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

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	BW	1	Total 1	Mg 1	0
88	Be	1	Total 1	Mg 1	0
88	Bl	1	Total 1	Mg 1	0
88	Bq	1	Total 1	Mg 1	0
88	Bt	1	Total 1	Mg 1	0
88	B0	1	Total 1	Mg 1	0
88	AA	102	Total 102	Mg 102	0

Continued on next page...

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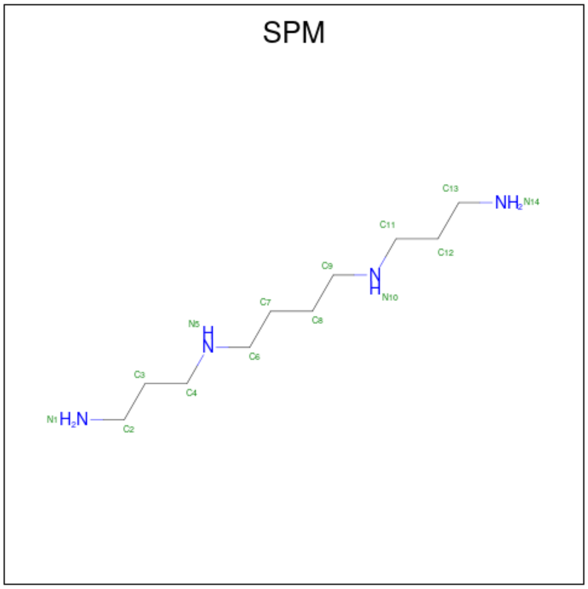
Mol	Chain	Residues	Atoms	AltConf
88	AB	1	Total Mg 1 1	0
88	AX	1	Total Mg 1 1	0
88	Ag	1	Total Mg 1 1	0
88	Am	1	Total Mg 1 1	0
88	An	1	Total Mg 1 1	0
88	BA	200	Total Mg 200 200	0
88	BB	1	Total Mg 1 1	0
88	BC	2	Total Mg 2 2	0
88	BD	3	Total Mg 3 3	0
88	BF	1	Total Mg 1 1	0
88	BJ	1	Total Mg 1 1	0
88	BP	3	Total Mg 3 3	0
88	BQ	1	Total Mg 1 1	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

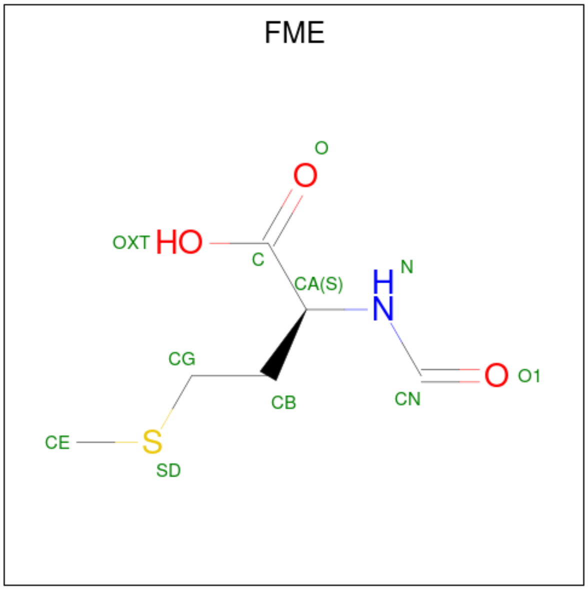
Mol	Chain	Residues	Atoms	AltConf
89	Bx	1	Total Zn 1 1	0
89	AR	1	Total Zn 1 1	0
89	Ac	1	Total Zn 1 1	0
89	Ap	1	Total Zn 1 1	0
89	B5	1	Total Zn 1 1	0
89	B9	1	Total Zn 1 1	0

- Molecule 90 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



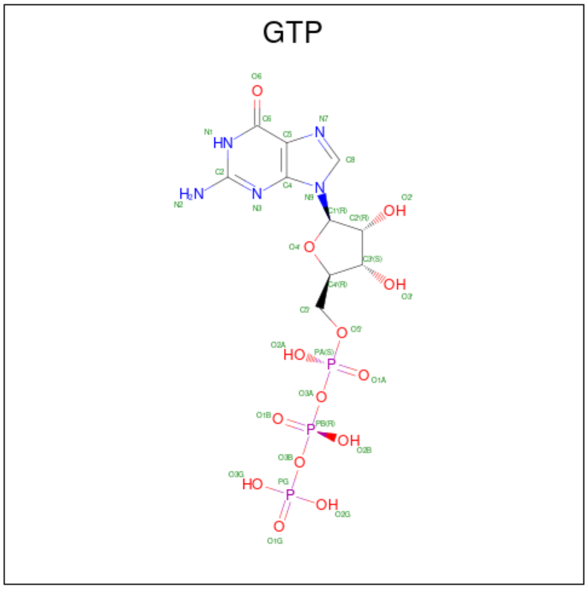
Mol	Chain	Residues	Atoms	AltConf
90	AA	1	Total C N 14 10 4	0
90	BA	1	Total C N 28 20 8	0
90	BA	1	Total C N 28 20 8	0

- Molecule 91 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$) (labeled as "Ligand of Interest" by depositor).



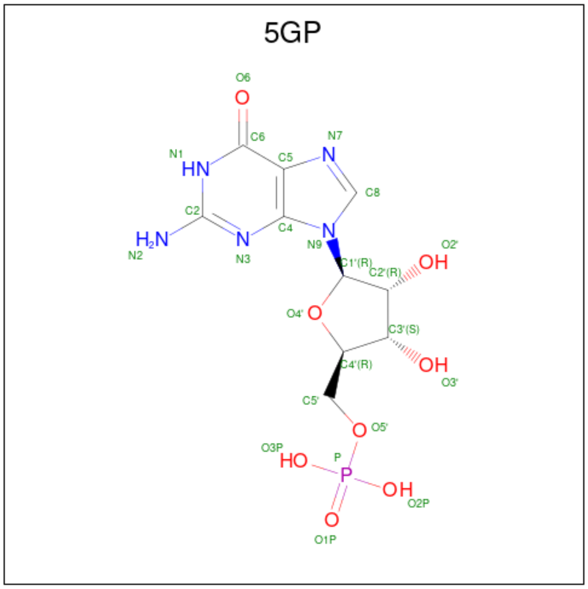
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
91	AV	1	10	6	1	2	1	0

- Molecule 92 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



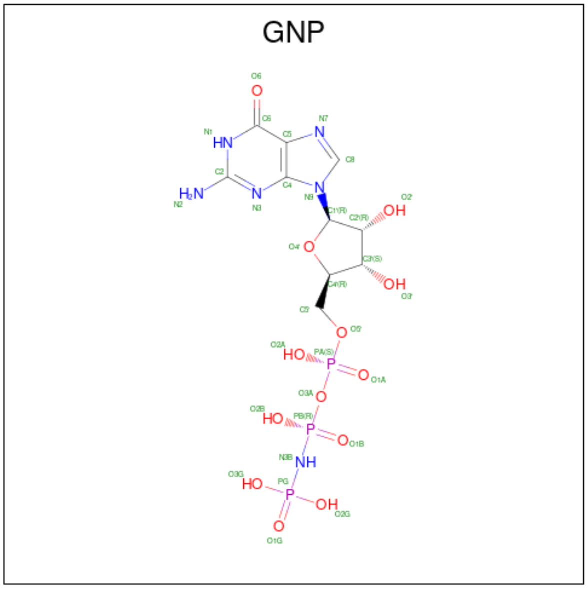
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
92	Ag	1	32	10	5	14	3	0

- Molecule 93 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



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

- Molecule 94 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
94	BC	1	Total 32	C 10	N 6	O 13	P 3	0

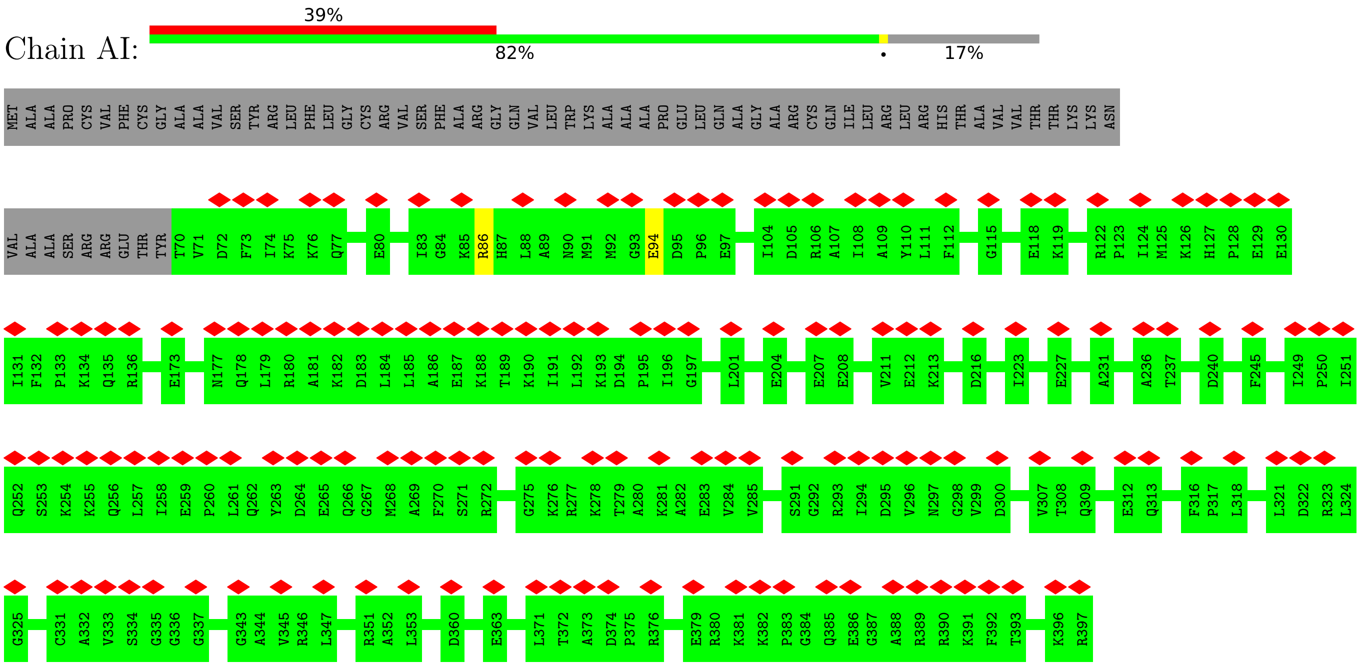
- Molecule 95 is water.

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

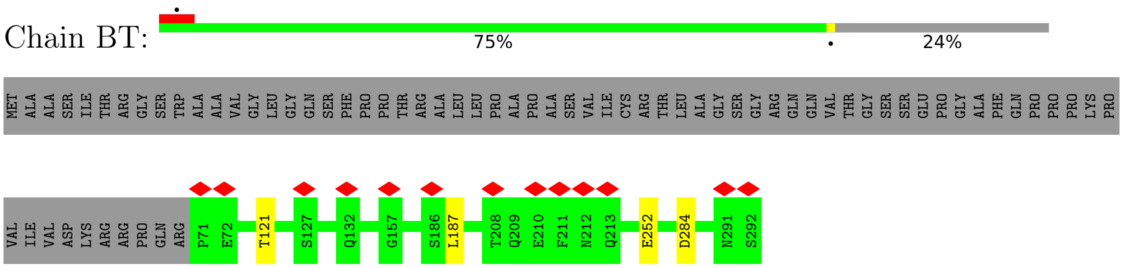
3 Residue-property plots ⓘ

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

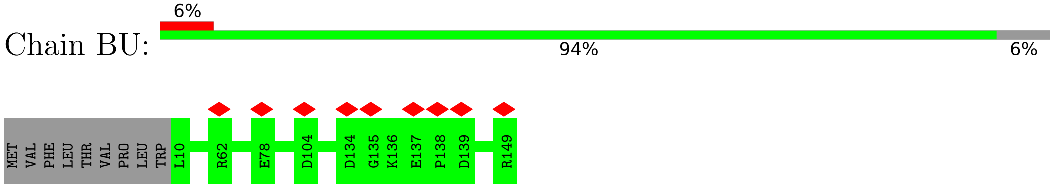
- Molecule 1: Uncharacterized protein



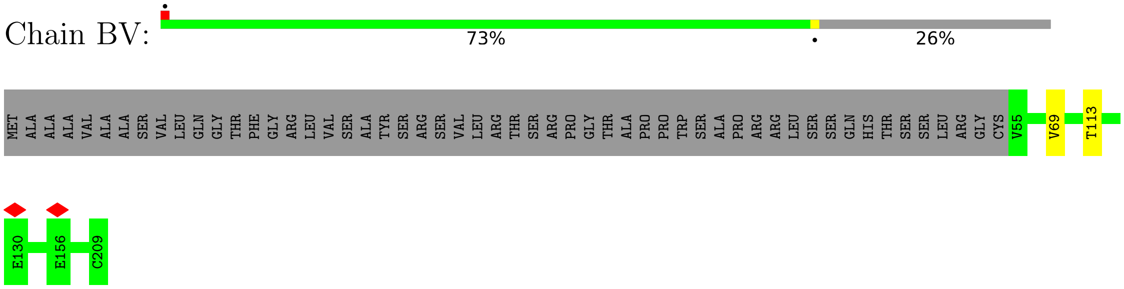
- Molecule 2: Mitochondrial ribosomal protein L19



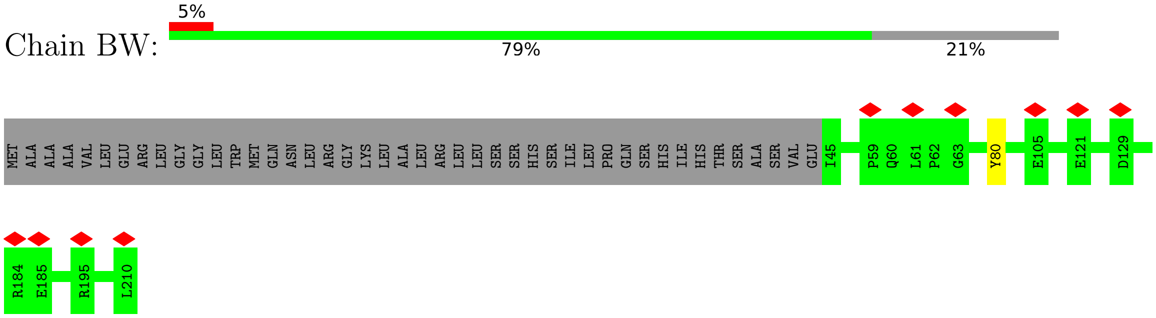
- Molecule 3: Mitochondrial ribosomal protein L20



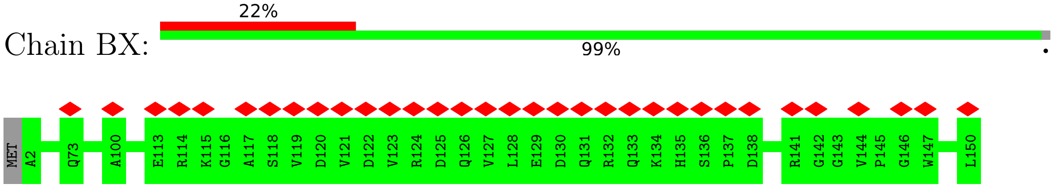
- Molecule 4: Mitochondrial ribosomal protein L21



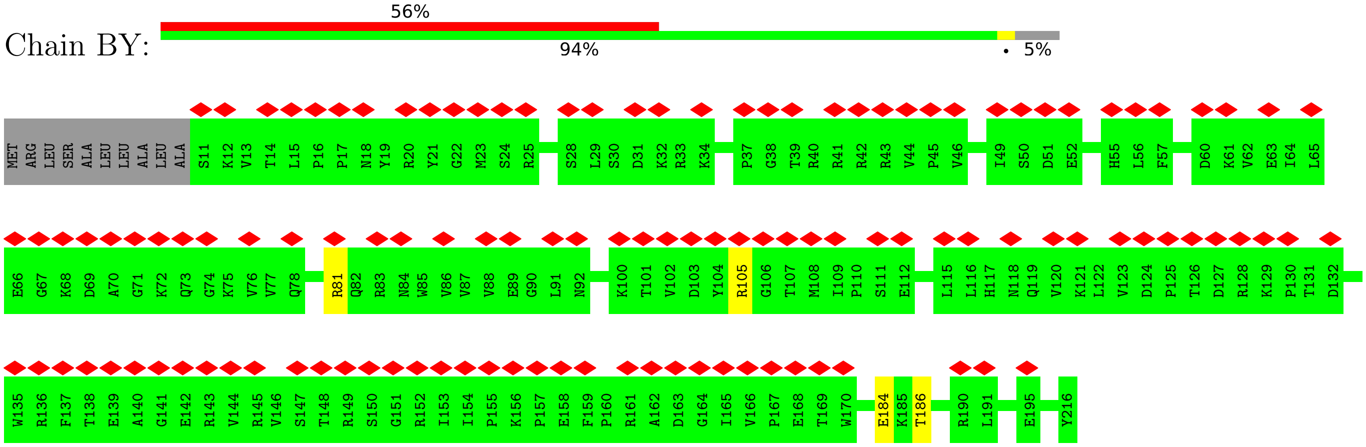
- Molecule 5: Uncharacterized protein



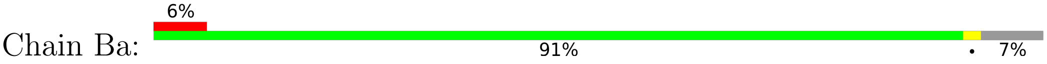
- Molecule 6: Uncharacterized protein

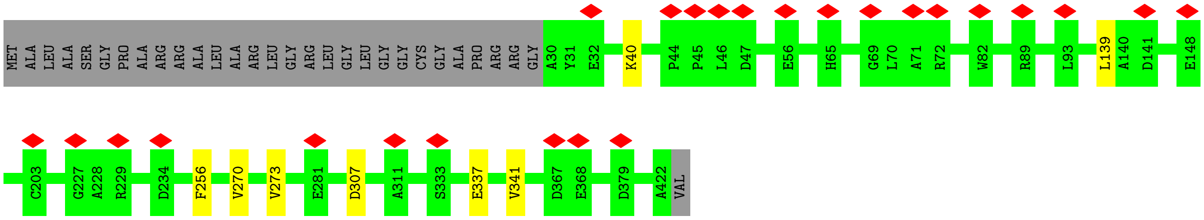


- Molecule 7: Uncharacterized protein



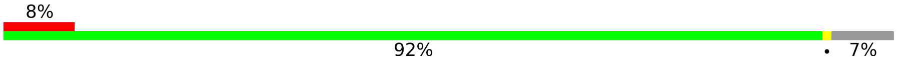
- Molecule 8: Mitochondrial ribosomal protein L37

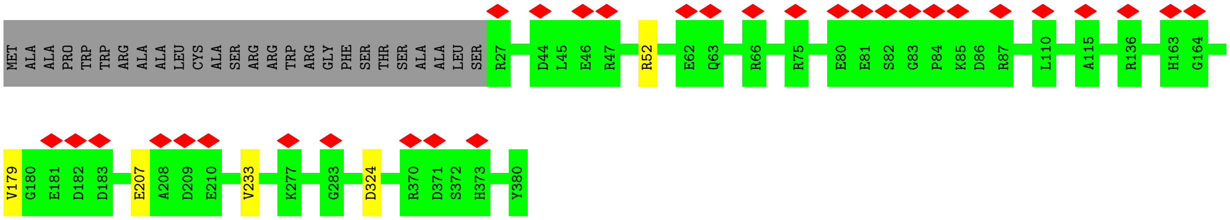




- Molecule 9: Mitochondrial ribosomal protein L38

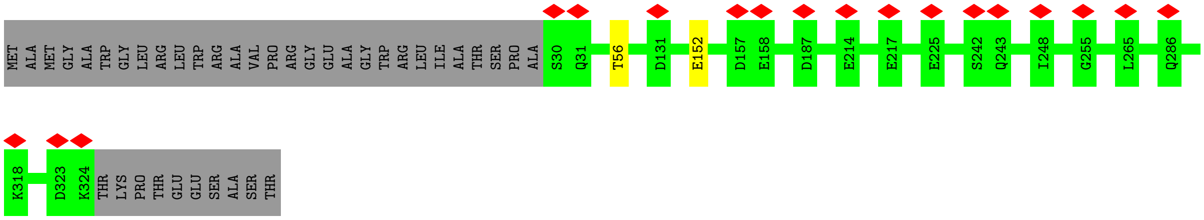
Chain Bb:





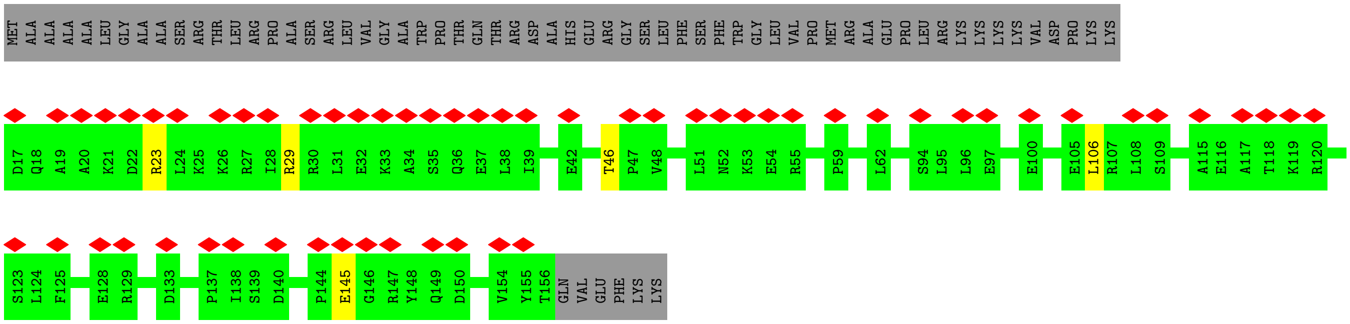
- Molecule 10: Mitochondrial ribosomal protein L39

Chain Bc:



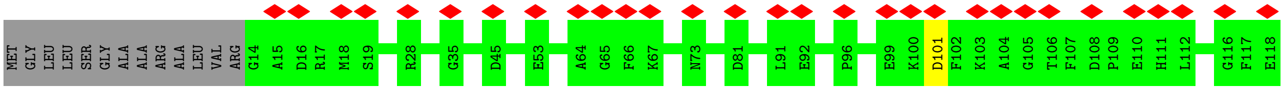
- Molecule 11: Uncharacterized protein

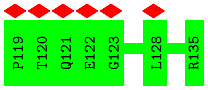
Chain Bd:



- Molecule 12: Mitochondrial ribosomal protein L41

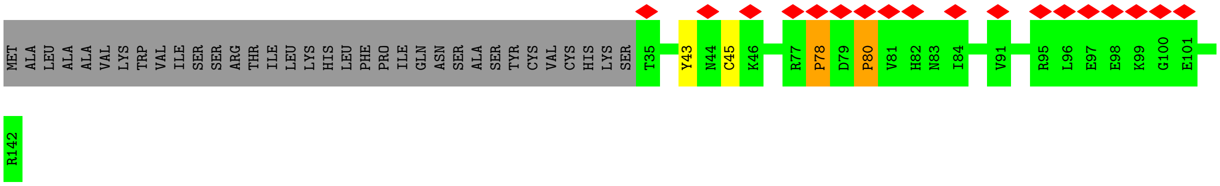
Chain Be:





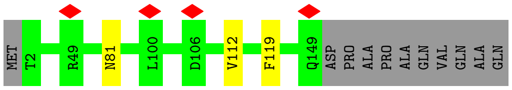
- Molecule 13: Uncharacterized protein

Chain Bf:



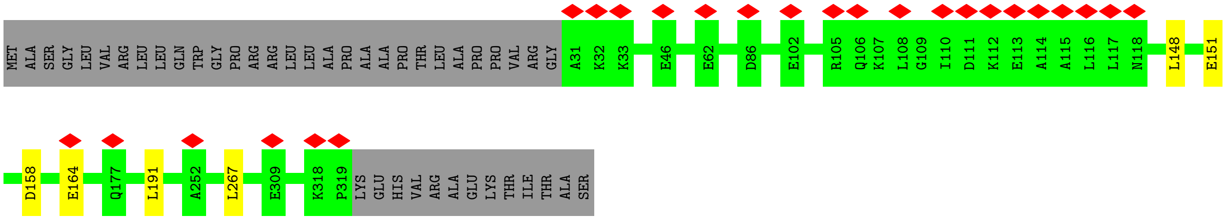
- Molecule 14: Mitochondrial ribosomal protein L43

Chain Bg:



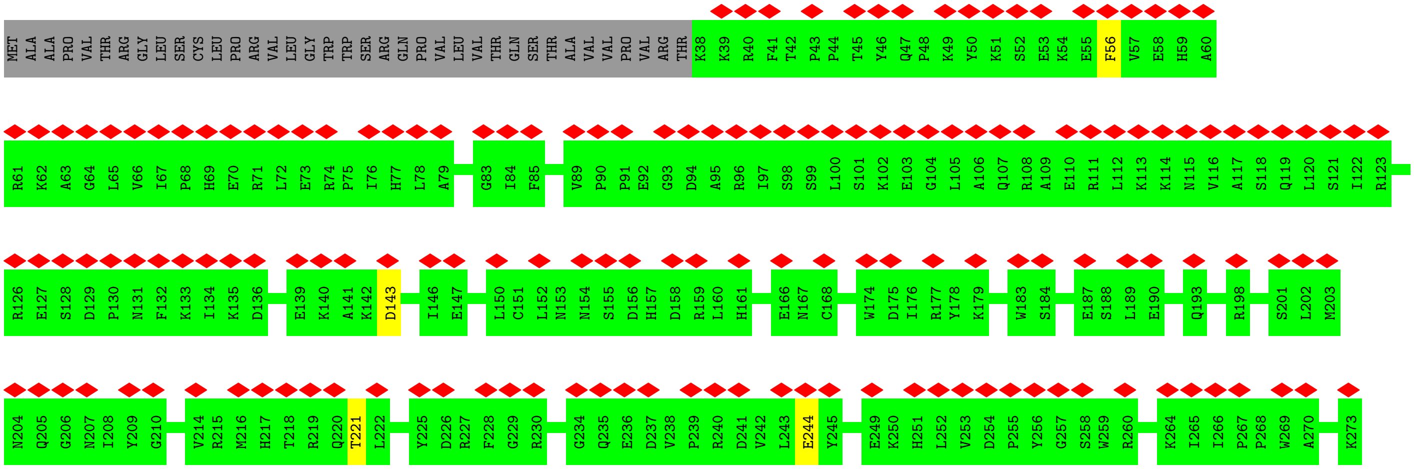
- Molecule 15: Uncharacterized protein

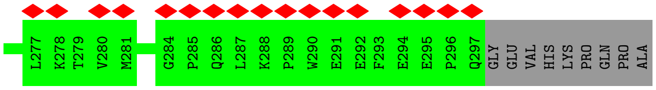
Chain Bh:



- Molecule 16: Mitochondrial ribosomal protein L45

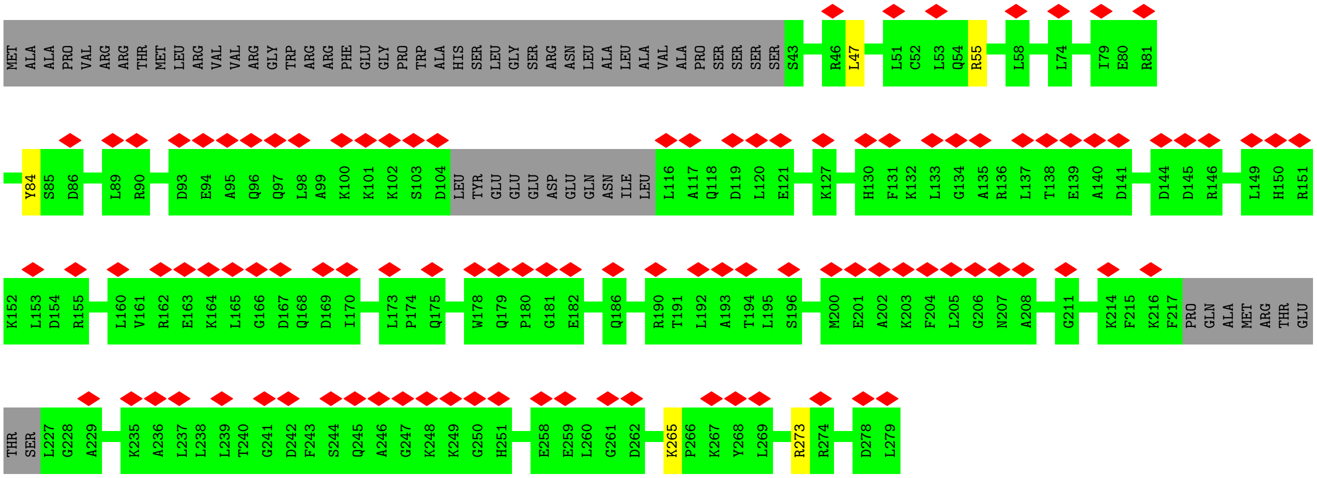
Chain Bi:





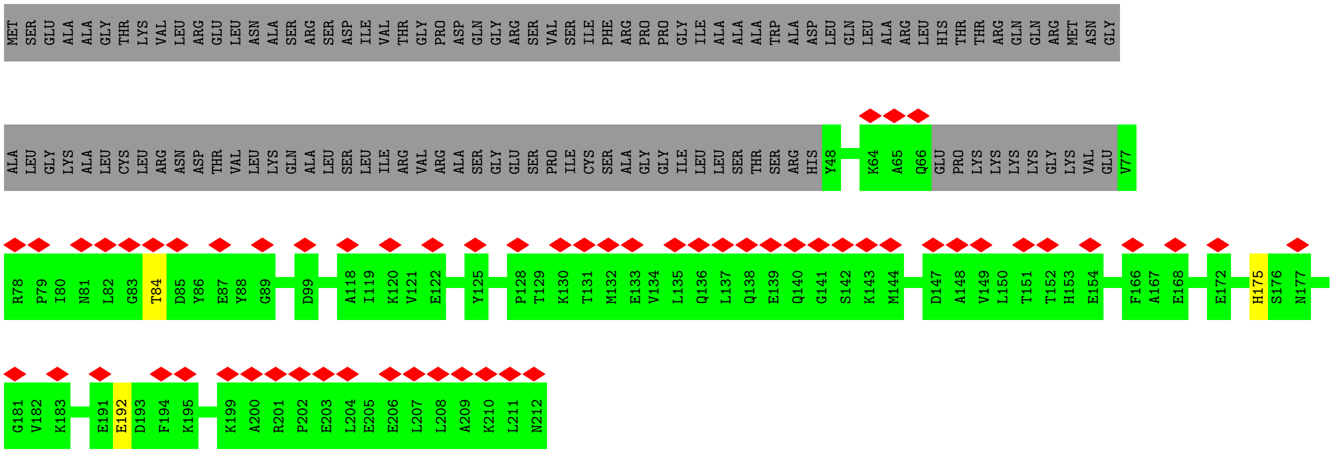
- Molecule 17: Mitochondrial ribosomal protein L46

Chain Bj:



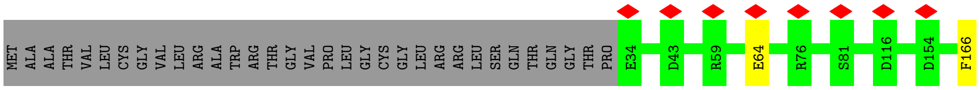
- Molecule 18: 39S ribosomal protein L48, mitochondrial

Chain Bk:



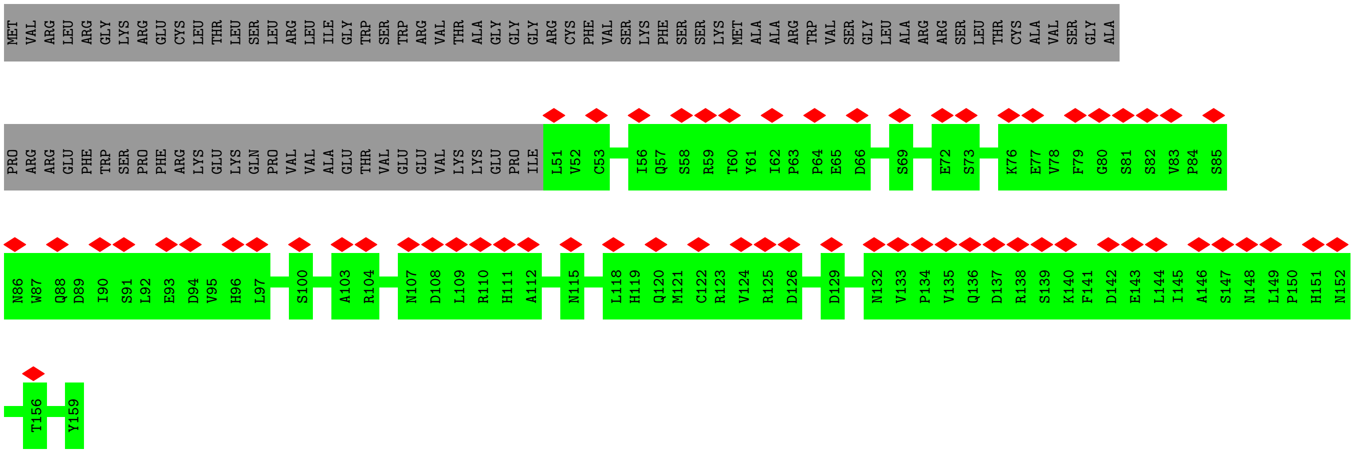
- Molecule 19: Mrpl34

Chain Bl:



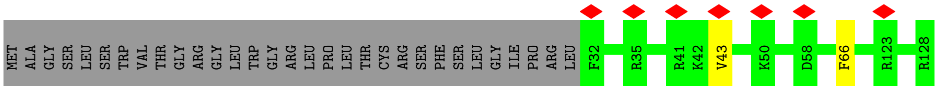
- Molecule 20: Mitochondrial ribosomal protein L50

Chain Bm:



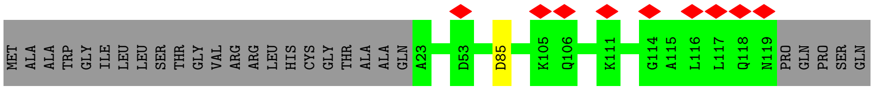
- Molecule 21: Mitochondrial ribosomal protein L51

Chain Bn:



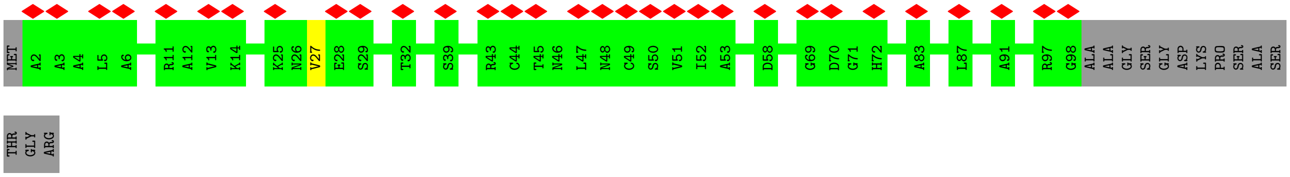
- Molecule 22: Uncharacterized protein

Chain Bo:



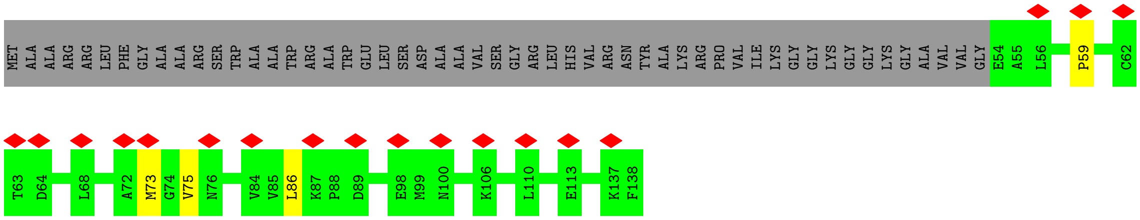
- Molecule 23: mL53

Chain Bp:

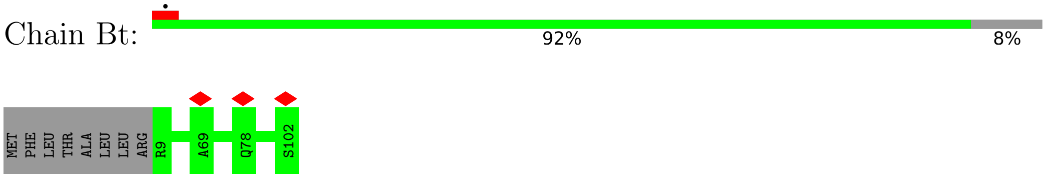


- Molecule 24: Uncharacterized protein

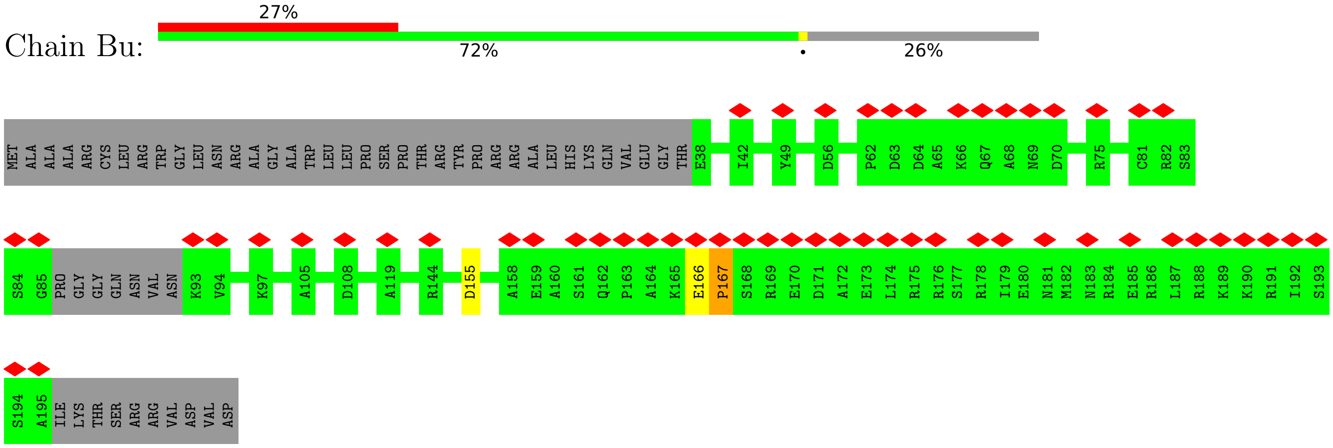
Chain Bq:



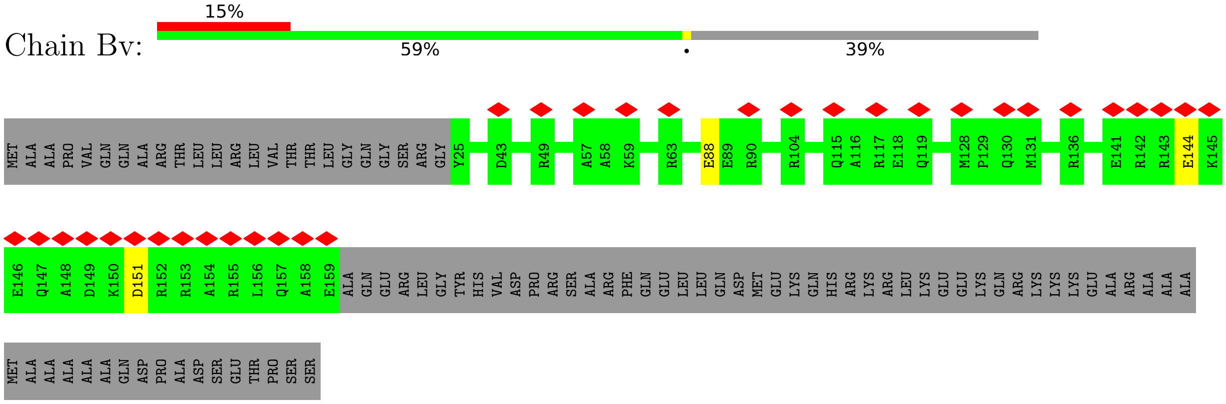
• Molecule 25: Mitochondrial ribosomal protein L57



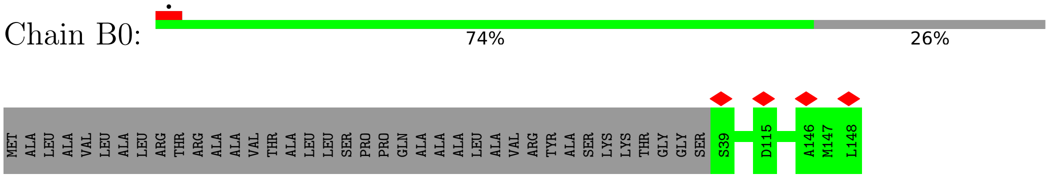
• Molecule 26: Uncharacterized protein



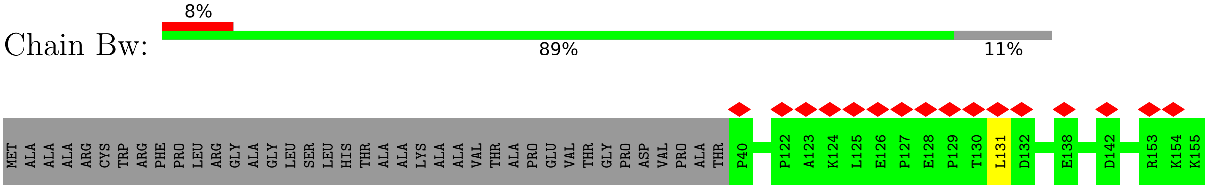
• Molecule 27: Uncharacterized protein

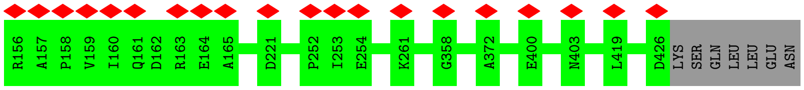


• Molecule 28: Mitochondrial ribosomal protein L27



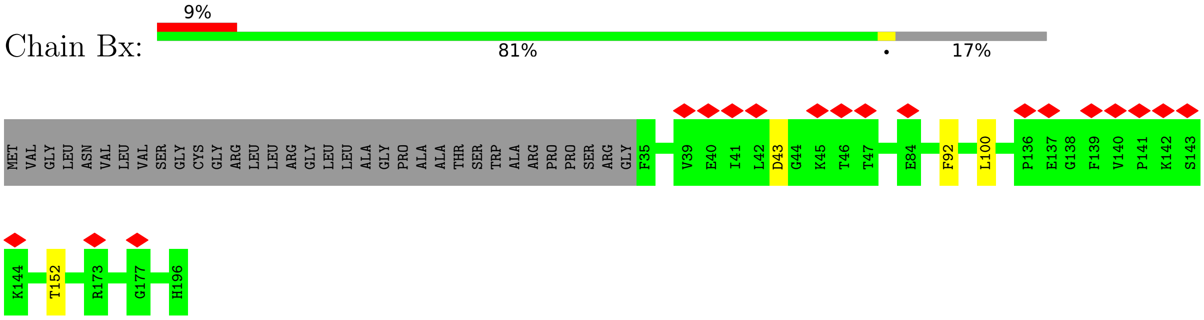
• Molecule 29: 39S ribosomal protein S30, mitochondrial





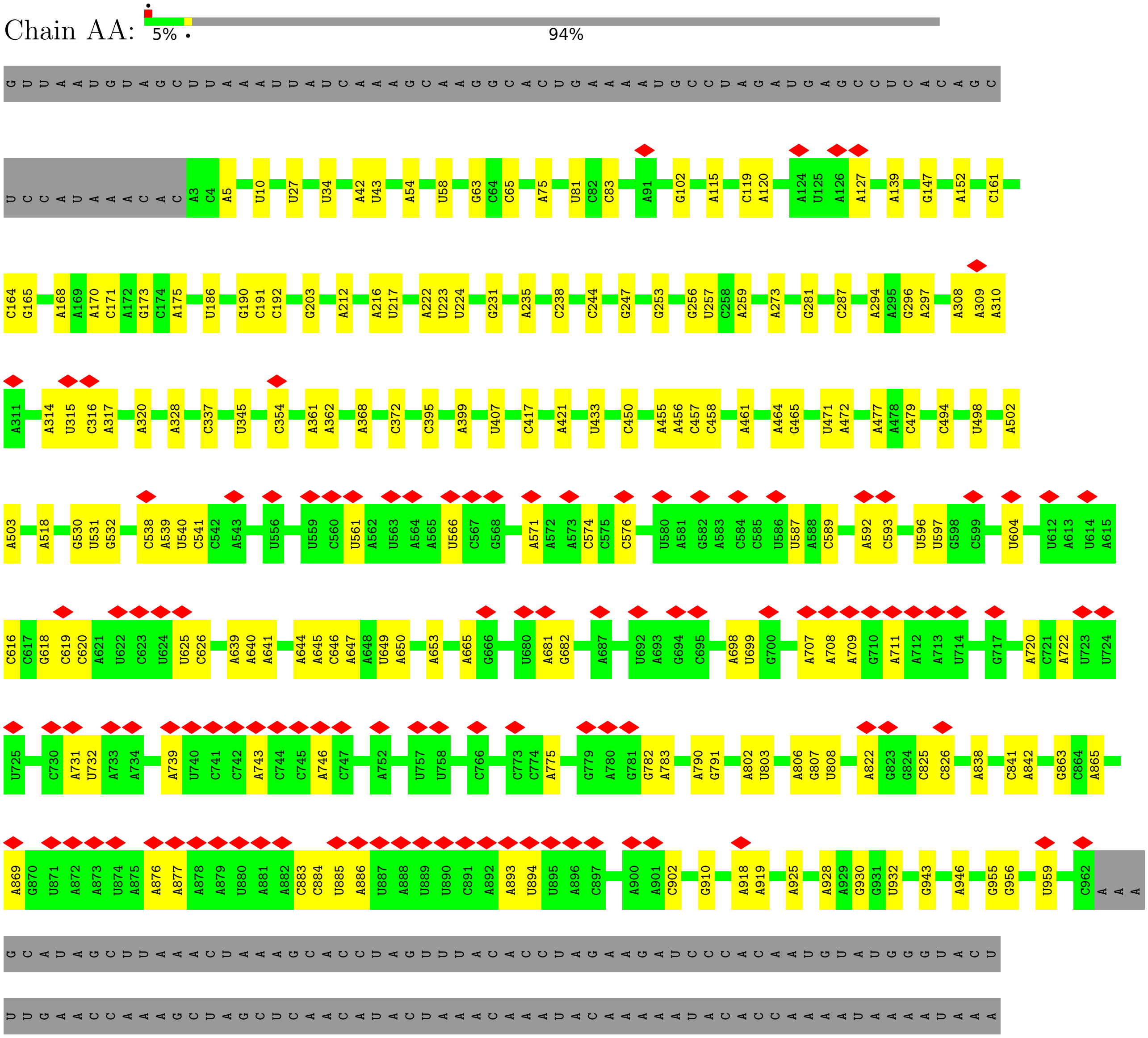
- Molecule 30: Mitochondrial ribosomal protein S18A

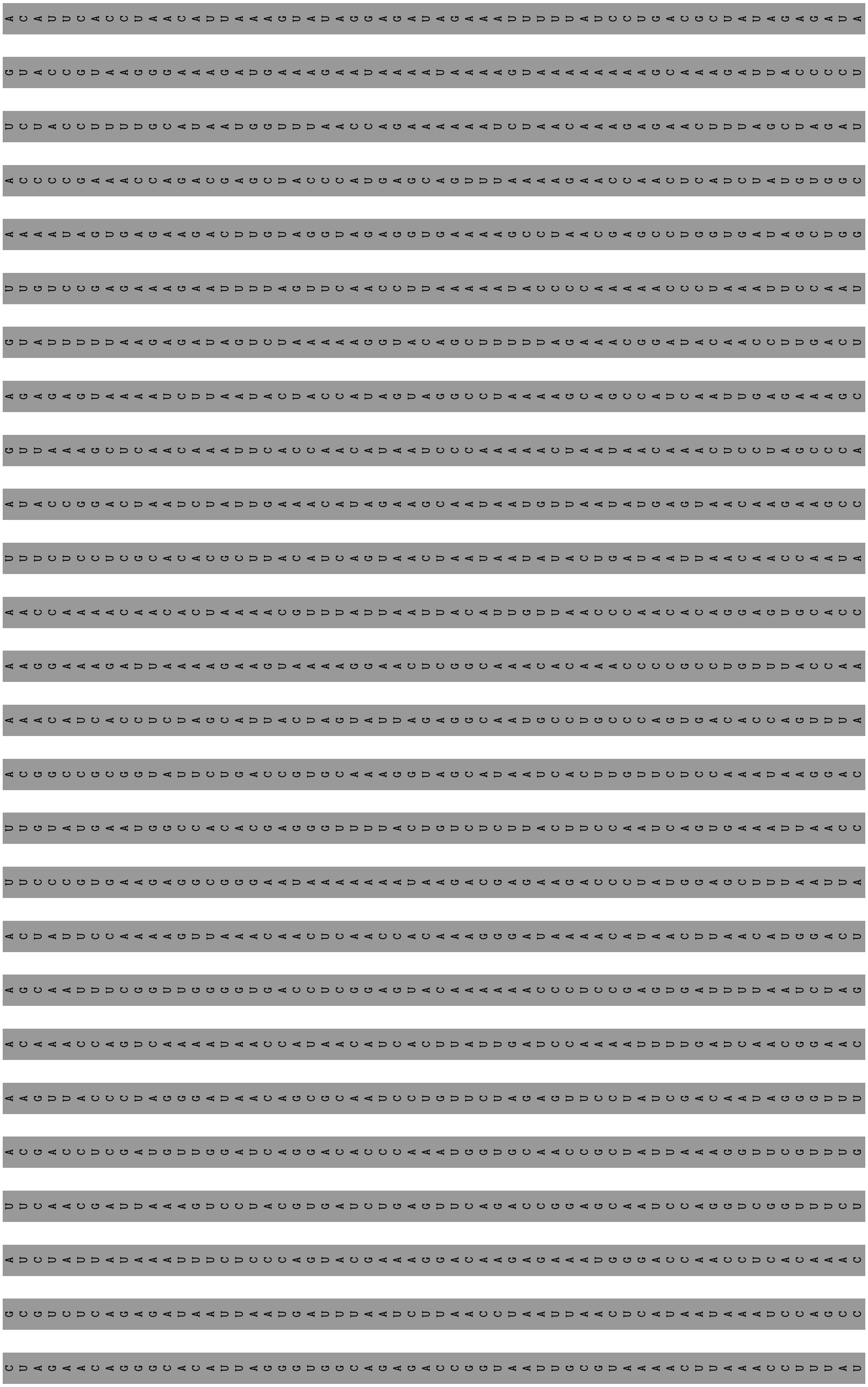
Chain Bx:



- Molecule 31: 12S rRNA

Chain AA:




A C A U U C A C C U A A C A U U A A A G U A U A G G A G A U A G A A A U U U U A U C C U G A C G C U A U A G A G A U A
G U A C C G U A A G G G A A A G A U G A A A G A A U A A A A U A A A A G U A A A A A A A A G C A A A G A U U A C C C C U
U C U A C C U U U U G C A U A A U G G U U U A A C C A G A A A A A A U C U A A C A A A G A G A A C U U U A G C U A G A U
A C C C C G A A A C C A G A C G A G C U A C C C A U G A G C A G U U U A A A A G A A C C A A C U C A U C U A U G U G G C
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A U A C C G G A C U A A U C U A U U G A A A C A U A G A A G C A A U A A U G U U A A U A U G A G U A A C A A G A A G C C
U U U C U C C U C G C A C A C G C U U A C A U C A G U A A C U A A U A A U A U A C U G A U A A U U A A C A A C C A A U A
A A C C A A A A C A A C A C U A A A A C G U U U A U U A A U U A C A U U G U U A A C C C A A C A C A G G A G U G C A C C
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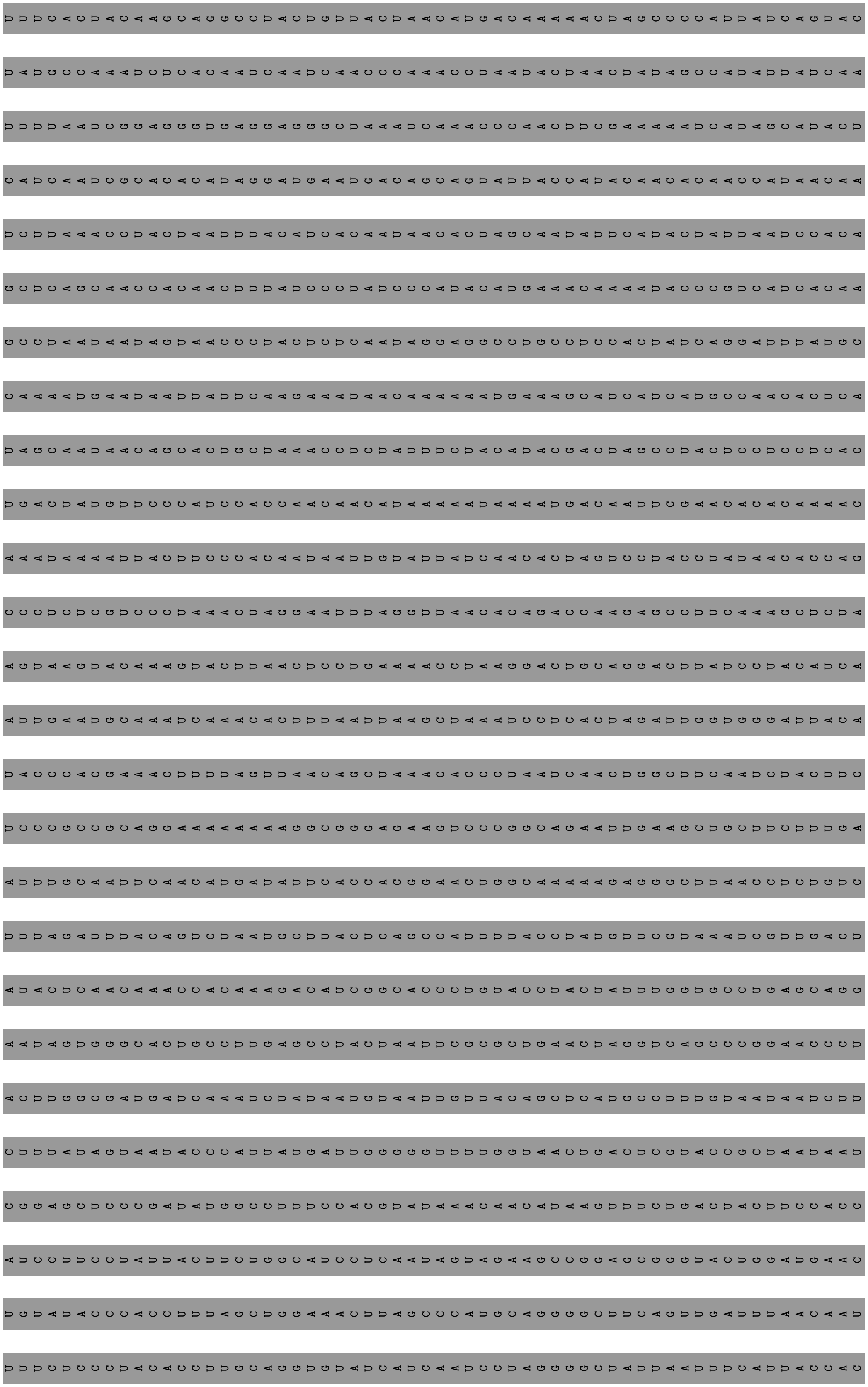
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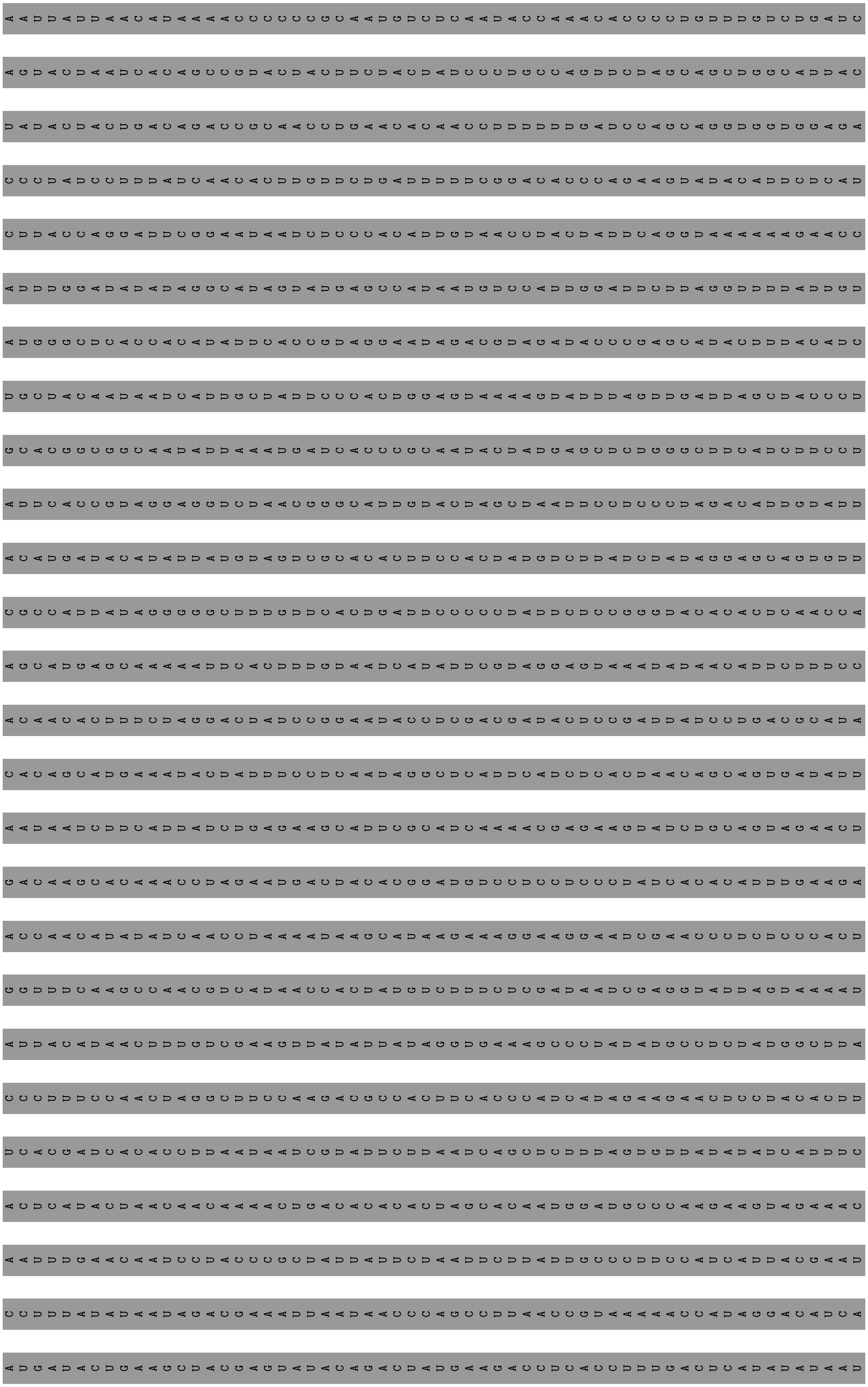
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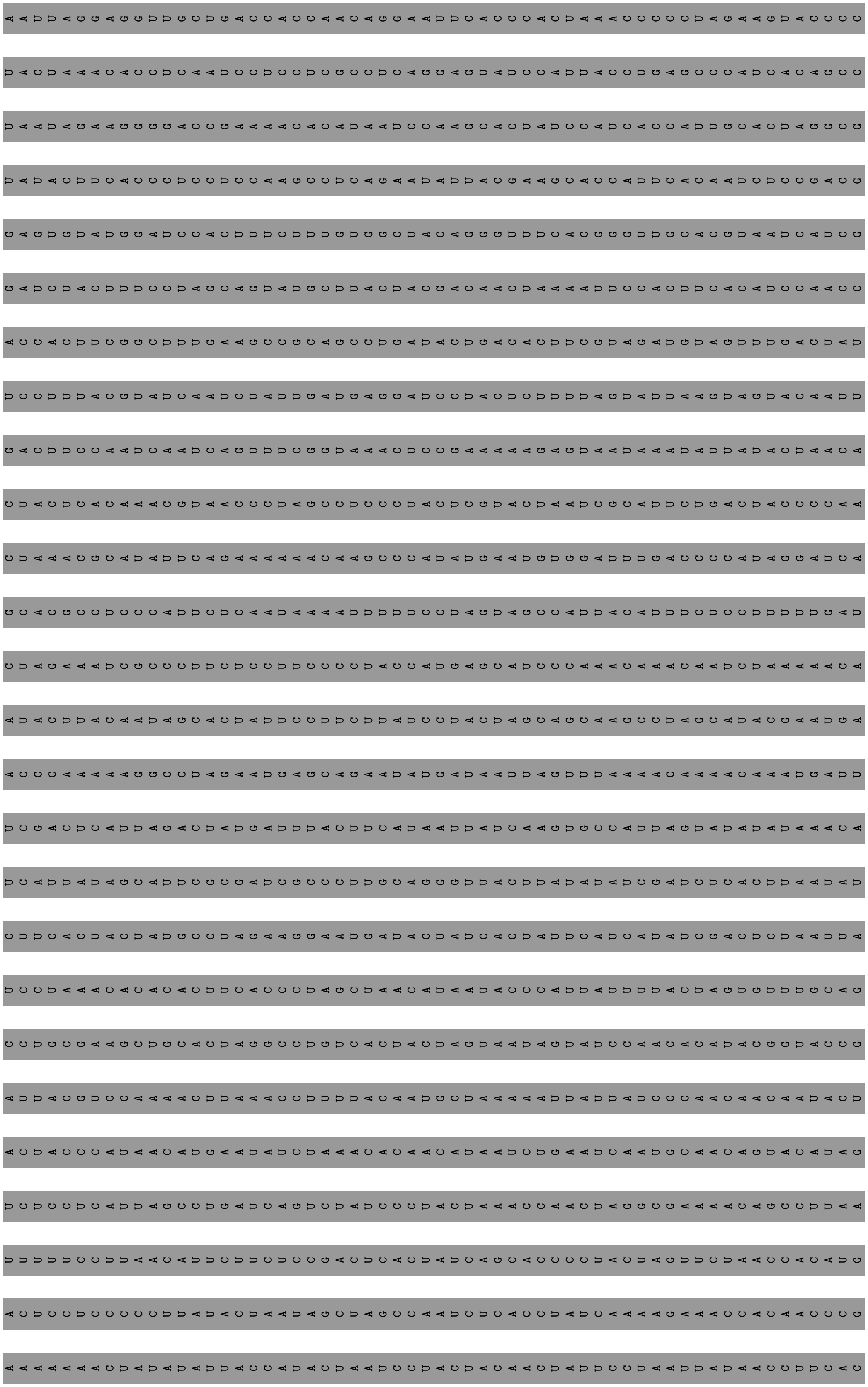

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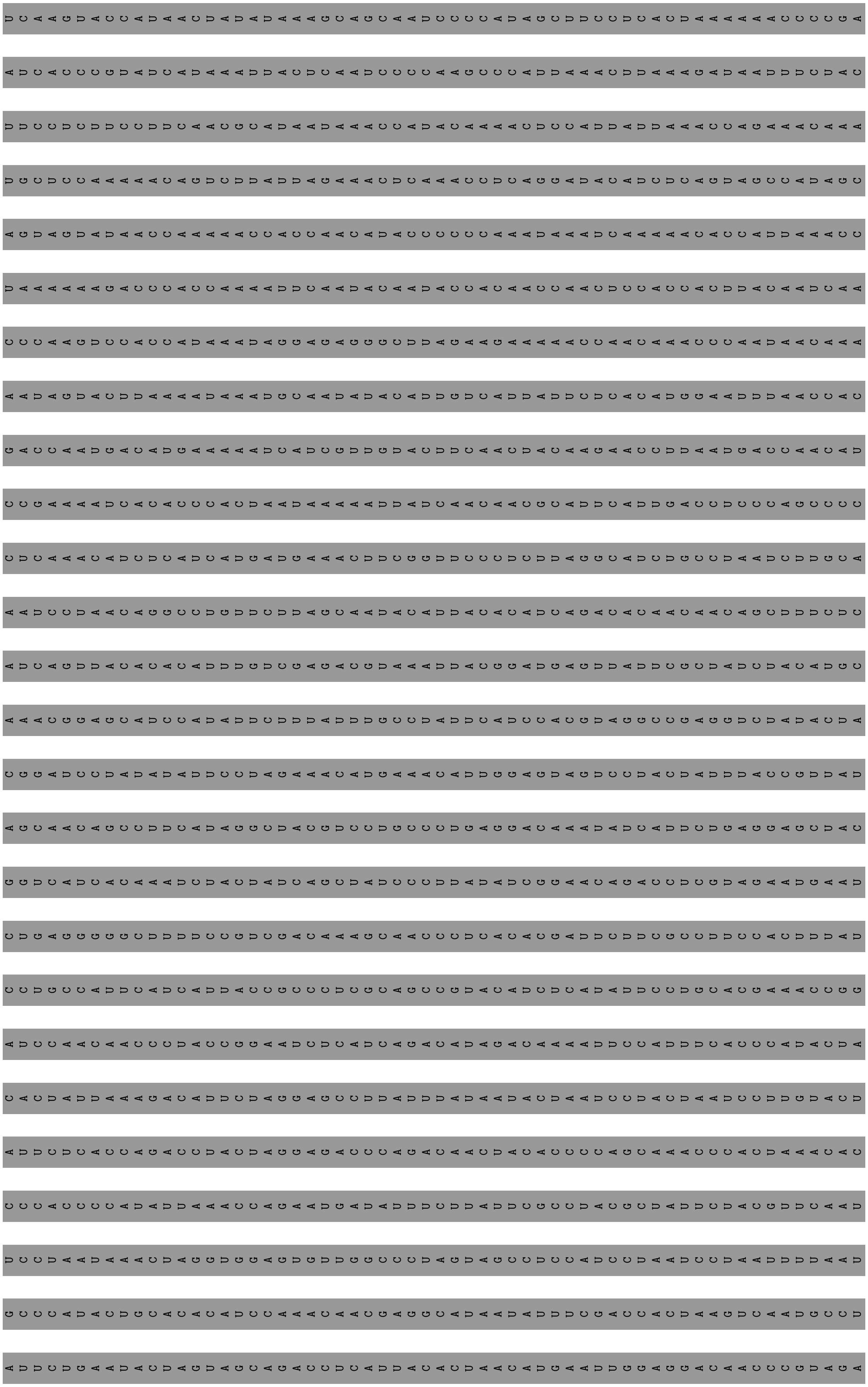
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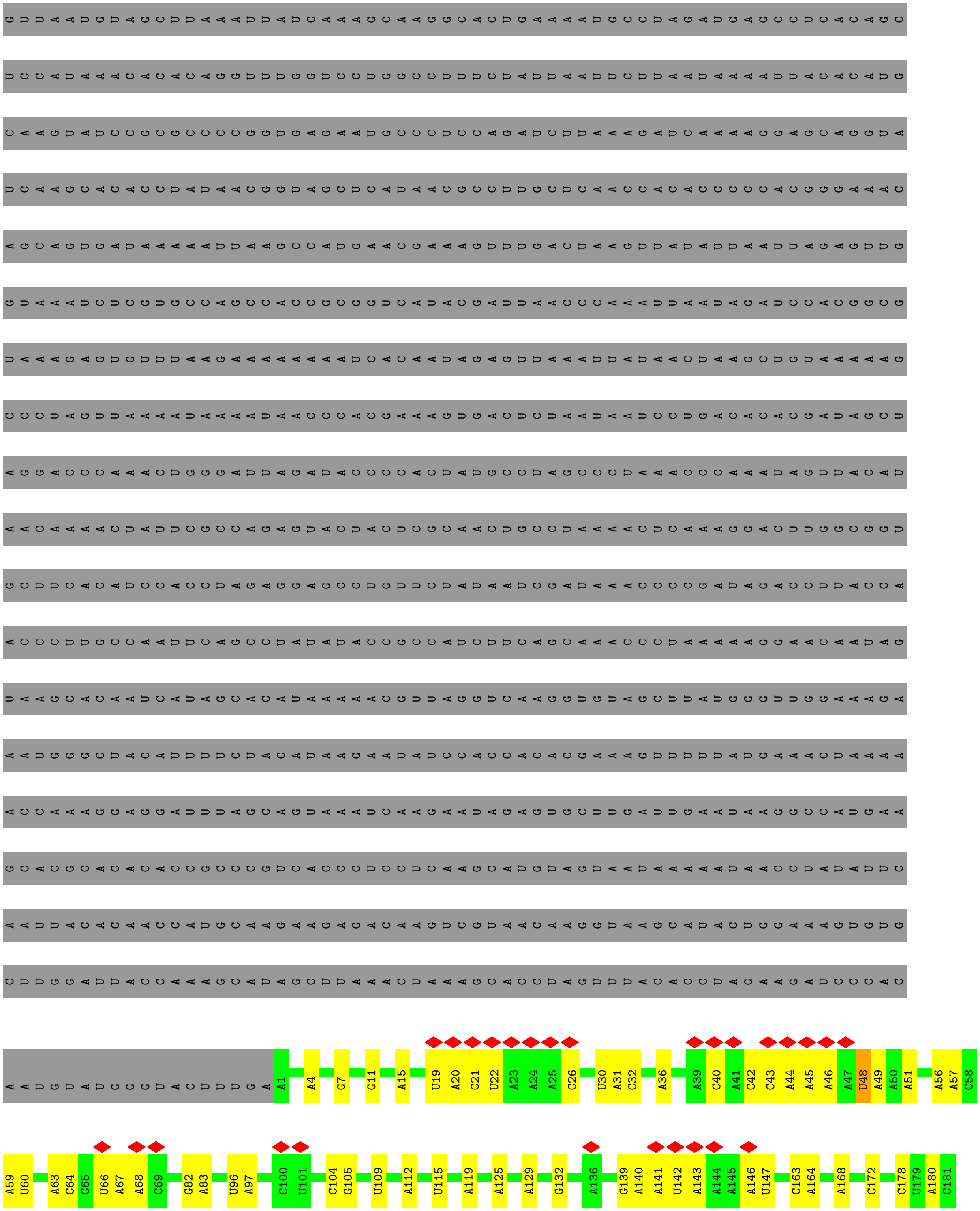

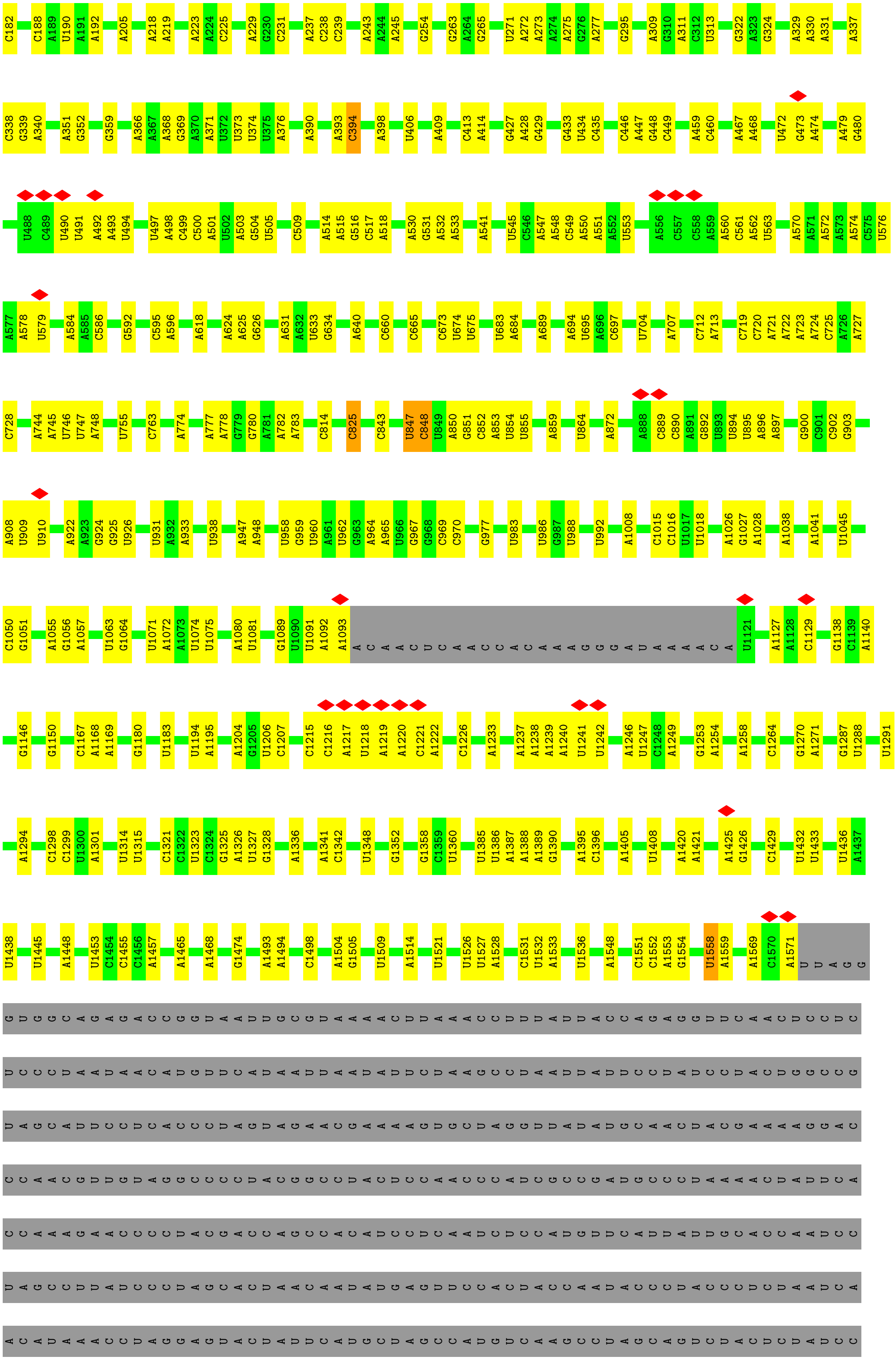
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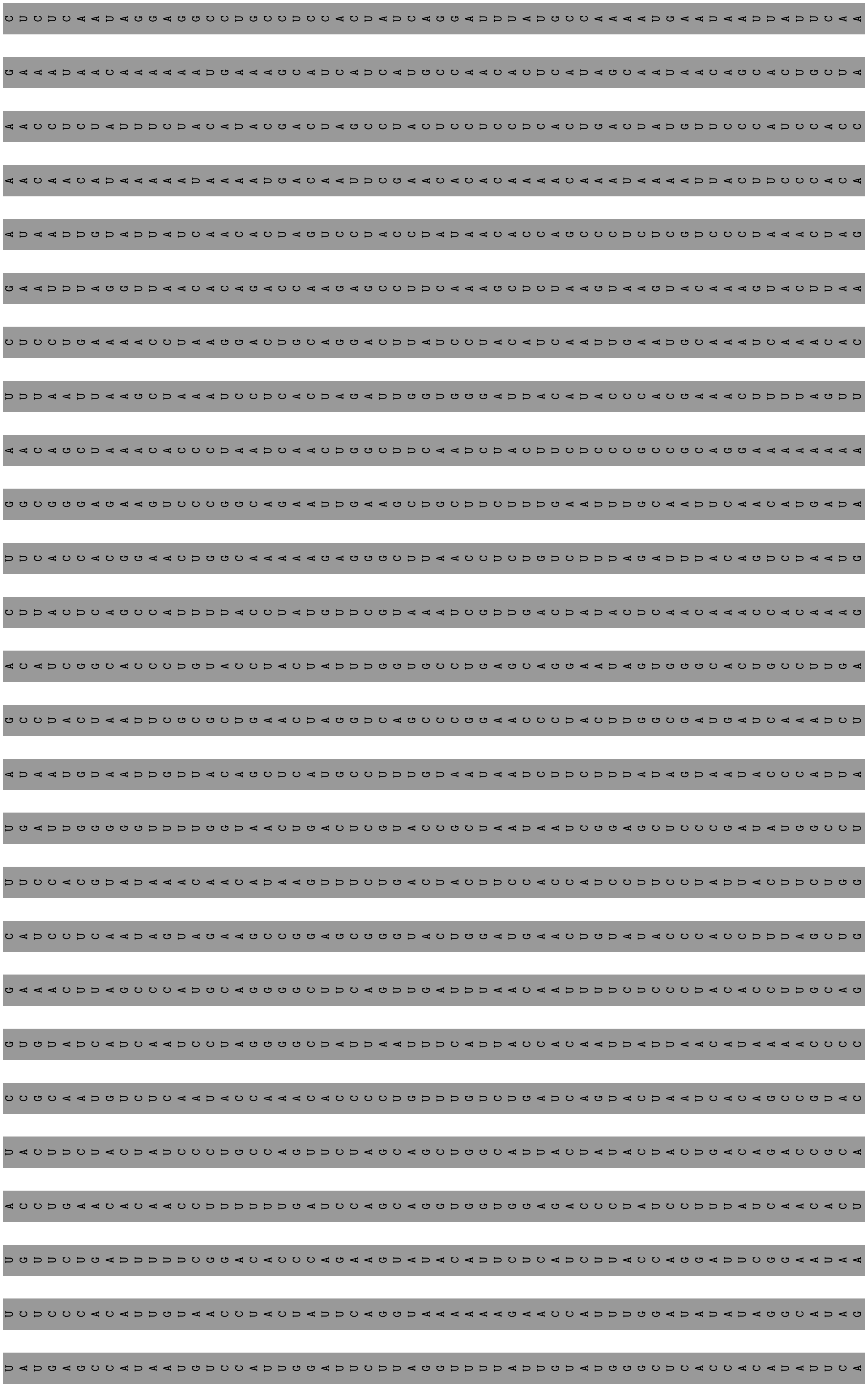
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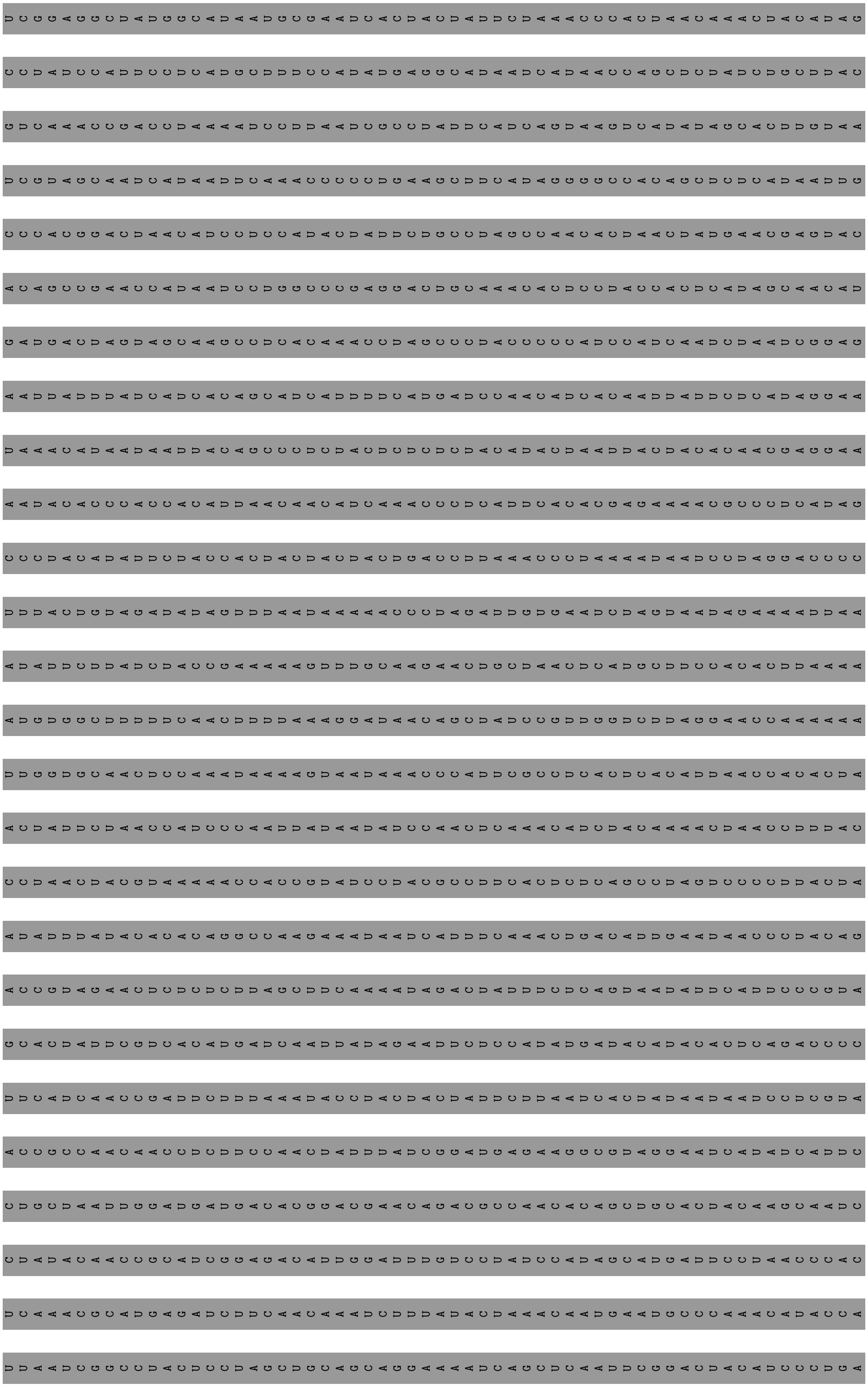
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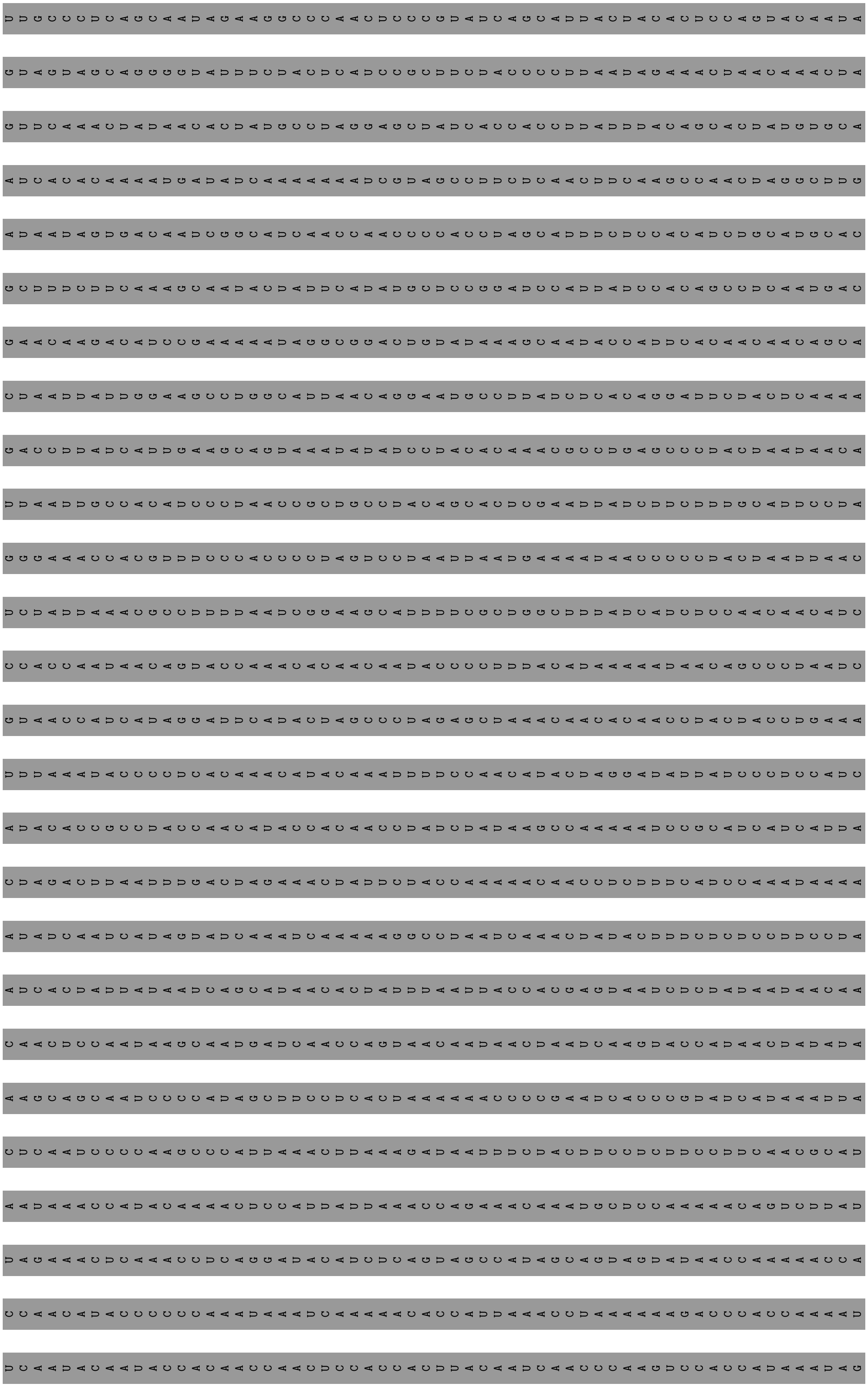
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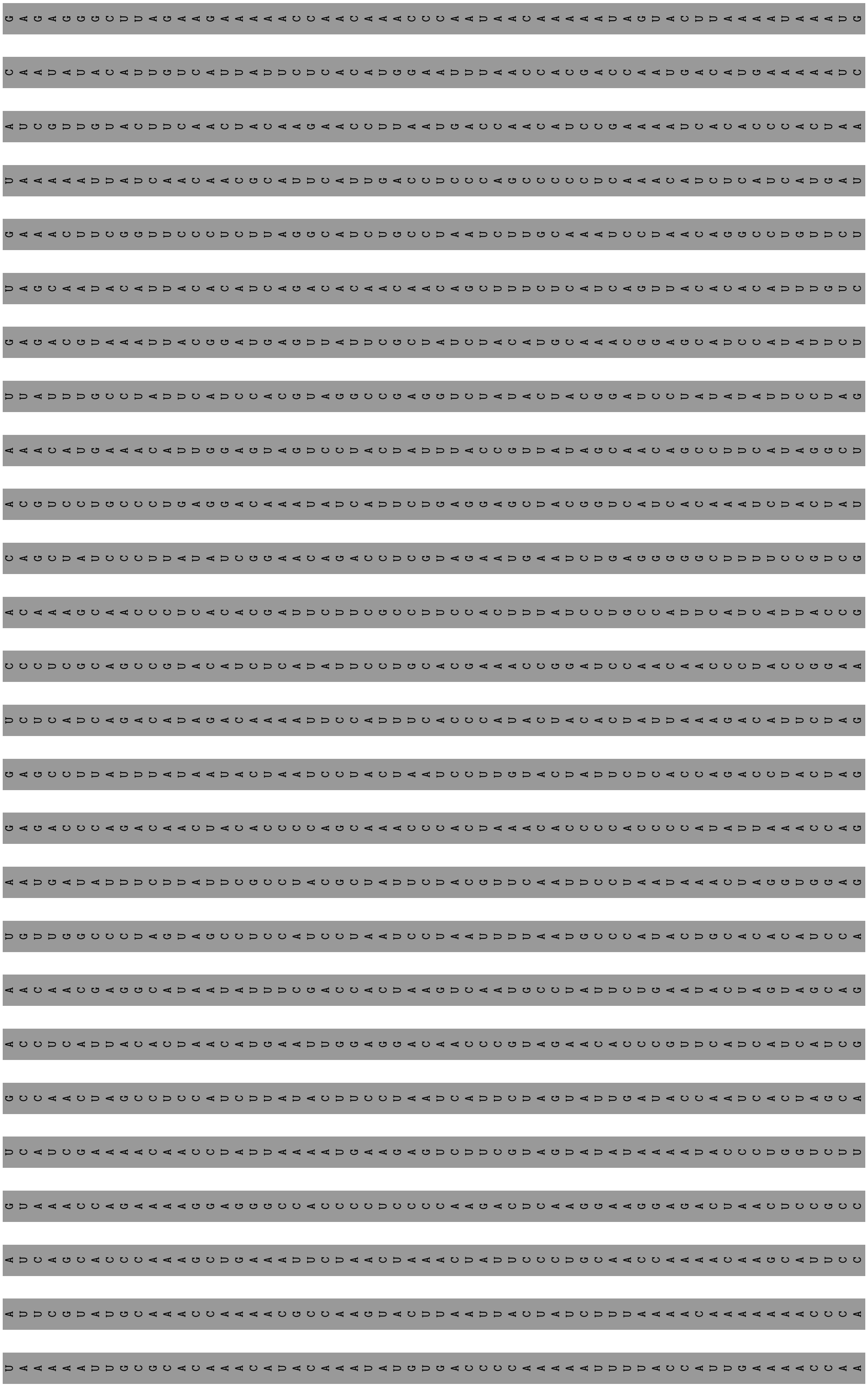
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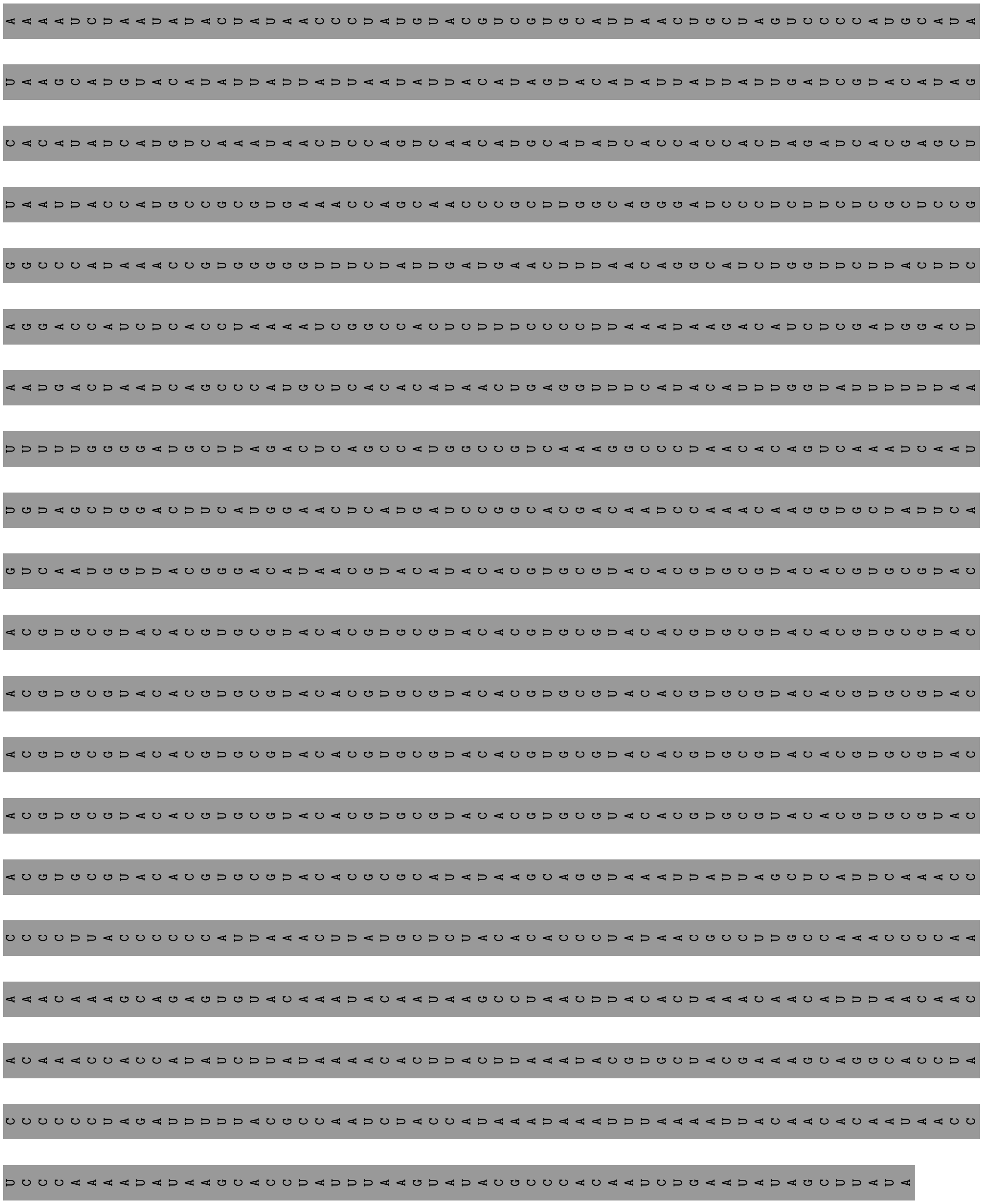
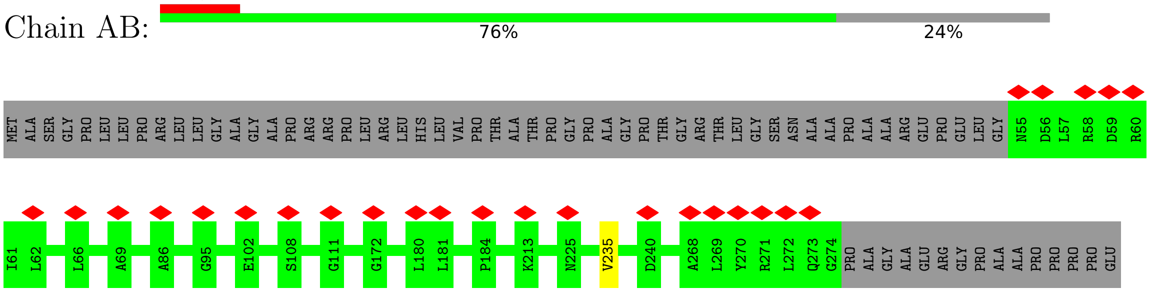


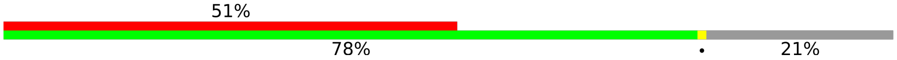
• Molecule 32: Mitochondrial ribosomal protein S2

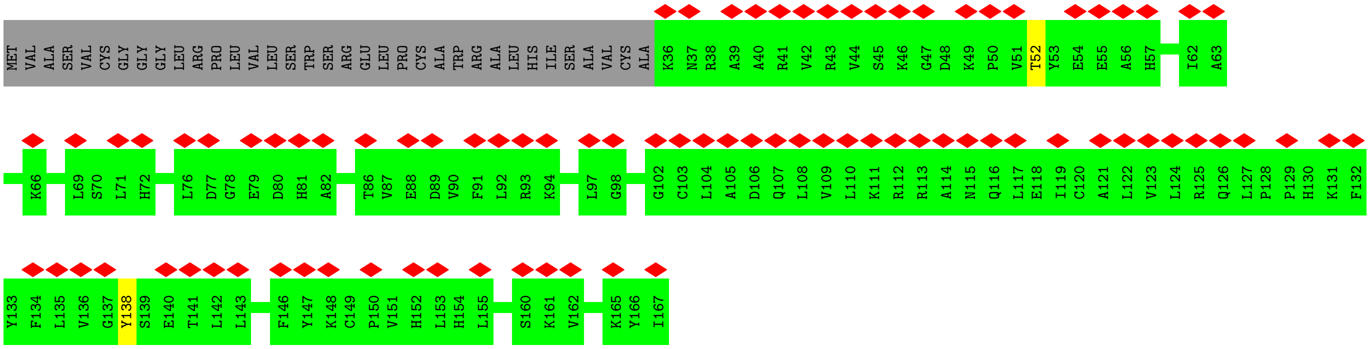
Chain AB:



- Molecule 33: Mitochondrial ribosomal protein S24

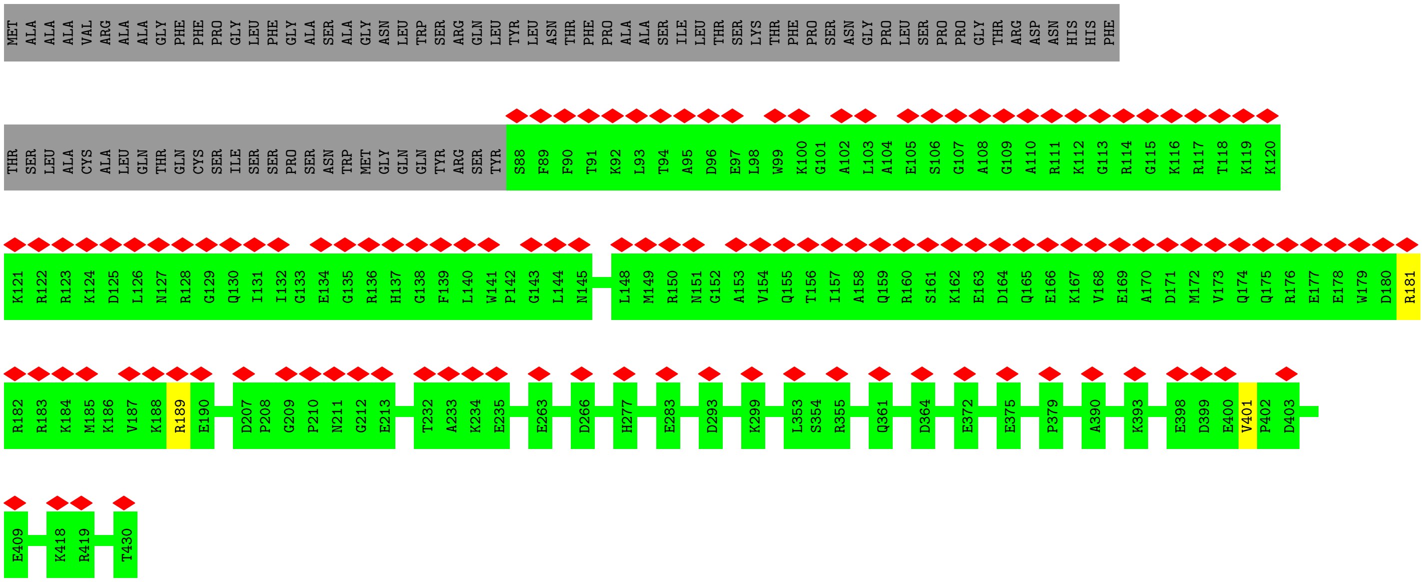
Chain AC:





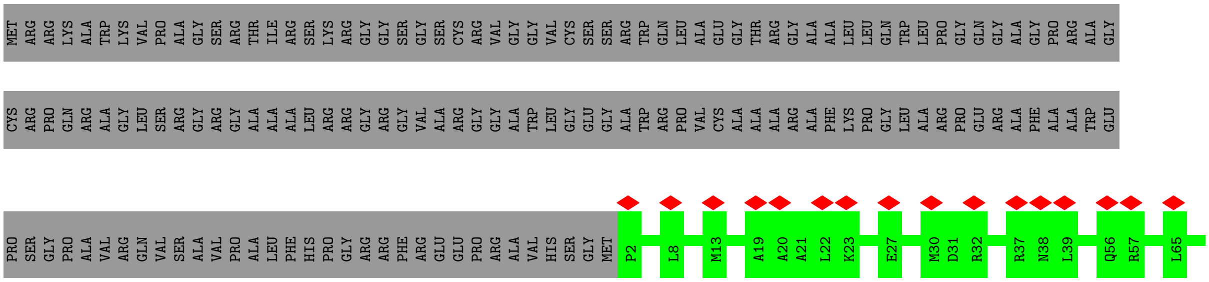
- Molecule 34: Mitochondrial ribosomal protein S5

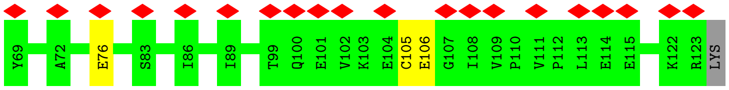
Chain AE:



- Molecule 35: Uncharacterized protein

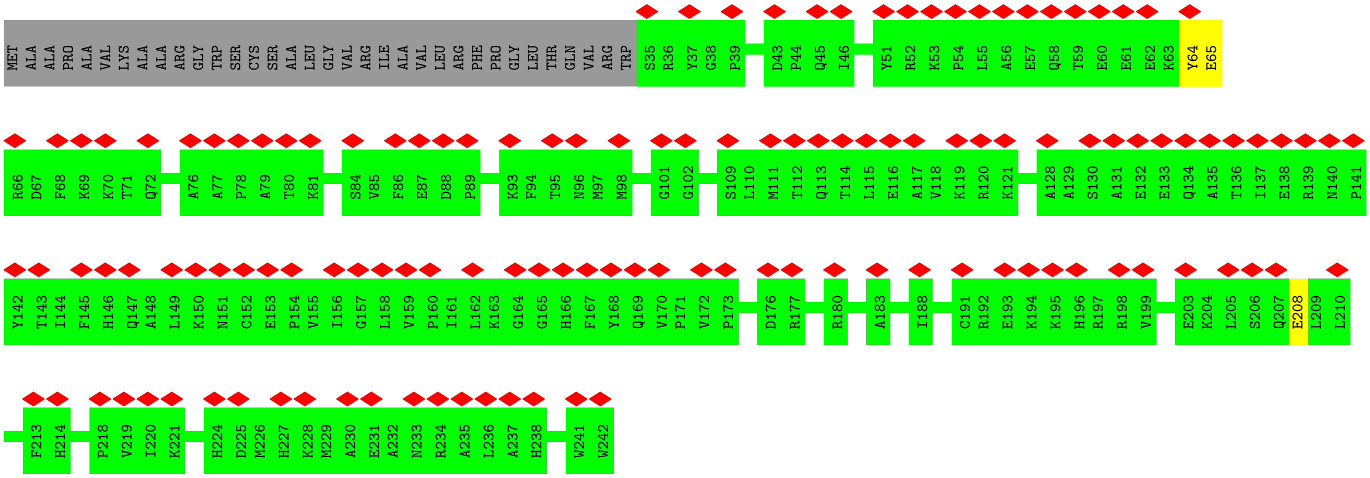
Chain AF:





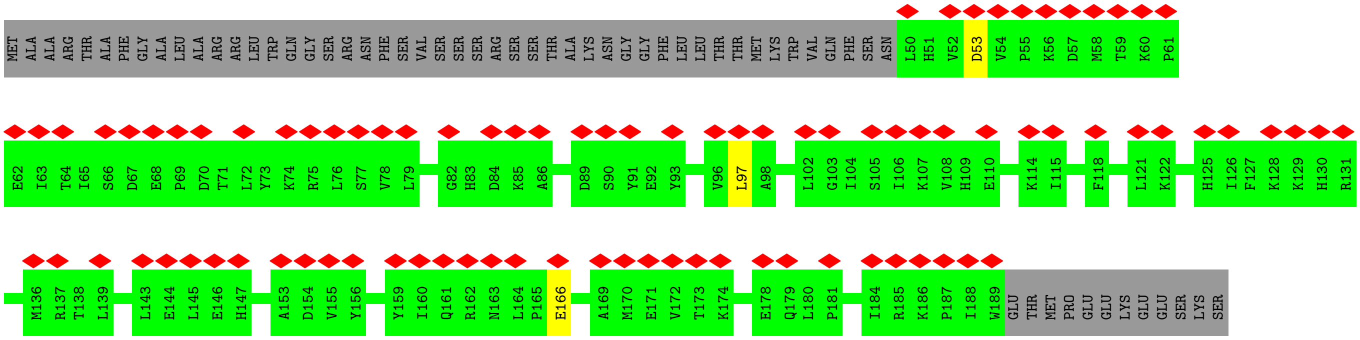
- Molecule 36: Mitochondrial ribosomal protein S7

Chain AG:



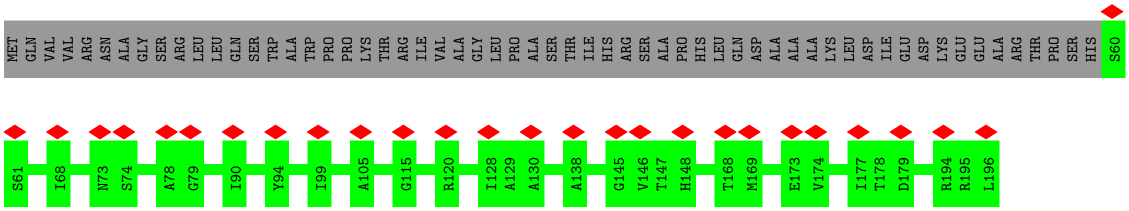
- Molecule 37: Mitochondrial ribosomal protein S10

Chain AJ:

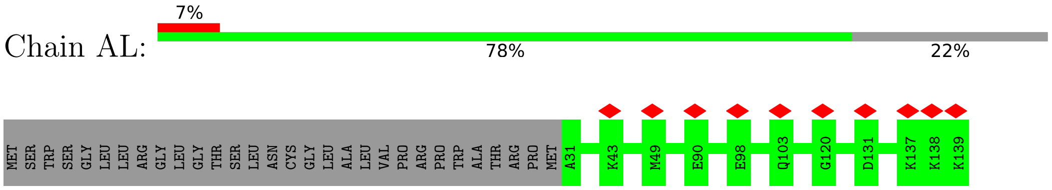


- Molecule 38: uS11m

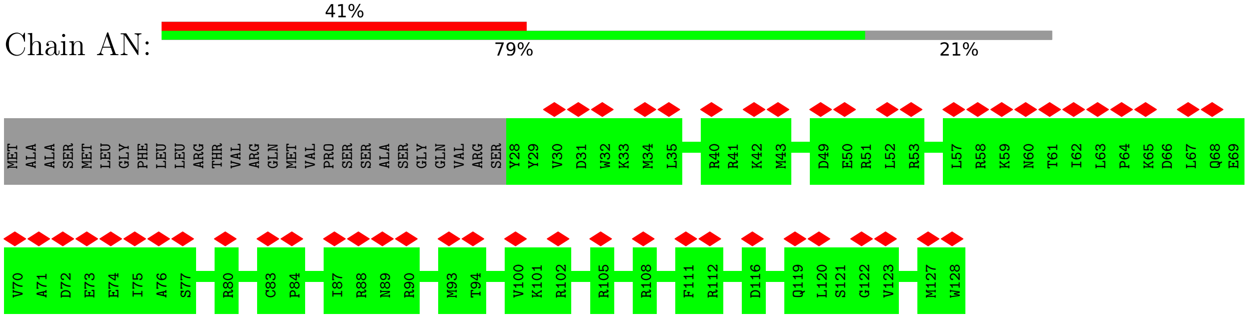
Chain AK:



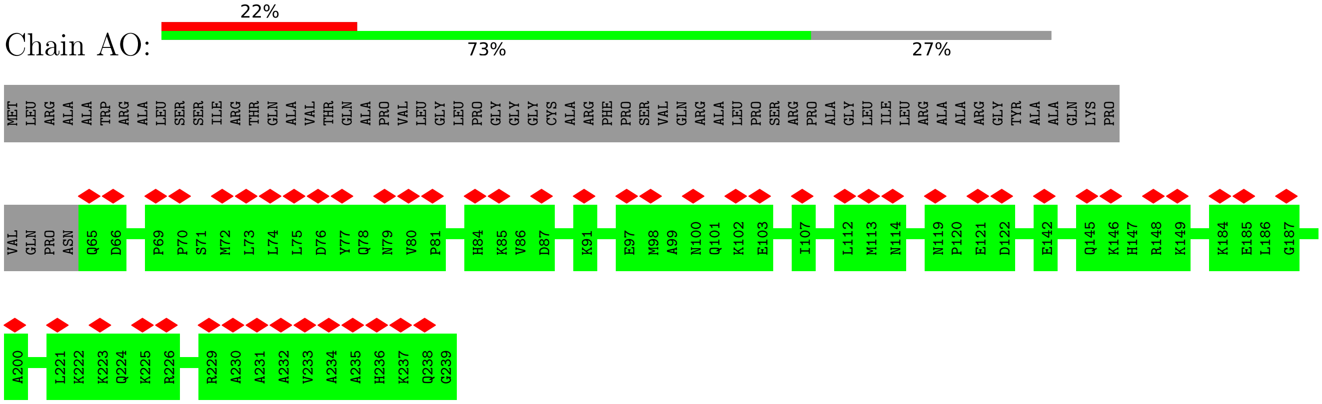
- Molecule 39: Mitochondrial ribosomal protein S12



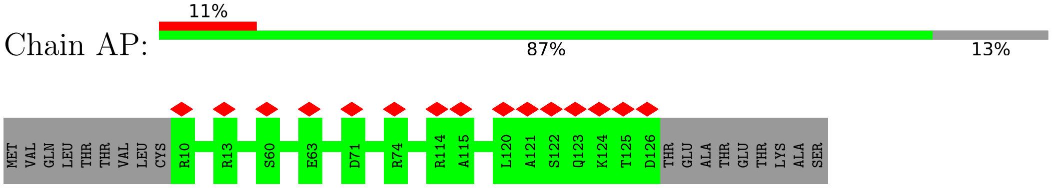
- Molecule 40: Mitochondrial ribosomal protein S14



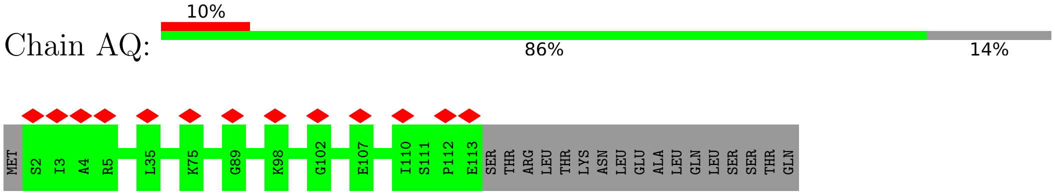
- Molecule 41: uS15m



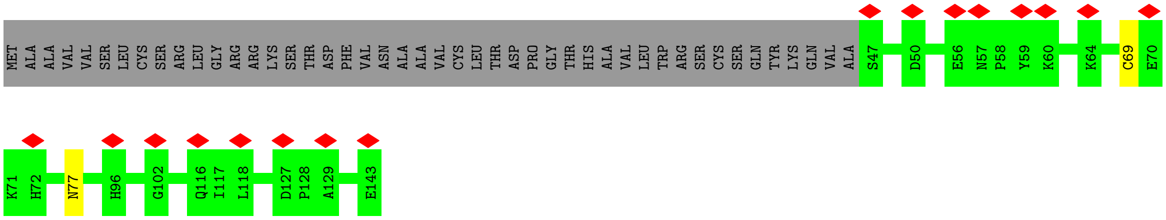
- Molecule 42: 28S ribosomal protein S16, mitochondrial



- Molecule 43: uS17m

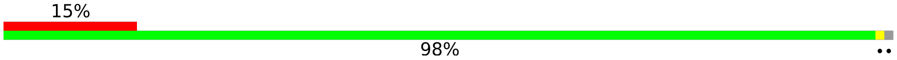


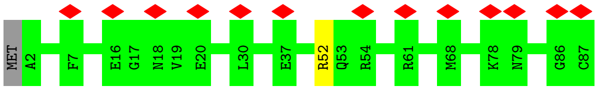
- Molecule 44: Mitochondrial ribosomal protein S18C



• Molecule 45: bS21m

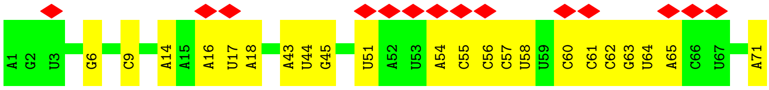
Chain AU:





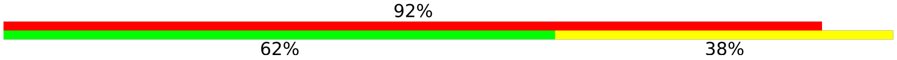
• Molecule 46: tRNAMet

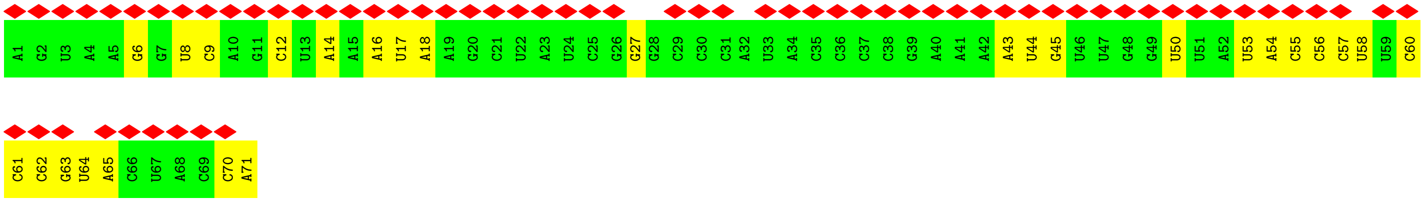
Chain AV:



• Molecule 46: tRNAMet

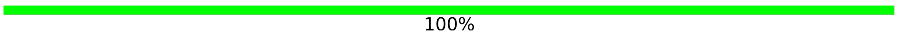
Chain AY:





• Molecule 47: mRNA

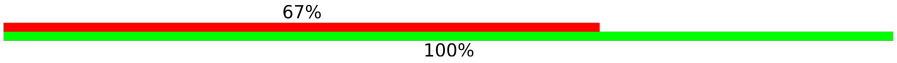
Chain AX:

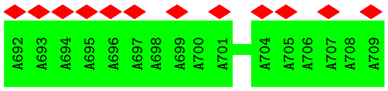


There are no outlier residues recorded for this chain.

• Molecule 48: unknown peptide

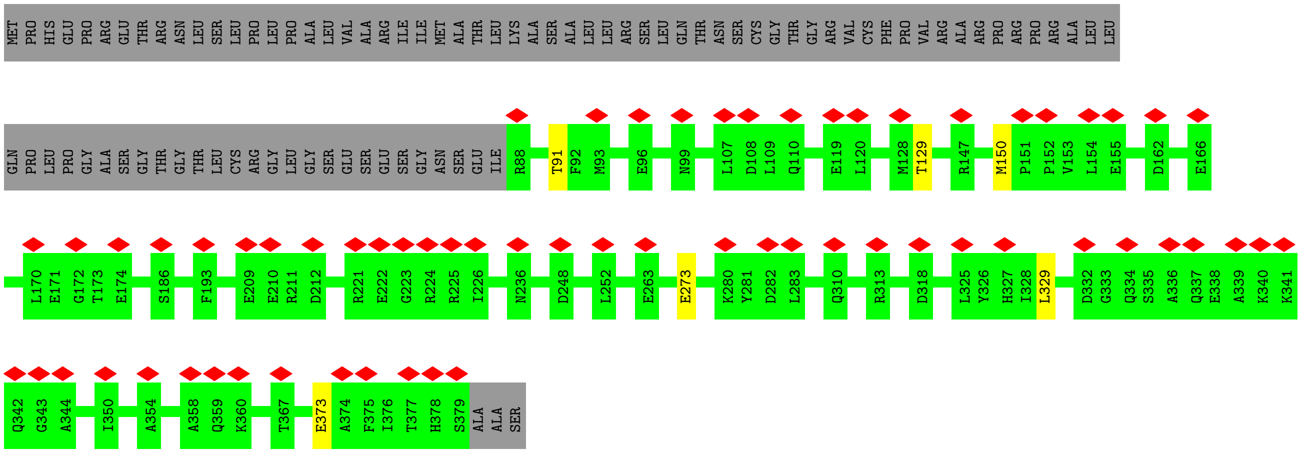
Chain AZ:





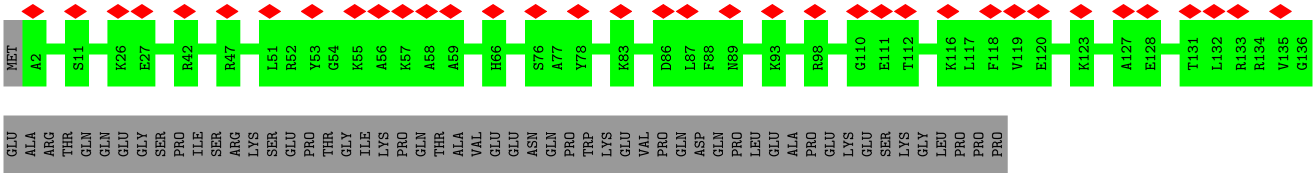
• Molecule 49: Mitochondrial ribosomal protein S22

Chain Aa:



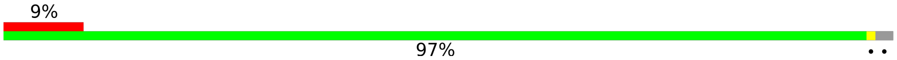
- Molecule 50: mS23

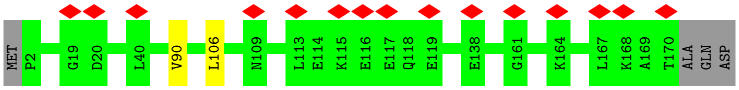
Chain Ab:



- Molecule 51: Mitochondrial ribosomal protein S25

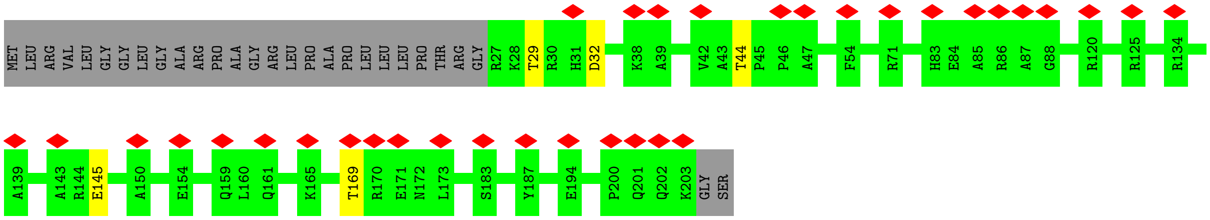
Chain Ac:





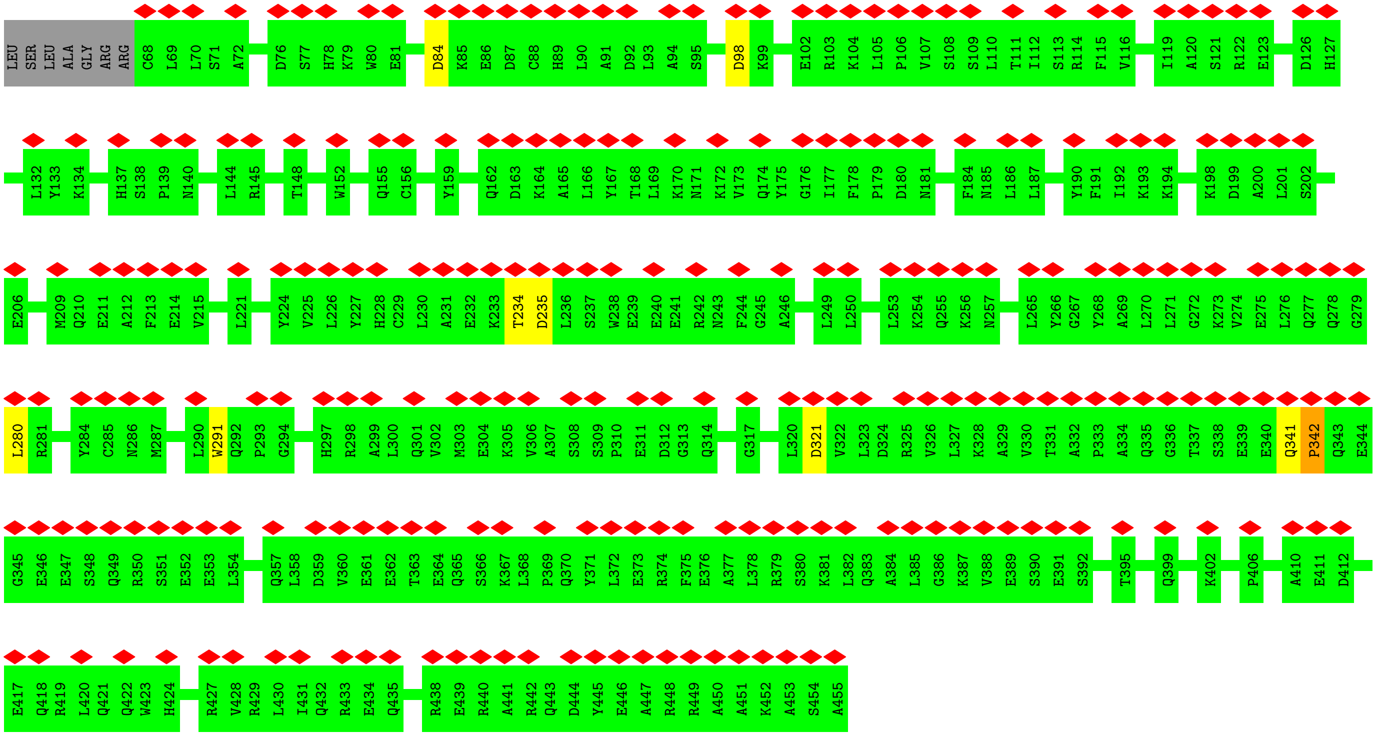
- Molecule 52: Mitochondrial ribosomal protein S26

Chain Ad:



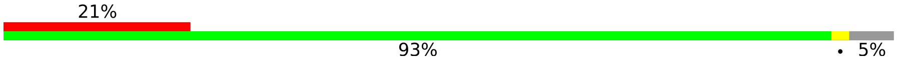
- Molecule 53: Mitochondrial ribosomal protein S27

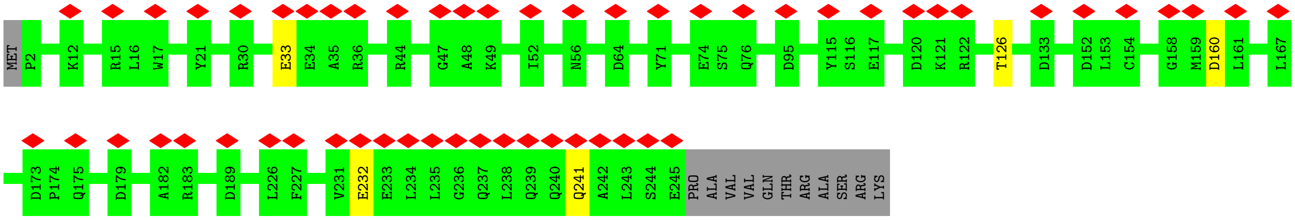
Chain Ae:



- Molecule 54: Mitochondrial ribosomal protein L28

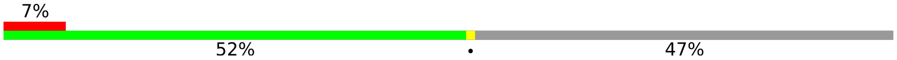
Chain B1:

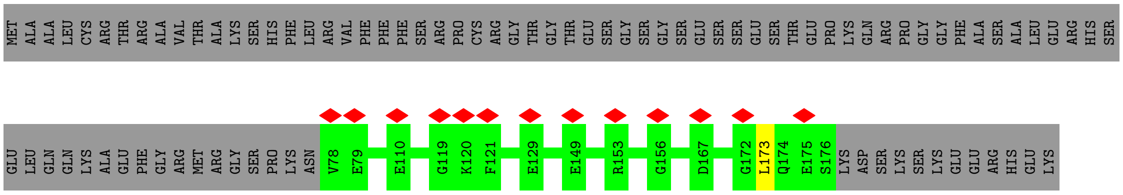




- Molecule 55: Mitoribosomal protein ms28, mrps28

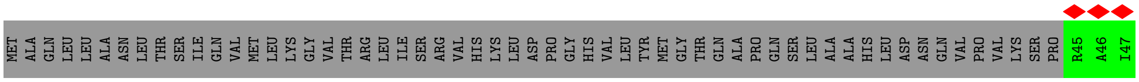
Chain Af:

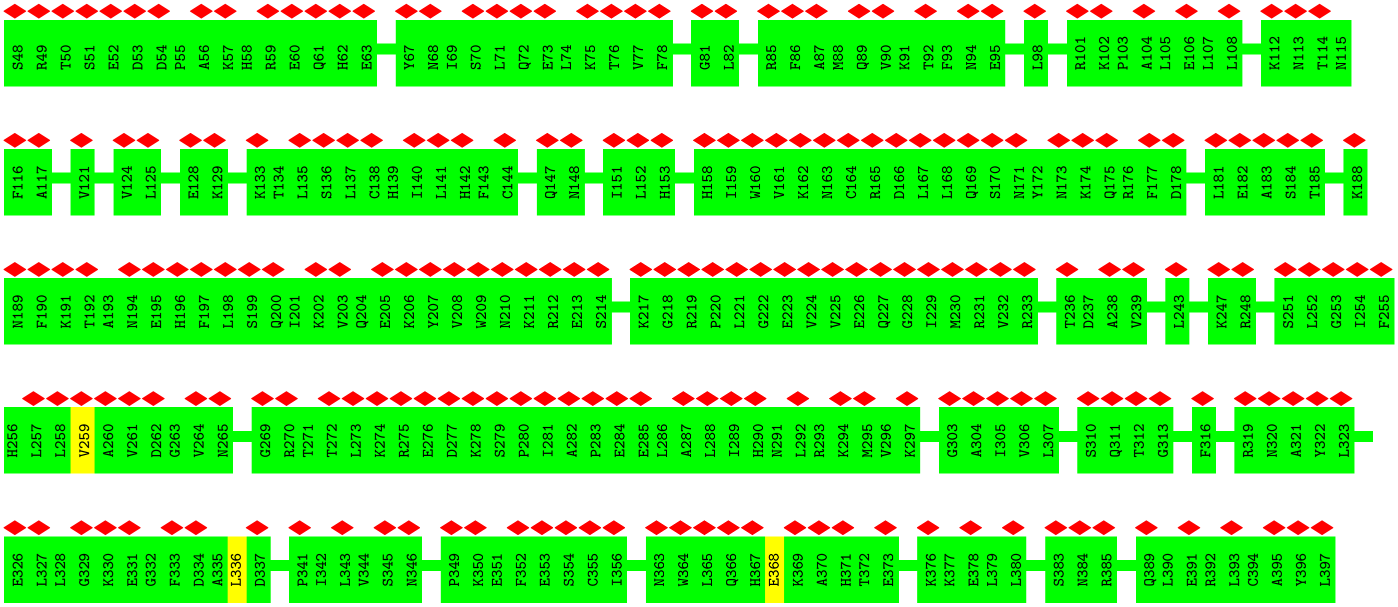




- Molecule 56: Death associated protein 3

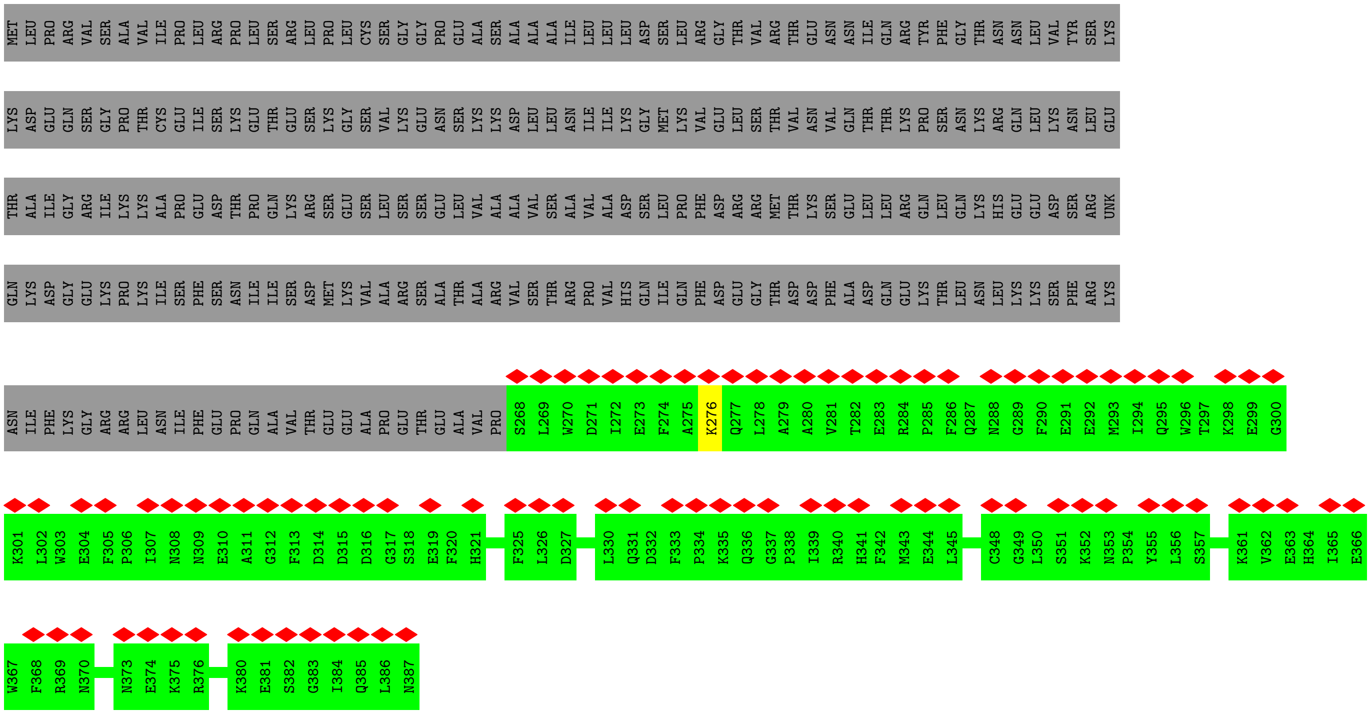
Chain Ag:





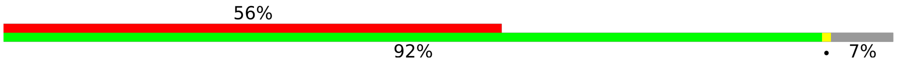
- Molecule 57: Mitochondrial ribosomal protein S31

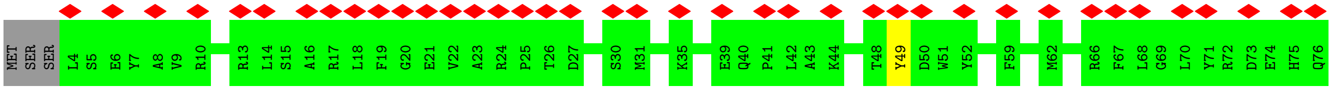
Chain Ah:

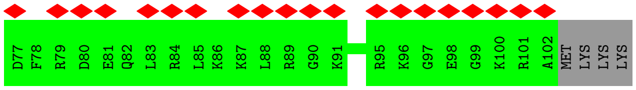


- Molecule 58: mS33

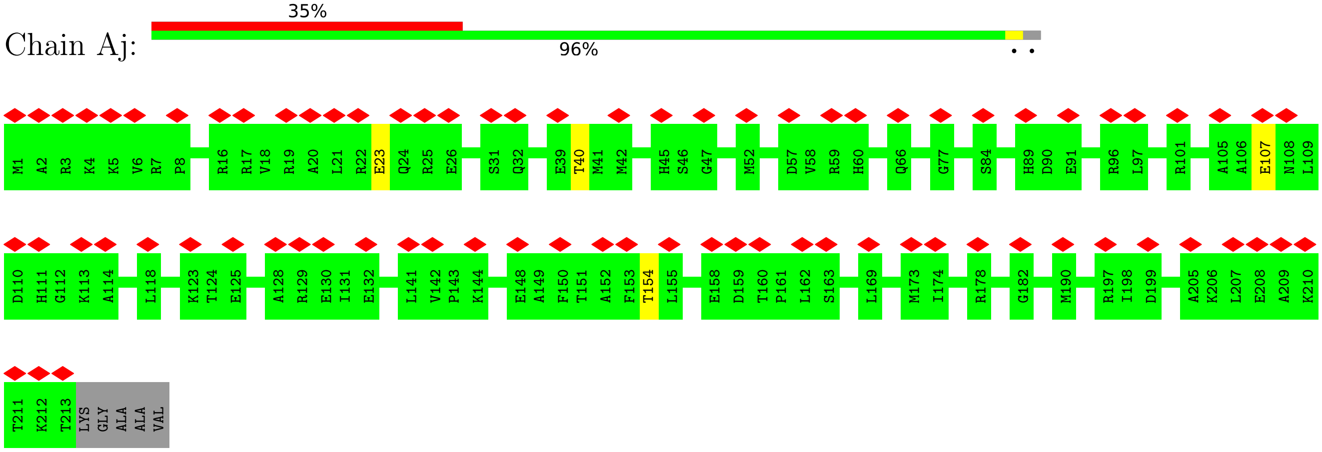
Chain Ai:



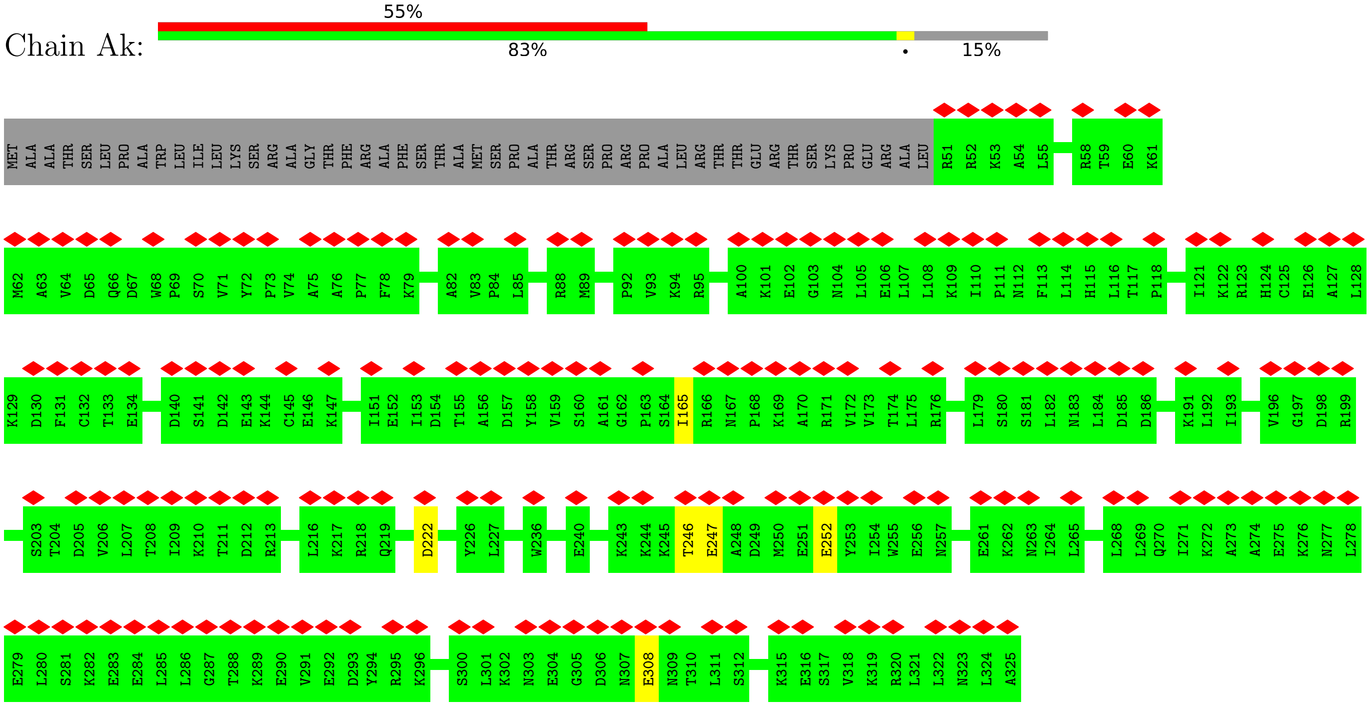




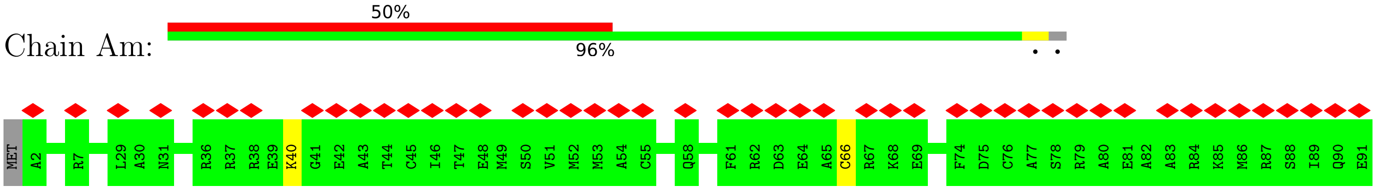
- Molecule 59: mS34

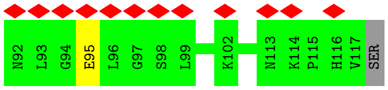


- Molecule 60: Mitochondrial ribosomal protein S35

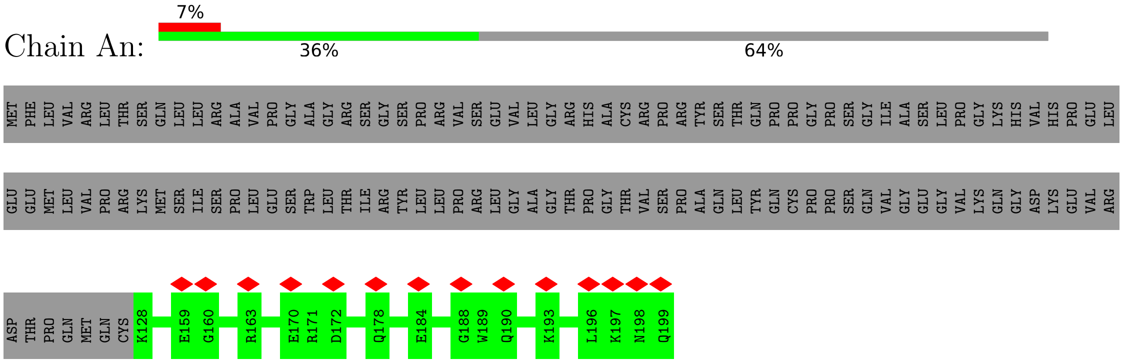


- Molecule 61: mS37

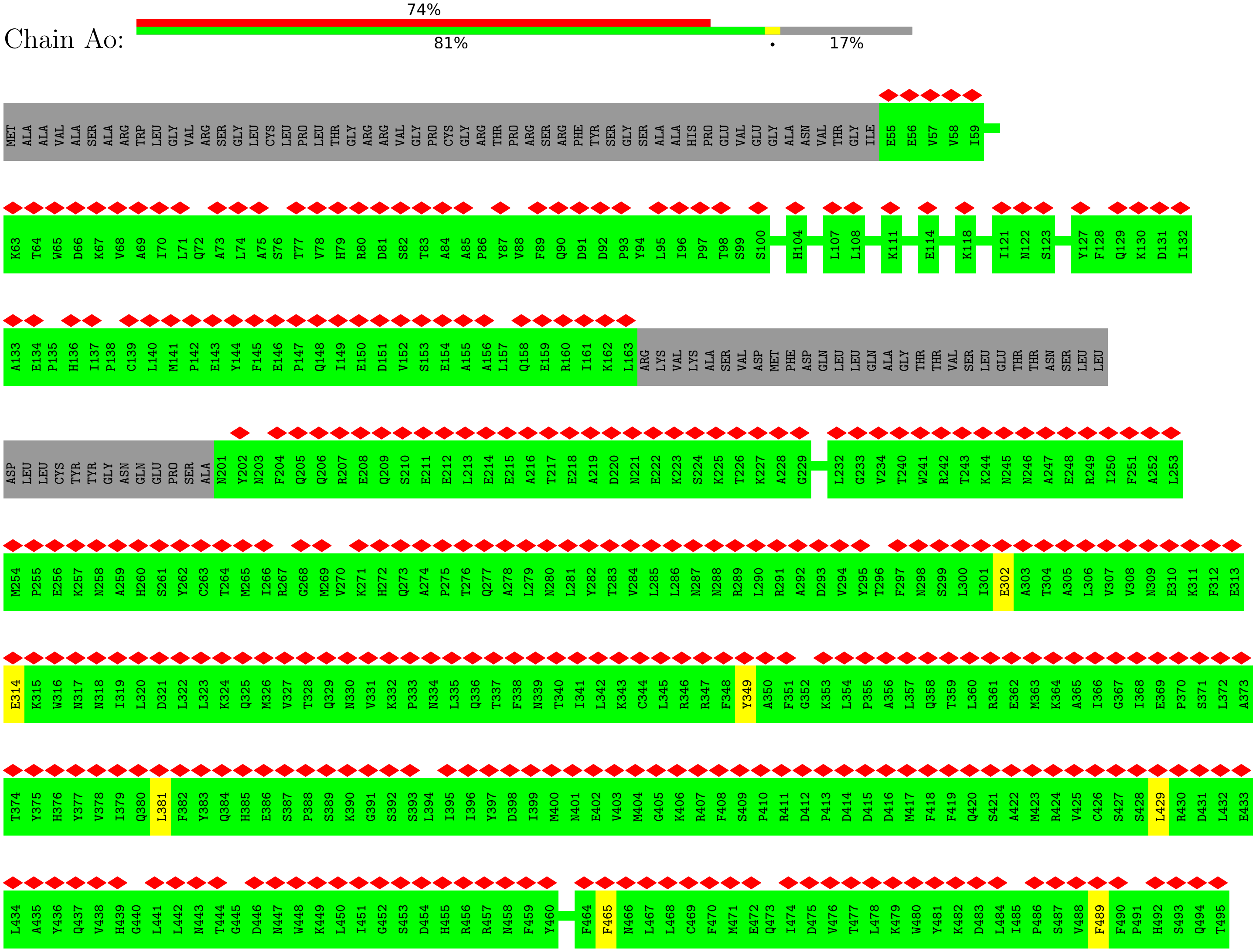




- Molecule 62: Aurora kinase A interacting protein 1

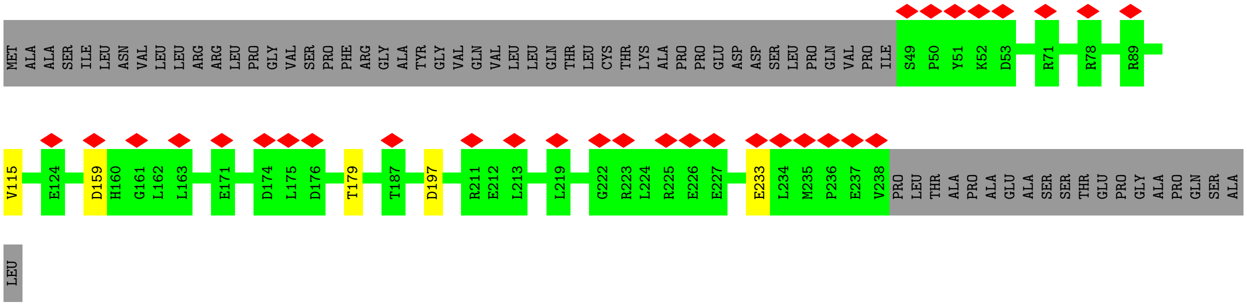


- Molecule 63: mS39



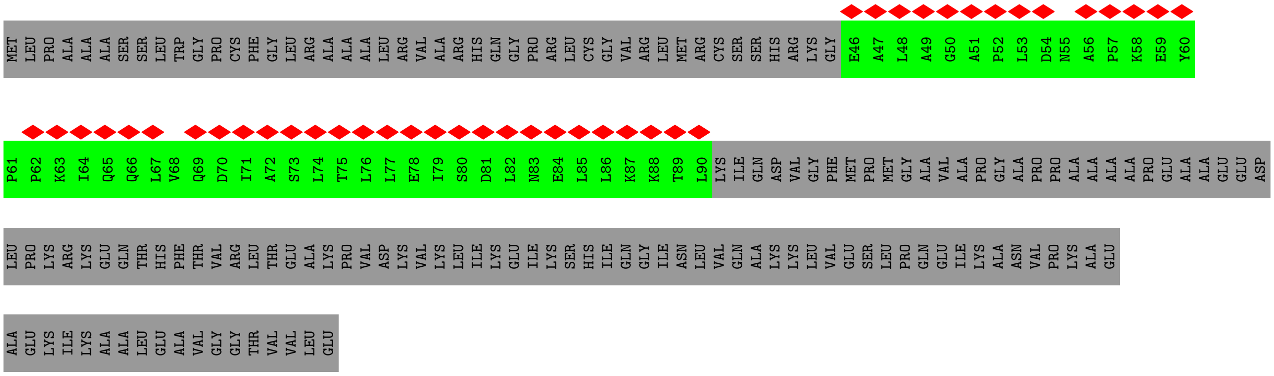
- Molecule 64: 28S ribosomal protein S18b, mitochondrial

Chain Ap:



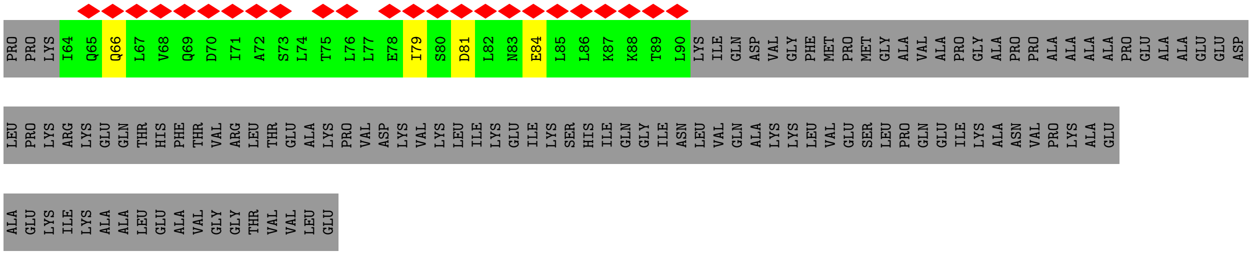
- Molecule 65: Mitochondrial ribosomal protein L12

Chain CL:

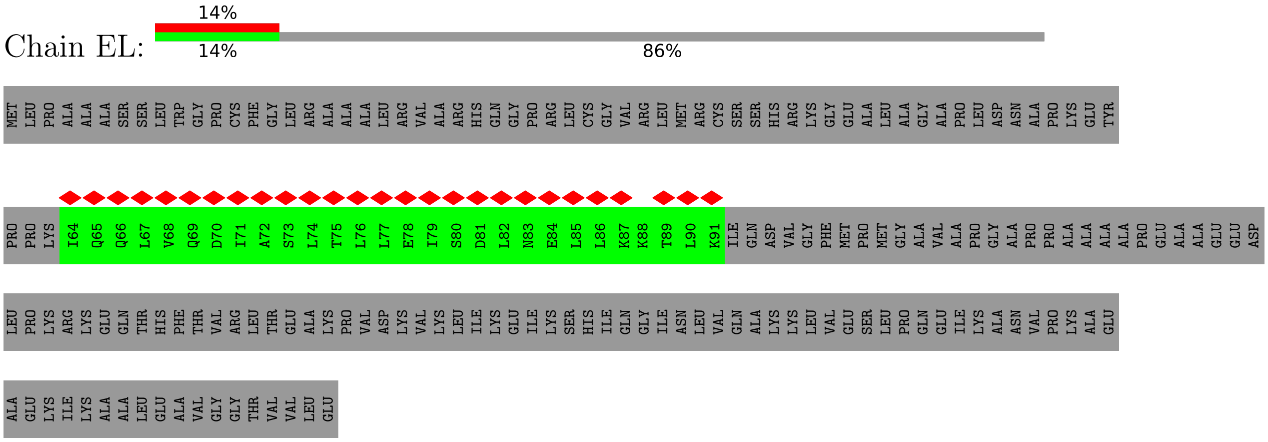


- Molecule 65: Mitochondrial ribosomal protein L12

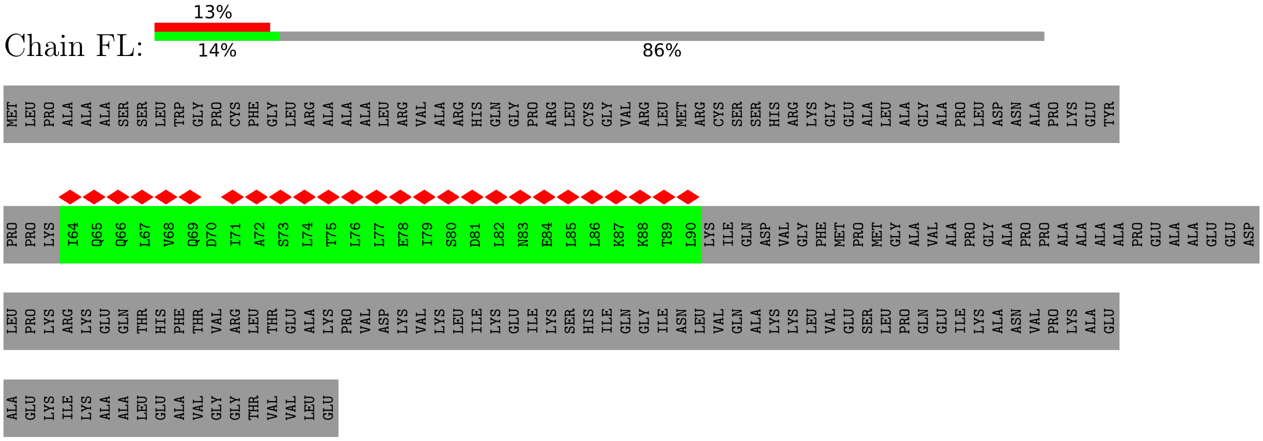
Chain DL:



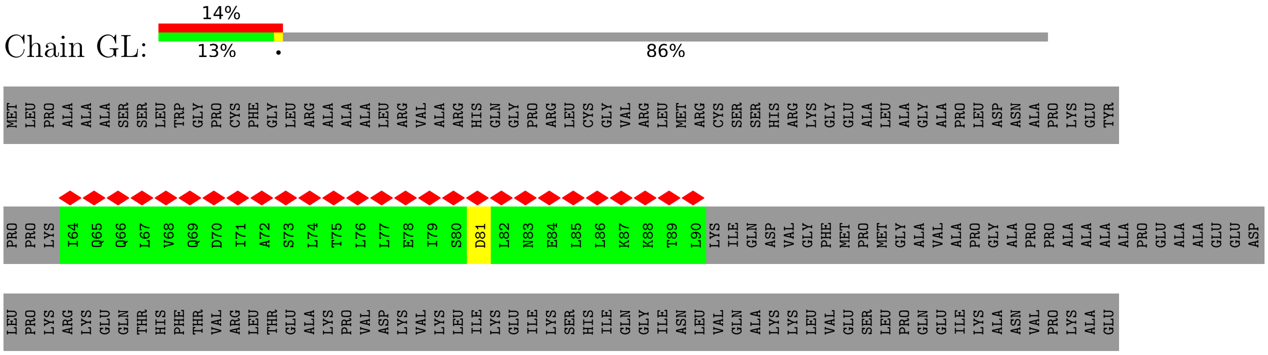
- Molecule 65: Mitochondrial ribosomal protein L12



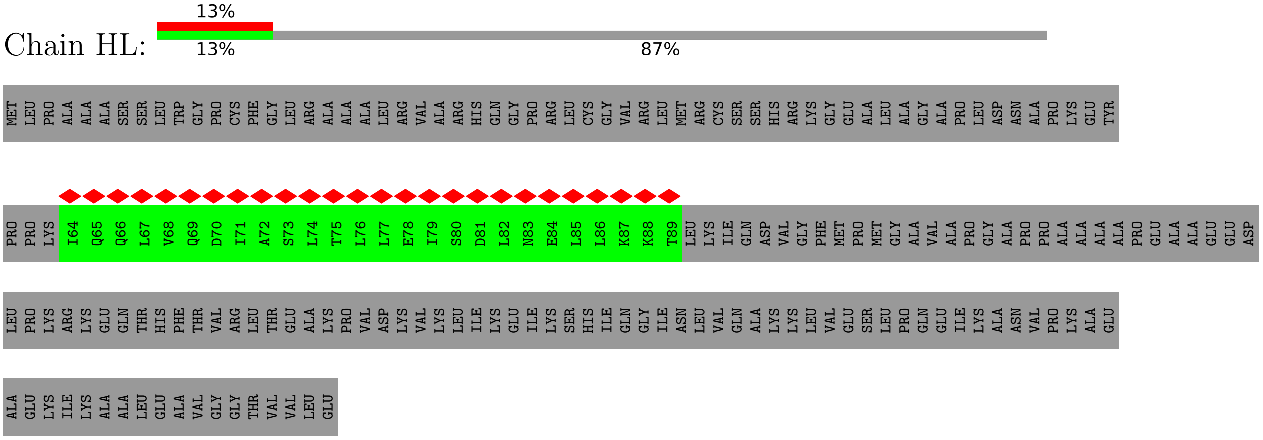
- Molecule 65: Mitochondrial ribosomal protein L12



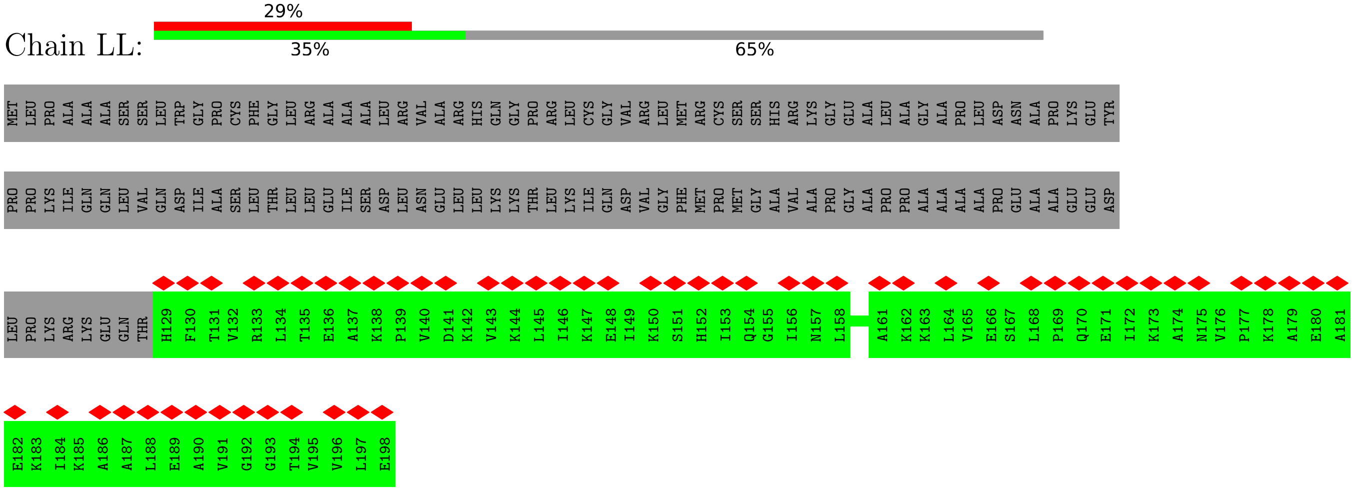
- Molecule 65: Mitochondrial ribosomal protein L12



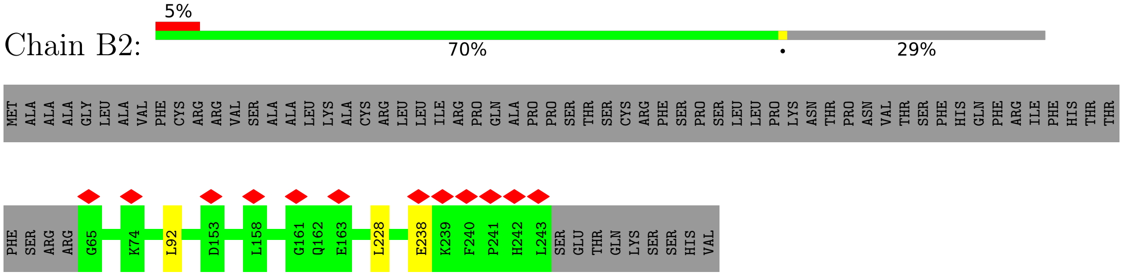
- Molecule 65: Mitochondrial ribosomal protein L12



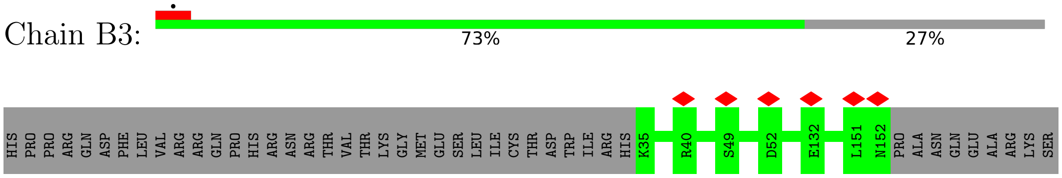
- Molecule 65: Mitochondrial ribosomal protein L12



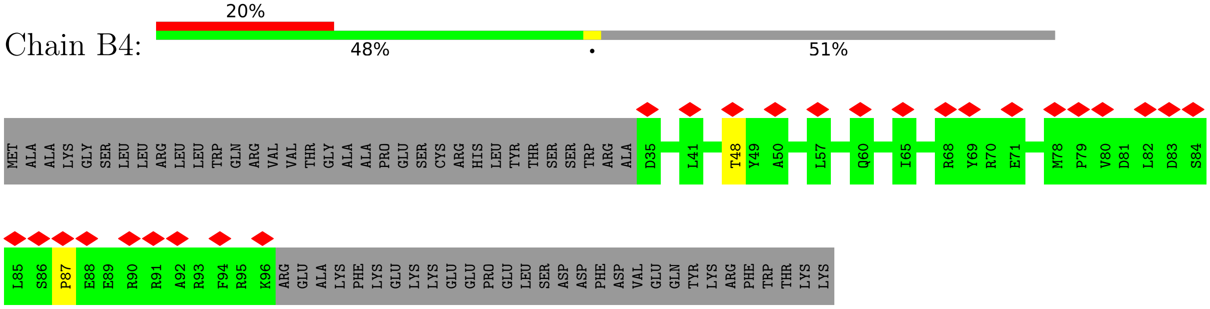
- Molecule 66: Mitochondrial ribosomal protein L47



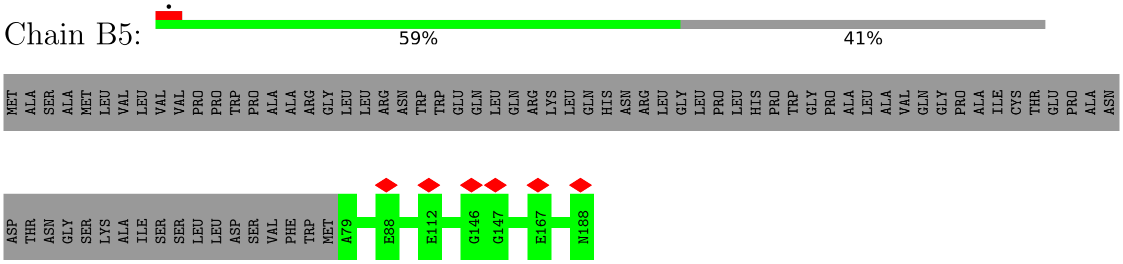
- Molecule 67: Uncharacterized protein



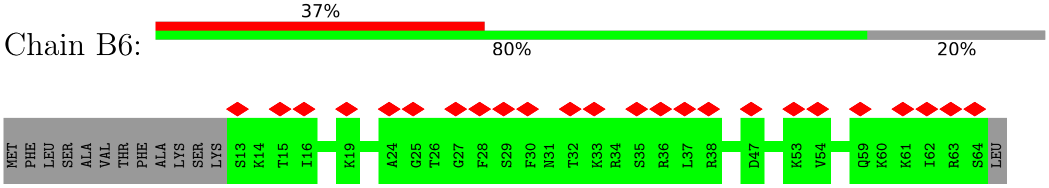
- Molecule 68: Uncharacterized protein



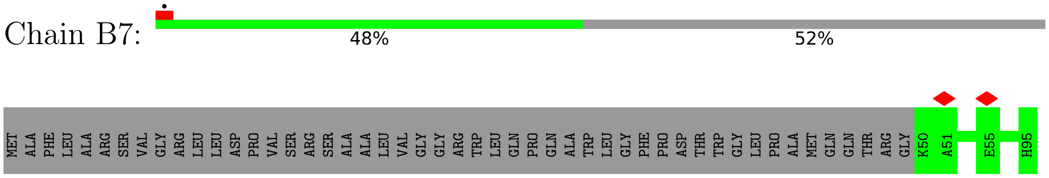
- Molecule 69: Uncharacterized protein



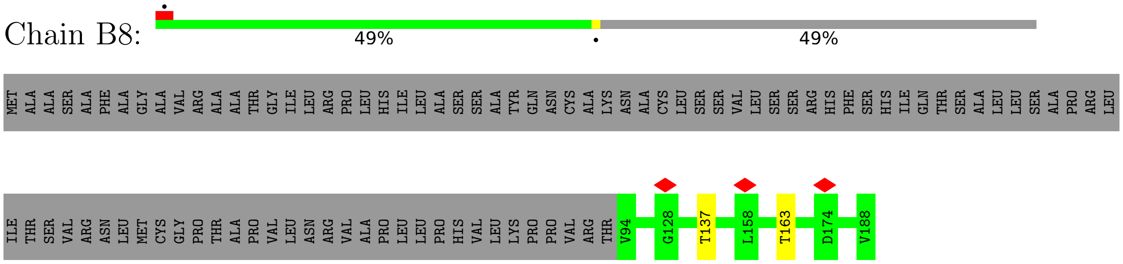
- Molecule 70: Uncharacterized protein



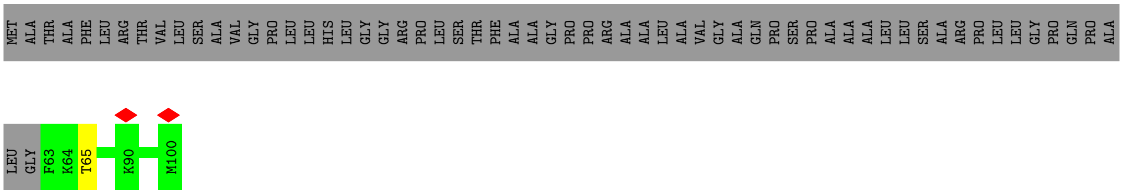
- Molecule 71: Mitochondrial ribosomal protein L34



- Molecule 72: Mitochondrial ribosomal protein L35

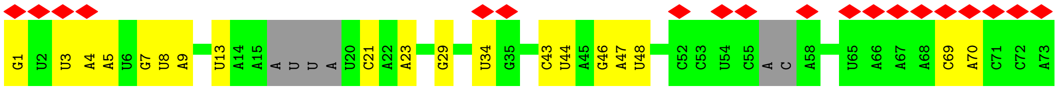


- Molecule 73: Ribosomal protein



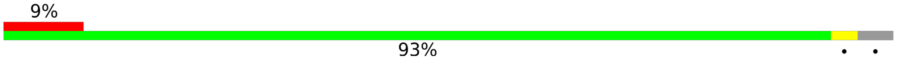
- Molecule 74: CP tRNA-Phe

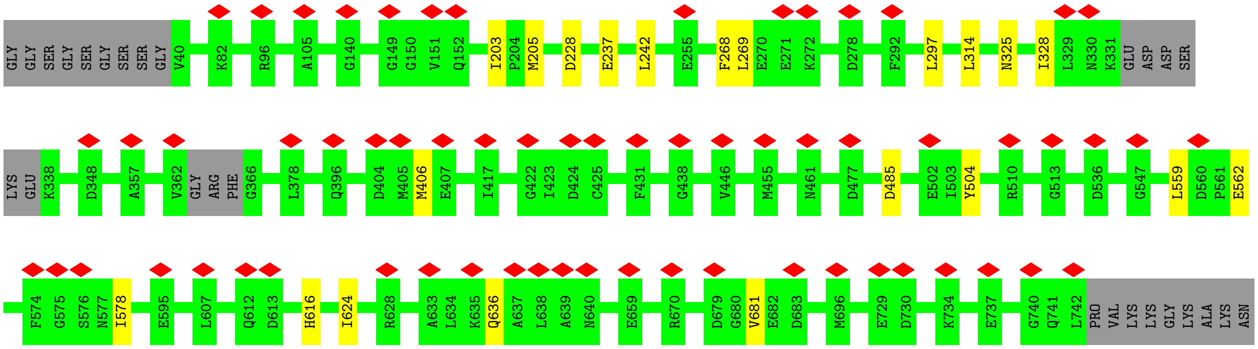
Chain BB:



- Molecule 75: Elongation factor G, mitochondrial

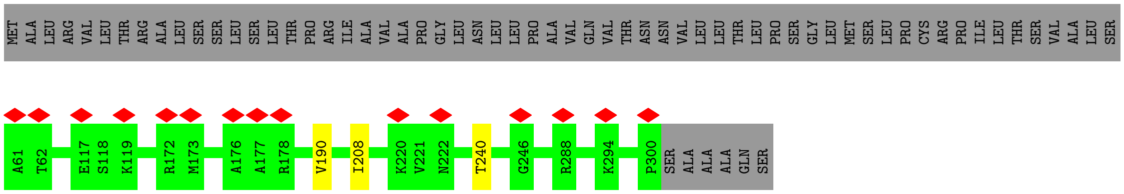
Chain BC:





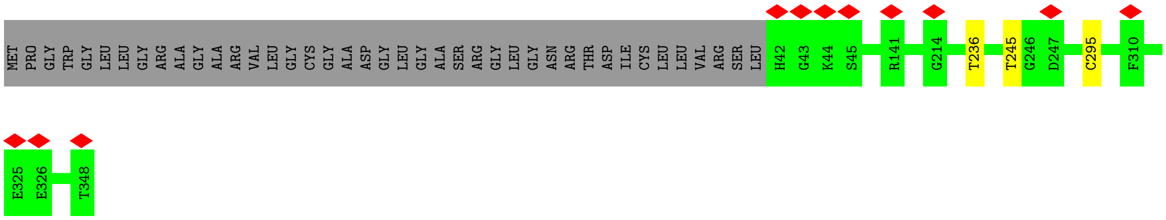
- Molecule 76: Uncharacterized protein

Chain BD:



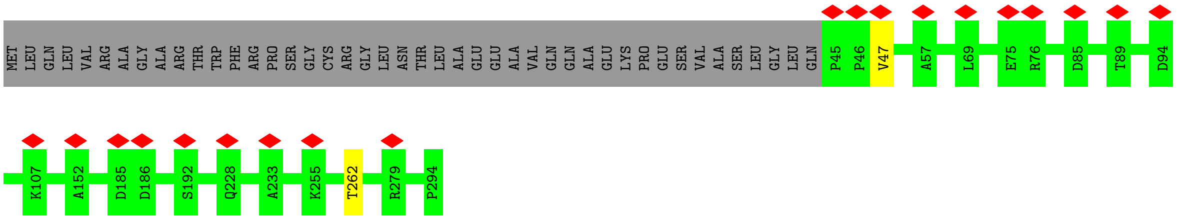
- Molecule 77: ICT1

Chain BE:



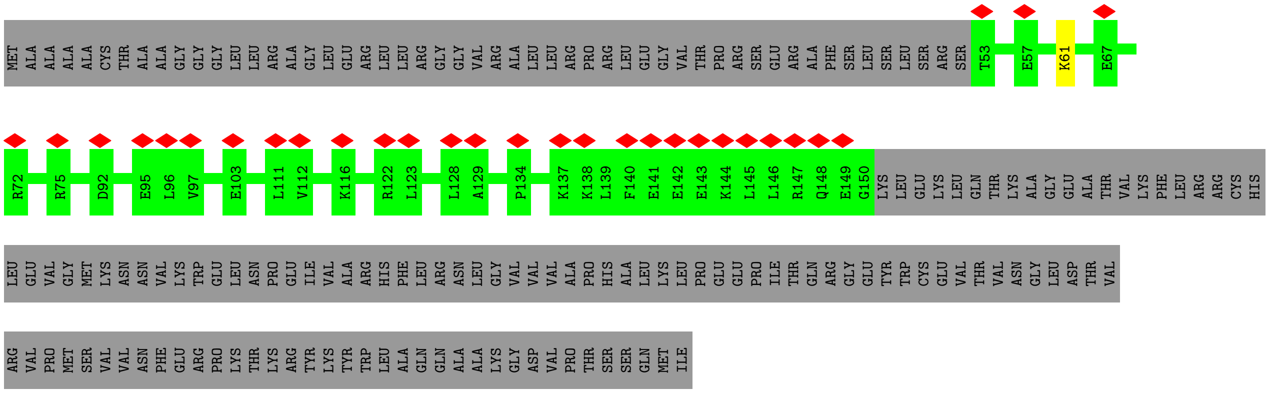
- Molecule 78: Mitochondrial ribosomal protein L4

Chain BF:



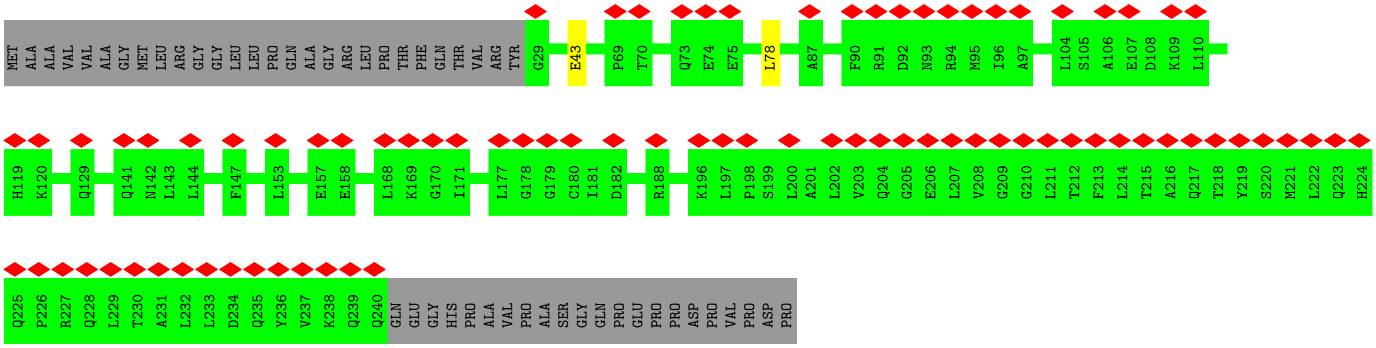
- Molecule 79: Mitochondrial ribosomal protein L9

Chain BI:



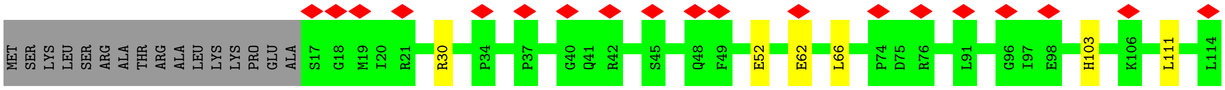
- Molecule 80: Mitochondrial ribosomal protein L10

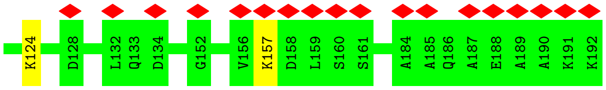
Chain BJ:



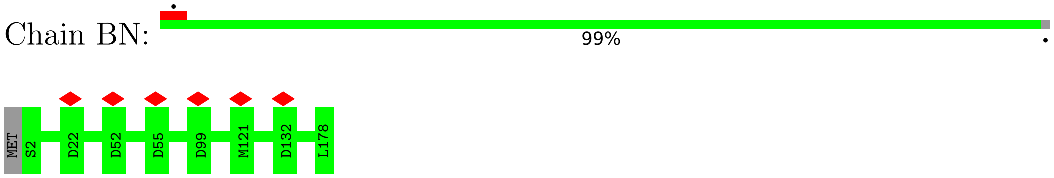
- Molecule 81: Mitochondrial ribosomal protein L11

Chain BK:

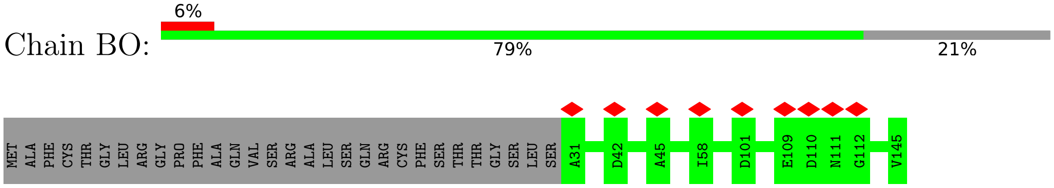




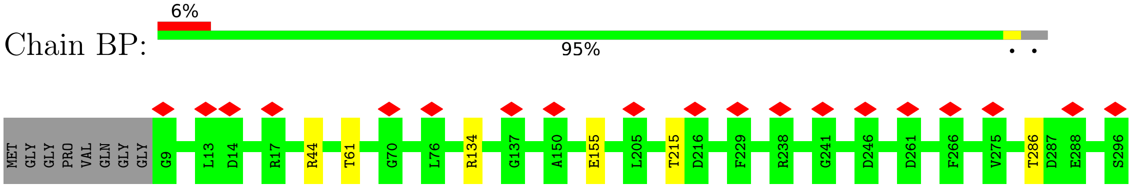
- Molecule 82: Uncharacterized protein



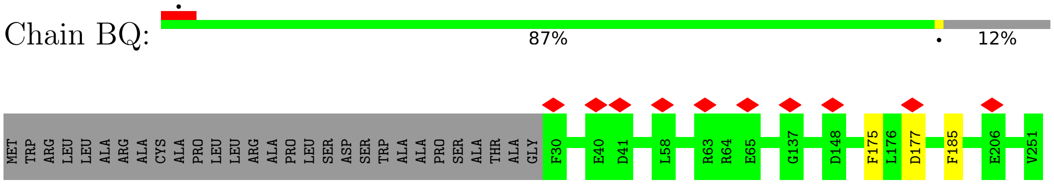
- Molecule 83: Uncharacterized protein



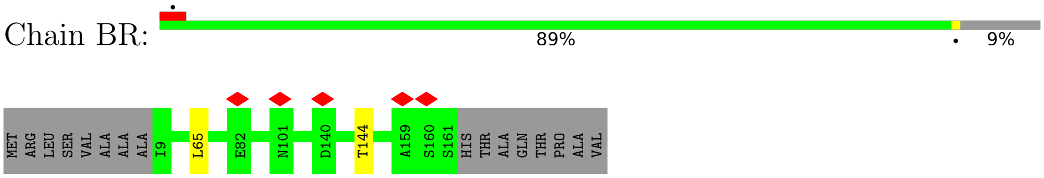
- Molecule 84: Uncharacterized protein



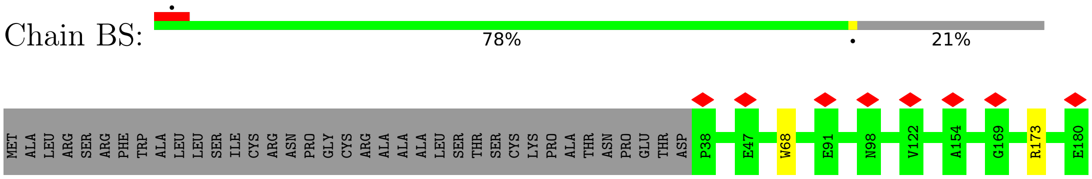
- Molecule 85: Uncharacterized protein



- Molecule 86: Uncharacterized protein



- Molecule 87: Mitochondrial ribosomal protein L18



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12858	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 $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.289	Depositor
Minimum map value	-0.162	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	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: MG, SPM, FME, GTP, GNP, 5GP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	AI	0.24	0/2707	0.38	0/3636
2	BT	0.24	0/1883	0.40	0/2540
3	BU	0.23	0/1179	0.36	0/1578
4	BV	0.24	0/1256	0.42	0/1706
5	BW	0.25	0/1407	0.38	0/1891
6	BX	0.25	0/1211	0.39	0/1646
7	BY	0.23	0/1719	0.41	0/2329
8	Ba	0.24	0/3267	0.40	0/4455
9	Bb	0.24	0/3047	0.39	0/4139
10	Bc	0.24	0/2464	0.38	0/3330
11	Bd	0.24	0/1203	0.38	0/1622
12	Be	0.25	0/1000	0.42	0/1345
13	Bf	0.25	0/851	0.50	2/1159 (0.2%)
14	Bg	0.24	0/1191	0.41	0/1614
15	Bh	0.24	0/2372	0.38	0/3211
16	Bi	0.24	0/2199	0.40	0/2980
17	Bj	0.23	0/1811	0.40	0/2436
18	Bk	0.24	0/1270	0.41	0/1714
19	Bl	0.25	0/1135	0.41	0/1549
20	Bm	0.23	0/917	0.36	0/1248
21	Bn	0.23	0/860	0.36	0/1150
22	Bo	0.24	0/787	0.36	0/1056
23	Bp	0.24	0/752	0.42	0/1013
24	Bq	0.23	0/717	0.43	1/971 (0.1%)
25	Bt	0.23	0/798	0.37	0/1073
26	Bu	0.23	0/1214	0.41	1/1630 (0.1%)
27	Bv	0.23	0/1157	0.35	0/1560
28	B0	0.25	0/880	0.40	0/1189
29	Bw	0.24	0/3206	0.39	0/4354
30	Bx	0.24	0/1364	0.40	0/1849
31	AA	0.18	0/22852	0.75	2/35580 (0.0%)
31	BA	0.21	0/36784	0.78	14/57270 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	AB	0.24	0/1804	0.39	0/2445
33	AC	0.24	0/1105	0.42	0/1496
34	AE	0.24	0/2785	0.40	0/3735
35	AF	0.24	0/999	0.41	0/1347
36	AG	0.24	0/1763	0.36	0/2368
37	AJ	0.23	0/1181	0.42	0/1597
38	AK	0.24	0/1027	0.42	0/1389
39	AL	0.24	0/858	0.42	0/1152
40	AN	0.22	0/874	0.37	0/1171
41	AO	0.23	0/1473	0.36	0/1970
42	AP	0.24	0/954	0.40	0/1284
43	AQ	0.24	0/894	0.42	0/1213
44	AR	0.24	0/802	0.39	0/1079
45	AU	0.23	0/745	0.35	0/993
46	AV	0.21	0/1673	0.91	3/2602 (0.1%)
46	AY	0.21	0/1673	0.93	4/2602 (0.2%)
47	AX	0.16	0/142	0.69	0/219
48	AZ	0.25	0/89	0.35	0/123
49	Aa	0.23	0/2428	0.38	0/3279
50	Ab	0.25	0/1126	0.38	0/1514
51	Ac	0.24	0/1399	0.41	0/1881
52	Ad	0.24	0/1490	0.35	0/2005
53	Ae	0.23	0/3171	0.40	1/4292 (0.0%)
54	B1	0.23	0/2093	0.37	0/2835
55	Af	0.24	0/790	0.43	0/1064
56	Ag	0.24	0/2945	0.40	0/3984
57	Ah	0.24	0/1045	0.36	0/1409
58	Ai	0.24	0/841	0.36	0/1121
59	Aj	0.23	0/1835	0.39	0/2484
60	Ak	0.23	0/2268	0.38	0/3069
61	Am	0.23	0/947	0.39	0/1268
62	An	0.22	0/650	0.35	0/858
63	Ao	0.24	0/4625	0.38	0/6267
64	Ap	0.23	0/1616	0.38	0/2195
65	CL	0.23	0/319	0.41	0/435
65	DL	0.22	0/212	0.41	0/286
65	EL	0.21	0/221	0.37	0/297
65	FL	0.21	0/212	0.36	0/286
65	GL	0.22	0/212	0.38	0/286
65	HL	0.22	0/204	0.40	0/275
65	LL	0.23	0/542	0.39	0/729
66	B2	0.24	0/1586	0.36	0/2123
67	B3	0.23	0/993	0.39	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
68	B4	0.22	0/481	0.46	1/653 (0.2%)
69	B5	0.24	0/917	0.39	0/1227
70	B6	0.23	0/430	0.41	0/570
71	B7	0.23	0/395	0.37	0/524
72	B8	0.24	0/853	0.39	0/1136
73	B9	0.23	0/342	0.39	0/450
74	BB	0.32	1/1595 (0.1%)	0.75	0/2475
75	BC	0.25	0/5522	0.42	0/7451
76	BD	0.24	0/1898	0.42	0/2555
77	BE	0.24	0/2493	0.41	0/3387
78	BF	0.23	0/2069	0.39	0/2816
79	BI	0.23	0/819	0.42	0/1101
80	BJ	0.24	0/1742	0.40	0/2358
81	BK	0.24	0/1359	0.39	0/1828
82	BN	0.24	0/1487	0.37	0/2017
83	BO	0.23	0/912	0.42	0/1231
84	BP	0.25	0/2368	0.40	0/3198
85	BQ	0.24	0/1850	0.40	0/2491
86	BR	0.23	0/1262	0.39	0/1700
87	BS	0.23	0/1197	0.41	0/1624
All	All	0.23	1/190062 (0.0%)	0.57	29/269983 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	BB	1	G	OP3-P	-10.69	1.48	1.61

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	AY	61	C	N3-C2-O2	-9.01	115.59	121.90
46	AY	57	C	N3-C2-O2	-8.77	115.76	121.90
46	AV	57	C	N3-C2-O2	-8.48	115.97	121.90
46	AV	61	C	N3-C2-O2	-7.83	116.42	121.90
31	AA	119	C	C2-N1-C1’	7.66	127.23	118.80
46	AY	61	C	N1-C2-O2	7.05	123.13	118.90
31	BA	1558	U	C2-N1-C1’	6.70	125.75	117.70
13	Bf	80	PRO	N-CA-CB	6.53	111.14	103.30
53	Ae	342	PRO	N-CA-CB	6.49	111.08	103.30
13	Bf	78	PRO	N-CA-CB	6.40	110.98	103.30
26	Bu	167	PRO	N-CA-CB	6.39	110.97	103.30
31	BA	1558	U	N1-C2-O2	6.15	127.11	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	BA	825	C	C2-N1-C1'	5.93	125.32	118.80
31	BA	1558	U	N3-C2-O2	-5.87	118.09	122.20
24	Bq	59	PRO	N-CA-CB	5.83	110.29	103.30
46	AV	61	C	N1-C2-O2	5.78	122.37	118.90
31	BA	848	C	C2-N1-C1'	5.63	125.00	118.80
68	B4	87	PRO	N-CA-CB	5.63	110.06	103.30
31	BA	890	C	N1-C2-O2	5.55	122.23	118.90
31	AA	119	C	C6-N1-C1'	-5.50	114.20	120.80
31	BA	48	U	OP1-P-O3'	5.44	117.17	105.20
31	BA	847	U	C2-N1-C1'	5.33	124.09	117.70
31	BA	394	C	N1-C2-O2	5.32	122.09	118.90
31	BA	48	U	P-O3'-C3'	5.32	126.08	119.70
31	BA	64	C	C2-N1-C1'	5.28	124.60	118.80
31	BA	890	C	C2-N1-C1'	5.25	124.58	118.80
31	BA	394	C	C2-N1-C1'	5.07	124.38	118.80
31	BA	825	C	N1-C2-O2	5.06	121.94	118.90
46	AY	57	C	N1-C2-O2	5.05	121.93	118.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	AI	326/397 (82%)	318 (98%)	8 (2%)	0	100	100
2	BT	220/292 (75%)	217 (99%)	3 (1%)	0	100	100
3	BU	138/149 (93%)	137 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	BV	153/209 (73%)	149 (97%)	4 (3%)	0	100	100
5	BW	164/210 (78%)	158 (96%)	6 (4%)	0	100	100
6	BX	147/150 (98%)	144 (98%)	3 (2%)	0	100	100
7	BY	204/216 (94%)	199 (98%)	5 (2%)	0	100	100
8	Ba	391/423 (92%)	379 (97%)	12 (3%)	0	100	100
9	Bb	352/380 (93%)	336 (96%)	16 (4%)	0	100	100
10	Bc	293/334 (88%)	279 (95%)	14 (5%)	0	100	100
11	Bd	138/206 (67%)	133 (96%)	5 (4%)	0	100	100
12	Be	120/135 (89%)	115 (96%)	5 (4%)	0	100	100
13	Bf	106/142 (75%)	101 (95%)	3 (3%)	2 (2%)	8	41
14	Bg	146/159 (92%)	135 (92%)	11 (8%)	0	100	100
15	Bh	287/332 (86%)	274 (96%)	13 (4%)	0	100	100
16	Bi	258/306 (84%)	249 (96%)	9 (4%)	0	100	100
17	Bj	211/279 (76%)	204 (97%)	7 (3%)	0	100	100
18	Bk	151/269 (56%)	146 (97%)	5 (3%)	0	100	100
19	Bl	131/166 (79%)	129 (98%)	2 (2%)	0	100	100
20	Bm	107/198 (54%)	104 (97%)	3 (3%)	0	100	100
21	Bn	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
22	Bo	95/124 (77%)	93 (98%)	2 (2%)	0	100	100
23	Bp	95/112 (85%)	91 (96%)	4 (4%)	0	100	100
24	Bq	83/138 (60%)	75 (90%)	8 (10%)	0	100	100
25	Bt	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
26	Bu	147/205 (72%)	140 (95%)	5 (3%)	2 (1%)	11	47
27	Bv	133/222 (60%)	133 (100%)	0	0	100	100
28	B0	108/148 (73%)	106 (98%)	2 (2%)	0	100	100
29	Bw	385/433 (89%)	363 (94%)	22 (6%)	0	100	100
30	Bx	160/196 (82%)	152 (95%)	8 (5%)	0	100	100
32	AB	218/289 (75%)	210 (96%)	8 (4%)	0	100	100
33	AC	130/167 (78%)	124 (95%)	6 (5%)	0	100	100
34	AE	341/430 (79%)	324 (95%)	17 (5%)	0	100	100
35	AF	120/276 (44%)	115 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	AG	206/242 (85%)	206 (100%)	0	0	100	100
37	AJ	138/200 (69%)	130 (94%)	8 (6%)	0	100	100
38	AK	135/196 (69%)	131 (97%)	4 (3%)	0	100	100
39	AL	107/139 (77%)	102 (95%)	5 (5%)	0	100	100
40	AN	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
41	AO	173/239 (72%)	169 (98%)	4 (2%)	0	100	100
42	AP	115/135 (85%)	112 (97%)	3 (3%)	0	100	100
43	AQ	110/130 (85%)	109 (99%)	1 (1%)	0	100	100
44	AR	95/143 (66%)	95 (100%)	0	0	100	100
45	AU	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
48	AZ	16/18 (89%)	16 (100%)	0	0	100	100
49	Aa	290/382 (76%)	286 (99%)	4 (1%)	0	100	100
50	Ab	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
51	Ac	167/173 (96%)	165 (99%)	2 (1%)	0	100	100
52	Ad	175/205 (85%)	174 (99%)	1 (1%)	0	100	100
53	Ae	386/455 (85%)	365 (95%)	19 (5%)	2 (0%)	29	68
54	B1	242/256 (94%)	242 (100%)	0	0	100	100
55	Af	97/188 (52%)	91 (94%)	6 (6%)	0	100	100
56	Ag	351/410 (86%)	337 (96%)	14 (4%)	0	100	100
57	Ah	118/387 (30%)	118 (100%)	0	0	100	100
58	Ai	97/106 (92%)	97 (100%)	0	0	100	100
59	Aj	211/218 (97%)	205 (97%)	6 (3%)	0	100	100
60	Ak	273/325 (84%)	267 (98%)	6 (2%)	0	100	100
61	Am	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
62	An	70/199 (35%)	69 (99%)	1 (1%)	0	100	100
63	Ao	564/692 (82%)	552 (98%)	12 (2%)	0	100	100
64	Ap	188/258 (73%)	181 (96%)	7 (4%)	0	100	100
65	CL	43/198 (22%)	40 (93%)	3 (7%)	0	100	100
65	DL	25/198 (13%)	25 (100%)	0	0	100	100
65	EL	26/198 (13%)	26 (100%)	0	0	100	100
65	FL	25/198 (13%)	24 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	GL	25/198 (13%)	25 (100%)	0	0	100	100
65	HL	24/198 (12%)	24 (100%)	0	0	100	100
65	LL	68/198 (34%)	67 (98%)	1 (2%)	0	100	100
66	B2	177/252 (70%)	176 (99%)	1 (1%)	0	100	100
67	B3	116/161 (72%)	113 (97%)	3 (3%)	0	100	100
68	B4	60/126 (48%)	52 (87%)	8 (13%)	0	100	100
69	B5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
70	B6	50/65 (77%)	50 (100%)	0	0	100	100
71	B7	44/95 (46%)	44 (100%)	0	0	100	100
72	B8	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
73	B9	36/100 (36%)	36 (100%)	0	0	100	100
75	BC	688/721 (95%)	641 (93%)	47 (7%)	0	100	100
76	BD	238/306 (78%)	229 (96%)	9 (4%)	0	100	100
77	BE	305/348 (88%)	287 (94%)	18 (6%)	0	100	100
78	BF	248/294 (84%)	243 (98%)	5 (2%)	0	100	100
79	BI	96/268 (36%)	95 (99%)	1 (1%)	0	100	100
80	BJ	210/262 (80%)	197 (94%)	13 (6%)	0	100	100
81	BK	174/192 (91%)	166 (95%)	8 (5%)	0	100	100
82	BN	175/178 (98%)	169 (97%)	6 (3%)	0	100	100
83	BO	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
84	BP	286/296 (97%)	274 (96%)	12 (4%)	0	100	100
85	BQ	220/251 (88%)	216 (98%)	4 (2%)	0	100	100
86	BR	151/169 (89%)	144 (95%)	7 (5%)	0	100	100
87	BS	141/180 (78%)	130 (92%)	11 (8%)	0	100	100
All	All	14964/20312 (74%)	14454 (97%)	504 (3%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	Bf	80	PRO
26	Bu	167	PRO
13	Bf	78	PRO
53	Ae	342	PRO
53	Ae	341	GLN

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Mol	Chain	Res	Type
26	Bu	166	GLU

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	AI	273/333 (82%)	271 (99%)	2 (1%)	84	90
2	BT	204/258 (79%)	200 (98%)	4 (2%)	55	73
3	BU	118/127 (93%)	118 (100%)	0	100	100
4	BV	136/178 (76%)	134 (98%)	2 (2%)	65	80
5	BW	144/180 (80%)	143 (99%)	1 (1%)	84	90
6	BX	116/134 (87%)	116 (100%)	0	100	100
7	BY	185/192 (96%)	181 (98%)	4 (2%)	52	70
8	Ba	348/365 (95%)	340 (98%)	8 (2%)	50	70
9	Bb	310/328 (94%)	305 (98%)	5 (2%)	62	79
10	Bc	271/299 (91%)	269 (99%)	2 (1%)	84	90
11	Bd	129/181 (71%)	124 (96%)	5 (4%)	32	57
12	Be	100/108 (93%)	99 (99%)	1 (1%)	76	86
13	Bf	80/133 (60%)	78 (98%)	2 (2%)	47	68
14	Bg	128/136 (94%)	125 (98%)	3 (2%)	50	70
15	Bh	251/284 (88%)	245 (98%)	6 (2%)	49	69
16	Bi	236/275 (86%)	232 (98%)	4 (2%)	60	78
17	Bj	190/242 (78%)	185 (97%)	5 (3%)	46	67
18	Bk	135/226 (60%)	132 (98%)	3 (2%)	52	70
19	Bl	122/147 (83%)	120 (98%)	2 (2%)	62	79
20	Bm	103/178 (58%)	103 (100%)	0	100	100
21	Bn	88/113 (78%)	86 (98%)	2 (2%)	50	70
22	Bo	77/97 (79%)	76 (99%)	1 (1%)	69	82
23	Bp	79/88 (90%)	78 (99%)	1 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Bq	70/114 (61%)	67 (96%)	3 (4%)	29	55
25	Bt	75/82 (92%)	75 (100%)	0	100	100
26	Bu	126/177 (71%)	125 (99%)	1 (1%)	81	89
27	Bv	115/183 (63%)	112 (97%)	3 (3%)	46	67
28	B0	90/115 (78%)	90 (100%)	0	100	100
29	Bw	340/373 (91%)	339 (100%)	1 (0%)	92	95
30	Bx	149/173 (86%)	145 (97%)	4 (3%)	44	66
32	AB	187/233 (80%)	186 (100%)	1 (0%)	88	93
33	AC	115/142 (81%)	113 (98%)	2 (2%)	60	78
34	AE	282/351 (80%)	279 (99%)	3 (1%)	73	84
35	AF	107/210 (51%)	104 (97%)	3 (3%)	43	65
36	AG	181/205 (88%)	178 (98%)	3 (2%)	60	78
37	AJ	130/180 (72%)	127 (98%)	3 (2%)	50	70
38	AK	103/151 (68%)	103 (100%)	0	100	100
39	AL	92/116 (79%)	92 (100%)	0	100	100
40	AN	92/114 (81%)	92 (100%)	0	100	100
41	AO	159/205 (78%)	159 (100%)	0	100	100
42	AP	97/113 (86%)	97 (100%)	0	100	100
43	AQ	97/114 (85%)	97 (100%)	0	100	100
44	AR	89/127 (70%)	87 (98%)	2 (2%)	52	70
45	AU	77/78 (99%)	76 (99%)	1 (1%)	69	82
49	Aa	258/330 (78%)	252 (98%)	6 (2%)	50	70
50	Ab	113/162 (70%)	113 (100%)	0	100	100
51	Ac	152/155 (98%)	150 (99%)	2 (1%)	69	82
52	Ad	149/168 (89%)	144 (97%)	5 (3%)	37	61
53	Ae	325/393 (83%)	318 (98%)	7 (2%)	52	70
54	B1	219/229 (96%)	214 (98%)	5 (2%)	50	70
55	Af	86/160 (54%)	85 (99%)	1 (1%)	71	83
56	Ag	312/361 (86%)	309 (99%)	3 (1%)	76	86
57	Ah	109/346 (32%)	108 (99%)	1 (1%)	78	87
58	Ai	86/93 (92%)	85 (99%)	1 (1%)	71	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	Aj	188/190 (99%)	184 (98%)	4 (2%)	53	71
60	Ak	249/289 (86%)	243 (98%)	6 (2%)	49	69
61	Am	100/102 (98%)	97 (97%)	3 (3%)	41	63
62	An	66/174 (38%)	66 (100%)	0	100	100
63	Ao	478/604 (79%)	467 (98%)	11 (2%)	50	70
64	Ap	170/225 (76%)	165 (97%)	5 (3%)	42	64
65	CL	30/157 (19%)	30 (100%)	0	100	100
65	DL	26/157 (17%)	22 (85%)	4 (15%)	2	16
65	EL	27/157 (17%)	27 (100%)	0	100	100
65	FL	26/157 (17%)	26 (100%)	0	100	100
65	GL	26/157 (17%)	25 (96%)	1 (4%)	33	58
65	HL	25/157 (16%)	25 (100%)	0	100	100
65	LL	59/157 (38%)	59 (100%)	0	100	100
66	B2	164/228 (72%)	161 (98%)	3 (2%)	59	76
67	B3	110/150 (73%)	110 (100%)	0	100	100
68	B4	45/114 (40%)	44 (98%)	1 (2%)	52	70
69	B5	99/163 (61%)	99 (100%)	0	100	100
70	B6	49/60 (82%)	49 (100%)	0	100	100
71	B7	41/78 (53%)	41 (100%)	0	100	100
72	B8	87/162 (54%)	85 (98%)	2 (2%)	50	70
73	B9	36/77 (47%)	35 (97%)	1 (3%)	43	65
75	BC	589/608 (97%)	568 (96%)	21 (4%)	35	60
76	BD	193/248 (78%)	190 (98%)	3 (2%)	62	79
77	BE	263/290 (91%)	260 (99%)	3 (1%)	73	84
78	BF	217/251 (86%)	215 (99%)	2 (1%)	78	87
79	BI	88/228 (39%)	87 (99%)	1 (1%)	73	84
80	BJ	192/230 (84%)	190 (99%)	2 (1%)	76	86
81	BK	138/151 (91%)	130 (94%)	8 (6%)	20	47
82	BN	156/157 (99%)	156 (100%)	0	100	100
83	BO	99/123 (80%)	99 (100%)	0	100	100
84	BP	245/249 (98%)	239 (98%)	6 (2%)	49	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
85	BQ	190/210 (90%)	187 (98%)	3 (2%)	62	79
86	BR	132/143 (92%)	130 (98%)	2 (2%)	65	80
87	BS	123/153 (80%)	121 (98%)	2 (2%)	62	79
All	All	13131/17311 (76%)	12913 (98%)	218 (2%)	62	78

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AI	86	ARG
1	AI	94	GLU
2	BT	121	THR
2	BT	187	LEU
2	BT	252	GLU
2	BT	284	ASP
4	BV	69	VAL
4	BV	113	THR
5	BW	80	TYR
7	BY	81	ARG
7	BY	105	ARG
7	BY	184	GLU
7	BY	186	THR
8	Ba	40	LYS
8	Ba	139	LEU
8	Ba	256	PHE
8	Ba	270	VAL
8	Ba	273	VAL
8	Ba	307	ASP
8	Ba	337	GLU
8	Ba	341	VAL
9	Bb	52	ARG
9	Bb	179	VAL
9	Bb	207	GLU
9	Bb	233	VAL
9	Bb	324	ASP
10	Bc	56	THR
10	Bc	152	GLU
11	Bd	23	ARG
11	Bd	29	ARG
11	Bd	46	THR
11	Bd	106	LEU
11	Bd	145	GLU

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Mol	Chain	Res	Type
12	Be	101	ASP
13	Bf	43	TYR
13	Bf	45	CYS
14	Bg	81	ASN
14	Bg	112	VAL
14	Bg	119	PHE
15	Bh	148	LEU
15	Bh	151	GLU
15	Bh	158	ASP
15	Bh	164	GLU
15	Bh	191	LEU
15	Bh	267	LEU
16	Bi	56	PHE
16	Bi	143	ASP
16	Bi	221	THR
16	Bi	244	GLU
17	Bj	47	LEU
17	Bj	55	ARG
17	Bj	84	TYR
17	Bj	265	LYS
17	Bj	273	ARG
18	Bk	84	THR
18	Bk	175	HIS
18	Bk	192	GLU
19	Bl	64	GLU
19	Bl	166	PHE
21	Bn	43	VAL
21	Bn	66	PHE
22	Bo	85	ASP
23	Bp	27	VAL
24	Bq	73	MET
24	Bq	75	VAL
24	Bq	86	LEU
26	Bu	155	ASP
27	Bv	88	GLU
27	Bv	144	GLU
27	Bv	151	ASP
29	Bw	131	LEU
30	Bx	43	ASP
30	Bx	92	PHE
30	Bx	100	LEU
30	Bx	152	THR

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Mol	Chain	Res	Type
32	AB	235	VAL
33	AC	52	THR
33	AC	138	TYR
34	AE	181	ARG
34	AE	189	ARG
34	AE	401	VAL
35	AF	76	GLU
35	AF	105	CYS
35	AF	106	GLU
36	AG	64	TYR
36	AG	65	GLU
36	AG	208	GLU
37	AJ	53	ASP
37	AJ	97	LEU
37	AJ	166	GLU
44	AR	69	CYS
44	AR	77	ASN
45	AU	52	ARG
49	Aa	91	THR
49	Aa	129	THR
49	Aa	150	MET
49	Aa	273	GLU
49	Aa	329	LEU
49	Aa	373	GLU
51	Ac	90	VAL
51	Ac	106	LEU
52	Ad	29	THR
52	Ad	32	ASP
52	Ad	44	THR
52	Ad	145	GLU
52	Ad	169	THR
53	Ae	84	ASP
53	Ae	98	ASP
53	Ae	234	THR
53	Ae	235	ASP
53	Ae	280	LEU
53	Ae	291	TRP
53	Ae	321	ASP
54	B1	33	GLU
54	B1	126	THR
54	B1	160	ASP
54	B1	232	GLU

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Mol	Chain	Res	Type
54	B1	241	GLN
55	Af	173	LEU
56	Ag	259	VAL
56	Ag	336	LEU
56	Ag	368	GLU
57	Ah	276	LYS
58	Ai	49	TYR
59	Aj	23	GLU
59	Aj	40	THR
59	Aj	107	GLU
59	Aj	154	THR
60	Ak	165	ILE
60	Ak	222	ASP
60	Ak	246	THR
60	Ak	247	GLU
60	Ak	252	GLU
60	Ak	308	GLU
61	Am	40	LYS
61	Am	66	CYS
61	Am	95	GLU
63	Ao	302	GLU
63	Ao	314	GLU
63	Ao	349	TYR
63	Ao	381	LEU
63	Ao	429	LEU
63	Ao	465	PHE
63	Ao	489	PHE
63	Ao	546	GLU
63	Ao	563	GLU
63	Ao	612	GLU
63	Ao	646	GLU
64	Ap	115	VAL
64	Ap	159	ASP
64	Ap	179	THR
64	Ap	197	ASP
64	Ap	233	GLU
65	DL	66	GLN
65	DL	79	ILE
65	DL	81	ASP
65	DL	84	GLU
65	GL	81	ASP
66	B2	92	LEU

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Mol	Chain	Res	Type
66	B2	228	LEU
66	B2	238	GLU
68	B4	48	THR
72	B8	137	THR
72	B8	163	THR
73	B9	65	THR
75	BC	203	ILE
75	BC	205	MET
75	BC	228	ASP
75	BC	237	GLU
75	BC	242	LEU
75	BC	268	PHE
75	BC	269	LEU
75	BC	297	LEU
75	BC	314	LEU
75	BC	325	ASN
75	BC	328	ILE
75	BC	406	MET
75	BC	485	ASP
75	BC	504	TYR
75	BC	559	LEU
75	BC	562	GLU
75	BC	578	ILE
75	BC	616	HIS
75	BC	624	ILE
75	BC	636	GLN
75	BC	681	VAL
76	BD	190	VAL
76	BD	208	ILE
76	BD	240	THR
77	BE	236	THR
77	BE	245	THR
77	BE	295	CYS
78	BF	47	VAL
78	BF	262	THR
79	BI	61	LYS
80	BJ	43	GLU
80	BJ	78	LEU
81	BK	30	ARG
81	BK	52	GLU
81	BK	62	GLU
81	BK	66	LEU

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Mol	Chain	Res	Type
81	BK	103	HIS
81	BK	111	LEU
81	BK	124	LYS
81	BK	157	LYS
84	BP	44	ARG
84	BP	61	THR
84	BP	134	ARG
84	BP	155	GLU
84	BP	215	THR
84	BP	286	THR
85	BQ	175	PHE
85	BQ	177	ASP
85	BQ	185	PHE
86	BR	65	LEU
86	BR	144	THR
87	BS	68	TRP
87	BS	173	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (243) such sidechains are listed below:

Mol	Chain	Res	Type
1	AI	101	GLN
1	AI	139	GLN
1	AI	156	GLN
1	AI	252	GLN
1	AI	319	HIS
2	BT	139	GLN
2	BT	153	ASN
2	BT	158	GLN
2	BT	172	GLN
2	BT	213	GLN
2	BT	219	GLN
3	BU	79	HIS
4	BV	104	HIS
4	BV	109	GLN
4	BV	122	ASN
5	BW	113	GLN
5	BW	171	HIS
6	BX	14	ASN
6	BX	35	GLN
8	Ba	108	HIS
8	Ba	119	GLN

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Mol	Chain	Res	Type
8	Ba	205	GLN
8	Ba	207	ASN
8	Ba	223	HIS
8	Ba	231	ASN
8	Ba	266	GLN
8	Ba	324	GLN
8	Ba	331	ASN
8	Ba	360	ASN
9	Bb	63	GLN
9	Bb	308	GLN
9	Bb	354	GLN
10	Bc	46	ASN
10	Bc	243	GLN
10	Bc	294	GLN
10	Bc	301	HIS
11	Bd	18	GLN
11	Bd	36	GLN
11	Bd	114	HIS
11	Bd	149	GLN
13	Bf	62	HIS
14	Bg	17	ASN
14	Bg	127	GLN
15	Bh	42	GLN
15	Bh	69	HIS
15	Bh	106	GLN
15	Bh	177	GLN
16	Bi	47	GLN
16	Bi	193	GLN
16	Bi	286	GLN
17	Bj	67	GLN
17	Bj	87	HIS
17	Bj	97	GLN
17	Bj	212	HIS
18	Bk	54	HIS
18	Bk	138	GLN
18	Bk	158	GLN
18	Bk	177	ASN
20	Bm	68	GLN
20	Bm	107	ASN
20	Bm	151	HIS
21	Bn	122	ASN
22	Bo	31	GLN

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Mol	Chain	Res	Type
22	Bo	69	GLN
22	Bo	100	GLN
23	Bp	15	GLN
23	Bp	35	GLN
23	Bp	93	HIS
24	Bq	71	HIS
25	Bt	30	GLN
25	Bt	34	ASN
25	Bt	91	GLN
26	Bu	67	GLN
26	Bu	145	ASN
27	Bv	107	GLN
27	Bv	112	GLN
27	Bv	138	GLN
28	B0	76	HIS
28	B0	107	ASN
29	Bw	65	GLN
29	Bw	87	GLN
29	Bw	226	GLN
29	Bw	234	GLN
29	Bw	381	ASN
29	Bw	385	ASN
29	Bw	414	GLN
30	Bx	130	ASN
30	Bx	164	ASN
32	AB	119	GLN
32	AB	133	HIS
32	AB	149	GLN
32	AB	238	ASN
33	AC	126	GLN
34	AE	175	GLN
34	AE	292	HIS
34	AE	317	HIS
34	AE	360	GLN
36	AG	122	GLN
36	AG	127	HIS
36	AG	140	ASN
36	AG	196	HIS
36	AG	215	ASN
37	AJ	51	HIS
37	AJ	125	HIS
37	AJ	163	ASN

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Mol	Chain	Res	Type
38	AK	73	ASN
38	AK	131	GLN
38	AK	185	HIS
38	AK	186	ASN
39	AL	35	GLN
39	AL	74	ASN
39	AL	77	ASN
39	AL	134	HIS
40	AN	117	HIS
40	AN	124	GLN
41	AO	84	HIS
41	AO	147	HIS
42	AP	28	ASN
42	AP	123	GLN
43	AQ	23	GLN
43	AQ	52	HIS
43	AQ	79	HIS
49	Aa	251	ASN
49	Aa	348	HIS
49	Aa	369	GLN
49	Aa	372	GLN
50	Ab	66	HIS
51	Ac	51	ASN
51	Ac	63	GLN
51	Ac	95	ASN
51	Ac	118	GLN
51	Ac	122	GLN
51	Ac	125	HIS
52	Ad	62	GLN
52	Ad	102	HIS
52	Ad	109	ASN
52	Ad	135	GLN
52	Ad	159	GLN
52	Ad	188	ASN
53	Ae	140	ASN
53	Ae	181	ASN
53	Ae	278	GLN
53	Ae	421	GLN
54	B1	27	HIS
54	B1	172	GLN
56	Ag	61	GLN
56	Ag	65	GLN

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Mol	Chain	Res	Type
56	Ag	68	ASN
56	Ag	179	GLN
56	Ag	200	GLN
56	Ag	204	GLN
56	Ag	298	ASN
56	Ag	311	GLN
56	Ag	362	ASN
56	Ag	366	GLN
56	Ag	386	ASN
56	Ag	389	GLN
57	Ah	309	ASN
57	Ah	321	HIS
57	Ah	331	GLN
57	Ah	364	HIS
57	Ah	370	ASN
59	Aj	88	GLN
59	Aj	177	GLN
60	Ak	263	ASN
60	Ak	270	GLN
61	Am	92	ASN
61	Am	113	ASN
63	Ao	158	GLN
63	Ao	260	HIS
63	Ao	288	ASN
63	Ao	325	GLN
63	Ao	336	GLN
63	Ao	473	GLN
63	Ao	542	GLN
63	Ao	593	GLN
63	Ao	629	GLN
64	Ap	152	GLN
64	Ap	160	HIS
64	Ap	181	HIS
64	Ap	221	GLN
65	DL	66	GLN
65	DL	83	ASN
65	FL	65	GLN
65	FL	83	ASN
66	B2	90	GLN
66	B2	218	GLN
69	B5	83	ASN
69	B5	90	ASN

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Mol	Chain	Res	Type
70	B6	23	GLN
72	B8	118	HIS
72	B8	154	GLN
75	BC	124	HIS
75	BC	154	GLN
75	BC	159	ASN
75	BC	330	ASN
75	BC	344	ASN
75	BC	349	ASN
75	BC	616	HIS
75	BC	617	HIS
75	BC	636	GLN
75	BC	640	ASN
75	BC	661	GLN
75	BC	733	ASN
76	BD	183	HIS
76	BD	228	GLN
77	BE	69	ASN
77	BE	128	HIS
77	BE	154	HIS
77	BE	281	ASN
77	BE	313	ASN
78	BF	74	GLN
78	BF	83	HIS
78	BF	97	HIS
79	BI	88	HIS
79	BI	121	ASN
79	BI	126	GLN
79	BI	136	ASN
80	BJ	41	HIS
80	BJ	93	ASN
80	BJ	151	ASN
80	BJ	223	GLN
80	BJ	235	GLN
81	BK	28	GLN
81	BK	133	GLN
82	BN	48	HIS
82	BN	74	GLN
82	BN	140	ASN
83	BO	33	GLN
83	BO	52	HIS
83	BO	89	HIS

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Mol	Chain	Res	Type
83	BO	103	ASN
83	BO	113	ASN
83	BO	142	GLN
84	BP	84	ASN
84	BP	94	GLN
84	BP	153	ASN
85	BQ	98	HIS
85	BQ	202	GLN
85	BQ	210	GLN
86	BR	148	GLN
87	BS	88	HIS
87	BS	142	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	AA	959/16770 (5%)	182 (18%)	2 (0%)
31	BA	1542/16770 (9%)	410 (26%)	1 (0%)
46	AV	70/71 (98%)	20 (28%)	0
46	AY	70/71 (98%)	24 (34%)	1 (1%)
47	AX	5/6 (83%)	0	0
74	BB	64/73 (87%)	18 (28%)	0
All	All	2710/33761 (8%)	654 (24%)	4 (0%)

All (654) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
31	AA	5	A
31	AA	10	U
31	AA	27	U
31	AA	34	U
31	AA	42	A
31	AA	43	U
31	AA	54	A
31	AA	58	U
31	AA	63	G
31	AA	65	C
31	AA	75	A
31	AA	81	U
31	AA	83	C
31	AA	102	G

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Mol	Chain	Res	Type
31	AA	115	A
31	AA	120	A
31	AA	127	A
31	AA	139	A
31	AA	147	G
31	AA	152	A
31	AA	161	C
31	AA	164	C
31	AA	165	G
31	AA	168	A
31	AA	170	A
31	AA	171	C
31	AA	173	G
31	AA	175	A
31	AA	186	U
31	AA	190	G
31	AA	191	C
31	AA	192	C
31	AA	203	G
31	AA	212	A
31	AA	216	A
31	AA	217	U
31	AA	222	A
31	AA	223	U
31	AA	224	U
31	AA	231	G
31	AA	235	A
31	AA	238	C
31	AA	244	C
31	AA	247	G
31	AA	253	G
31	AA	256	G
31	AA	257	U
31	AA	259	A
31	AA	273	A
31	AA	281	G
31	AA	287	C
31	AA	294	A
31	AA	296	G
31	AA	297	A
31	AA	308	A
31	AA	309	A

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Mol	Chain	Res	Type
31	AA	310	A
31	AA	314	A
31	AA	315	U
31	AA	316	C
31	AA	317	A
31	AA	320	A
31	AA	328	A
31	AA	337	C
31	AA	345	U
31	AA	354	C
31	AA	361	A
31	AA	362	A
31	AA	368	A
31	AA	372	C
31	AA	395	C
31	AA	399	A
31	AA	407	U
31	AA	417	C
31	AA	421	A
31	AA	433	U
31	AA	450	C
31	AA	455	A
31	AA	456	A
31	AA	457	C
31	AA	458	C
31	AA	461	A
31	AA	464	A
31	AA	465	G
31	AA	471	U
31	AA	472	A
31	AA	477	A
31	AA	479	C
31	AA	494	C
31	AA	498	U
31	AA	502	A
31	AA	503	A
31	AA	518	A
31	AA	531	U
31	AA	532	G
31	AA	538	C
31	AA	539	A
31	AA	540	U

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Mol	Chain	Res	Type
31	AA	541	C
31	AA	561	U
31	AA	566	U
31	AA	571	A
31	AA	574	C
31	AA	576	C
31	AA	587	U
31	AA	589	C
31	AA	592	A
31	AA	593	C
31	AA	596	U
31	AA	597	U
31	AA	604	U
31	AA	616	C
31	AA	618	G
31	AA	619	C
31	AA	620	C
31	AA	625	U
31	AA	626	C
31	AA	639	A
31	AA	640	A
31	AA	641	A
31	AA	644	A
31	AA	645	A
31	AA	646	C
31	AA	647	A
31	AA	649	U
31	AA	650	A
31	AA	653	A
31	AA	665	A
31	AA	681	A
31	AA	682	G
31	AA	698	A
31	AA	699	U
31	AA	707	A
31	AA	708	A
31	AA	709	A
31	AA	711	A
31	AA	720	A
31	AA	722	A
31	AA	731	A
31	AA	732	U

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Mol	Chain	Res	Type
31	AA	739	A
31	AA	743	A
31	AA	746	A
31	AA	775	A
31	AA	782	G
31	AA	783	A
31	AA	790	A
31	AA	791	G
31	AA	802	A
31	AA	803	U
31	AA	806	A
31	AA	807	G
31	AA	808	U
31	AA	822	A
31	AA	826	C
31	AA	838	A
31	AA	841	C
31	AA	842	A
31	AA	863	G
31	AA	865	A
31	AA	869	A
31	AA	876	A
31	AA	877	A
31	AA	883	C
31	AA	884	C
31	AA	885	U
31	AA	886	A
31	AA	893	A
31	AA	894	U
31	AA	902	C
31	AA	910	G
31	AA	918	A
31	AA	919	A
31	AA	925	A
31	AA	928	A
31	AA	930	G
31	AA	932	U
31	AA	943	G
31	AA	946	A
31	AA	955	G
31	AA	956	G
31	AA	959	U

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Mol	Chain	Res	Type
46	AV	6	G
46	AV	9	C
46	AV	14	A
46	AV	16	A
46	AV	17	U
46	AV	18	A
46	AV	43	A
46	AV	44	U
46	AV	45	G
46	AV	51	U
46	AV	54	A
46	AV	55	C
46	AV	56	C
46	AV	58	U
46	AV	60	C
46	AV	62	C
46	AV	63	G
46	AV	64	U
46	AV	65	A
46	AV	71	A
46	AY	6	G
46	AY	8	U
46	AY	9	C
46	AY	12	C
46	AY	14	A
46	AY	16	A
46	AY	17	U
46	AY	18	A
46	AY	27	G
46	AY	43	A
46	AY	45	G
46	AY	50	U
46	AY	53	U
46	AY	54	A
46	AY	55	C
46	AY	56	C
46	AY	58	U
46	AY	60	C
46	AY	62	C
46	AY	63	G
46	AY	64	U
46	AY	65	A

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Mol	Chain	Res	Type
46	AY	70	C
46	AY	71	A
31	BA	4	A
31	BA	7	G
31	BA	11	G
31	BA	15	A
31	BA	19	U
31	BA	20	A
31	BA	21	C
31	BA	22	U
31	BA	26	C
31	BA	30	U
31	BA	31	A
31	BA	32	C
31	BA	36	A
31	BA	40	C
31	BA	42	C
31	BA	43	C
31	BA	44	A
31	BA	45	A
31	BA	46	A
31	BA	49	A
31	BA	51	A
31	BA	56	A
31	BA	57	A
31	BA	59	A
31	BA	60	U
31	BA	63	A
31	BA	66	U
31	BA	67	A
31	BA	68	A
31	BA	82	G
31	BA	83	A
31	BA	96	U
31	BA	97	A
31	BA	104	C
31	BA	105	G
31	BA	109	U
31	BA	112	A
31	BA	115	U
31	BA	119	A
31	BA	125	A

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Mol	Chain	Res	Type
31	BA	129	A
31	BA	132	G
31	BA	139	G
31	BA	140	A
31	BA	141	A
31	BA	142	U
31	BA	143	A
31	BA	146	A
31	BA	147	U
31	BA	163	C
31	BA	164	A
31	BA	168	A
31	BA	172	C
31	BA	178	C
31	BA	180	A
31	BA	182	C
31	BA	188	C
31	BA	190	U
31	BA	192	A
31	BA	205	A
31	BA	218	A
31	BA	219	A
31	BA	223	A
31	BA	225	C
31	BA	229	A
31	BA	231	C
31	BA	237	A
31	BA	238	C
31	BA	239	C
31	BA	243	A
31	BA	245	A
31	BA	254	G
31	BA	263	G
31	BA	265	G
31	BA	271	U
31	BA	272	A
31	BA	273	A
31	BA	275	A
31	BA	277	A
31	BA	295	G
31	BA	309	A
31	BA	311	A

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Mol	Chain	Res	Type
31	BA	313	U
31	BA	322	G
31	BA	324	G
31	BA	329	A
31	BA	330	A
31	BA	331	A
31	BA	337	A
31	BA	338	C
31	BA	339	G
31	BA	340	A
31	BA	351	A
31	BA	352	G
31	BA	359	G
31	BA	366	A
31	BA	368	A
31	BA	369	G
31	BA	371	A
31	BA	373	U
31	BA	374	U
31	BA	376	A
31	BA	390	A
31	BA	393	A
31	BA	394	C
31	BA	398	A
31	BA	406	U
31	BA	409	A
31	BA	413	C
31	BA	414	A
31	BA	427	G
31	BA	428	A
31	BA	429	G
31	BA	433	G
31	BA	434	U
31	BA	435	C
31	BA	446	C
31	BA	447	A
31	BA	448	G
31	BA	449	C
31	BA	459	A
31	BA	460	C
31	BA	467	A
31	BA	468	A

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Mol	Chain	Res	Type
31	BA	472	U
31	BA	473	G
31	BA	474	A
31	BA	479	A
31	BA	480	G
31	BA	490	U
31	BA	491	U
31	BA	492	A
31	BA	493	A
31	BA	494	U
31	BA	497	U
31	BA	498	A
31	BA	499	C
31	BA	500	C
31	BA	501	A
31	BA	503	A
31	BA	504	G
31	BA	505	U
31	BA	509	C
31	BA	514	A
31	BA	515	A
31	BA	516	G
31	BA	517	C
31	BA	518	A
31	BA	530	A
31	BA	531	G
31	BA	532	A
31	BA	533	A
31	BA	541	A
31	BA	545	U
31	BA	547	A
31	BA	548	A
31	BA	549	C
31	BA	550	A
31	BA	551	A
31	BA	553	U
31	BA	560	A
31	BA	561	C
31	BA	562	A
31	BA	563	U
31	BA	570	A
31	BA	572	A

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Mol	Chain	Res	Type
31	BA	574	A
31	BA	576	U
31	BA	578	A
31	BA	579	U
31	BA	584	A
31	BA	586	C
31	BA	592	G
31	BA	595	C
31	BA	596	A
31	BA	618	A
31	BA	624	A
31	BA	625	A
31	BA	626	G
31	BA	631	A
31	BA	633	U
31	BA	634	G
31	BA	640	A
31	BA	660	C
31	BA	665	C
31	BA	673	C
31	BA	674	U
31	BA	675	U
31	BA	683	U
31	BA	684	A
31	BA	689	A
31	BA	694	A
31	BA	695	U
31	BA	697	C
31	BA	704	U
31	BA	707	A
31	BA	712	C
31	BA	713	A
31	BA	719	C
31	BA	720	C
31	BA	721	A
31	BA	722	A
31	BA	723	A
31	BA	724	A
31	BA	725	C
31	BA	727	A
31	BA	728	C
31	BA	744	A

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Mol	Chain	Res	Type
31	BA	745	A
31	BA	746	U
31	BA	747	U
31	BA	748	A
31	BA	755	U
31	BA	763	C
31	BA	774	A
31	BA	777	A
31	BA	778	A
31	BA	780	G
31	BA	782	A
31	BA	783	A
31	BA	814	C
31	BA	825	C
31	BA	843	C
31	BA	847	U
31	BA	848	C
31	BA	850	A
31	BA	851	G
31	BA	852	C
31	BA	853	A
31	BA	854	U
31	BA	855	U
31	BA	859	A
31	BA	864	U
31	BA	872	A
31	BA	889	C
31	BA	892	G
31	BA	894	U
31	BA	895	U
31	BA	896	A
31	BA	897	A
31	BA	900	G
31	BA	902	C
31	BA	903	G
31	BA	908	A
31	BA	909	U
31	BA	910	U
31	BA	922	A
31	BA	924	G
31	BA	925	G
31	BA	926	U

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Mol	Chain	Res	Type
31	BA	931	U
31	BA	933	A
31	BA	938	U
31	BA	947	A
31	BA	948	A
31	BA	958	U
31	BA	959	G
31	BA	960	U
31	BA	962	U
31	BA	964	A
31	BA	965	A
31	BA	967	G
31	BA	969	C
31	BA	970	C
31	BA	977	G
31	BA	983	U
31	BA	986	U
31	BA	988	U
31	BA	992	U
31	BA	1008	A
31	BA	1015	C
31	BA	1016	C
31	BA	1018	U
31	BA	1026	A
31	BA	1027	G
31	BA	1028	A
31	BA	1038	A
31	BA	1041	A
31	BA	1045	U
31	BA	1050	C
31	BA	1051	G
31	BA	1055	A
31	BA	1056	G
31	BA	1057	A
31	BA	1063	U
31	BA	1064	G
31	BA	1071	U
31	BA	1072	A
31	BA	1074	U
31	BA	1075	U
31	BA	1080	A
31	BA	1081	U

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Mol	Chain	Res	Type
31	BA	1089	G
31	BA	1091	U
31	BA	1092	A
31	BA	1093	A
31	BA	1127	A
31	BA	1129	C
31	BA	1138	G
31	BA	1140	A
31	BA	1146	G
31	BA	1150	G
31	BA	1167	C
31	BA	1168	A
31	BA	1169	A
31	BA	1180	G
31	BA	1183	U
31	BA	1194	U
31	BA	1195	A
31	BA	1204	A
31	BA	1206	U
31	BA	1207	C
31	BA	1215	C
31	BA	1216	C
31	BA	1217	A
31	BA	1218	U
31	BA	1219	A
31	BA	1220	A
31	BA	1221	C
31	BA	1222	A
31	BA	1226	C
31	BA	1233	A
31	BA	1237	A
31	BA	1238	A
31	BA	1239	A
31	BA	1240	A
31	BA	1241	U
31	BA	1242	U
31	BA	1246	A
31	BA	1247	U
31	BA	1249	A
31	BA	1253	G
31	BA	1254	A
31	BA	1258	A

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Mol	Chain	Res	Type
31	BA	1264	C
31	BA	1270	G
31	BA	1271	A
31	BA	1287	G
31	BA	1288	U
31	BA	1291	U
31	BA	1294	A
31	BA	1298	C
31	BA	1299	C
31	BA	1301	A
31	BA	1314	U
31	BA	1315	U
31	BA	1321	C
31	BA	1323	U
31	BA	1325	G
31	BA	1326	A
31	BA	1327	U
31	BA	1328	G
31	BA	1336	A
31	BA	1341	A
31	BA	1342	C
31	BA	1348	U
31	BA	1352	G
31	BA	1358	G
31	BA	1360	U
31	BA	1385	U
31	BA	1386	U
31	BA	1387	A
31	BA	1388	A
31	BA	1389	A
31	BA	1390	G
31	BA	1395	A
31	BA	1396	C
31	BA	1405	A
31	BA	1408	U
31	BA	1420	A
31	BA	1421	A
31	BA	1425	A
31	BA	1426	G
31	BA	1429	C
31	BA	1432	U
31	BA	1433	U

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Mol	Chain	Res	Type
31	BA	1436	U
31	BA	1438	U
31	BA	1445	U
31	BA	1448	A
31	BA	1453	U
31	BA	1455	C
31	BA	1457	A
31	BA	1465	A
31	BA	1468	A
31	BA	1474	G
31	BA	1493	A
31	BA	1494	A
31	BA	1498	C
31	BA	1504	A
31	BA	1505	G
31	BA	1509	U
31	BA	1514	A
31	BA	1521	U
31	BA	1526	U
31	BA	1527	U
31	BA	1528	A
31	BA	1531	C
31	BA	1532	U
31	BA	1533	A
31	BA	1536	U
31	BA	1548	A
31	BA	1551	C
31	BA	1552	C
31	BA	1553	A
31	BA	1554	G
31	BA	1558	U
31	BA	1559	A
31	BA	1569	A
31	BA	1571	A
74	BB	3	U
74	BB	4	A
74	BB	5	A
74	BB	7	G
74	BB	8	U
74	BB	9	A
74	BB	13	U
74	BB	21	C

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Mol	Chain	Res	Type
74	BB	23	A
74	BB	29	G
74	BB	34	U
74	BB	43	C
74	BB	44	U
74	BB	46	G
74	BB	47	A
74	BB	48	U
74	BB	69	C
74	BB	70	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	AA	530	G
31	AA	825	C
46	AY	44	U
31	BA	48	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 338 ligands modelled in this entry, 331 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
90	SPM	AA	16801	-	13,13,13	0.33	0	12,12,12	0.80	0
92	GTP	Ag	500	88	26,34,34	1.10	2 (7%)	32,54,54	1.65	7 (21%)
94	GNP	BC	802	88	29,34,34	1.60	7 (24%)	33,54,54	2.15	7 (21%)
91	FME	AV	101	46	8,9,10	0.96	0	7,9,11	0.89	0
90	SPM	BA	15902	-	13,13,13	0.34	0	12,12,12	0.76	0
90	SPM	BA	15903	-	13,13,13	0.34	0	12,12,12	0.78	0
93	5GP	BA	15901	88	22,26,26	1.26	2 (9%)	26,40,40	1.24	4 (15%)

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
90	SPM	AA	16801	-	-	2/11/11/11	-
92	GTP	Ag	500	88	-	1/18/38/38	0/3/3/3
94	GNP	BC	802	88	-	9/14/38/38	0/3/3/3
91	FME	AV	101	46	-	3/7/9/11	-
90	SPM	BA	15902	-	-	1/11/11/11	-
90	SPM	BA	15903	-	-	1/11/11/11	-
93	5GP	BA	15901	88	-	0/6/26/26	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
94	BC	802	GNP	PB-O3A	4.53	1.64	1.59
93	BA	15901	5GP	C5-C6	-4.14	1.39	1.47
92	Ag	500	GTP	C5-C6	-3.91	1.39	1.47
94	BC	802	GNP	C6-N1	3.11	1.38	1.33
94	BC	802	GNP	PB-O1B	3.05	1.51	1.46
94	BC	802	GNP	PG-N3B	2.98	1.71	1.63
93	BA	15901	5GP	C6-N1	-2.56	1.34	1.37
94	BC	802	GNP	PG-O1G	2.53	1.50	1.46
92	Ag	500	GTP	C2-N3	2.22	1.38	1.33
94	BC	802	GNP	PB-O2B	-2.15	1.51	1.56
94	BC	802	GNP	C5-C6	2.04	1.44	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
94	BC	802	GNP	C5-C6-N1	-8.44	111.89	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
94	BC	802	GNP	C2-N1-C6	5.86	125.24	115.93
92	Ag	500	GTP	PA-O3A-PB	-3.91	119.41	132.83
92	Ag	500	GTP	PB-O3B-PG	-3.83	119.67	132.83
92	Ag	500	GTP	C5-C6-N1	3.27	119.73	113.95
92	Ag	500	GTP	C3'-C2'-C1'	3.27	105.91	100.98
93	BA	15901	5GP	C5-C6-N1	3.12	119.45	113.95
92	Ag	500	GTP	C8-N7-C5	3.10	108.90	102.99
92	Ag	500	GTP	C2-N1-C6	-2.99	119.59	125.10
94	BC	802	GNP	N3-C2-N1	-2.77	123.53	127.22
94	BC	802	GNP	PB-O3A-PA	-2.54	123.67	132.62
94	BC	802	GNP	C4-C5-C6	-2.53	118.39	120.80
93	BA	15901	5GP	C8-N7-C5	2.31	107.39	102.99
93	BA	15901	5GP	C2-N1-C6	-2.26	120.93	125.10
94	BC	802	GNP	O1B-PB-N3B	-2.17	108.57	111.77
93	BA	15901	5GP	O6-C6-C5	-2.17	120.14	124.37
94	BC	802	GNP	C2-N3-C4	-2.16	112.89	115.36
92	Ag	500	GTP	O6-C6-C5	-2.11	120.25	124.37

There are no chirality outliers.

All (17) torsion outliers are listed below:

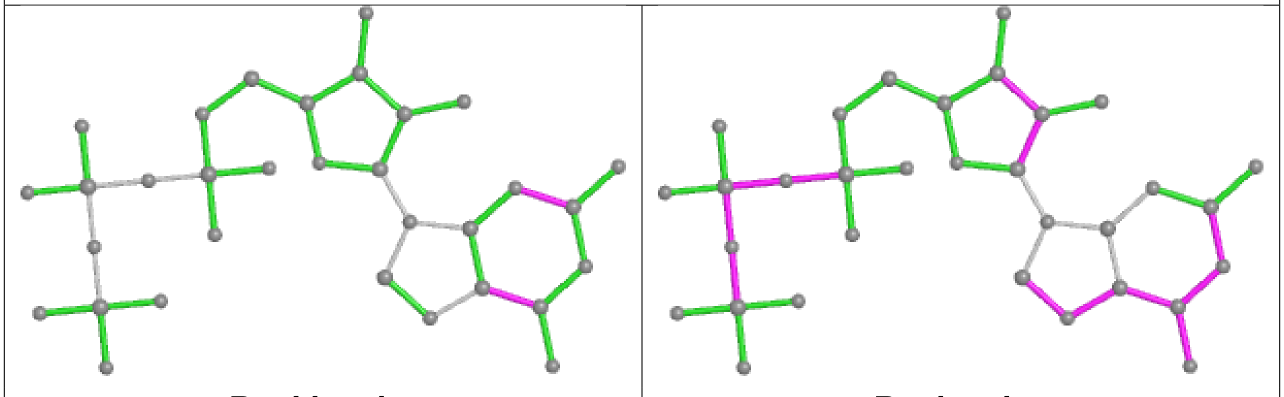
Mol	Chain	Res	Type	Atoms
91	AV	101	FME	N-CA-CB-CG
94	BC	802	GNP	PB-N3B-PG-O1G
94	BC	802	GNP	PG-N3B-PB-O1B
94	BC	802	GNP	PA-O3A-PB-O1B
94	BC	802	GNP	PA-O3A-PB-O2B
94	BC	802	GNP	C5'-O5'-PA-O3A
94	BC	802	GNP	C5'-O5'-PA-O2A
94	BC	802	GNP	O4'-C4'-C5'-O5'
90	BA	15903	SPM	N5-C6-C7-C8
90	AA	16801	SPM	C8-C9-N10-C11
94	BC	802	GNP	C3'-C4'-C5'-O5'
91	AV	101	FME	CB-CG-SD-CE
94	BC	802	GNP	C5'-O5'-PA-O1A
91	AV	101	FME	C-CA-CB-CG
92	Ag	500	GTP	C4'-C5'-O5'-PA
90	AA	16801	SPM	C7-C6-N5-C4
90	BA	15902	SPM	C8-C9-N10-C11

There are no ring outliers.

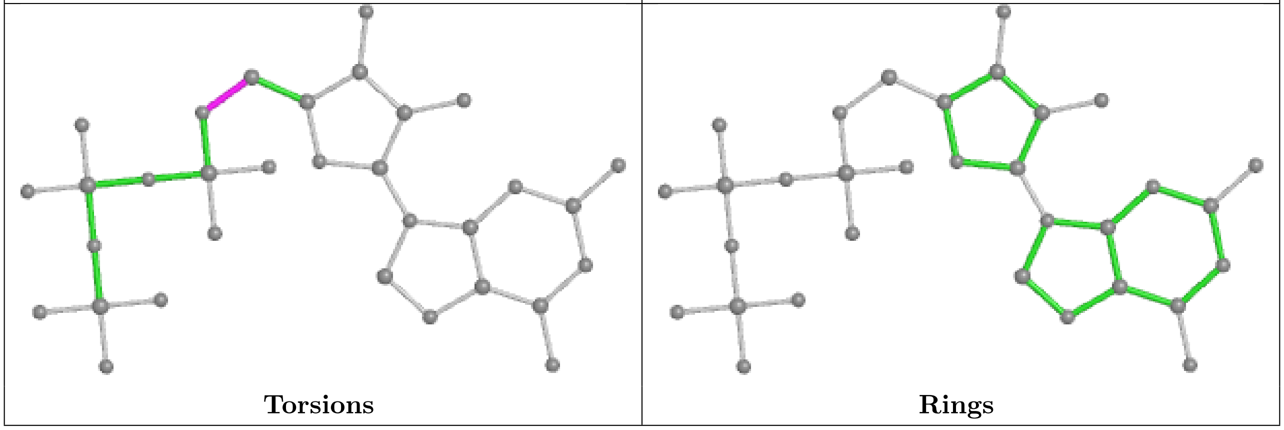
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 GTP Ag 500

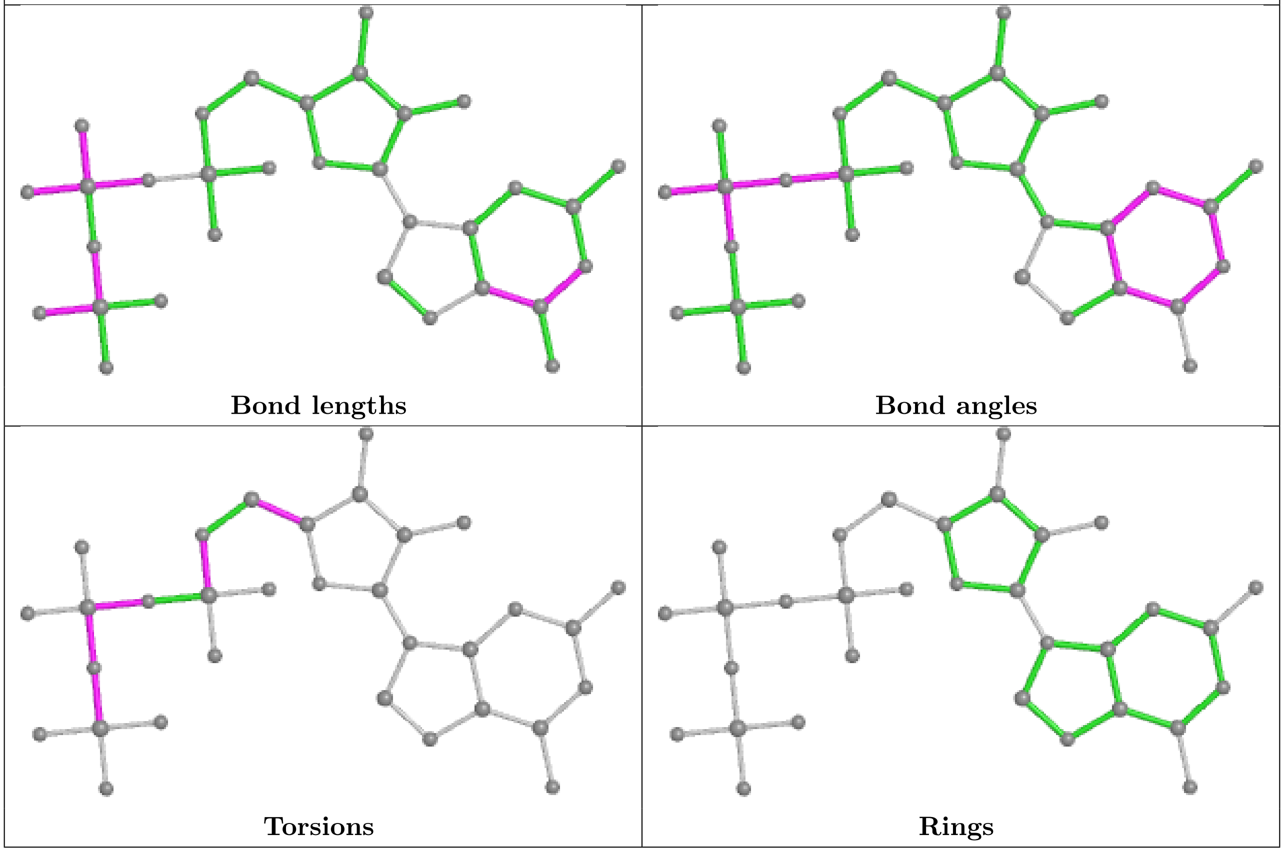


Bond lengths **Bond angles**



Torsions **Rings**

Ligand GNP BC 802



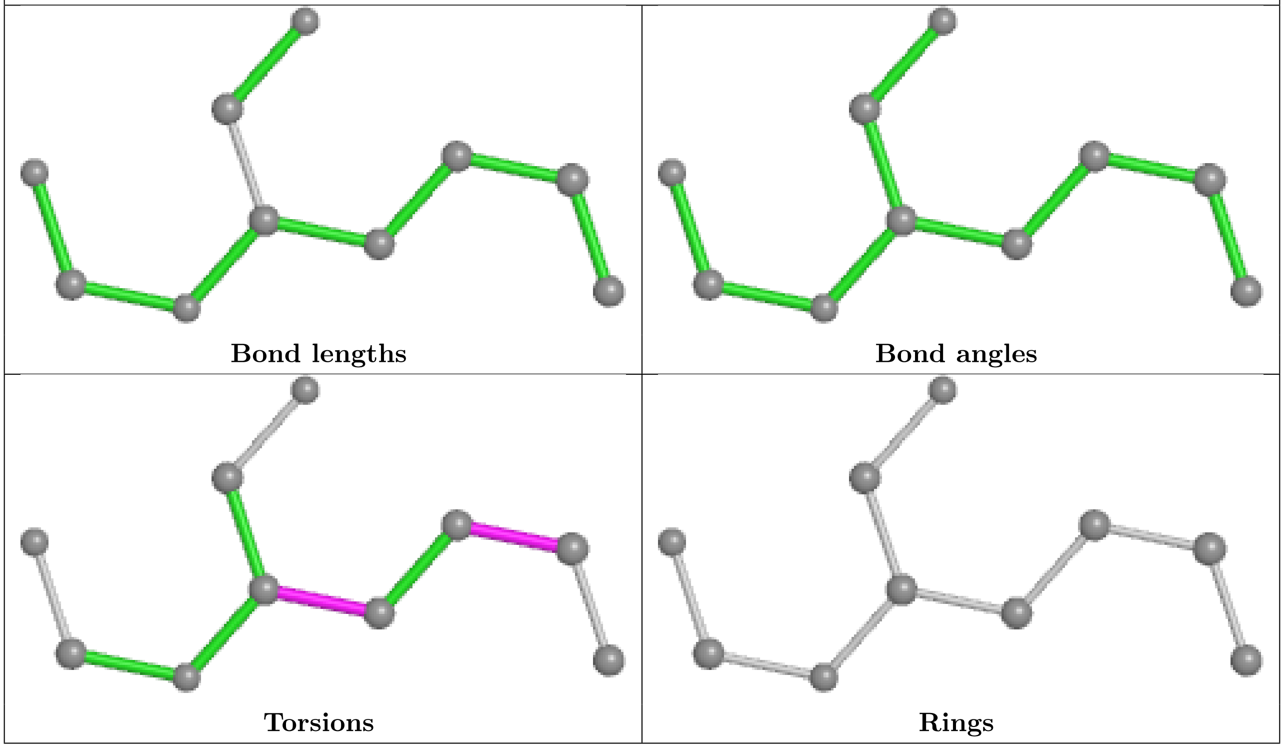
Bond lengths

Bond angles

Torsions

Rings

Ligand FME AV 101

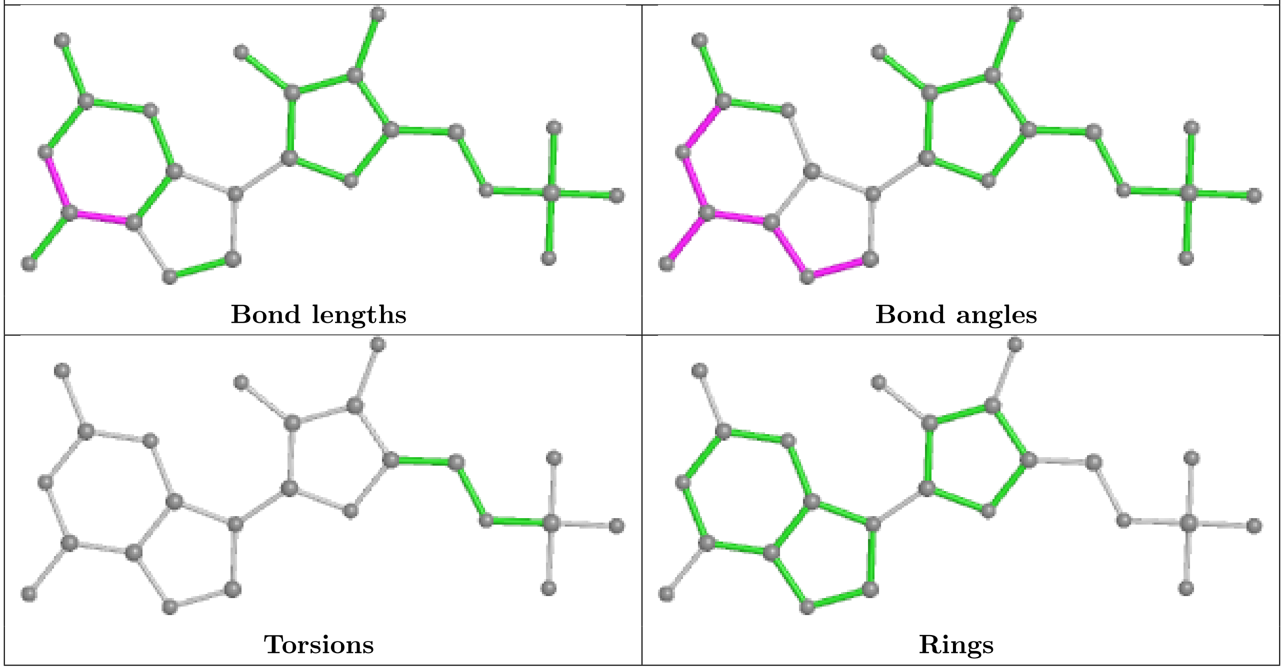


Bond lengths

Bond angles

Torsions

Rings



Ligand 5GP BA 15901

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
63	Ao	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ao	234:VAL	C	240:THR	N	8.13

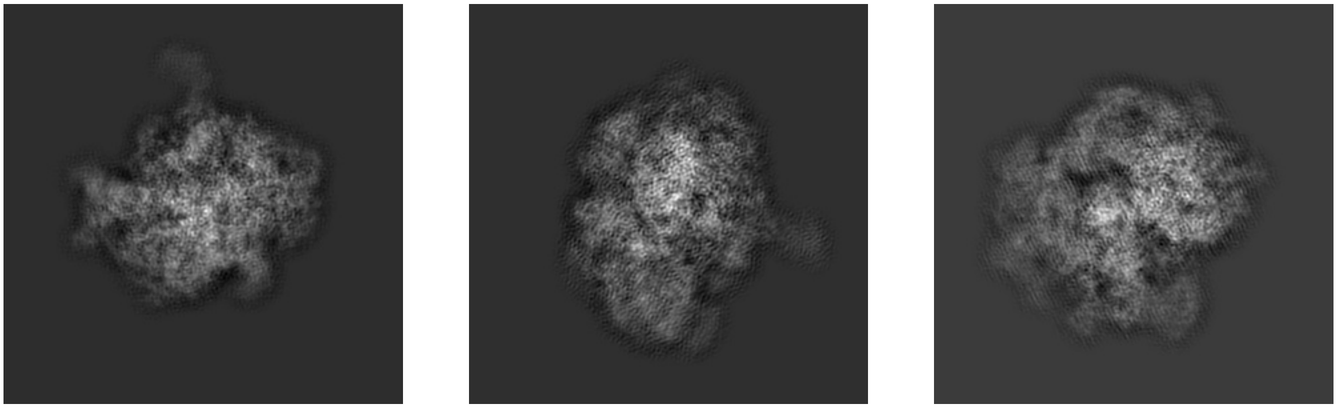
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10779. 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.

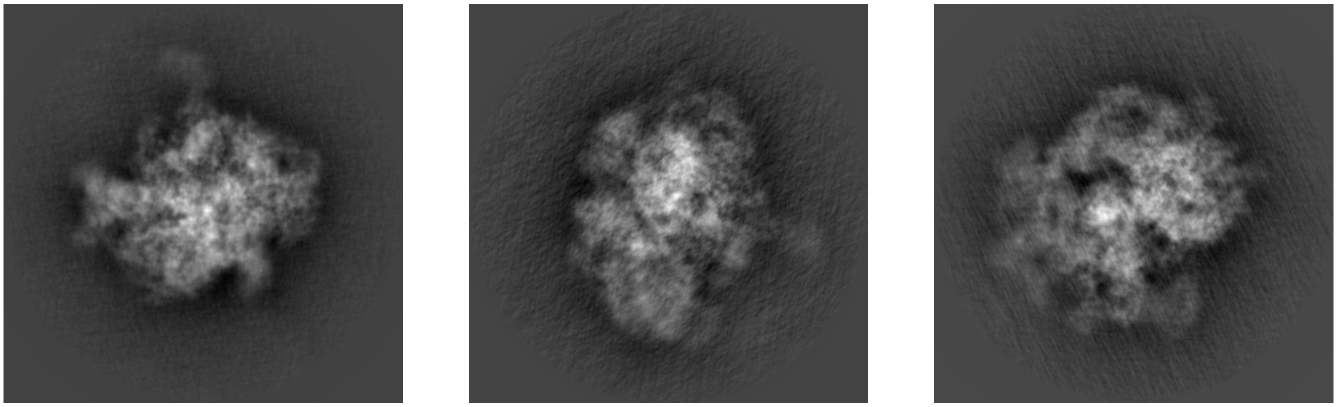
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

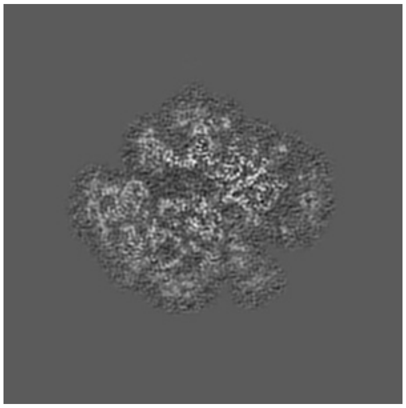


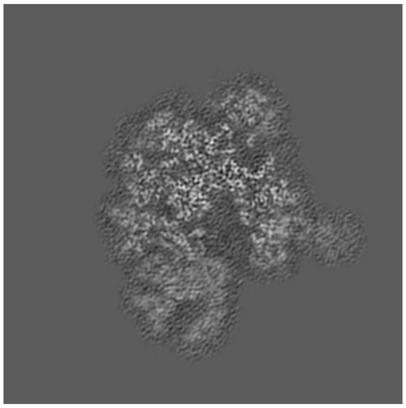
X Y Z

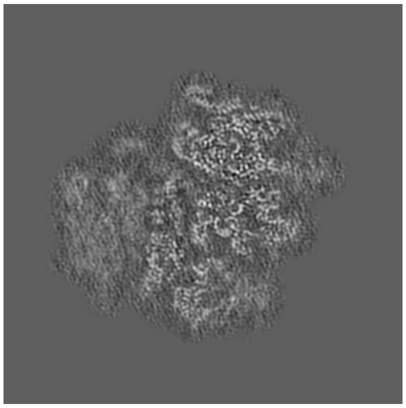
The images above show the map projected in three orthogonal directions.

6.2 Central slices

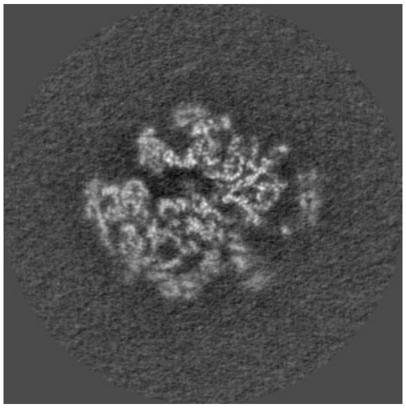
6.2.1 Primary map

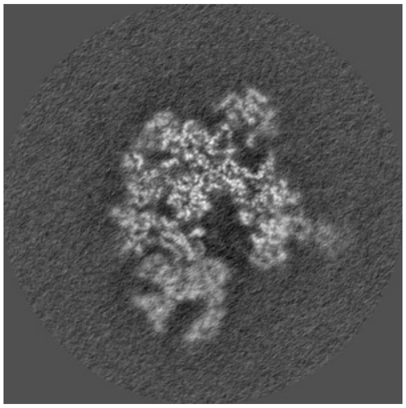

X Index: 160

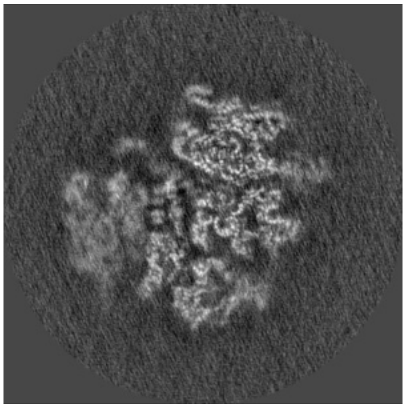

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

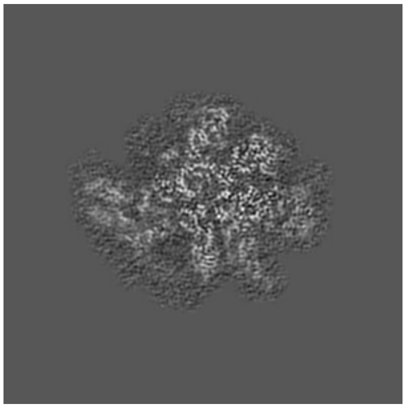

Y Index: 160


Z Index: 160

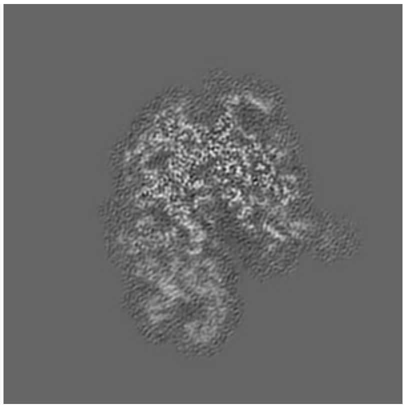
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

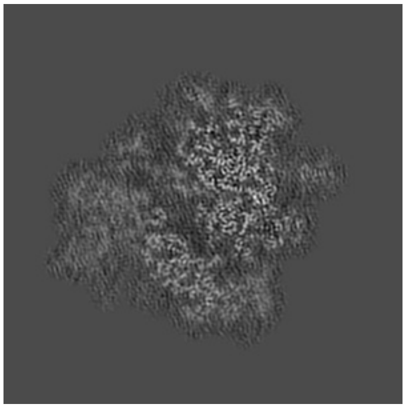
6.3.1 Primary map



X Index: 168

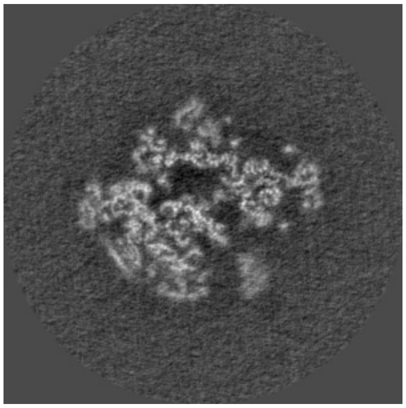


Y Index: 166

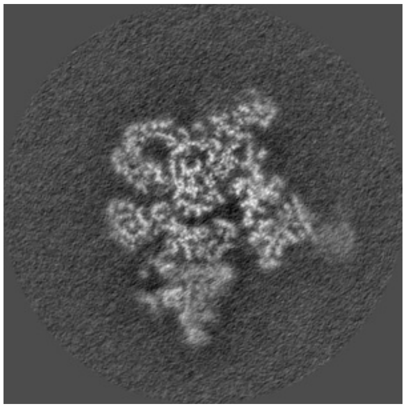


Z Index: 166

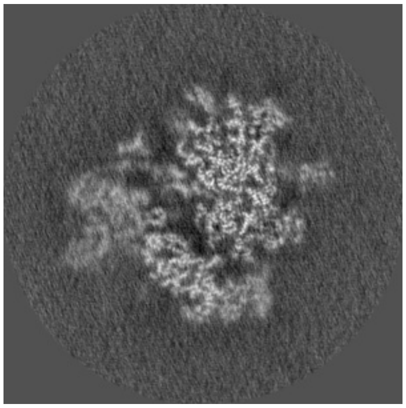
6.3.2 Raw map



X Index: 154



Y Index: 150



Z Index: 166

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

6.4 Orthogonal surface views

6.4.1 Primary map

X

Y

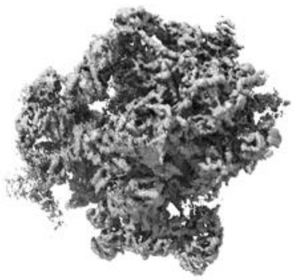
Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X

Y



Z

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

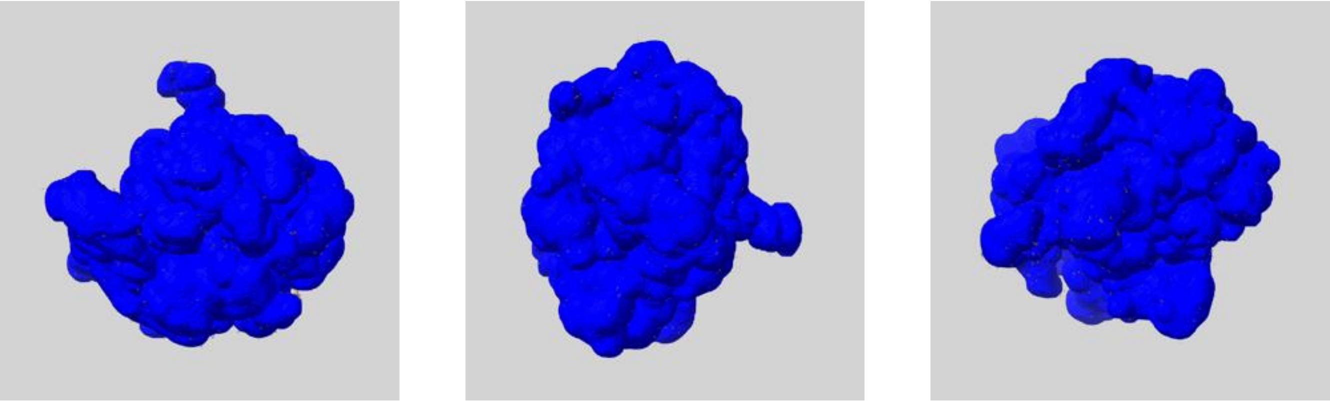
6.5 Mask visualisation ⓘ

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

A mask typically either:

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

6.5.1 emd_10779_msk_1.map ⓘ

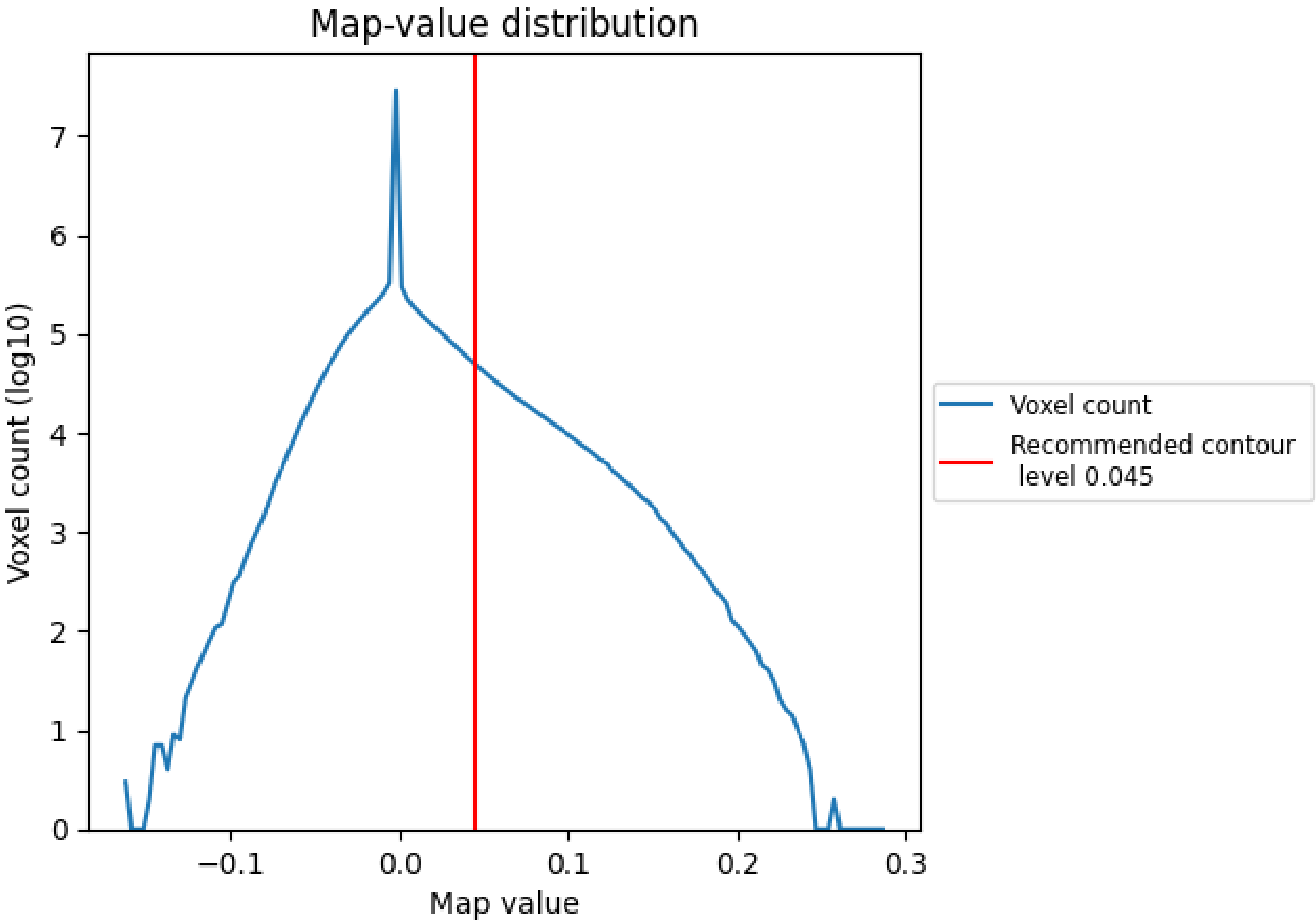


X Y Z

7 Map analysis ⓘ

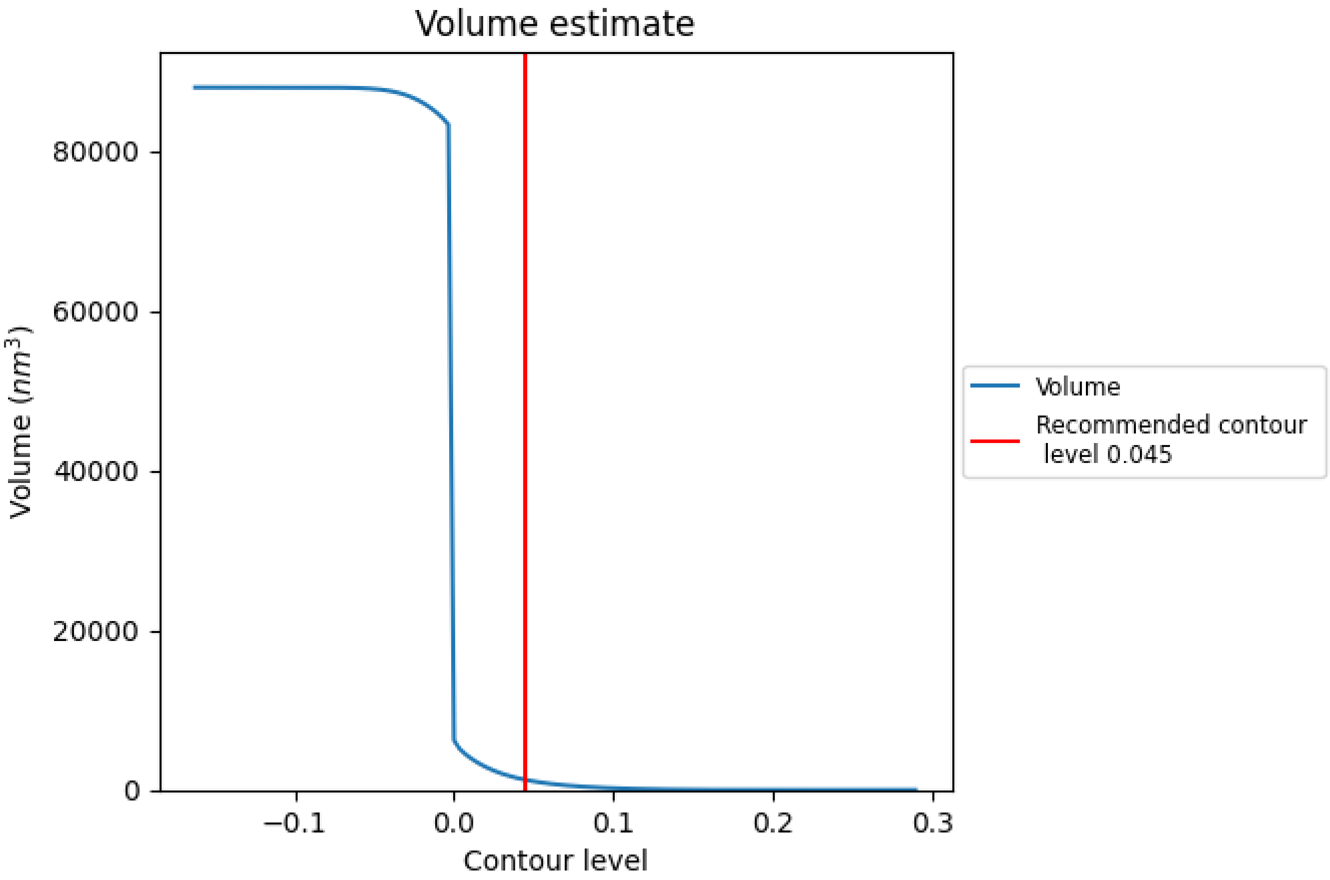
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

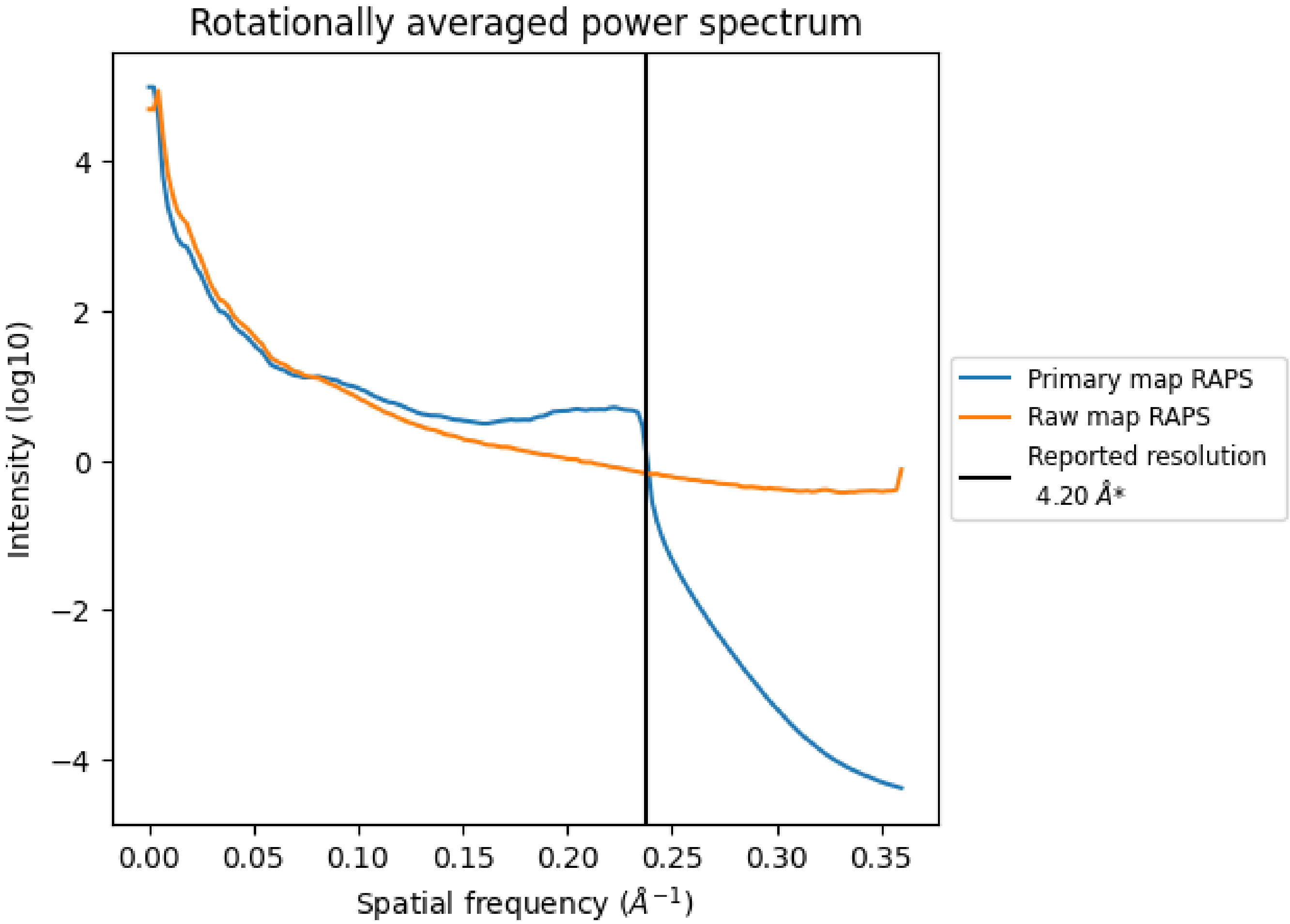
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1253 nm^3; this corresponds to an approximate mass of 1132 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 ⓘ

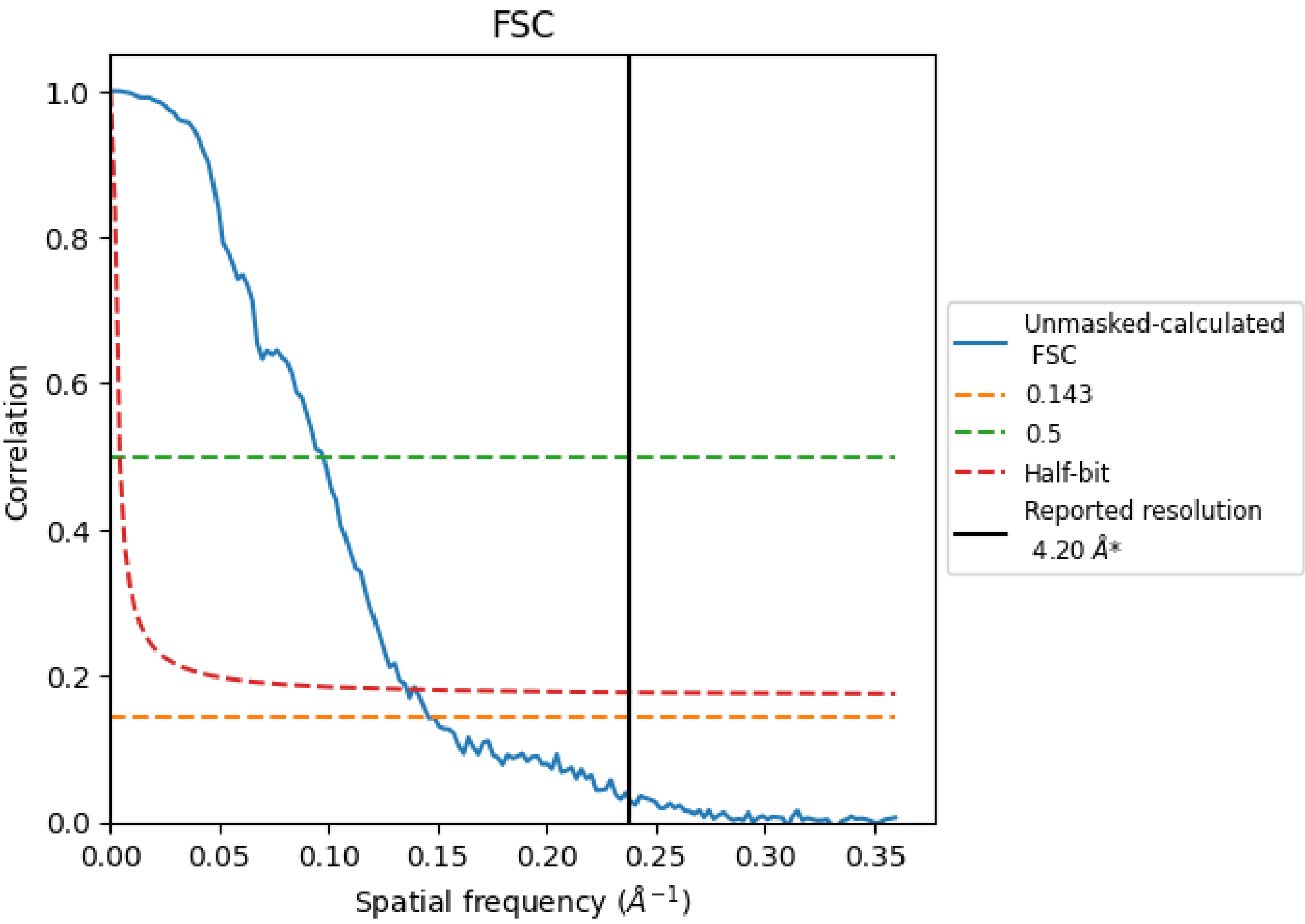


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.238 $Å^{-1}$

8.2 Resolution estimates ⓘ

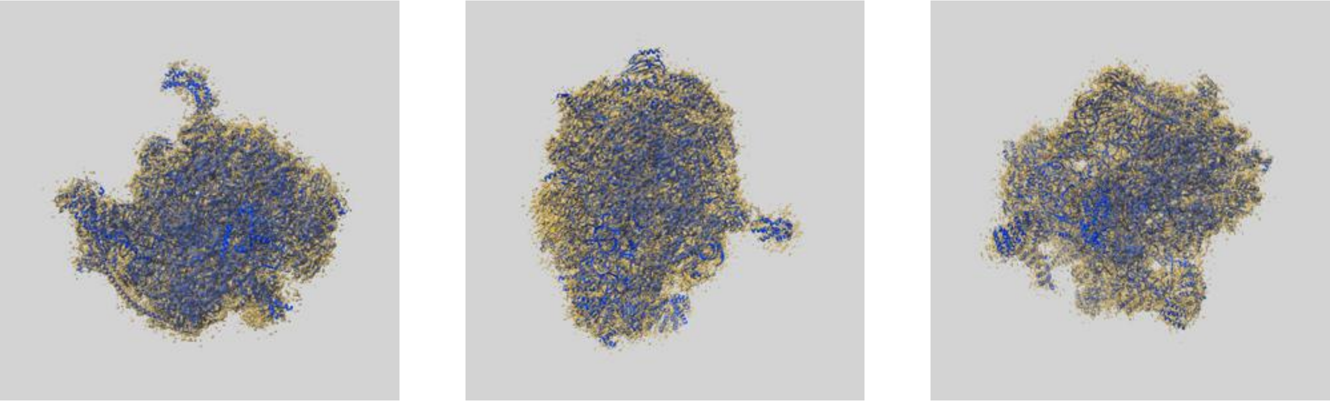
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.85	10.27	7.36

*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 6.85 differs from the reported value 4.2 by more than 10 %

9 Map-model fit

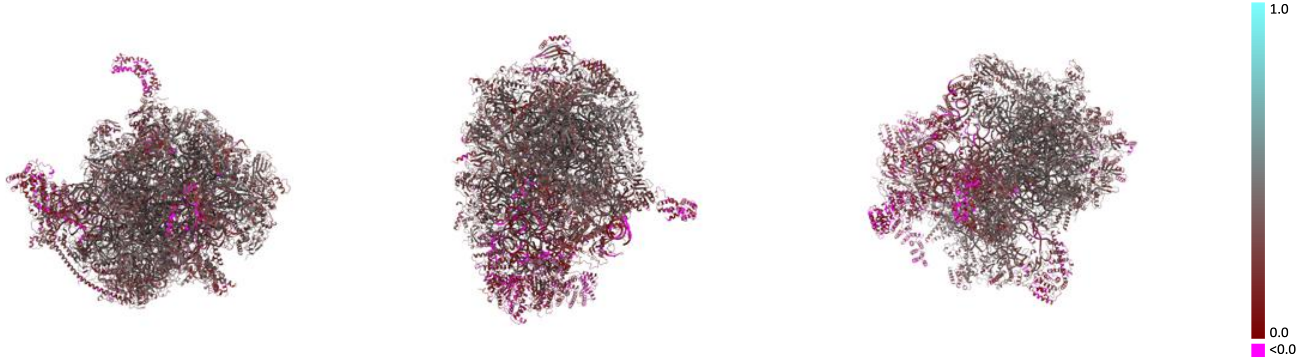
This section contains information regarding the fit between EMDB map EMD-10779 and PDB model 6YDW. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay


X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

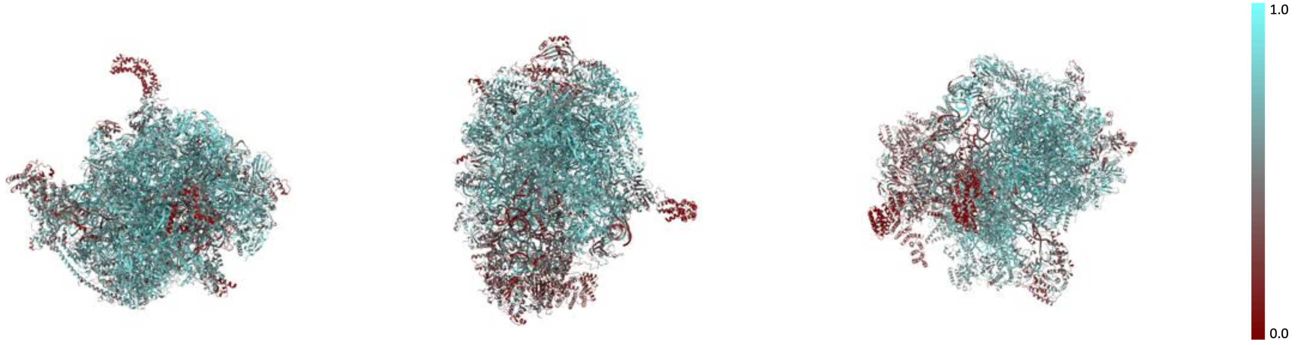
9.2 Q-score mapped to coordinate model



X Y Z

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

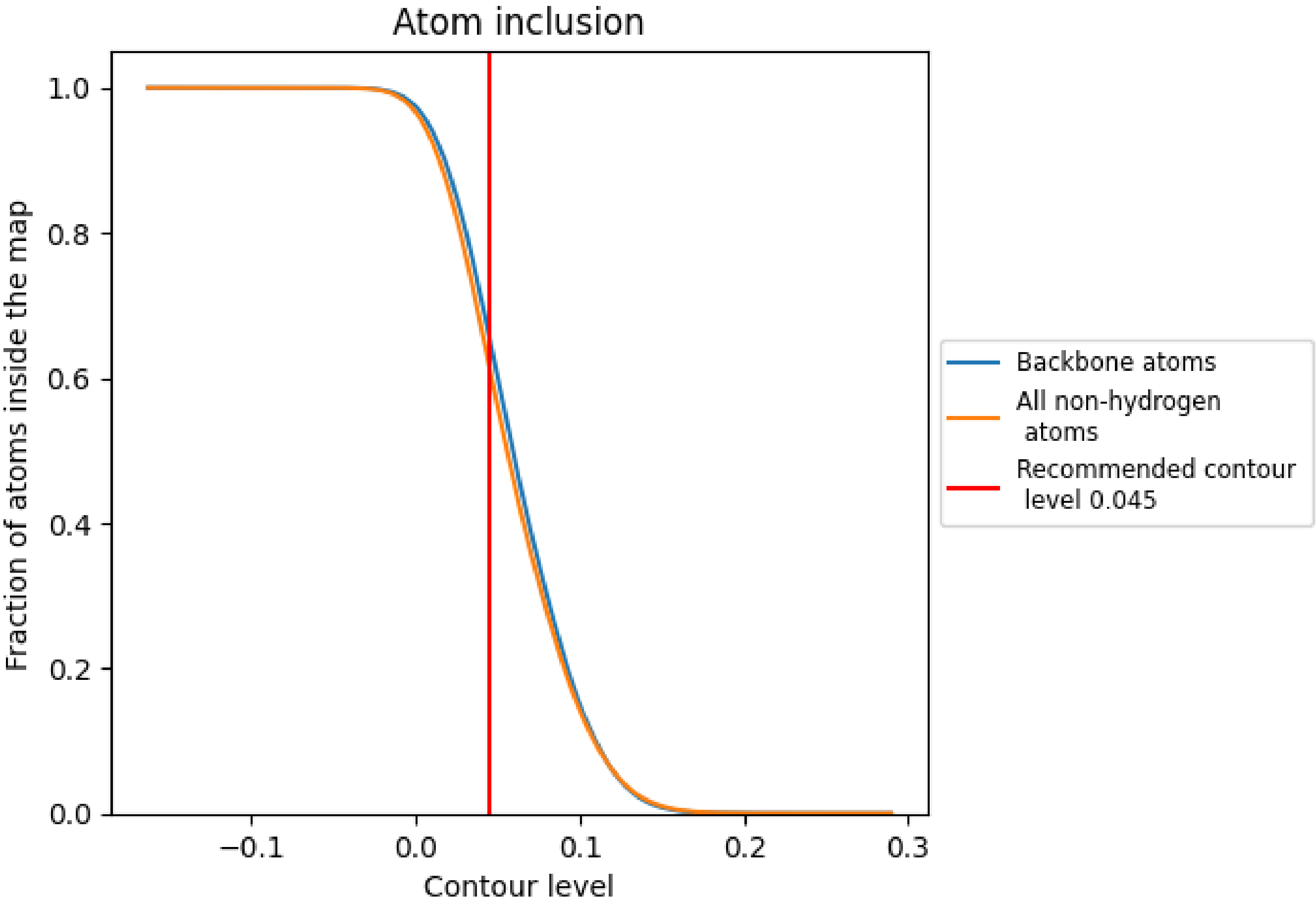
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.045).

9.4 Atom inclusion ⓘ



At the recommended contour level, 66% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6163	0.3100
AA	0.7160	0.3050
AB	0.6284	0.3230
AC	0.3194	0.2000
AE	0.4732	0.3040
AF	0.5388	0.2990
AG	0.3429	0.1640
AI	0.4422	0.2460
AJ	0.3431	0.2150
AK	0.5648	0.3020
AL	0.6435	0.4010
AN	0.3926	0.2180
AO	0.5290	0.2940
AP	0.6474	0.3250
AQ	0.6326	0.3610
AR	0.5977	0.3150
AU	0.6261	0.3520
AV	0.6021	0.2450
AX	0.6667	0.3200
AY	0.2069	0.1010
AZ	0.3889	0.1530
Aa	0.5865	0.2900
Ab	0.5555	0.2810
Ac	0.6283	0.3450
Ad	0.5915	0.2550
Ae	0.3385	0.1420
Af	0.5851	0.3250
Ag	0.3156	0.1270
Ah	0.2600	0.1710
Ai	0.3426	0.2060
Aj	0.4881	0.2530
Ak	0.3237	0.1790
Am	0.3947	0.2510
An	0.5869	0.3470
Ao	0.1451	0.0880

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Chain	Atom inclusion	Q-score
Ap	0.6182	0.3150
B0	0.7328	0.4150
B1	0.5971	0.3470
B2	0.6687	0.3460
B3	0.7250	0.4110
B4	0.4967	0.2140
B5	0.6866	0.3720
B6	0.4519	0.2850
B7	0.7317	0.4100
B8	0.6964	0.4170
B9	0.7539	0.4190
BA	0.8231	0.3750
BB	0.6394	0.2140
BC	0.6489	0.3510
BD	0.6955	0.3900
BE	0.7114	0.3890
BF	0.6827	0.3830
BI	0.5327	0.3160
BJ	0.4620	0.2430
BK	0.5948	0.2900
BN	0.7449	0.4160
BO	0.6414	0.4040
BP	0.7025	0.3790
BQ	0.7110	0.3970
BR	0.7108	0.3900
BS	0.6980	0.3500
BT	0.6735	0.3730
BU	0.7173	0.3910
BV	0.7322	0.4080
BW	0.7008	0.4040
BX	0.6288	0.3680
BY	0.3635	0.2760
Ba	0.6845	0.3490
Bb	0.6926	0.3390
Bc	0.6643	0.3290
Bd	0.4513	0.1900
Be	0.5556	0.3240
Bf	0.6741	0.3510
Bg	0.7130	0.4040
Bh	0.6939	0.3450
Bi	0.2991	0.2280
Bj	0.4431	0.1670

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Chain	Atom inclusion	Q-score
Bk	0.4649	0.2380
Bl	0.7353	0.3890
Bm	0.3853	0.2860
Bn	0.6923	0.3910
Bo	0.7190	0.3680
Bp	0.5249	0.2570
Bq	0.6268	0.2870
Bt	0.7329	0.3940
Bu	0.5087	0.2650
Bv	0.5631	0.2700
Bw	0.6791	0.3480
Bx	0.6962	0.3650
CL	0.0886	0.0840
DL	0.1737	0.1540
EL	0.0811	0.0630
FL	0.0845	0.0830
GL	0.0469	0.0660
HL	0.0488	0.1430
LL	0.2000	0.1800