Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 09:26 pm BST

PDB ID	:	7ANE / pdb_00007ane
EMDB ID	:	EMD-11829
Title	:	Leishmania Major mitochondrial ribosome
Authors	:	Soufari, H.; Waltz, F.; Parrot, C.; Bochler, A.; Hashem, Y.
Deposited on	:	2020-10-11
Resolution	:	3.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

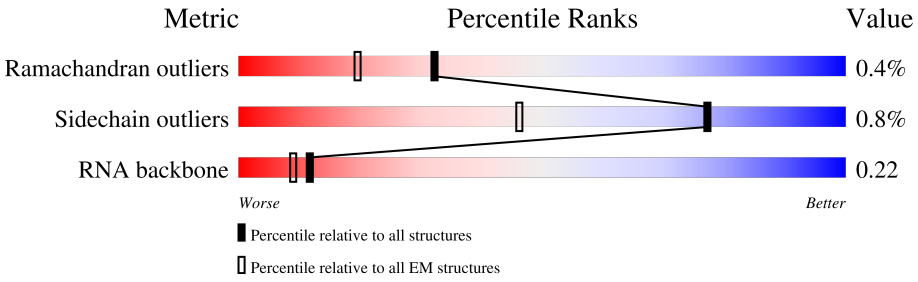
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	18998	94%
1	2	18998	97%
2	h	166	16% 95% 5%
3	aw	139	24% 100%
4	m	325	24% 88% 11%
5	f	371	15% 39% 60%
6	s	179	25% 92% 8%
7	au	247	32% 96%

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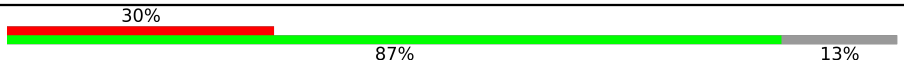
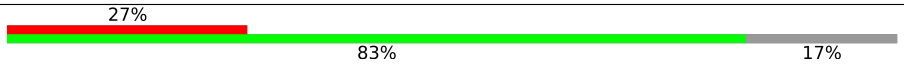
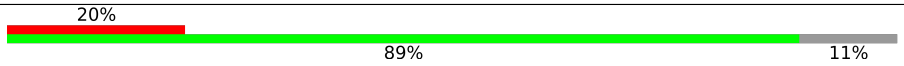
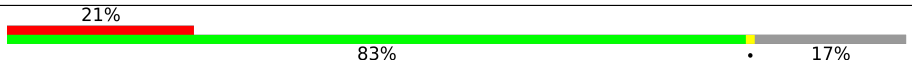
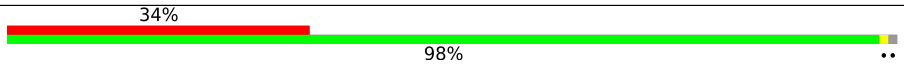
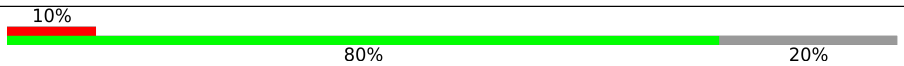
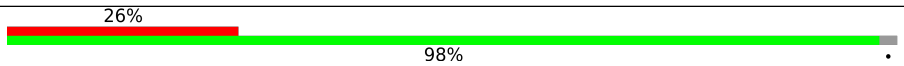
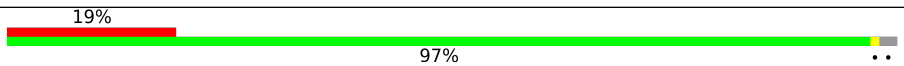
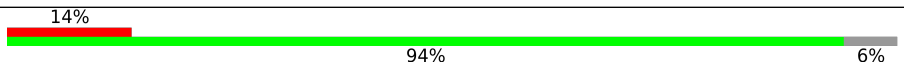
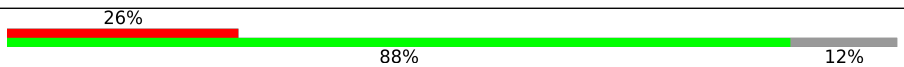
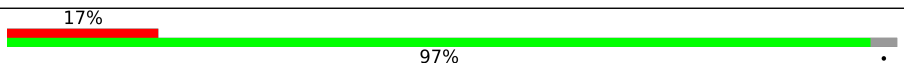
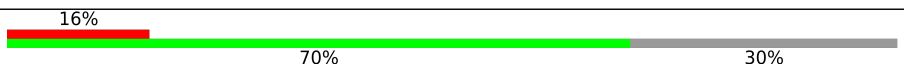
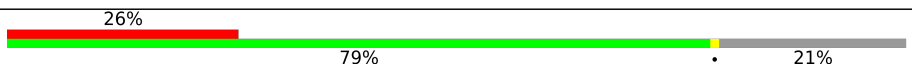
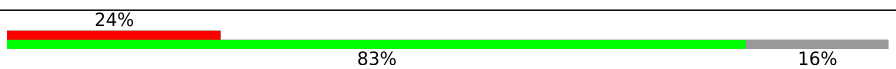
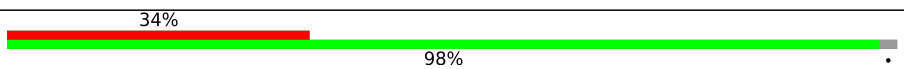
Mol	Chain	Length	Quality of chain
8	am	313	
9	n	171	
10	ae	655	
11	ay	169	
12	ag	564	
13	aj	397	
14	e	822	
15	d	351	
16	az	163	
17	ax	184	
18	r	467	
19	af	835	
20	u	890	
21	aa	1813	
22	ab	1177	
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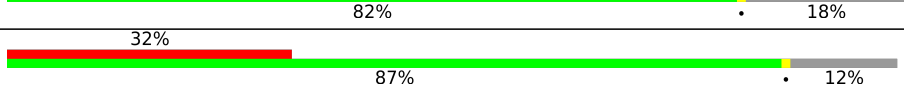
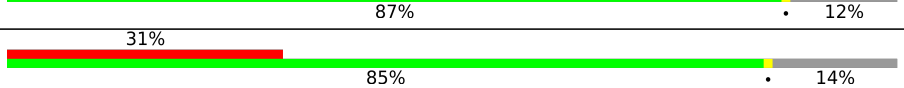
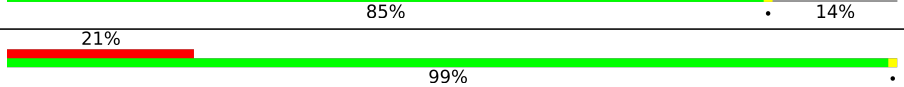
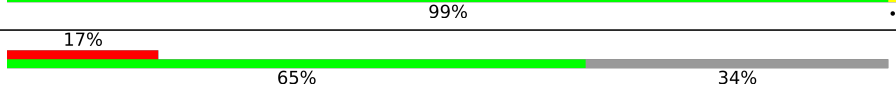
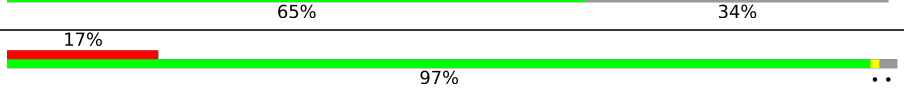
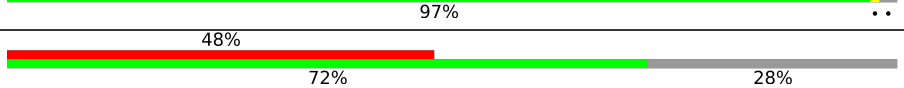
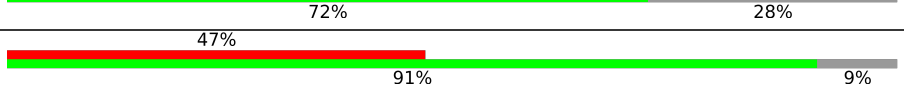
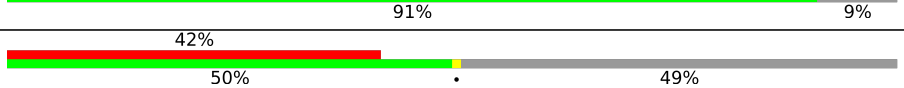
24	ac	1267	
25	ad	811	
26	an	302	
27	ao	291	
28	ap	245	
29	aq	295	
30	as	270	
31	at	397	
32	y	485	

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Mol	Chain	Length	Quality of chain
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34	v	214	
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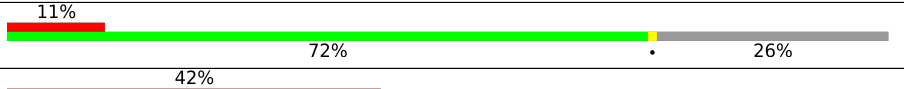
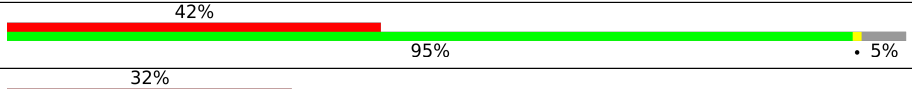
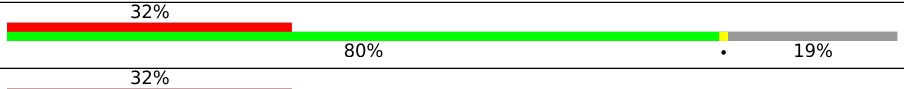
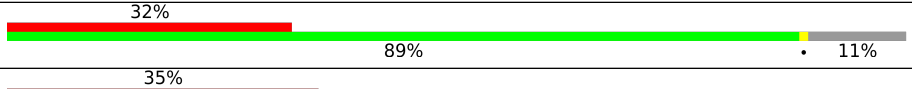
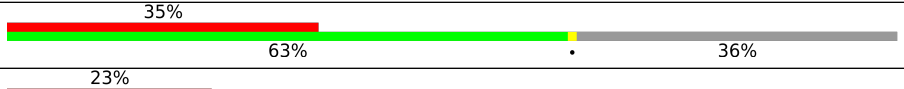
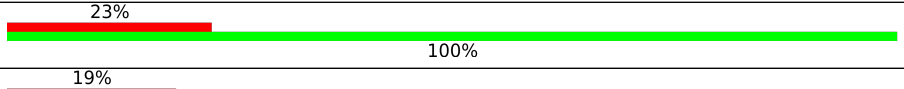
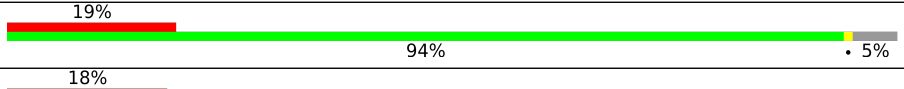
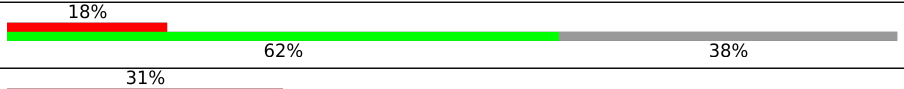
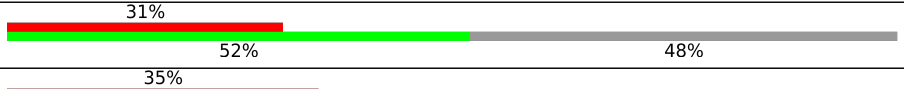
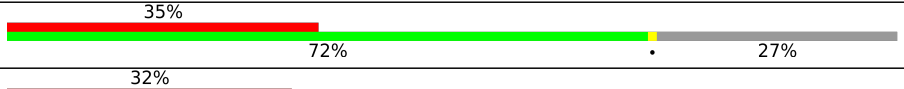
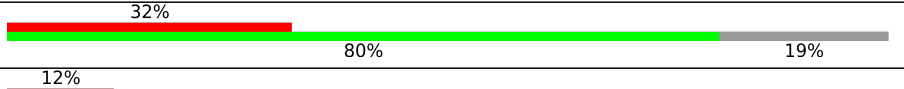
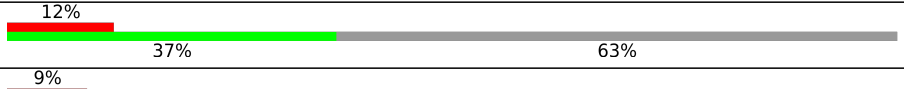
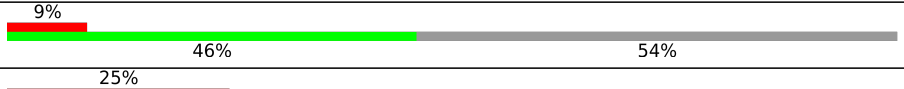
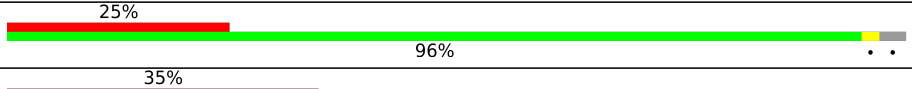
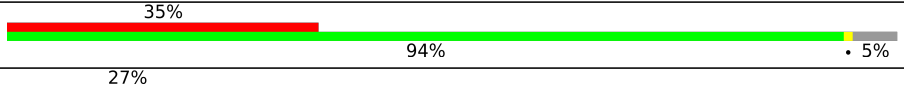
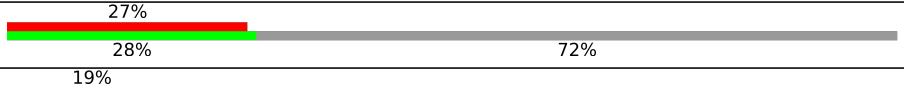
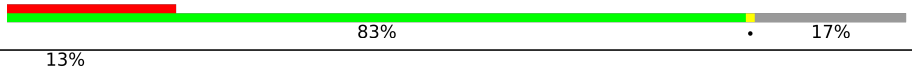
36	p	321	
37	j	189	
38	l	677	
39	ar	282	
40	av	236	
41	ai	379	
42	x	268	
43	i	429	
44	g	192	
45	o	604	
46	c	311	
47	k	312	
48	q	425	
49	b	159	
50	a	431	
51	ba	94	
52	z	1169	
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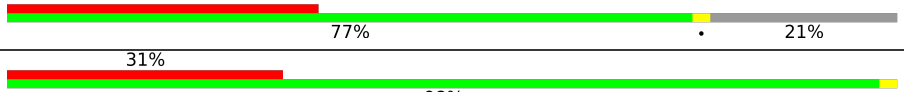
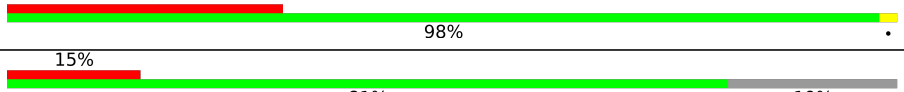
54	A	466	
55	B	435	
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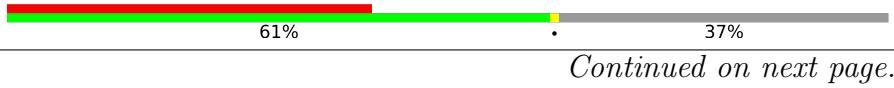
57	D	204	

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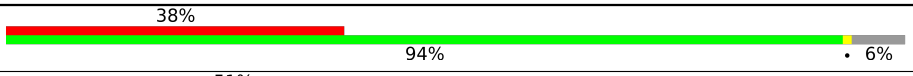
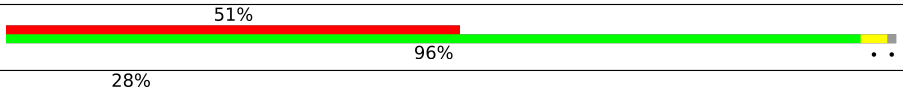
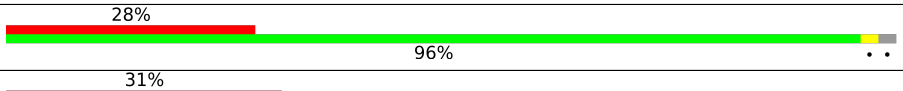
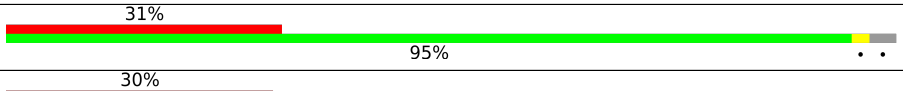
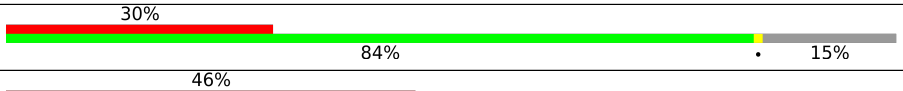
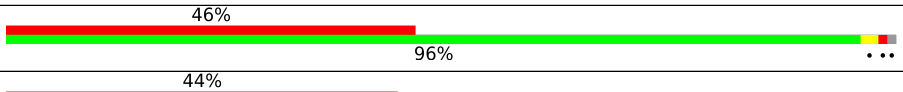
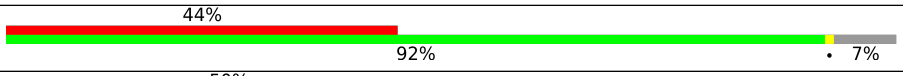
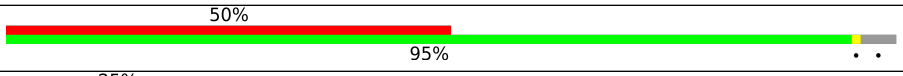
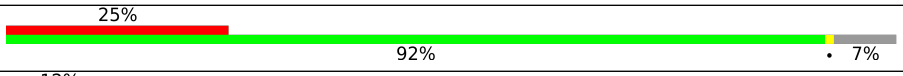
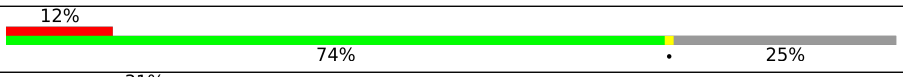
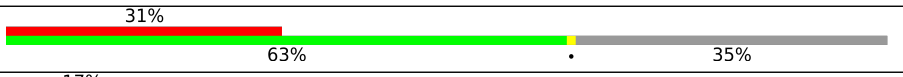
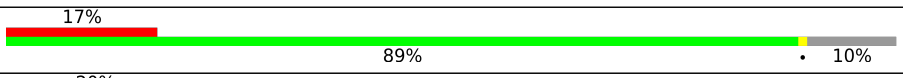
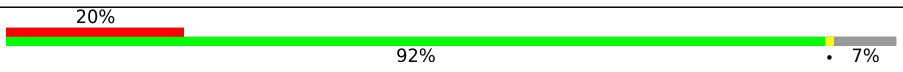
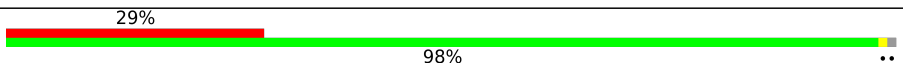
Mol	Chain	Length	Quality of chain
58	E	345	
59	F	171	
60	G	373	
61	H	167	
62	I	304	
63	J	143	
64	K	193	
65	L	185	
66	M	278	
67	N	251	
68	O	475	
69	P	184	
70	Q	233	
71	R	479	
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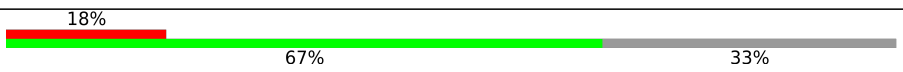
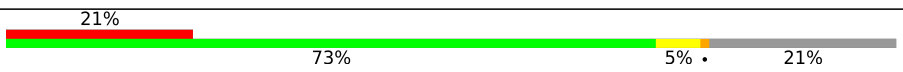
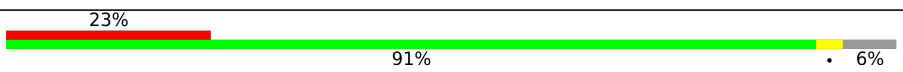
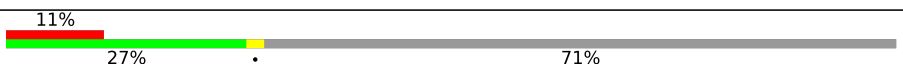
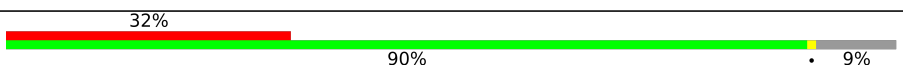
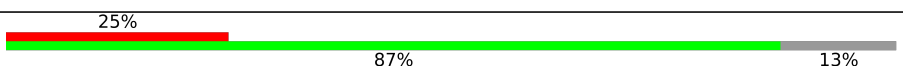
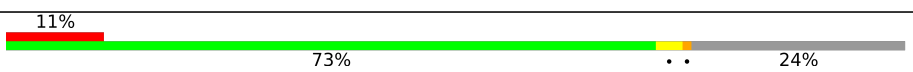
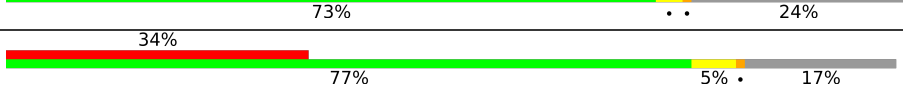
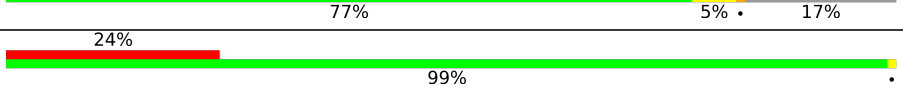
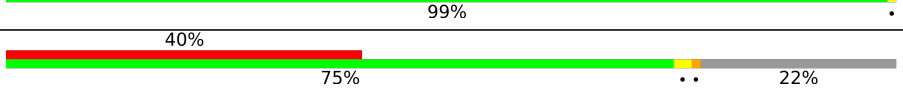
73	T	82	
74	U	117	
75	V	150	
76	W	185	
77	X	512	
78	Y	292	
79	Z	197	
80	BA	167	
81	UA	203	
82	BB	156	

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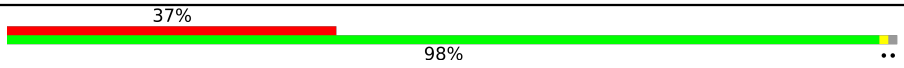
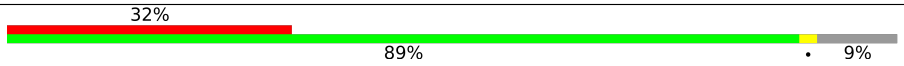
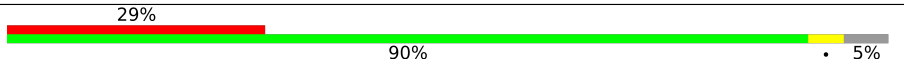
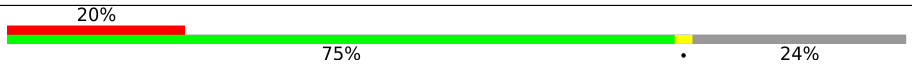
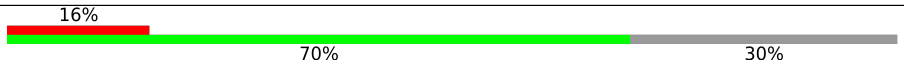
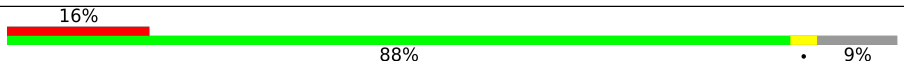
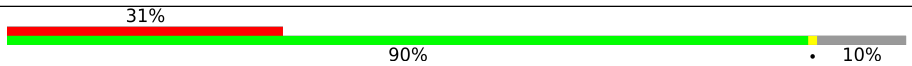
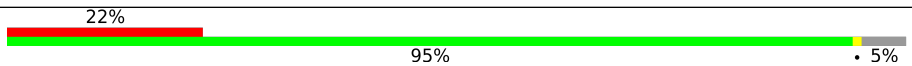
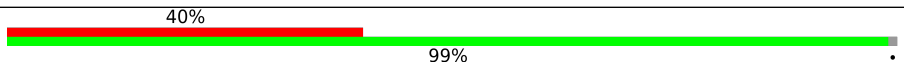
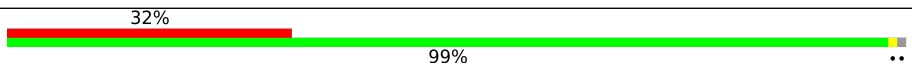
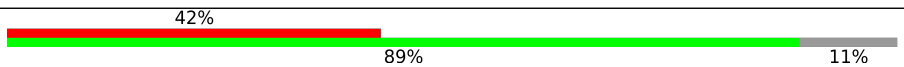
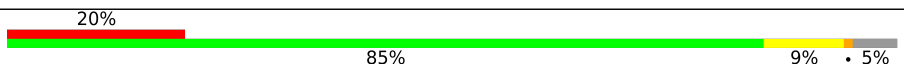
Mol	Chain	Length	Quality of chain
83	Aw	187	
84	Bj	185	
85	An	331	
86	Al	346	
87	BI	266	
88	Az	152	
89	At	183	
90	BC	147	
91	Ab	262	
92	Ai	479	
93	Ap	240	
94	Au	186	
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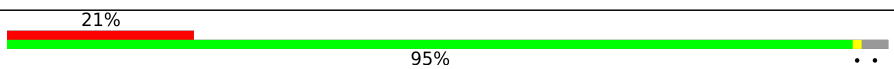
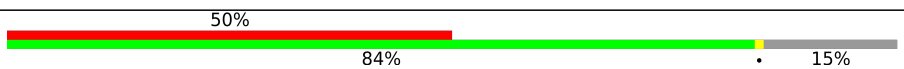
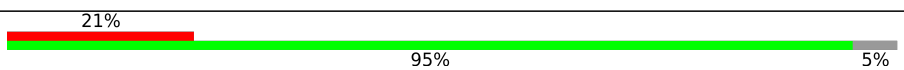
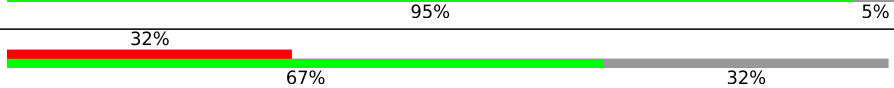
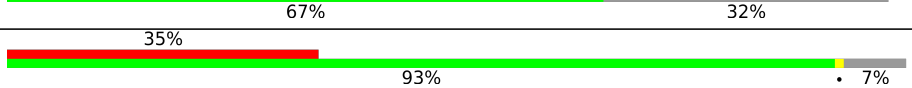
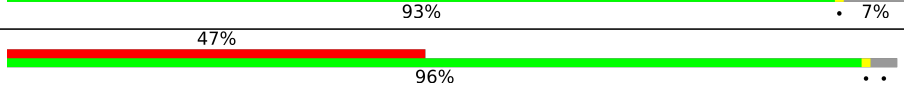
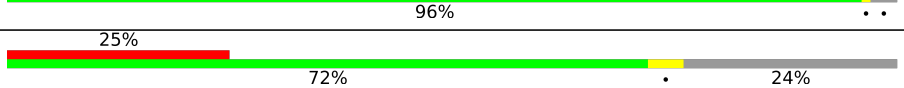
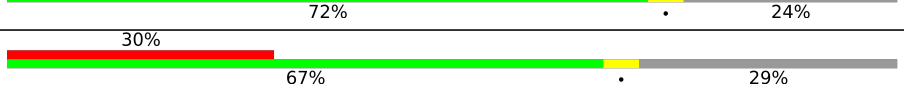
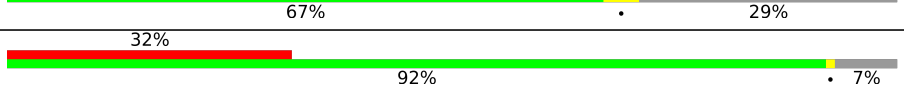
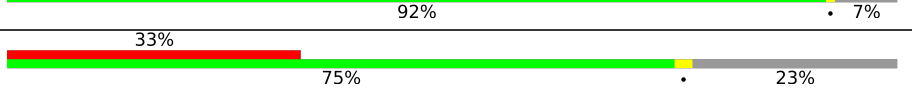
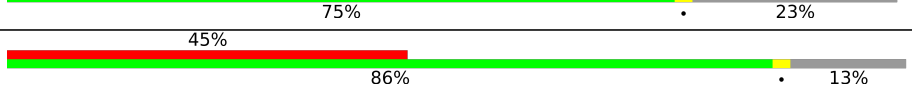
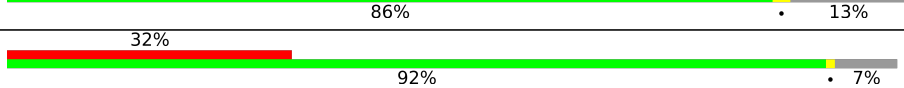
96	Ao	284	
97	BM	457	
98	Ar	205	
99	Aj	503	
100	BH	229	
101	Am	340	
102	Aq	341	
103	BE	118	
104	Ak	323	
105	BP	254	
106	Ad	237	
107	BF	109	

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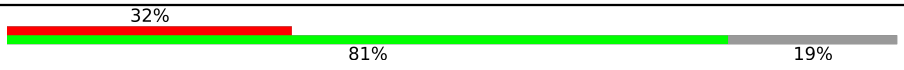
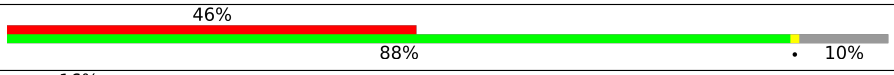
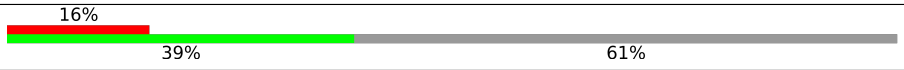
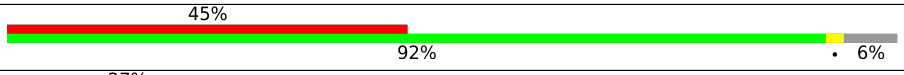
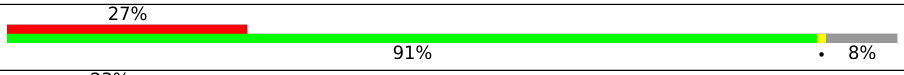
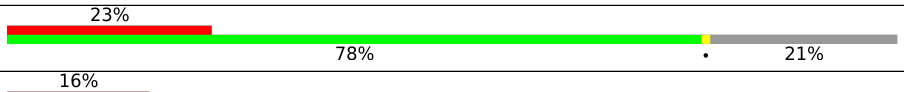
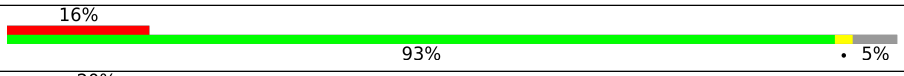
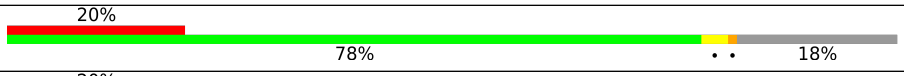
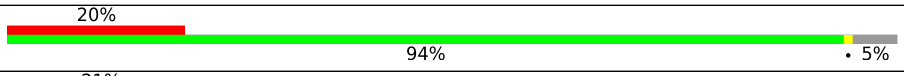
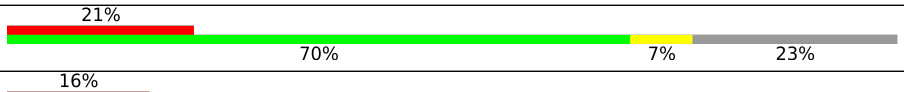
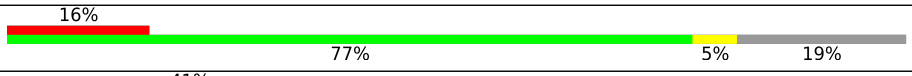
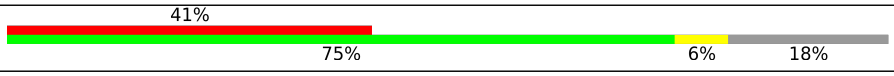
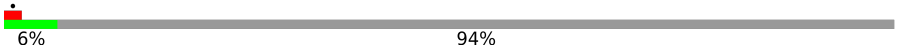
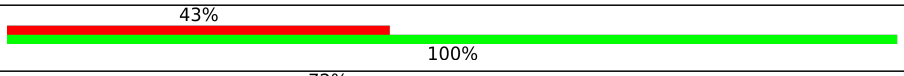
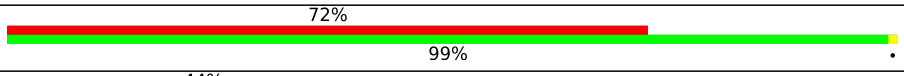
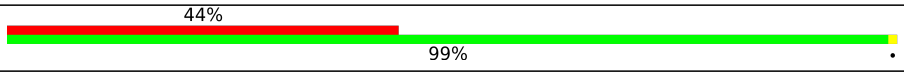
Mol	Chain	Length	Quality of chain
108	Av	192	
109	Af	155	
110	As	249	
111	Ae	311	
112	Ac	291	
113	Ah	570	
114	BD	102	
115	Ay	174	
116	Ag	244	
117	Ax	216	
118	BL	380	
119	BO	190	
120	BG	1347	
121	UB	67	
122	UC	144	
123	UD	95	

2 Entry composition (i)

There are 126 unique types of molecules in this entry. The entry contains 303111 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 RNA chain called Large ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	604	Total 12723	C 5725	N 2119	O 4275	P 604	0	0
1	1	1084	Total 22858	C 10292	N 3832	O 7650	P 1084	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	612	U	A	conflict	GB 1756572068
2	613	U	A	conflict	GB 1756572068
2	615	U	G	conflict	GB 1756572068
1	1840	U	A	conflict	GB 1756572068
1	1841	U	A	conflict	GB 1756572068
1	1843	U	G	conflict	GB 1756572068

- Molecule 2 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	h	157	Total 1311	C 831	N 248	O 224	S 8	0	0

- Molecule 3 is a protein called mS69.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aw	139	Total 1144	C 723	N 209	O 204	S 8	0	0

- Molecule 4 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	m	288	Total 2368	C 1495	N 435	O 427	S 11	0	0

- Molecule 5 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	148	Total	C	N	O	S	0	0
			1213	764	231	216	2		

- Molecule 6 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	s	165	Total	C	N	O	S	0	0
			1349	852	251	239	7		

- Molecule 7 is a protein called Rhodanese domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	au	239	Total	C	N	O	S	0	0
			2066	1322	366	368	10		

- Molecule 8 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	am	272	Total	C	N	O	S	0	0
			2198	1398	404	386	10		

- Molecule 9 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	n	142	Total	C	N	O	S	0	0
			1176	760	210	201	5		

- Molecule 10 is a protein called mS53.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	ae	584	Total	C	N	O	S	0	0
			4593	2888	856	830	19		

- Molecule 11 is a protein called mS71.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	ay	141	Total	C	N	O	S	0	0
			1187	756	222	204	5		

- Molecule 12 is a protein called mS55.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	ag	557	Total	C	N	O	S	0	0
			4521	2827	849	821	24		

- Molecule 13 is a protein called mS57.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	aj	316	Total	C	N	O	S	0	0
			2560	1643	449	453	15		

- Molecule 14 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	e	809	Total	C	N	O	S	0	0
			6413	4040	1128	1218	27		

- Molecule 15 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	d	343	Total	C	N	O	S	0	0
			2715	1716	474	511	14		

- Molecule 16 is a protein called mS72.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	az	154	Total	C	N	O	S	0	0
			1301	834	246	214	7		

- Molecule 17 is a protein called mS70.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	ax	161	Total	C	N	O	S	0	0
			1356	864	261	224	7		

- Molecule 18 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	451	Total	C	N	O	S	0	0
			3703	2380	646	660	17		

- Molecule 19 is a protein called Excreted/secreted protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	af	585	Total 4698	C 2963	N 853	O 857	S 25	0	0

- Molecule 20 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	u	706	Total 5564	C 3497	N 1017	O 1025	S 25	0	0

- Molecule 21 is a protein called mS48.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	aa	1514	Total 12070	C 7616	N 2166	O 2249	S 39	0	0

- Molecule 22 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	ab	1151	Total 9209	C 5726	N 1711	O 1744	S 28	0	0

- Molecule 23 is a protein called mS58.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	ak	268	Total 2141	C 1337	N 403	O 394	S 7	0	0

- Molecule 24 is a protein called mS50.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	ac	1116	Total 8700	C 5454	N 1568	O 1644	S 34	0	0

- Molecule 25 is a protein called mS51.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	ad	694	Total 5676	C 3607	N 1012	O 1023	S 34	0	0

- Molecule 26 is a protein called mS60.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	an	302	Total	C	N	O	S	0	0
			2480	1560	484	427	9		

- Molecule 27 is a protein called mS61.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	ao	191	Total	C	N	O	S	0	0
			1535	980	271	274	10		

- Molecule 28 is a protein called mS62.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	ap	240	Total	C	N	O	S	0	0
			1893	1180	341	360	12		

- Molecule 29 is a protein called mS63.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	aq	212	Total	C	N	O	S	0	0
			1794	1147	318	320	9		

- Molecule 30 is a protein called mS65.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	as	247	Total	C	N	O	S	0	0
			1954	1246	352	348	8		

- Molecule 31 is a protein called mS66.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	at	204	Total	C	N	O	S	0	0
			1631	1008	313	300	10		

- Molecule 32 is a protein called mS43.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	y	283	Total	C	N	O	S	0	0
			2152	1345	395	398	14		

- Molecule 33 is a protein called Protein FYV4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	w	155	Total	C	N	O	S	0	0
			1279	815	227	233	4		

- Molecule 34 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	v	63	Total	C	N	O	S	0	0
			486	294	89	97	6		

- Molecule 35 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	t	226	Total	C	N	O	S	0	0
			1776	1128	308	336	4		

- Molecule 36 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	p	236	Total	C	N	O	S	0	0
			1954	1241	346	360	7		

- Molecule 37 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	180	Total	C	N	O	S	0	0
			1506	963	280	254	9		

- Molecule 38 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	545	Total	C	N	O	S	0	0
			4438	2809	821	796	12		

- Molecule 39 is a protein called AKAP7_NLS domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	ar	252	Total	C	N	O	S	0	0
			1993	1249	376	356	12		

- Molecule 40 is a protein called Ubiquitin-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	av	150	Total	C	N	O	S	0	0
			1237	777	219	236	5		

- Molecule 41 is a protein called mS56.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	ai	379	Total	C	N	O	S	0	0
			3068	1957	534	565	12		

- Molecule 42 is a protein called Putative superoxide dismutase.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	x	255	Total	C	N	O	S	0	0
			2034	1299	351	375	9		

- Molecule 43 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	267	Total	C	N	O	S	0	0
			2221	1406	403	402	10		

- Molecule 44 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	g	99	Total	C	N	O	S	0	0
			818	513	161	141	3		

- Molecule 45 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	438	Total	C	N	O	S	0	0
			3736	2395	658	664	19		

- Molecule 46 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	c	251	Total	C	N	O	S	0	0
			2038	1279	379	370	10		

- Molecule 47 is a protein called 30S Ribosomal protein S17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	k	116	Total	C	N	O	S	0	0
			951	614	169	163	5		

- Molecule 48 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	196	Total	C	N	O	S	0	0
			1699	1077	317	297	8		

- Molecule 49 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	b	155	Total	C	N	O	S	0	0
			1290	816	232	238	4		

- Molecule 50 is a protein called Ribosomal_S5_C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	a	408	Total	C	N	O	S	0	0
			3298	2084	610	587	17		

- Molecule 51 is a protein called mS73.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	ba	26	Total	C	N	O	S	0	0
			223	147	36	39	1		

- Molecule 52 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	z	971	Total	C	N	O	S	0	0
			7713	4847	1378	1454	34		

- Molecule 53 is a protein called uS3m.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	bd	41	Total	C	N	O	0	0
			350	245	52	53		

- Molecule 54 is a protein called Ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	A	368	Total	C	N	O	S	0	0
			2996	1929	496	556	15		

- Molecule 55 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B	435	Total	C	N	O	S	0	0
			3513	2237	615	642	19		

- Molecule 56 is a protein called RIBOSOMAL_L9 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	C	212	Total	C	N	O	S	0	0
			1772	1144	303	321	4		

- Molecule 57 is a protein called uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	D	128	Total	C	N	O	S	0	0
			1036	656	198	177	5		

- Molecule 58 is a protein called Putative ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	E	326	Total	C	N	O	S	0	0
			2668	1704	480	470	14		

- Molecule 59 is a protein called 50S ribosomal protein L13-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	F	170	Total	C	N	O	S	0	0
			1435	919	261	243	12		

- Molecule 60 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	G	365	Total	C	N	O	S	0	0
			3012	1917	555	531	9		

- Molecule 61 is a protein called Ribosomal_L16 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	H	162	Total	C	N	O	S	0	0
			1305	836	239	226	4		

- Molecule 62 is a protein called Putative 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	I	257	Total	C	N	O	S	0	0
			2153	1362	406	372	13		

- Molecule 63 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	J	141	Total	C	N	O	S	0	0
			1146	727	211	202	6		

- Molecule 64 is a protein called bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	K	179	Total	C	N	O	S	0	0
			1467	910	289	258	10		

- Molecule 65 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	L	178	Total	C	N	O	S	0	0
			1419	907	257	250	5		

- Molecule 66 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	M	259	Total	C	N	O	S	0	0
			2116	1345	385	371	15		

- Molecule 67 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	N	189	Total	C	N	O	S	0	0
			1599	1031	296	269	3		

- Molecule 68 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	O	307	Total	C	N	O	S	0	0
			2537	1600	455	475	7		

- Molecule 69 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	P	165	Total	C	N	O	S	0	0
			1367	856	266	238	7		

- Molecule 70 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Q	217	Total	C	N	O	S	0	0
			1785	1127	331	316	11		

- Molecule 71 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	R	472	Total	C	N	O	S	0	0
			3755	2377	662	704	12		

- Molecule 72 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	S	150	Total	C	N	O	S	0	0
			1244	782	247	207	8		

- Molecule 73 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	T	55	Total	C	N	O	S	0	0
			487	311	93	78	5		

- Molecule 74 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	U	92	Total	C	N	O	S	0	0
			744	472	142	125	5		

- Molecule 75 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	V	141	Total	C	N	O	S	0	0
			1202	755	242	197	8		

- Molecule 76 is a protein called bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	W	54	Total	C	N	O	S	0	0
			465	299	89	74	3		

- Molecule 77 is a protein called mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	X	468	Total	C	N	O	S	0	0
			3733	2365	657	694	17		

- Molecule 78 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Y	255	Total	C	N	O	S	0	0
			2067	1287	373	402	5		

- Molecule 79 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Z	150	Total	C	N	O	S	0	0
			1223	784	224	211	4		

- Molecule 80 is a protein called mL94.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	BA	138	Total	C	N	O	S	0	0
			1038	648	188	197	5		

- Molecule 81 is a protein called UA.

Mol	Chain	Residues	Atoms				AltConf	Trace
81	UA	203	Total	C	N	O	0	0
			1015	609	203	203		

- Molecule 82 is a protein called mL95.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	BB	122	Total	C	N	O	0	0
			1028	663	189	176		

- Molecule 83 is a protein called mL89.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Aw	185	Total	C	N	O	S	0	0
			1509	949	289	268	3		

- Molecule 84 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bj	168	Total	C	N	O	S	0	0
			1358	865	255	231	7		

- Molecule 85 is a protein called mL76.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	An	314	Total	C	N	O	S	0	0
			2605	1643	487	470	5		

- Molecule 86 is a protein called mL74.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Al	264	Total	C	N	O	S	0	0
			2152	1371	374	399	8		

- Molecule 87 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	BI	186	Total	C	N	O	S	0	0
			1409	895	242	264	8		

- Molecule 88 is a protein called mL93.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	Az	138	Total	C	N	O	S	0	0
			1215	782	216	211	6		

- Molecule 89 is a protein called mL86.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	At	165	Total	C	N	O	S	0	0
			1346	824	260	254	8		

- Molecule 90 is a protein called mL96.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	BC	140	Total	C	N	O	S	0	0
			1114	693	205	207	9		

- Molecule 91 is a protein called L51_S25_CI-B8 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	Ab	260	Total	C	N	O	S	0	0
			2185	1365	416	397	7		

- Molecule 92 is a protein called mL69.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	Ai	476	Total	C	N	O	S	0	0
			3789	2419	654	694	22		

- Molecule 93 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	Ap	214	Total	C	N	O	S	0	0
			1775	1111	327	328	9		

- Molecule 94 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
94	Au	176	Total	C	N	O	S	0	0
			1490	945	292	245	8		

- Molecule 95 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
95	Aa	178	Total	C	N	O	S	0	0
			1417	884	270	256	7		

- Molecule 96 is a protein called mL79.

Mol	Chain	Residues	Atoms					AltConf	Trace
96	Ao	275	Total	C	N	O	S	0	0
			2276	1433	429	402	12		

- Molecule 97 is a protein called mL70.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	BM	389	Total	C	N	O	S	0	0
			3069	1954	548	551	16		

- Molecule 98 is a protein called mL84.

Mol	Chain	Residues	Atoms					AltConf	Trace
98	Ar	195	Total	C	N	O	S	0	0
			1644	1054	295	288	7		

- Molecule 99 is a protein called mL72.

Mol	Chain	Residues	Atoms					AltConf	Trace
99	Aj	341	Total	C	N	O	S	0	0
			2766	1756	508	491	11		

- Molecule 100 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
100	BH	214	Total	C	N	O	S	0	0
			1659	1050	290	310	9		

- Molecule 101 is a protein called mL75.

Mol	Chain	Residues	Atoms					AltConf	Trace
101	Am	330	Total	C	N	O	S	0	0
			2708	1727	491	474	16		

- Molecule 102 is a protein called mL82.

Mol	Chain	Residues	Atoms					AltConf	Trace
102	Aq	258	Total	C	N	O	S	0	0
			2074	1296	406	360	12		

- Molecule 103 is a protein called mL98.

Mol	Chain	Residues	Atoms				AltConf	Trace
103	BE	84	Total 700	C 447	N 125	O 128	0	0

- Molecule 104 is a protein called mL73.

Mol	Chain	Residues	Atoms					AltConf	Trace
104	Ak	300	Total 2352	C 1489	N 421	O 429	S 13	0	0

- Molecule 105 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
105	BP	195	Total 1593	C 1014	N 288	O 288	S 3	0	0

- Molecule 106 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
106	Ad	207	Total 1632	C 1049	N 289	O 286	S 8	0	0

- Molecule 107 is a protein called mL99.

Mol	Chain	Residues	Atoms					AltConf	Trace
107	BF	101	Total 851	C 530	N 165	O 154	S 2	0	0

- Molecule 108 is a protein called mL88.

Mol	Chain	Residues	Atoms					AltConf	Trace
108	Av	155	Total 1300	C 828	N 230	O 234	S 8	0	0

- Molecule 109 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
109	Af	139	Total 1132	C 709	N 215	O 207	S 1	0	0

- Molecule 110 is a protein called mL85.

Mol	Chain	Residues	Atoms					AltConf	Trace
110	As	97	Total	C	N	O	S	0	0
			787	495	139	148	5		

- Molecule 111 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
111	Ae	291	Total	C	N	O	S	0	0
			2359	1526	418	404	11		

- Molecule 112 is a protein called MRP-L46 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
112	Ac	268	Total	C	N	O	S	0	0
			2174	1375	389	405	5		

- Molecule 113 is a protein called mL68.

Mol	Chain	Residues	Atoms					AltConf	Trace
113	Ah	452	Total	C	N	O	S	0	0
			3686	2338	651	679	18		

- Molecule 114 is a protein called mL97.

Mol	Chain	Residues	Atoms					AltConf	Trace
114	BD	97	Total	C	N	O	S	0	0
			807	499	160	140	8		

- Molecule 115 is a protein called C2H2-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
115	Ay	142	Total	C	N	O	S	0	0
			1226	774	228	217	7		

- Molecule 116 is a protein called mL59/64.

Mol	Chain	Residues	Atoms					AltConf	Trace
116	Ag	231	Total	C	N	O	S	0	0
			1916	1211	356	340	9		

- Molecule 117 is a protein called LIM zinc-binding domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
117	Ax	167	Total	C	N	O	S	0	0
			1388	876	268	233	11		

- Molecule 118 is a protein called Putative ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
118	BL	309	Total	C	N	O	S	0	0
			2497	1594	464	427	12		

- Molecule 119 is a protein called Putative ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
119	BO	155	Total	C	N	O	S	0	0
			1239	772	253	205	9		

- Molecule 120 is a protein called mL100.

Mol	Chain	Residues	Atoms					AltConf	Trace
120	BG	85	Total	C	N	O	S	0	0
			643	400	122	115	6		

- Molecule 121 is a protein called UB.

Mol	Chain	Residues	Atoms				AltConf	Trace
121	UB	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 122 is a protein called UC.

Mol	Chain	Residues	Atoms				AltConf	Trace
122	UC	144	Total	C	N	O	0	0
			720	432	144	144		

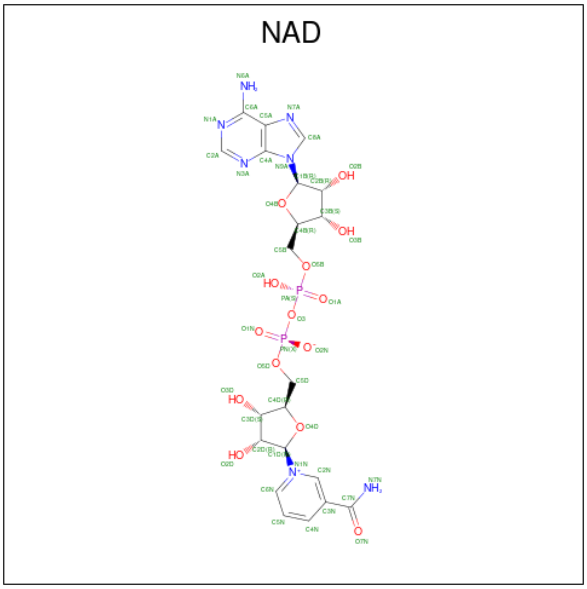
- Molecule 123 is a protein called UD.

Mol	Chain	Residues	Atoms				AltConf	Trace
123	UD	95	Total	C	N	O	0	0
			475	285	95	95		

- Molecule 124 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
124	T	1	Total Zn 1 1	0
124	W	1	Total Zn 1 1	0
124	BD	1	Total Zn 1 1	0
124	Ax	2	Total Zn 2 2	0
124	BG	1	Total Zn 1 1	0

- Molecule 125 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 126 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

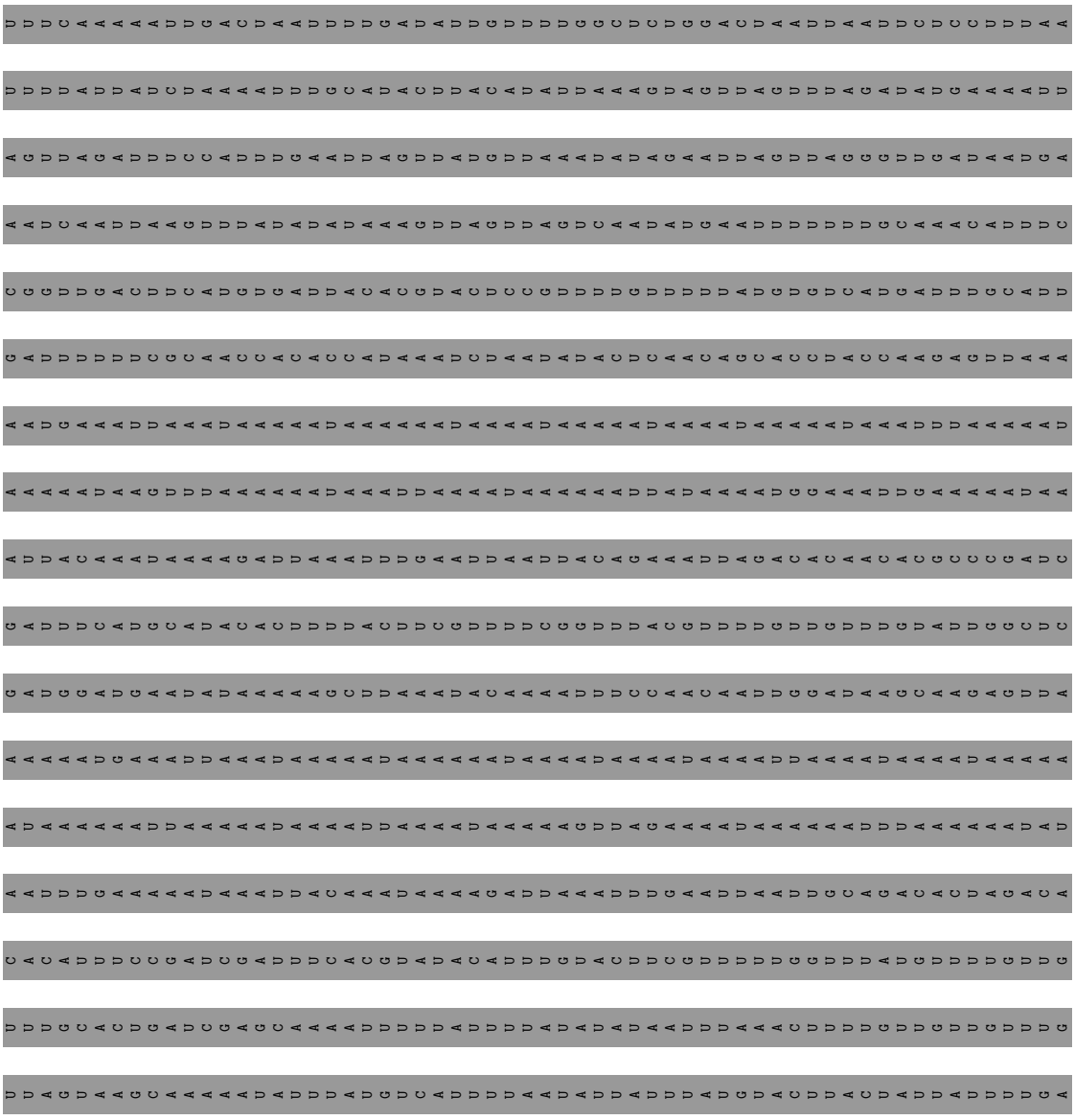
Mol	Chain	Residues	Atoms	AltConf
126	1	2	Total Mg 2 2	0

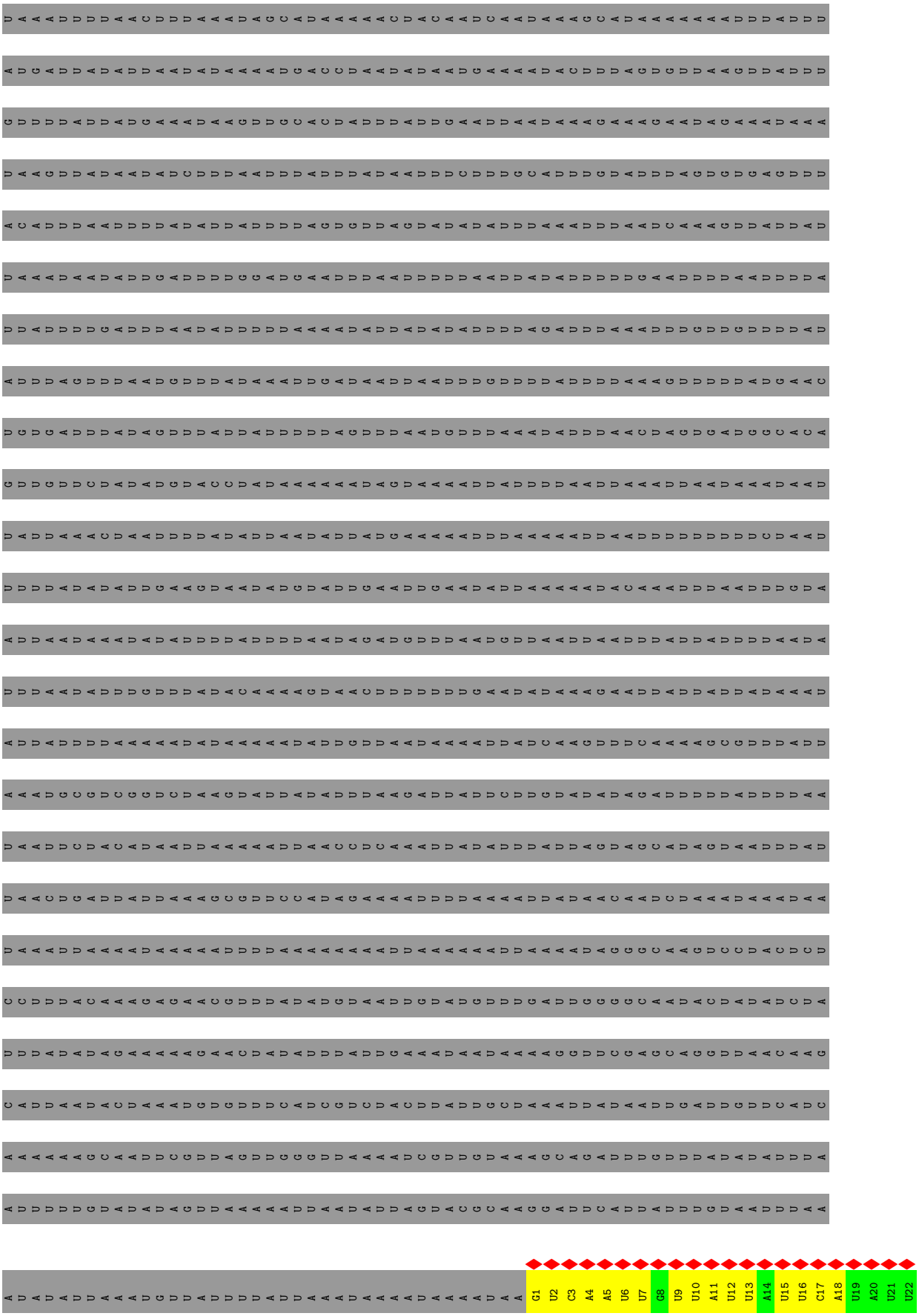
3 Residue-property plots (i)

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

- Molecule 1: Large ribosomal RNA

Chain 2: 97%

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A4
A5
U6
U7
G8
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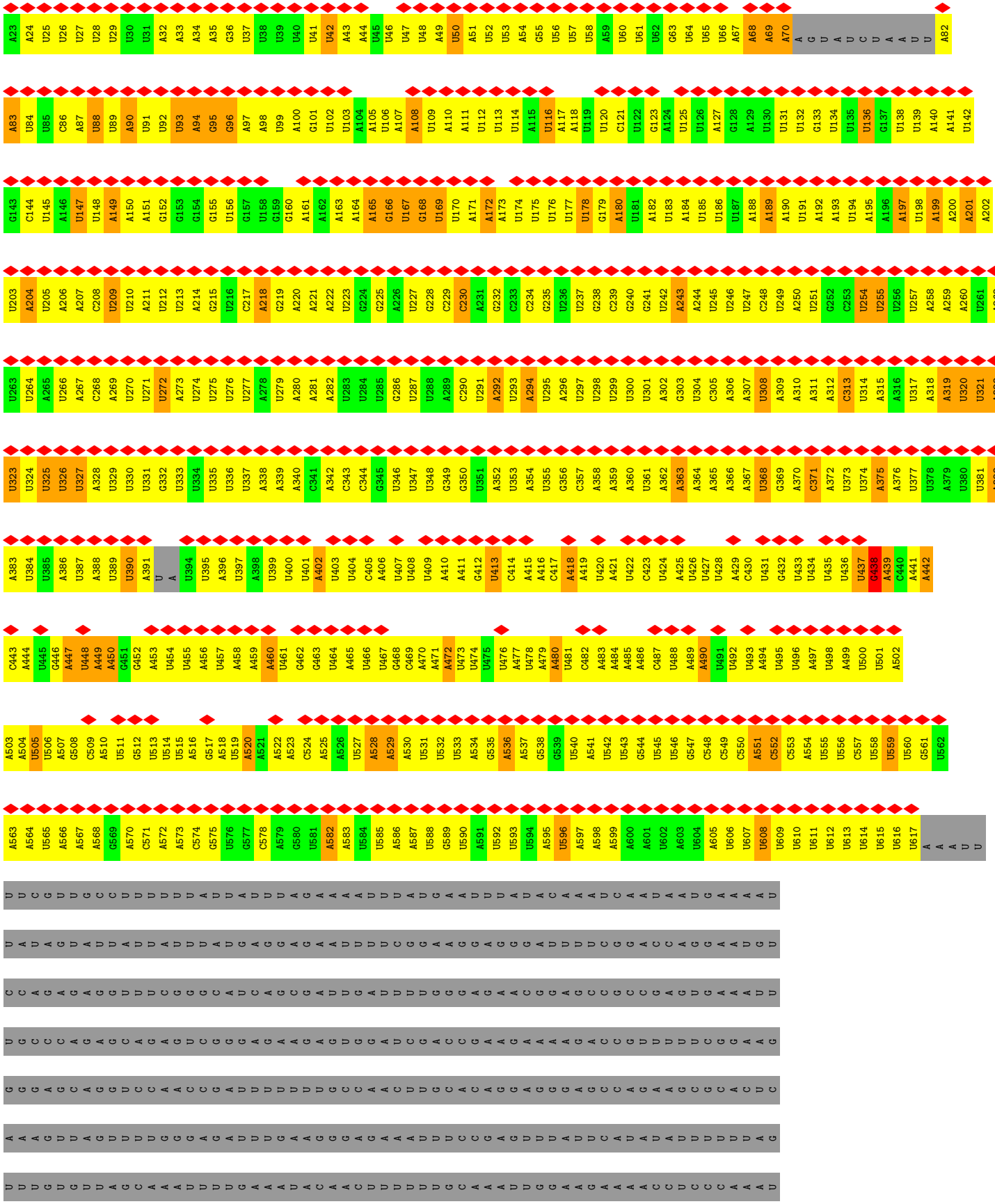
U21
U22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A83 U84 U85 C86 A87 U88 U89 A90 U91 U92 U93 A94 G95 G96 A97 A98 U99 A100 G101 U102 U103 A104 A105 U106 A107 A108 U109 A110 A111 U112 U113 U114 A115 U116 A117 A118 U119 U120 C121 U122 G123 A124 U125 U126 A127 G128 A129 U130 U131 U132 G133 U134 U135 U136 G137 U138 U139 A140 A141 U142
G143 C144 U145 A146 U147 U148 A149 A150 A151 G152 G153 G154 G155 U156 G157 U158 G159 G160 A161 A162 A163 A164 A165 G166 U167 G168 U169 U170 A171 A172 A173 U174 U175 U176 U177 U178 G179 A180 U181 A182 U183 A184 U185 U186 U187 A188 A189 A190 U191 A192 A193 U194 A195 A196 A197 U198 A199 A200 A201 A202
U203 A204 U205 A206 A207 C208 U209 U210 A211 U212 U213 A214 G215 U216 C217 A218 G219 A220 A221 A222 U223 G224 G225 A226 U227 G228 C229 C230 A231 G232 C233 C234 G235 U236 U237 G238 C239 G240 G241 U242 A243 A244 U245 U246 U247 C248 U249 A250 U251 G252 C253 U254 U255 U256 U257 A258 A259 A260 U261 A262
U263 U264 A265 U266 A267 C268 A269 U270 U271 U272 A273 U274 U275 U276 U277 A278 U279 A280 A281 A282 U283 U284 U285 G286 U287 U288 A289 C290 U291 A292 U293 A294 U295 A296 U297 U298 U299 U300 U301 A302 G303 U304 C305 A306 A307 U308 A309 A310 A311 A312 C313 U314 A315 A316 U317 A318 A319 U320 U321 A322
U323 U324 U325 U326 U327 A328 U329 U330 U331 G332 U333 U334 U335 U336 U337 A338 A339 A340 C341 A342 C343 C344 G345 U346 U347 U348 G349 G350 U351 A352 U353 A354 U355 G356 C357 A358 A359 A360 U361 A362 A363 A364 A365 A366 A367 U368 G369 A370 C371 A372 U373 U374 A375 A376 U377 U378 A379 U380 U381 A382
A383 U384 U385 A386 U387 A388 U389 U390 A391 U A U394 U395 A396 U397 A398 U399 U400 U401 A402 U403 U404 C405 A406 U407 U408 U409 A410 A411 G412 U413 C414 A415 A416 C417 A418 A419 U420 A421 U422 C423 U424 A425 U426 U427 U428 A429 C430 U431 G432 U433 U434 U435 U436 U437 G438 A439 C440 A441 A442
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A503 A504 U505 U506 A507 G508 C509 A510 U511 G512 U513 U514 U515 A516 G517 A518 U519 A520 A521 A522 A523 C524 A525 A526 U527 A528 A529 A530 U531 U532 U533 A534 G535 A536 A537 G538 G539 U540 A541 U542 U543 G544 U545 U546 G547 C548 C549 C550 A551 C552 C553 A554 U555 U556 C557 U558 U559 U560 G561 U562
A563 A564 U565 A566 A567 A568 G569 A570 C571 A572 A573 C574 G575 U576 G577 C578 A579 G580 U581 A582 A583 U584 U585 A586 A587 U588 G589 U590 A591 U592 U593 U594 A595 U596 A597 A598 A599 A600 A601 U602 A603 U604 A605 U606 U607 U608 U609 U610 U611 U612 U613 U614 U615 U616 U617 A A A U U
U U U G U G U A A G C U U U U A U U A U A U U A U U A U U A A A A A U U U U C C A A U G A A A A U
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U G C C A G G C A A G U U G A C G G G A A C C C G G A A A C G G A A G A C C C G U C G A A U U G
G G A A G C A G U C C A A G U U U U G C C A A G G A A A U C G A C C C A G U U C G C G A A C U C
A A A G G U U A G U U U U G A A G G A A G U U G G A A U C A A C A A U A U C A G U U U U U U U A G
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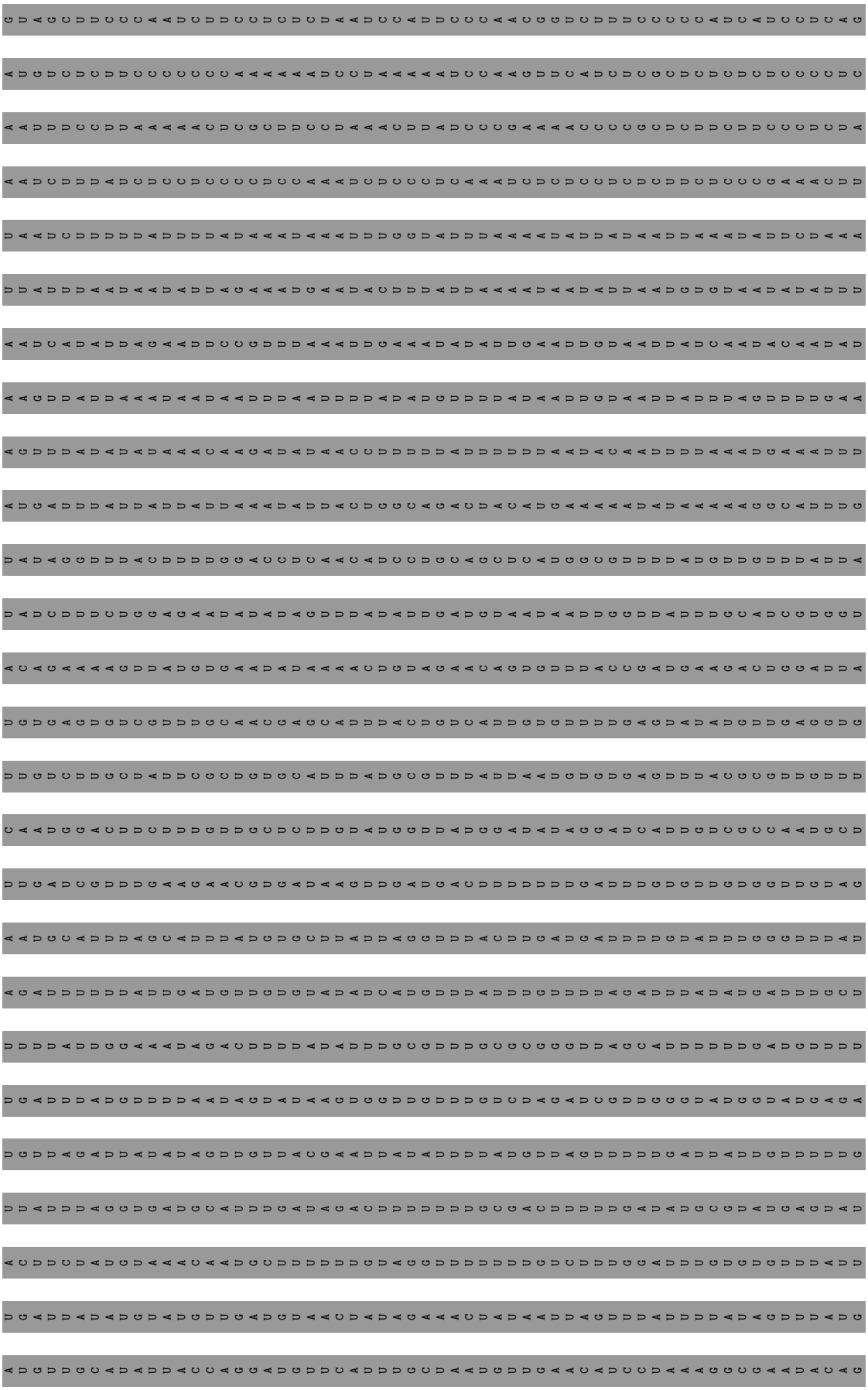
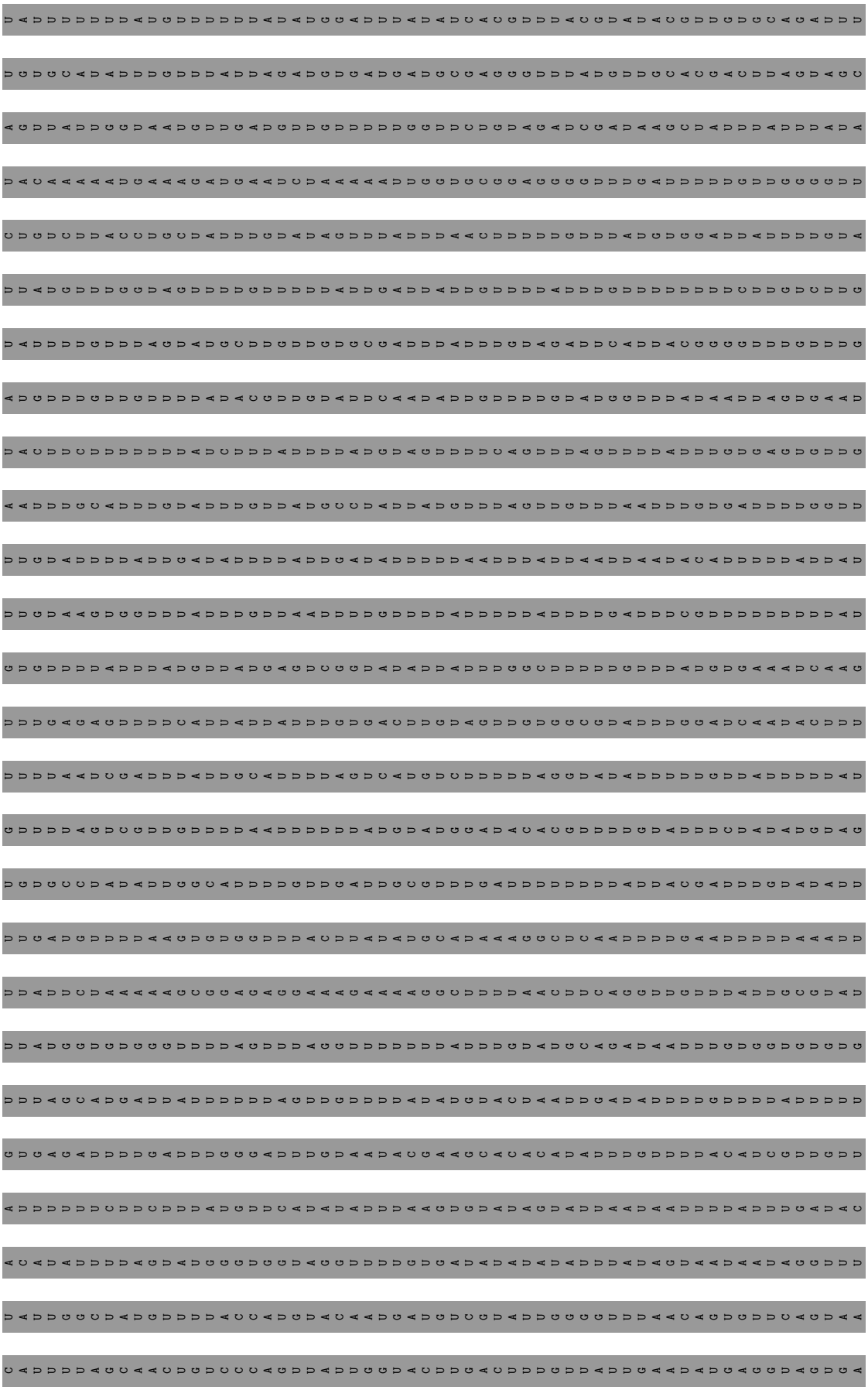
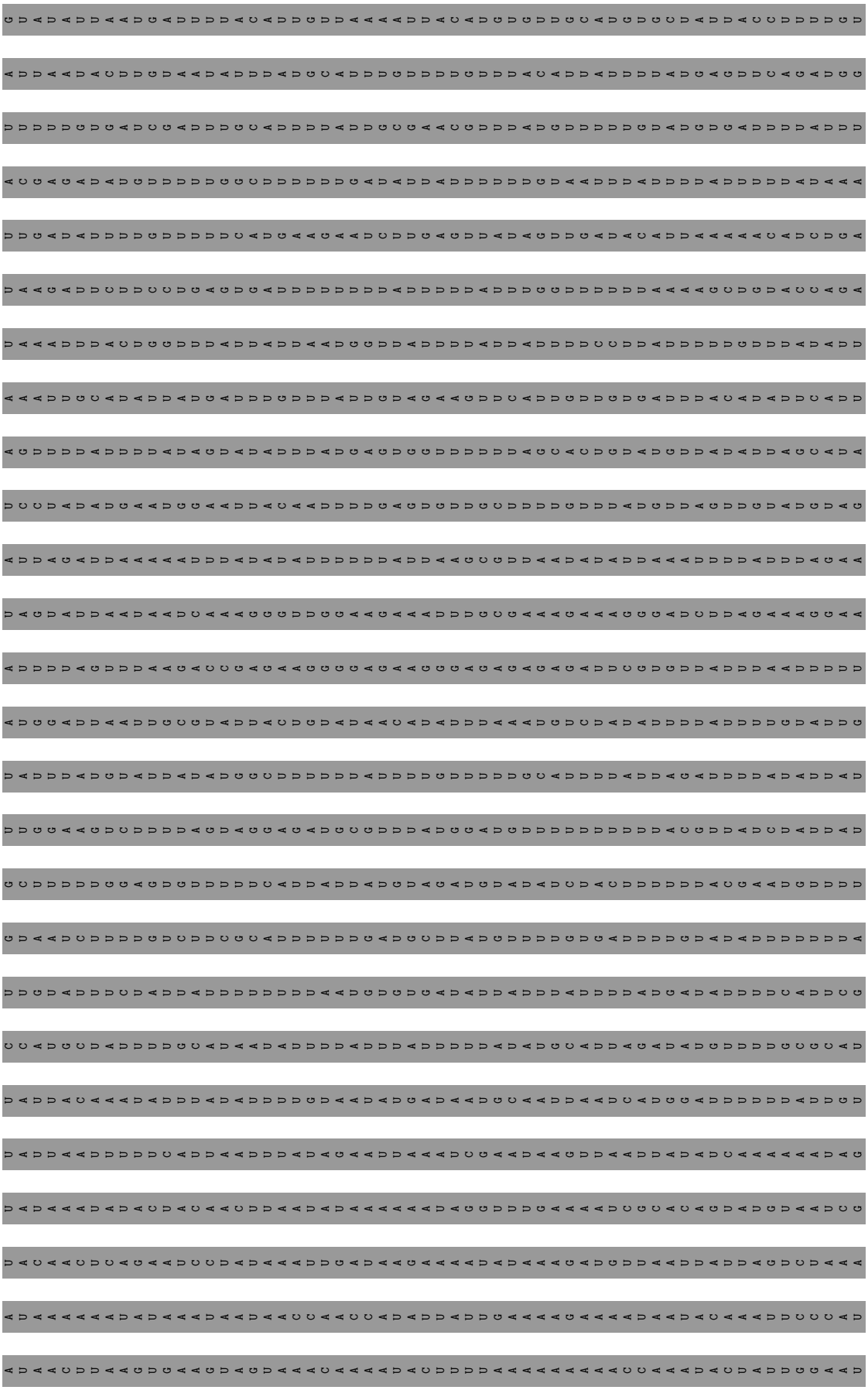
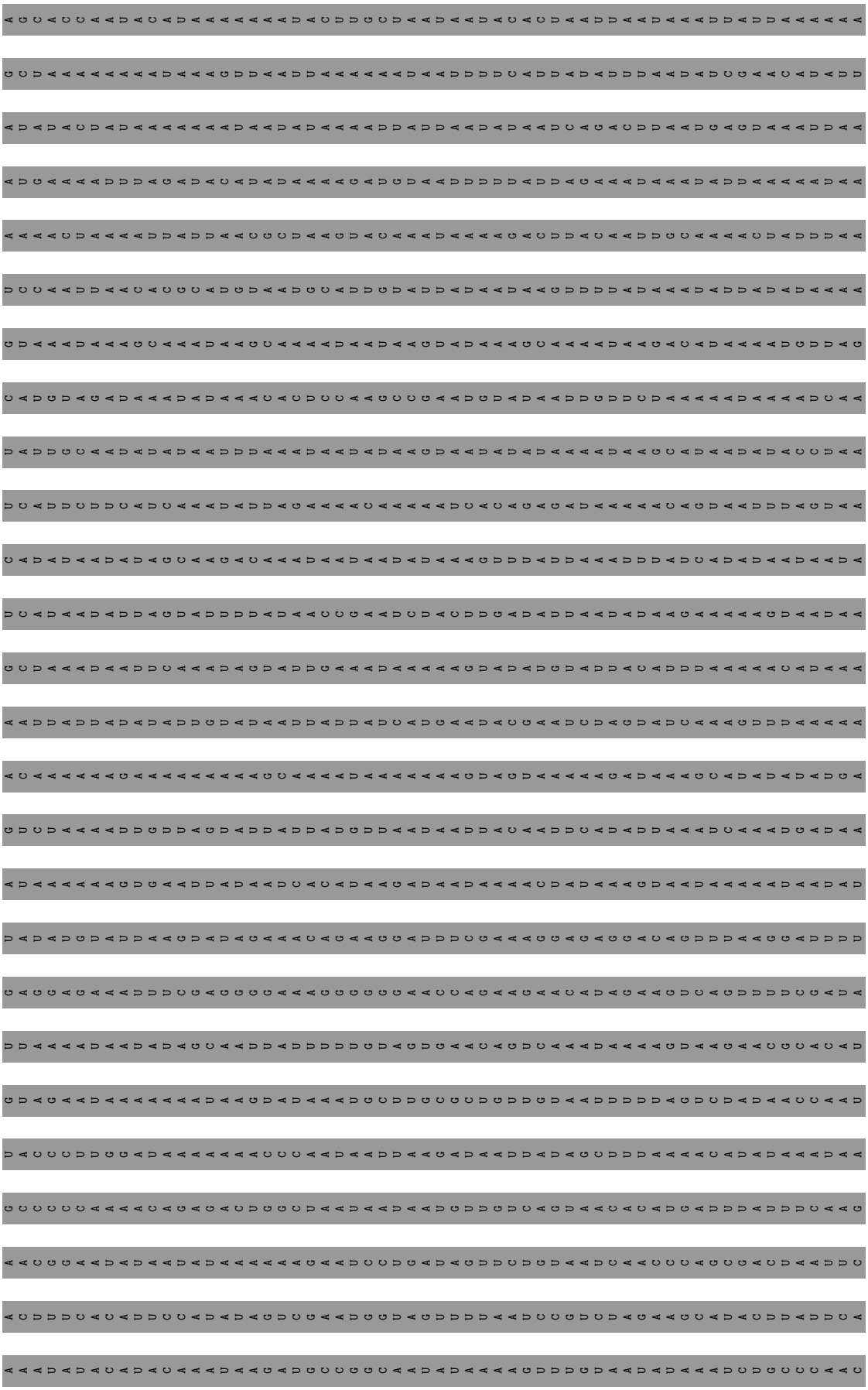
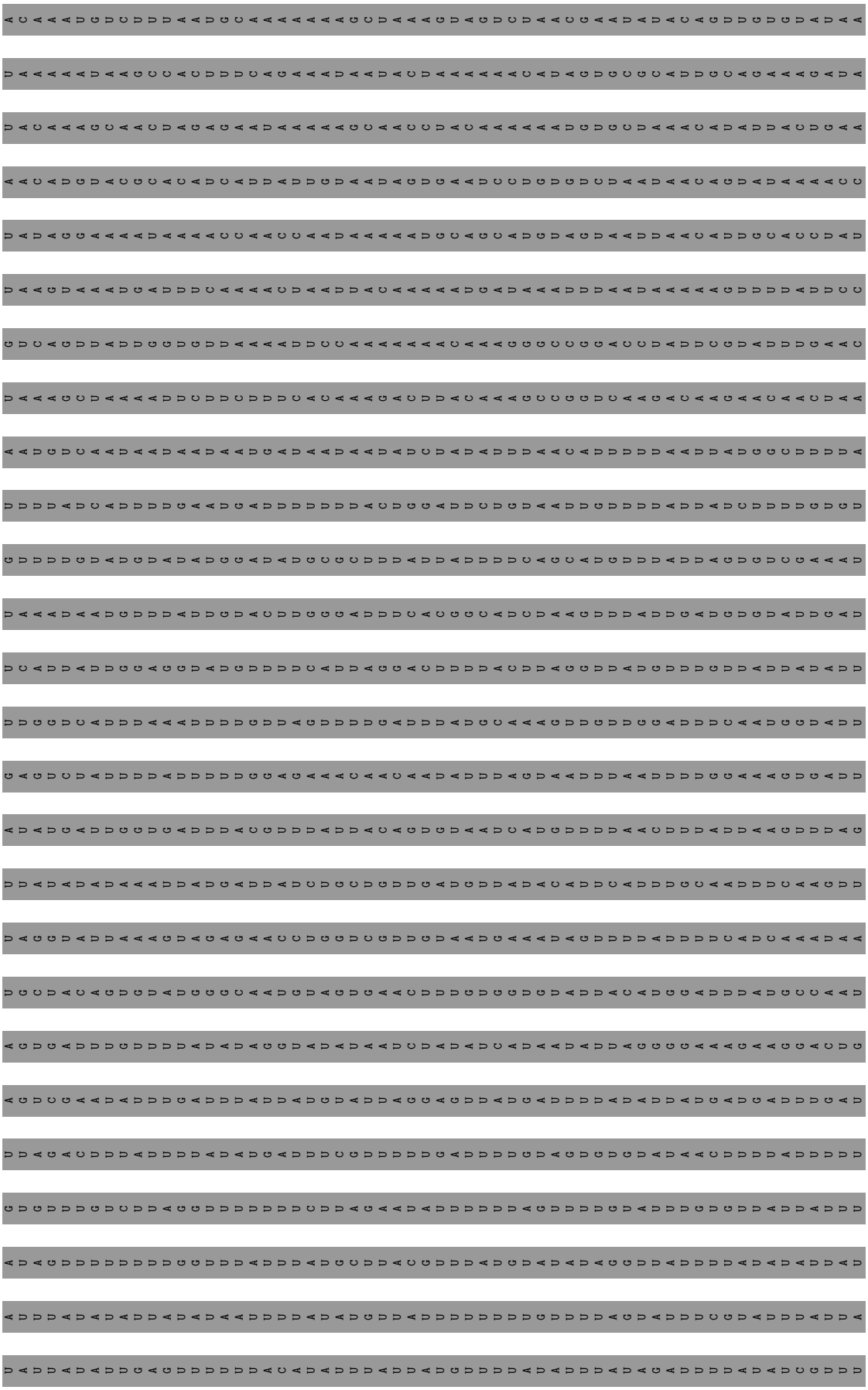
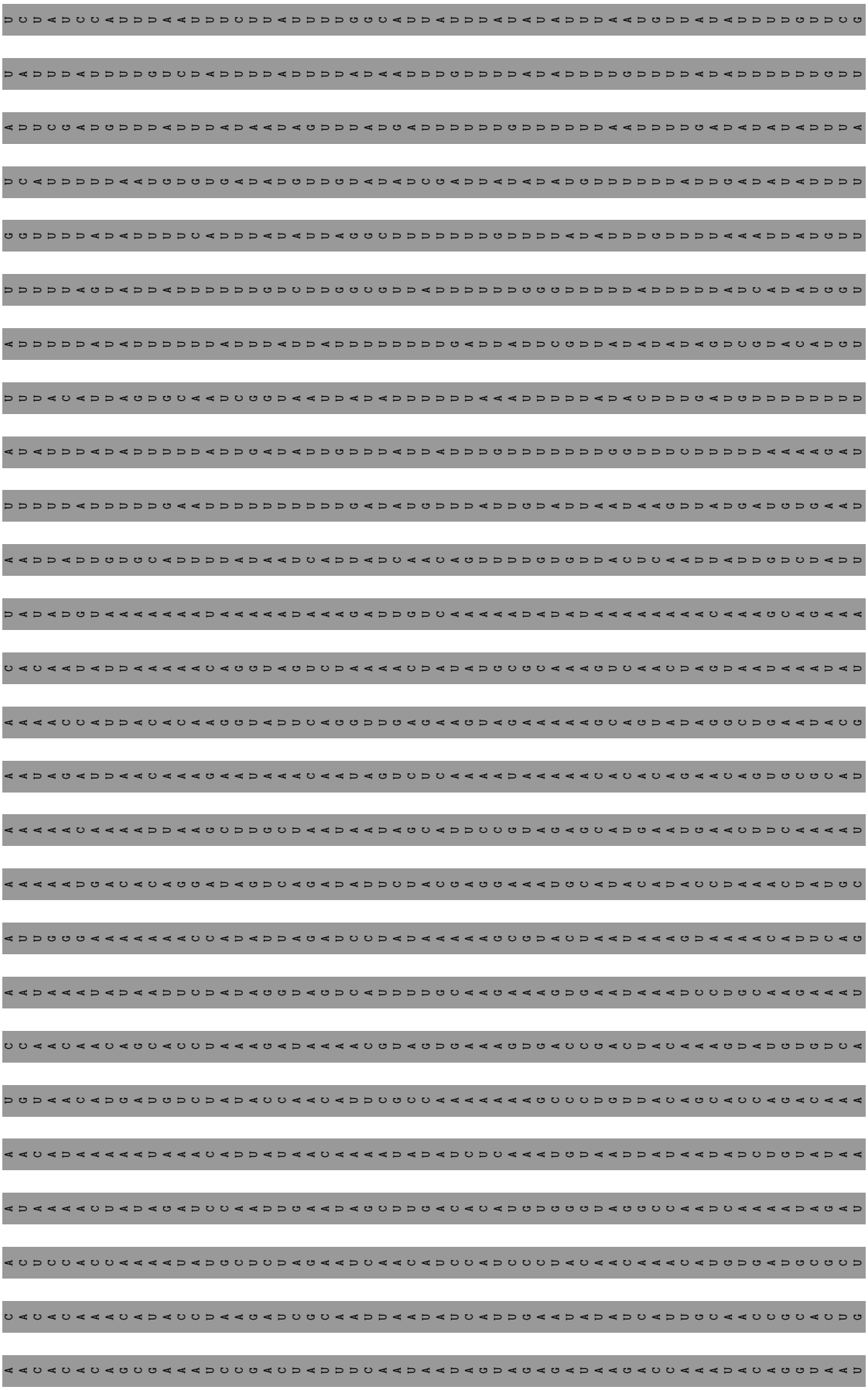


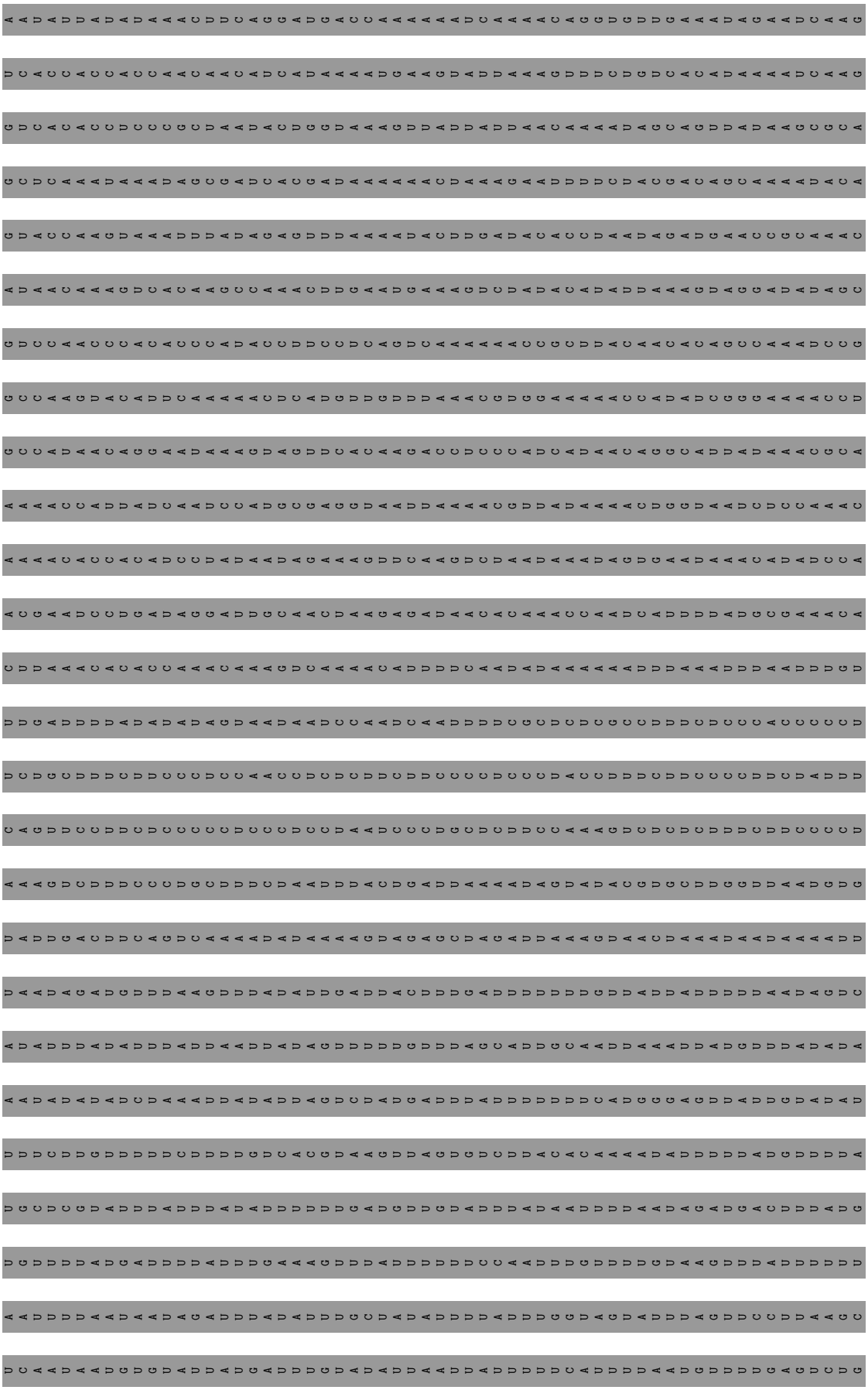


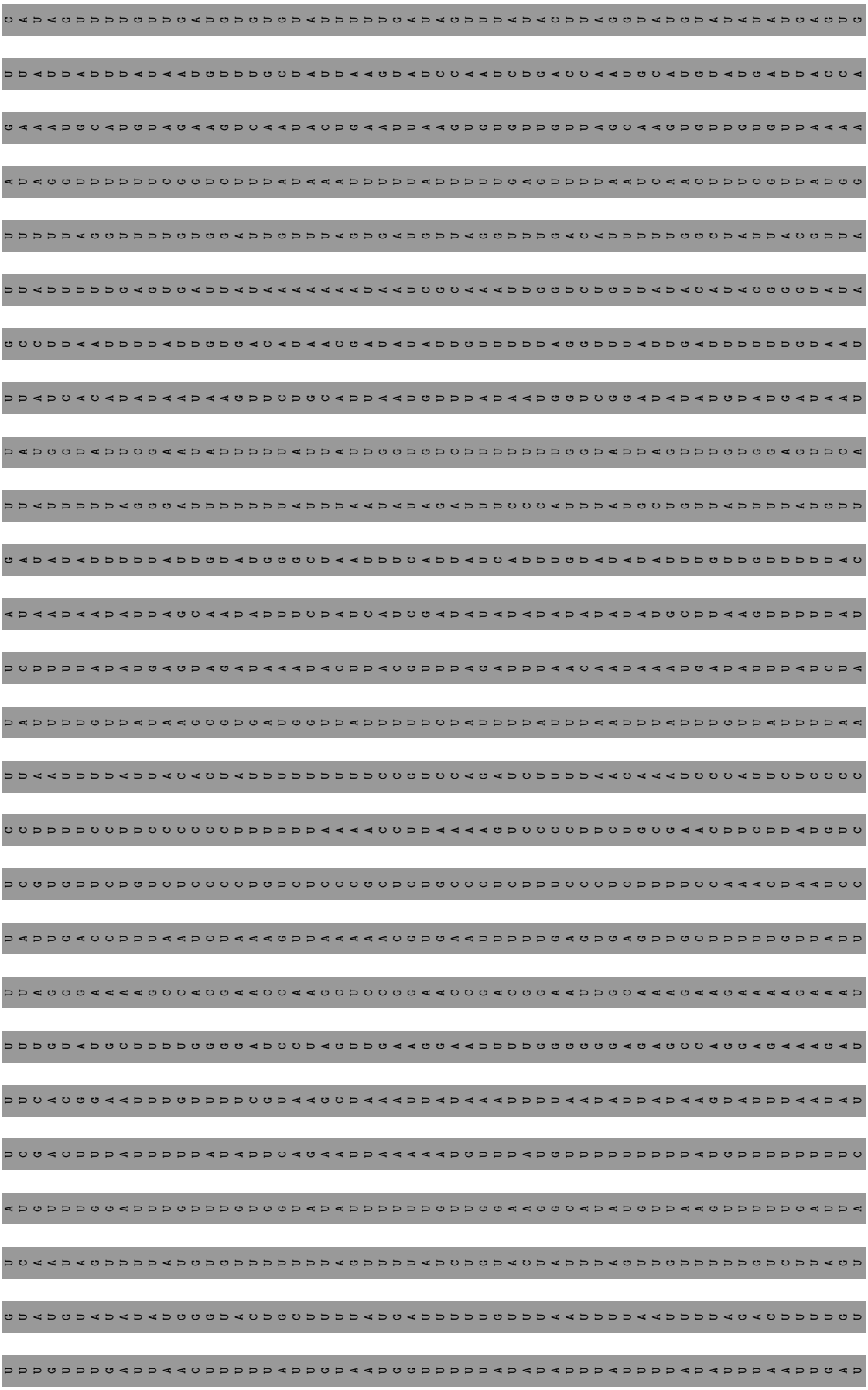


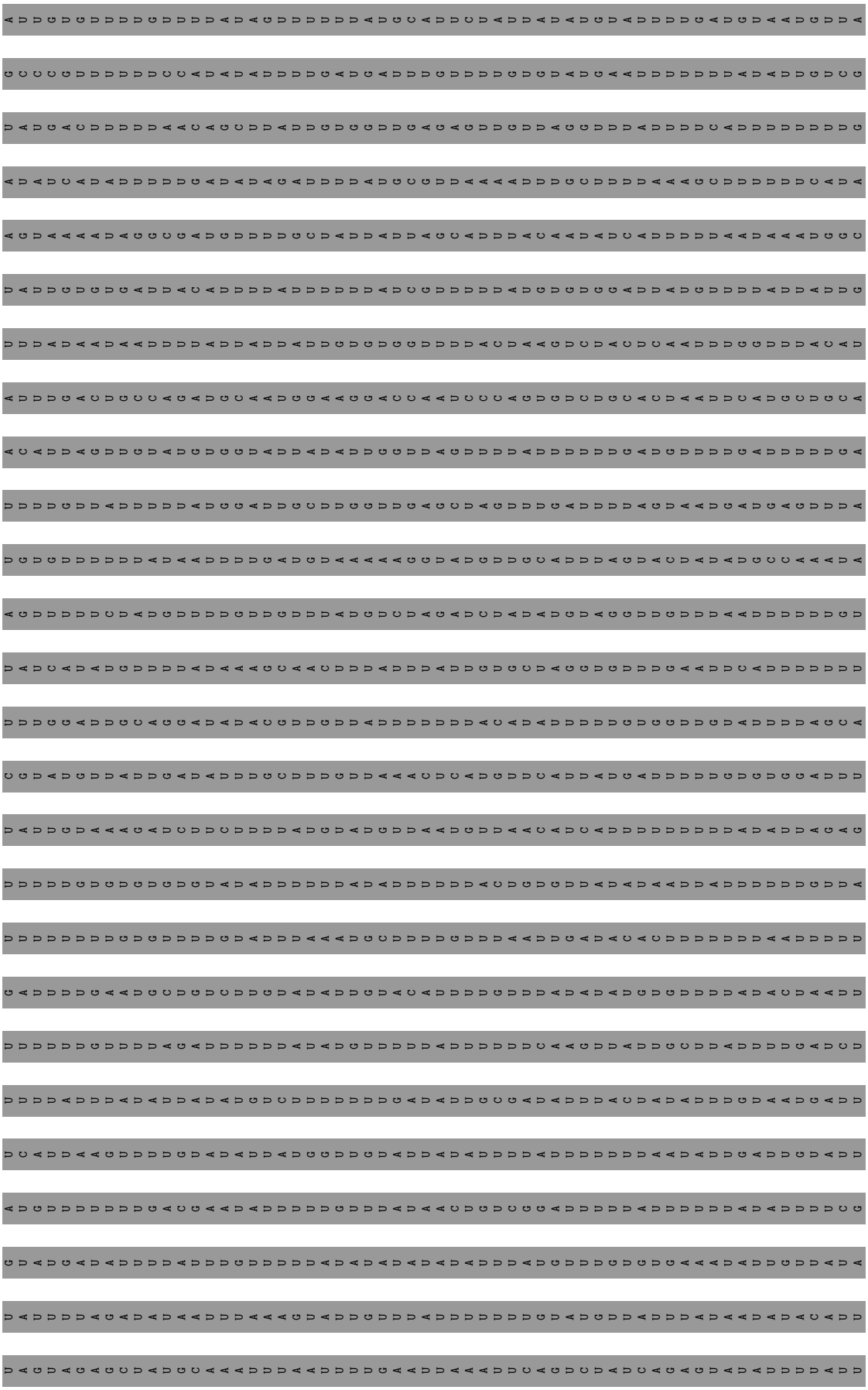


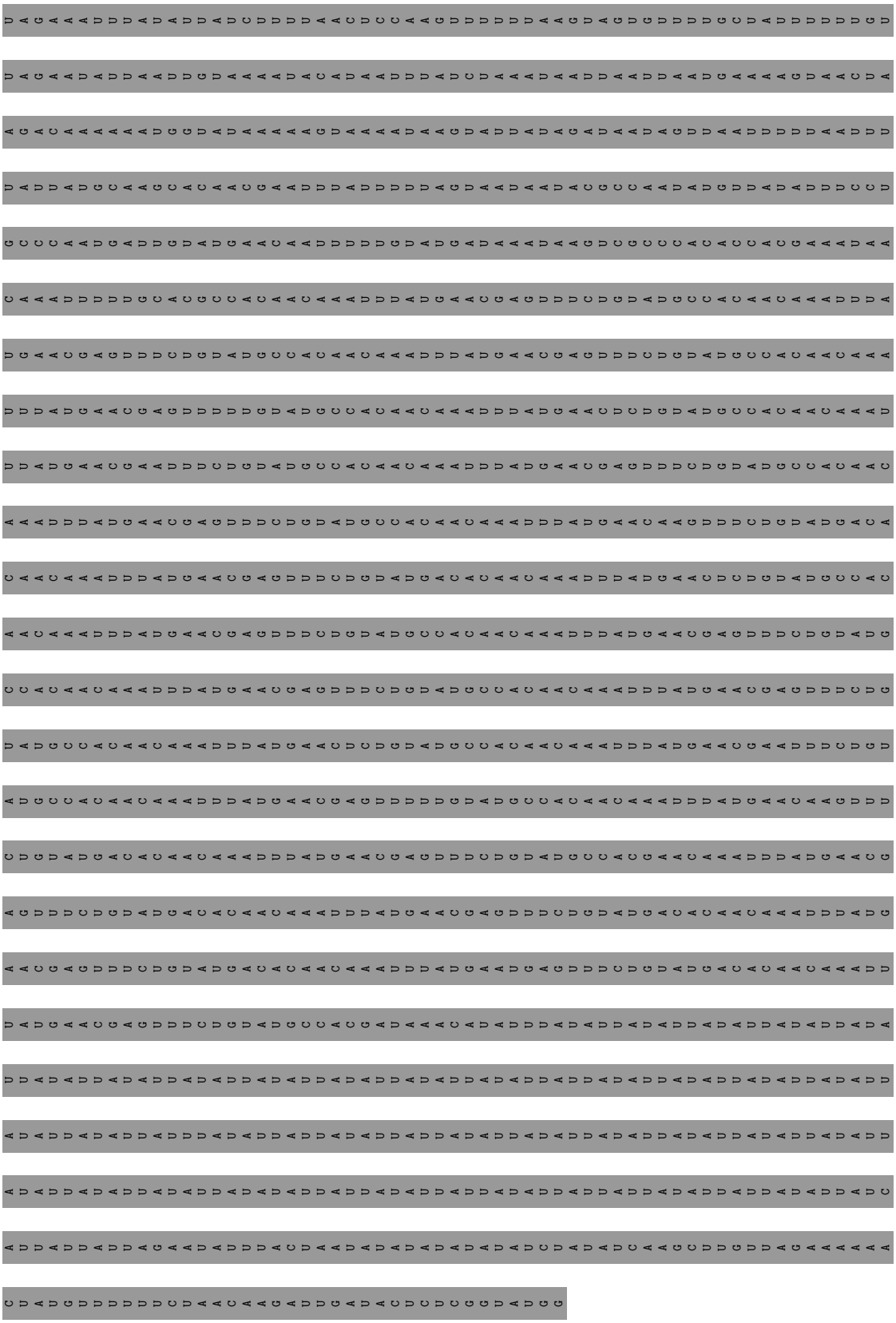




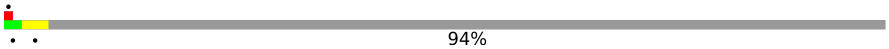


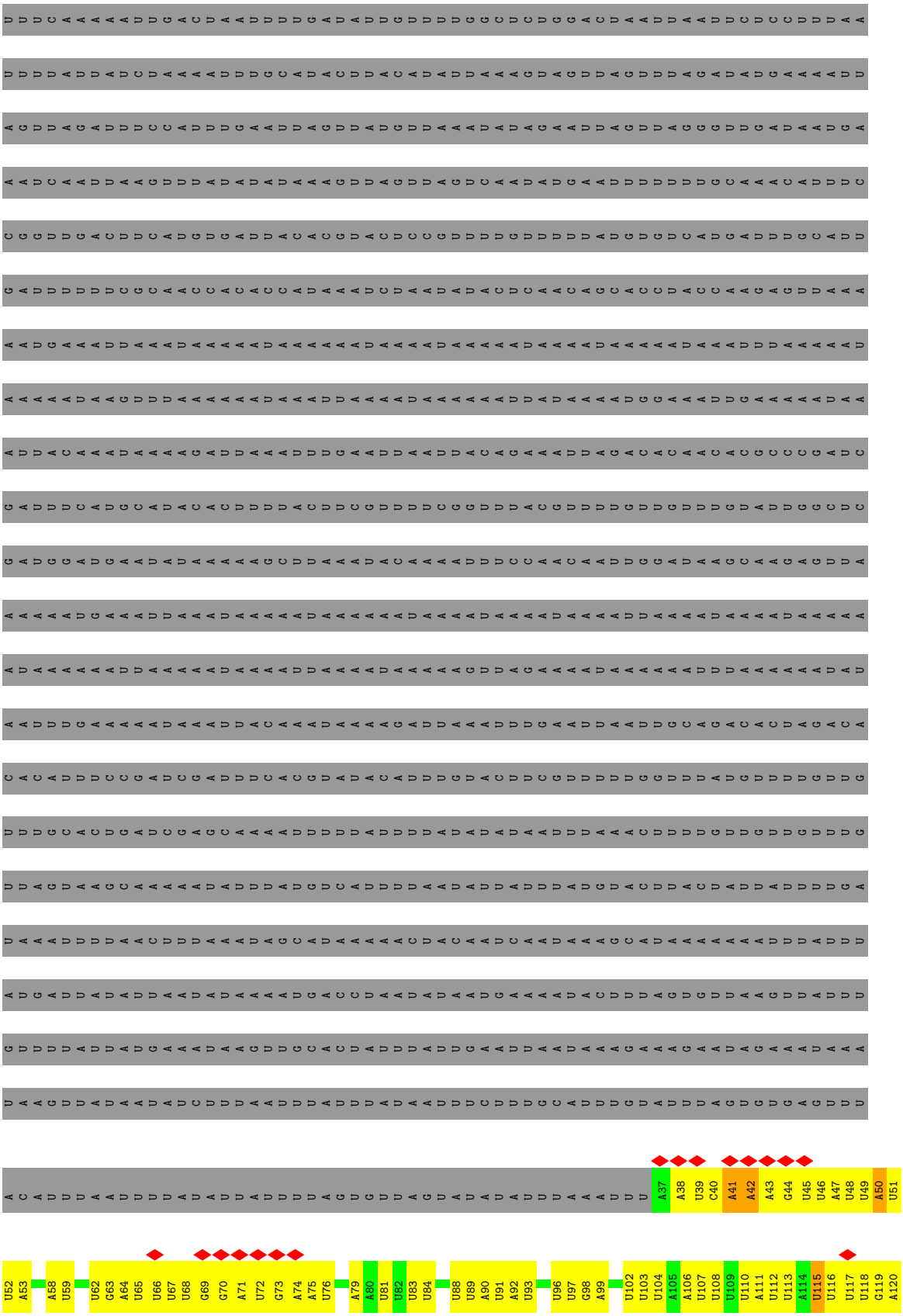






• Molecule 1: Large ribosomal RNA

Chain 1: 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A53
A58
U59
U62
G63
A64
U65
U66
U67
U68
G69
G70
A71
U72
G73
A74
A75
U76
A79
A80
U81
U82
U83
U84
U88
U89
A90
U91
A92
U93
U96
U97
G98
A99
U102
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U104
A105
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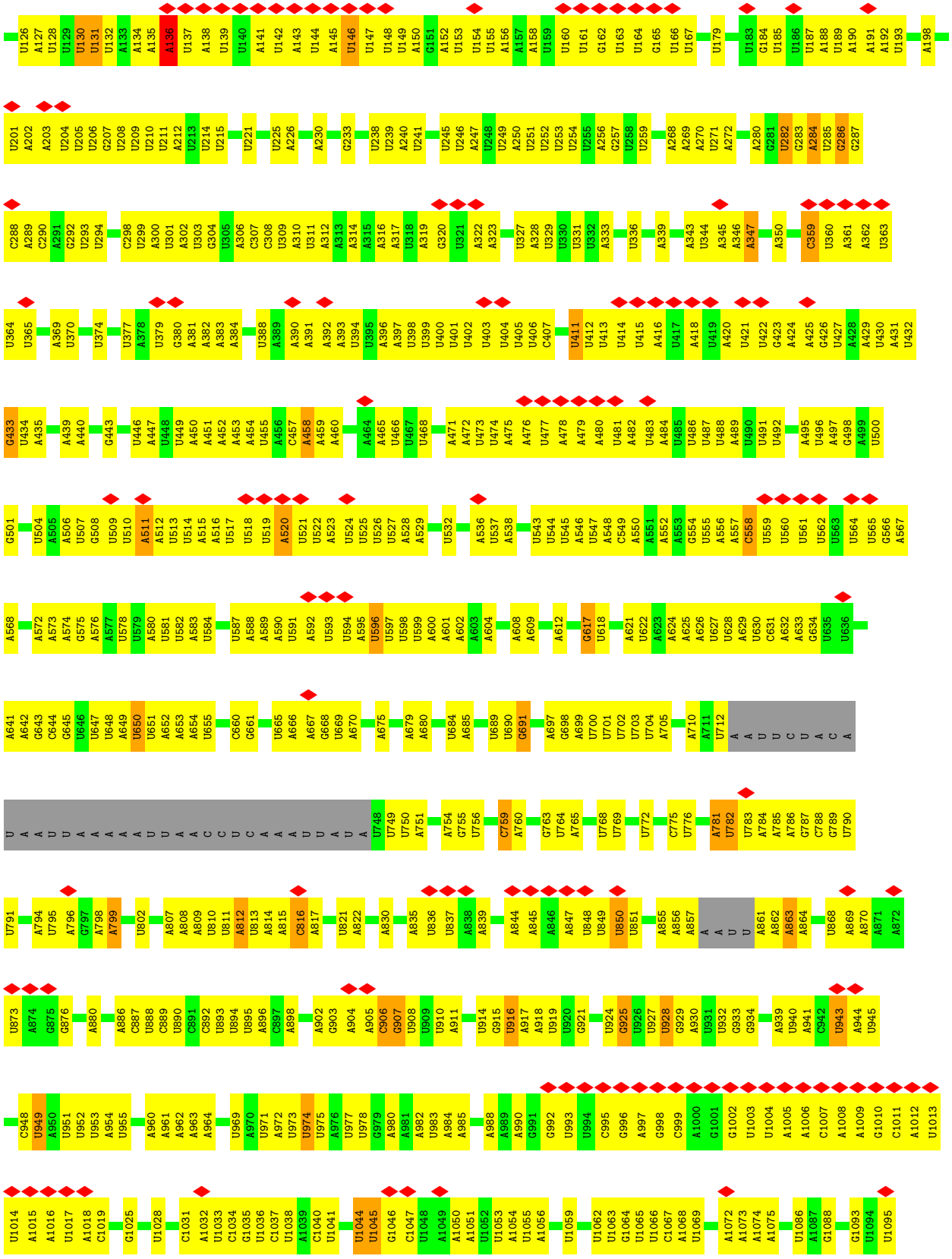

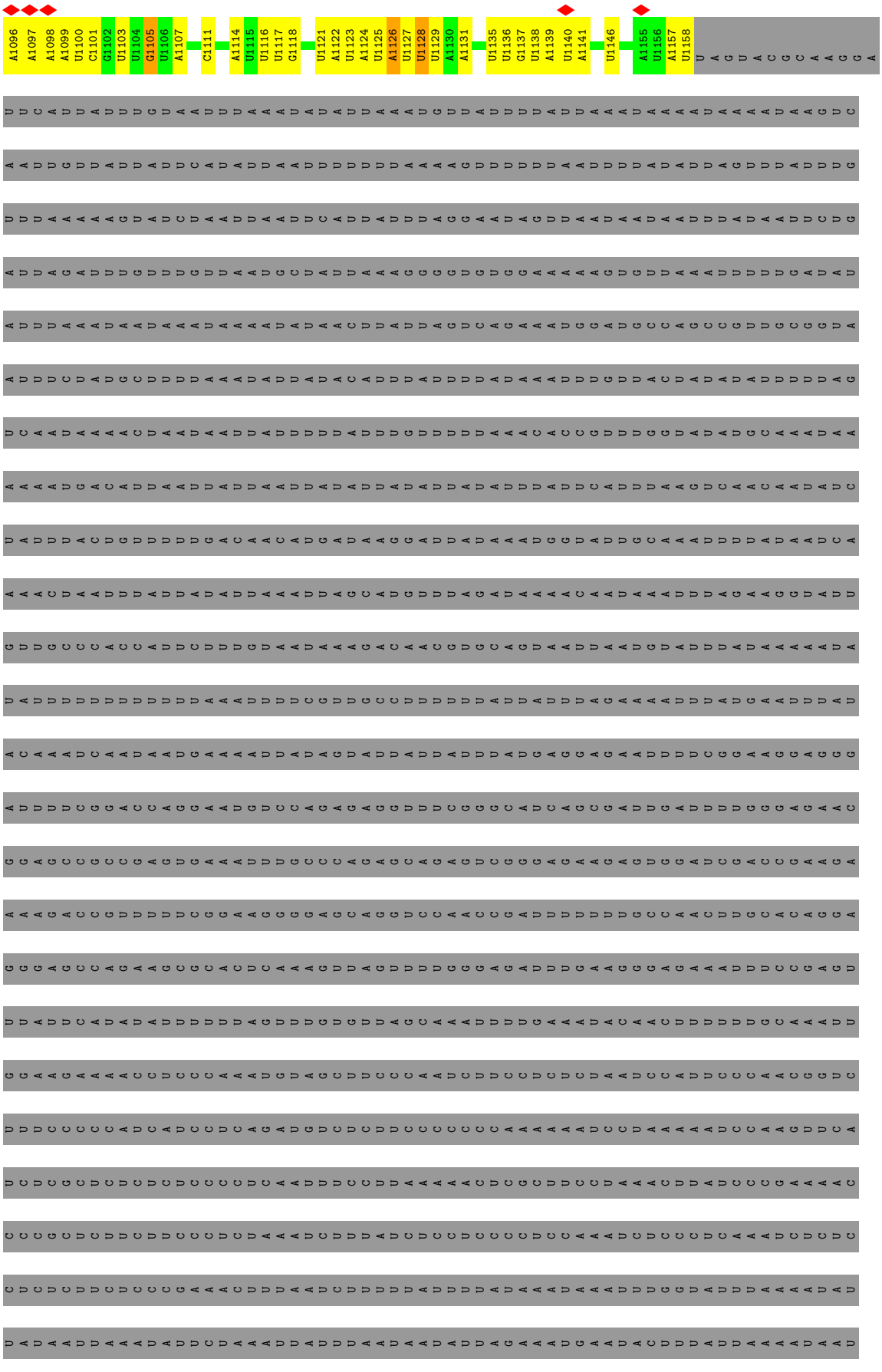
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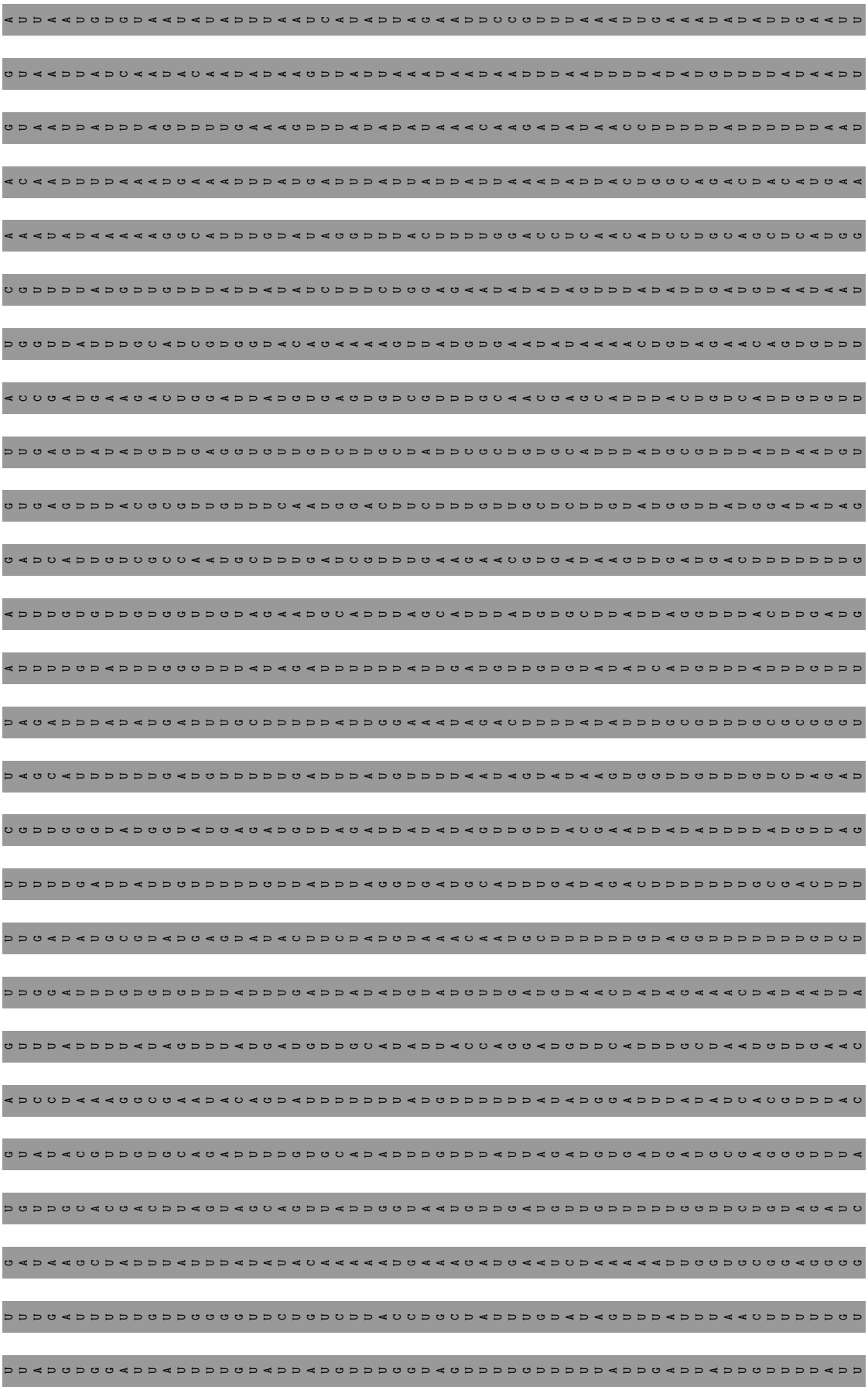
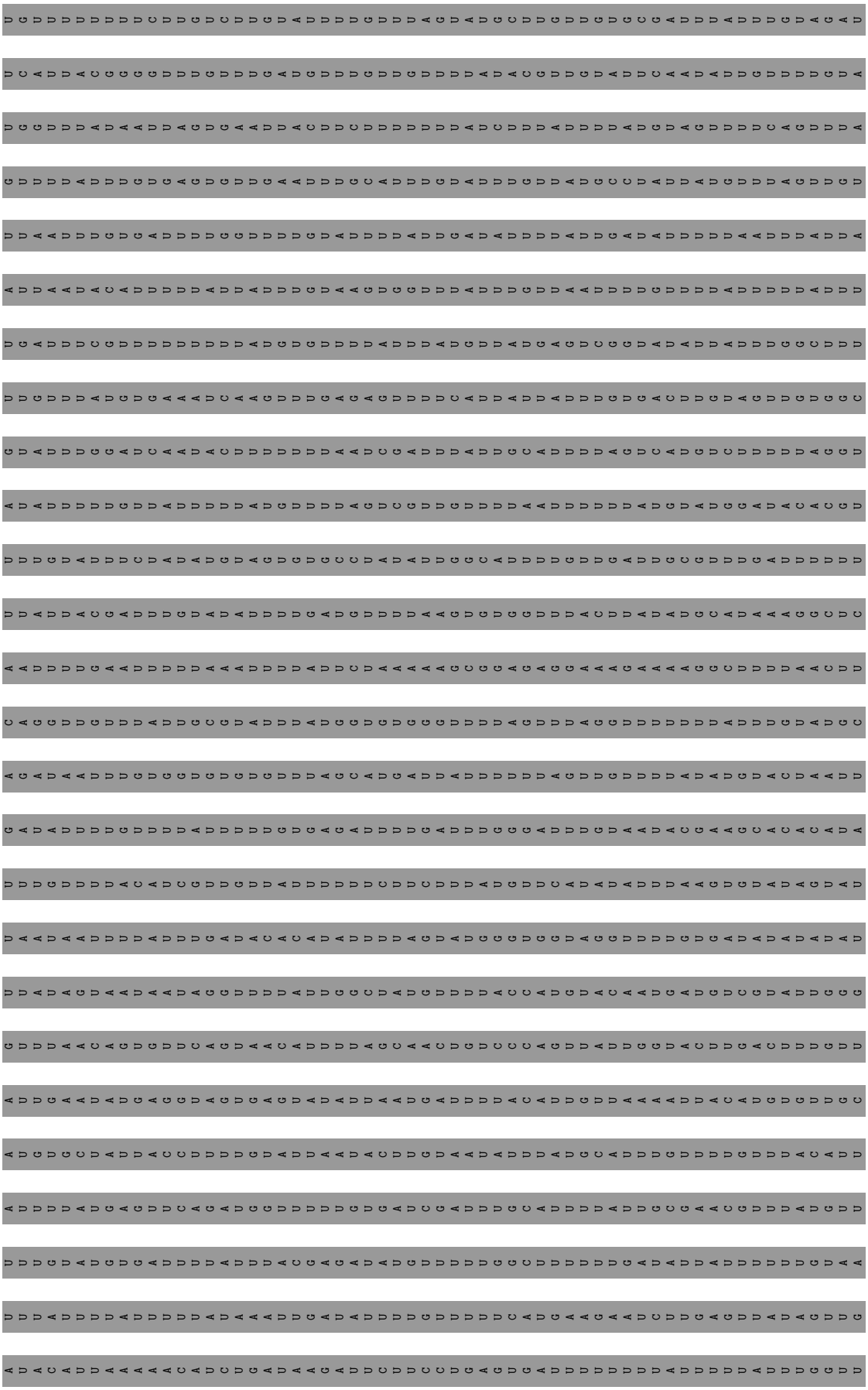
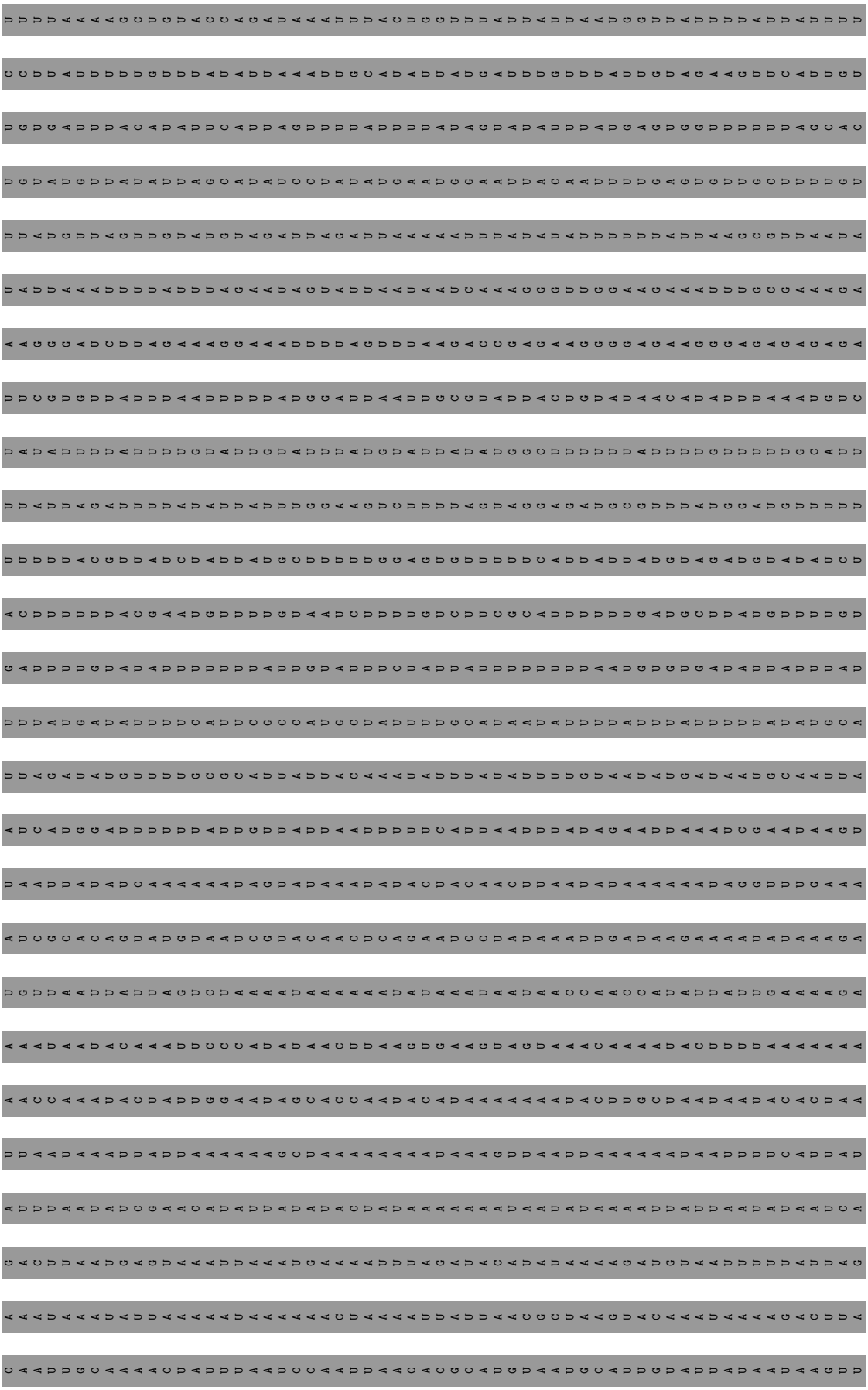
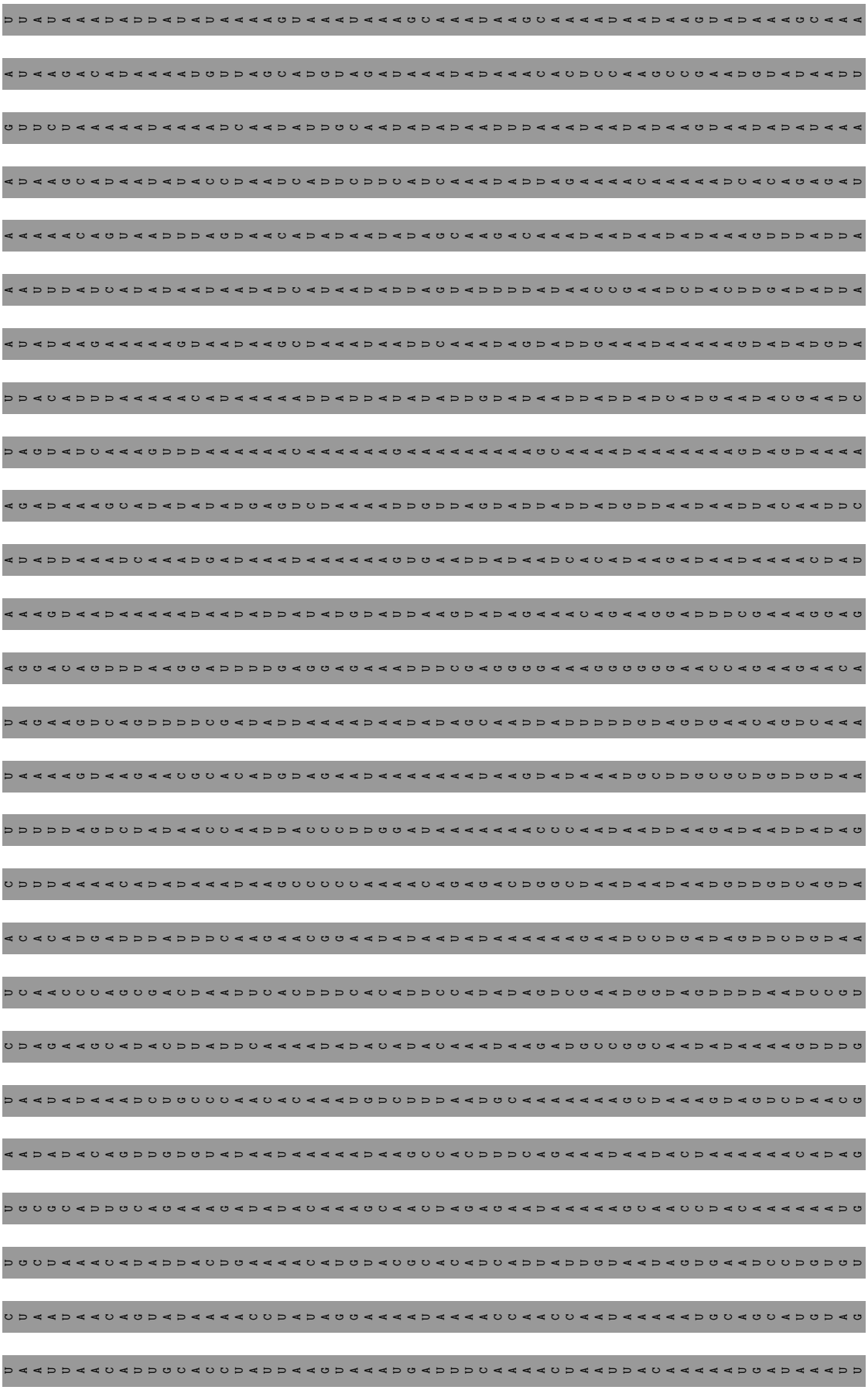
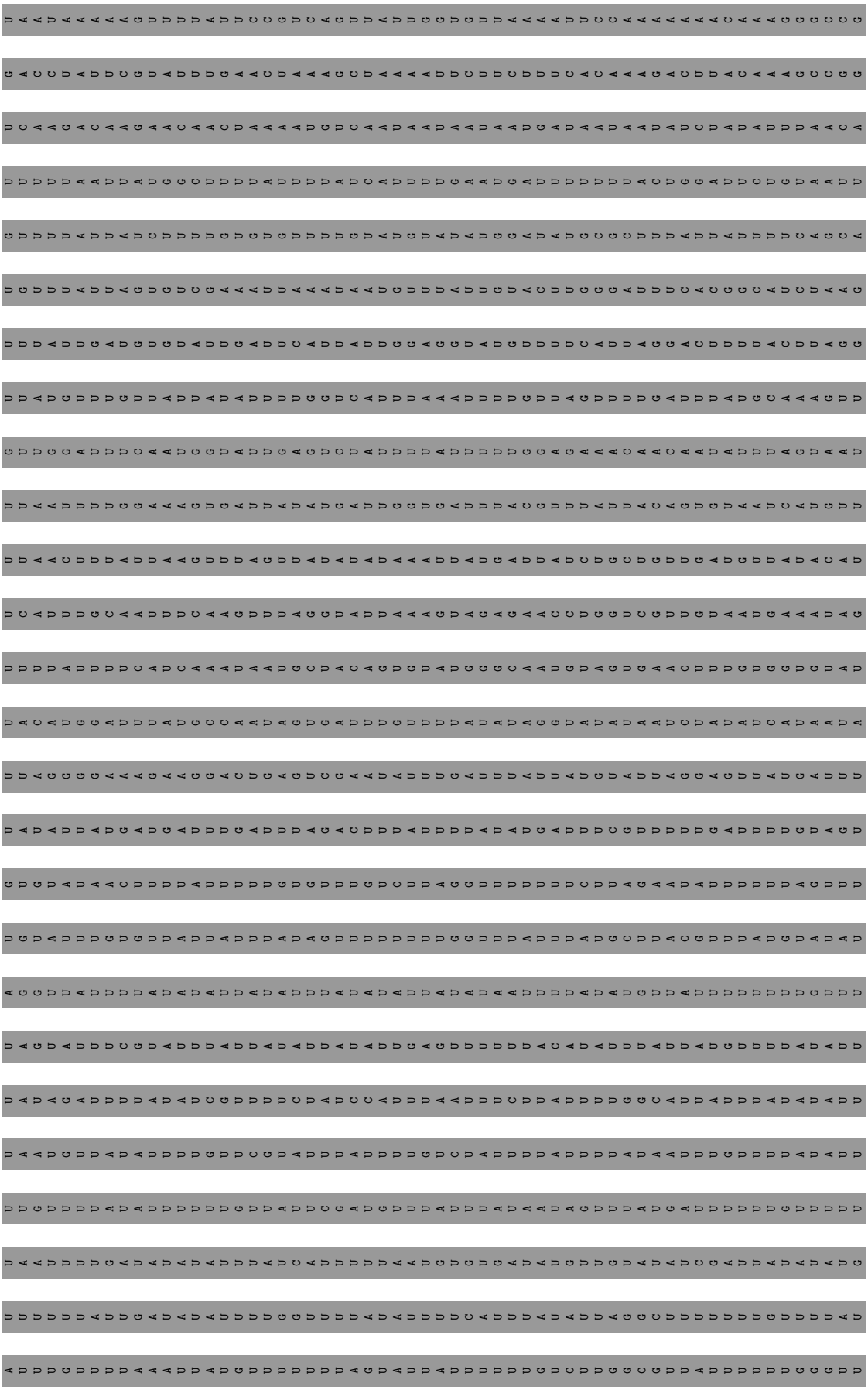
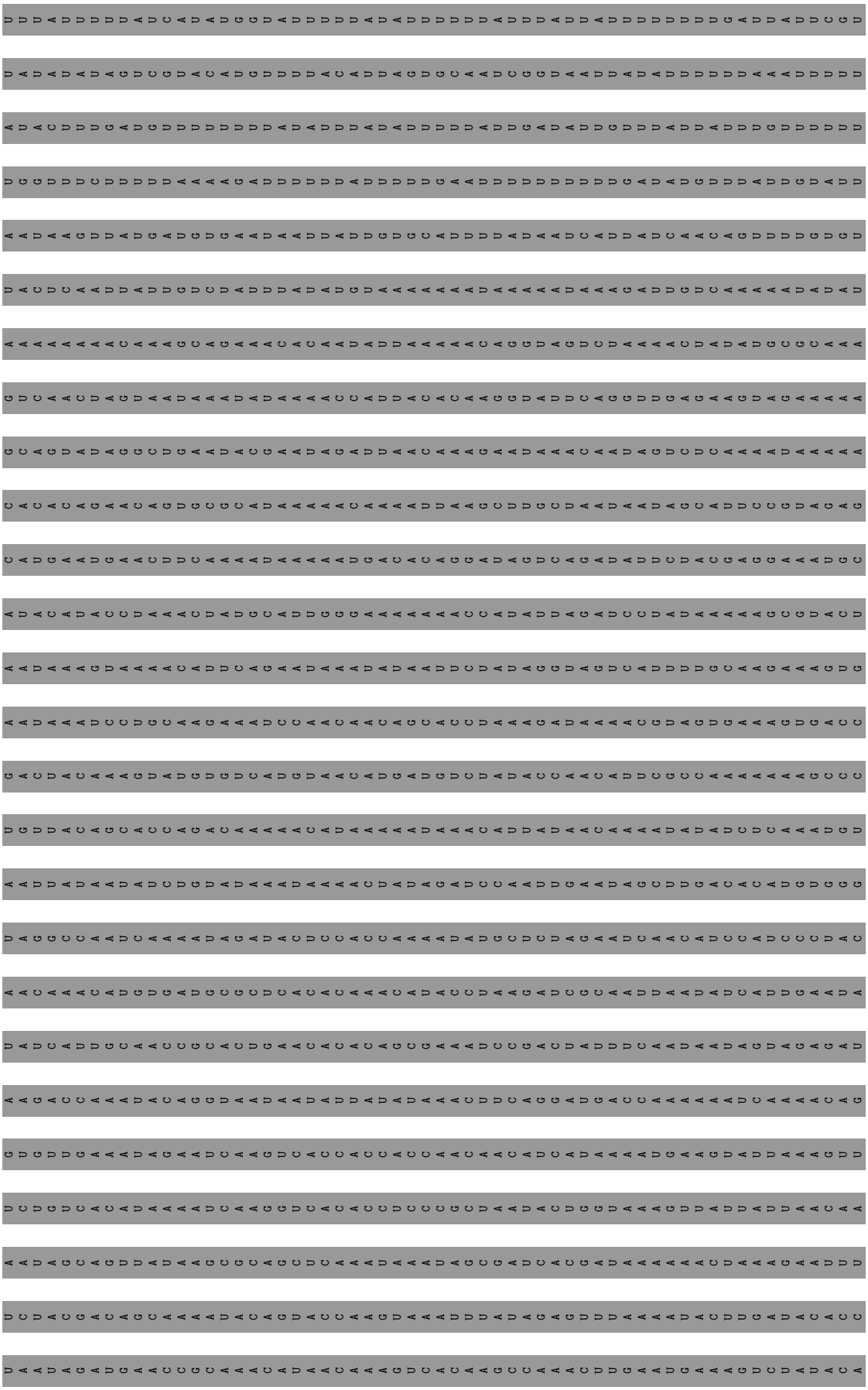


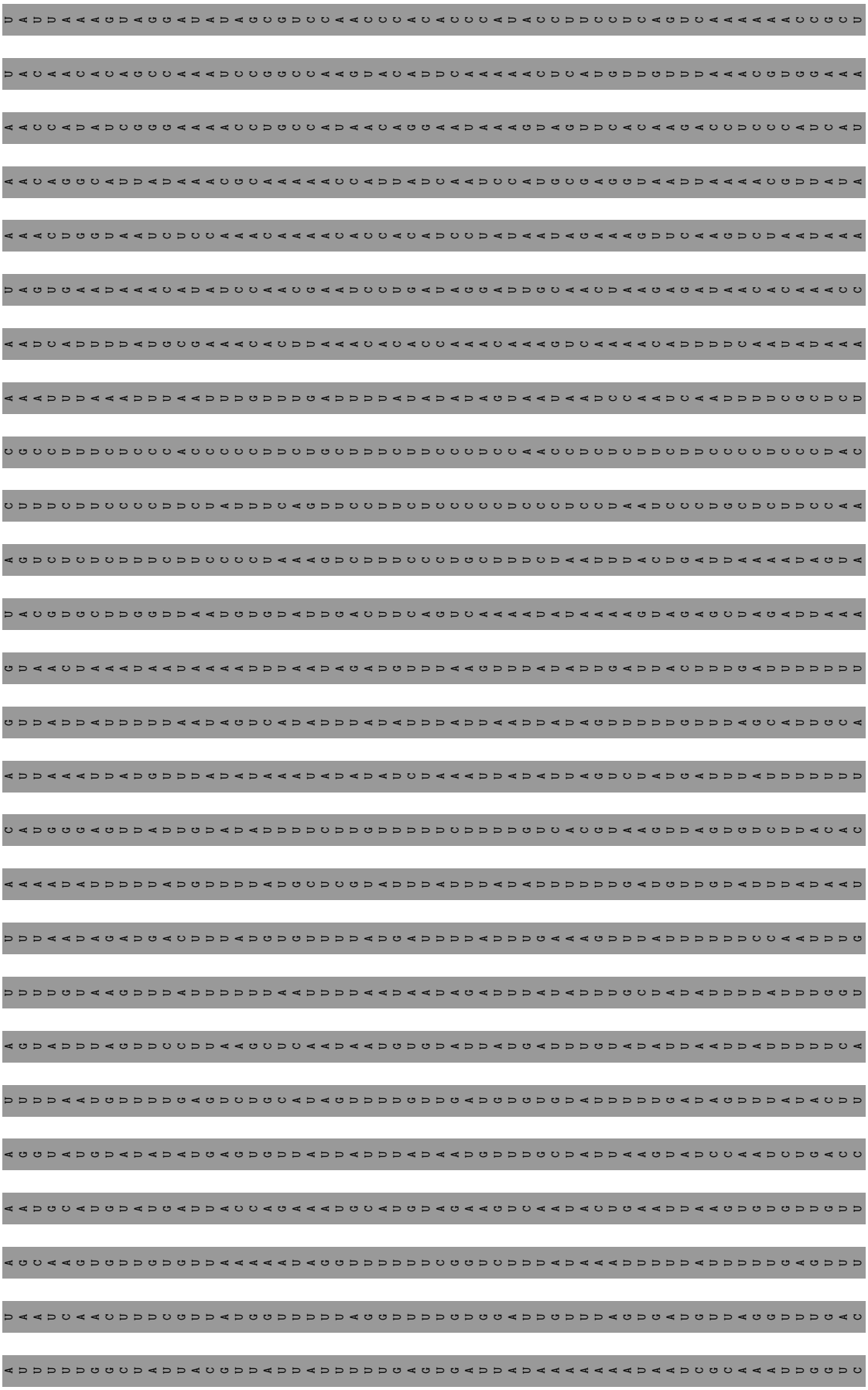


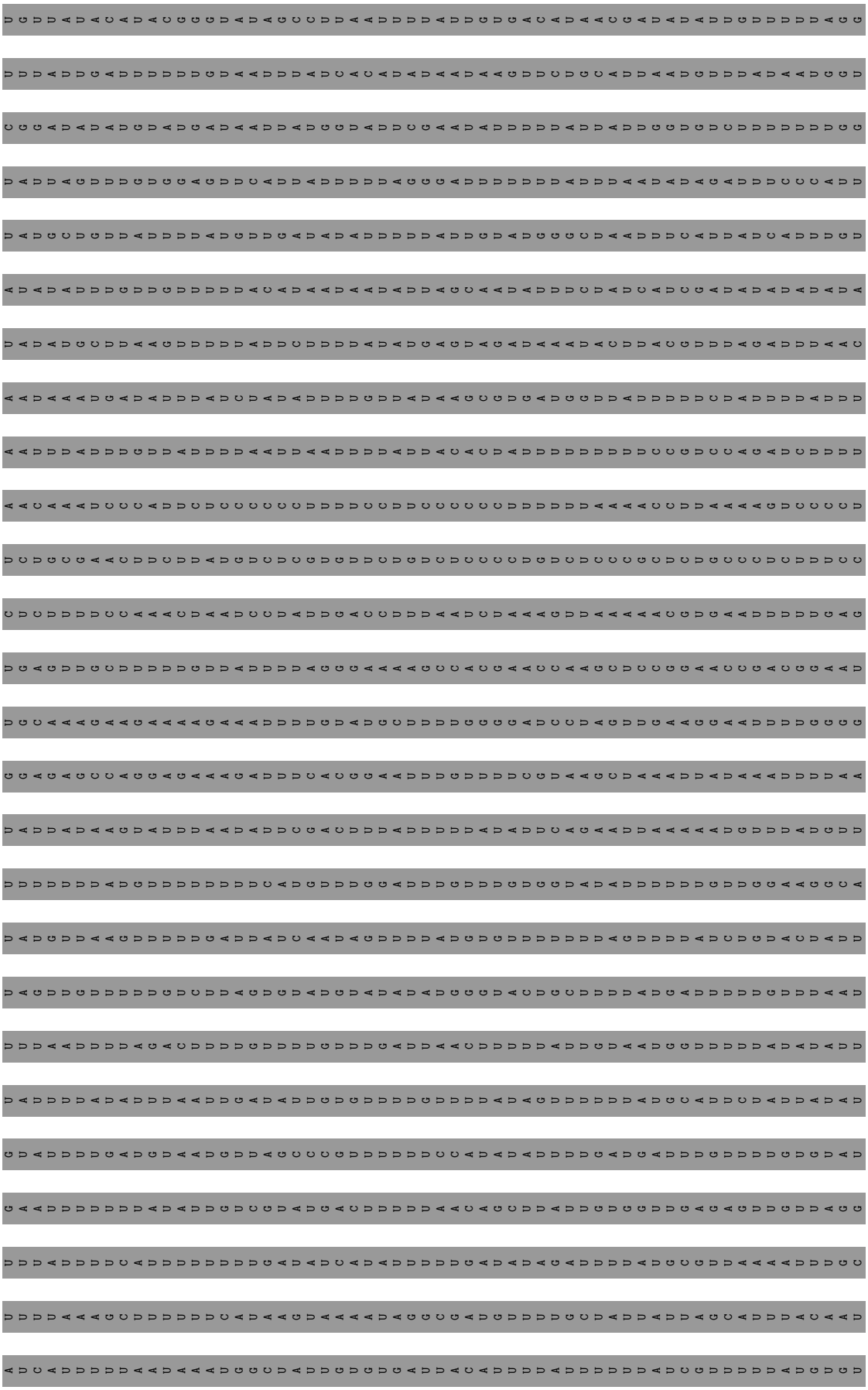


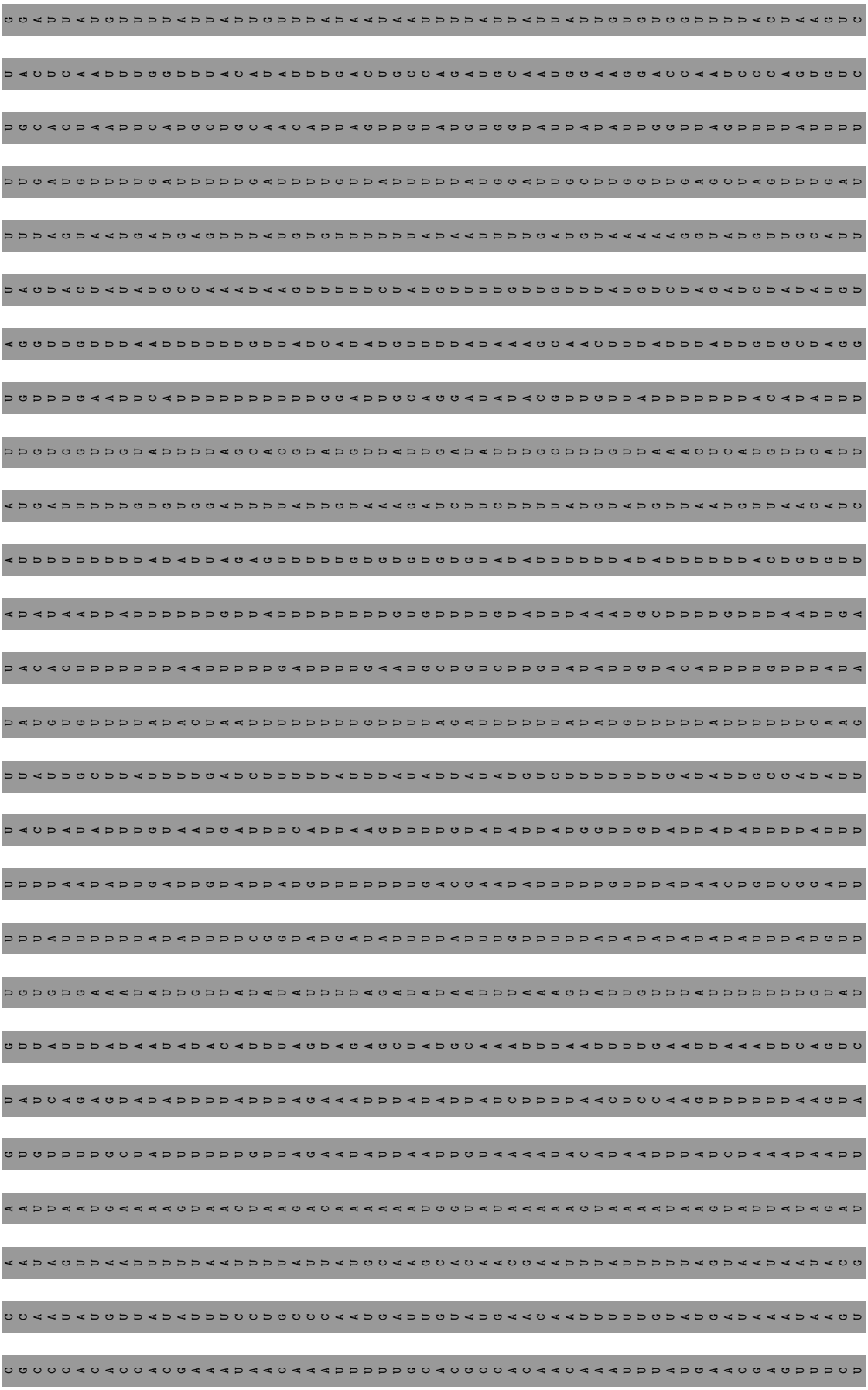


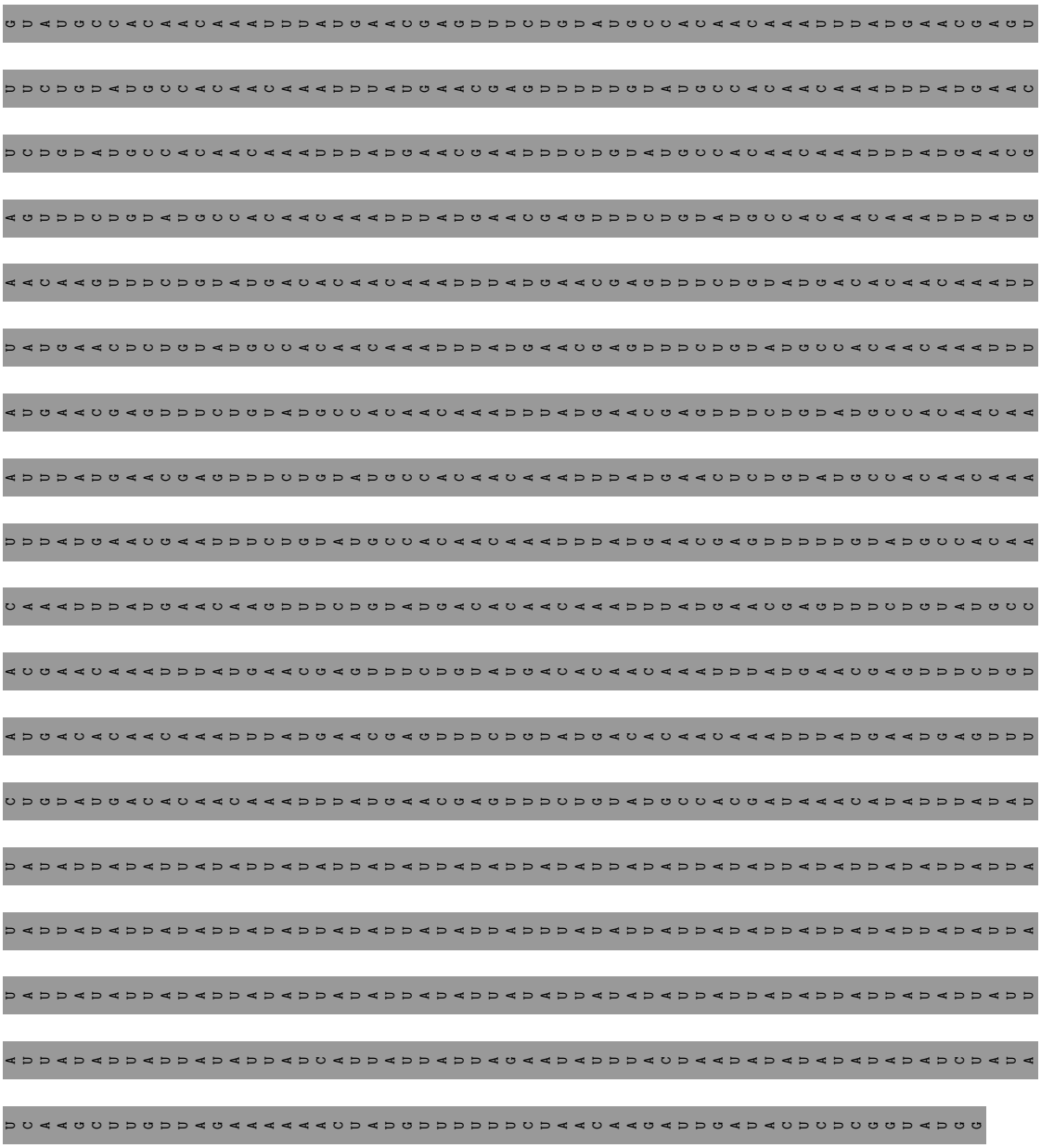






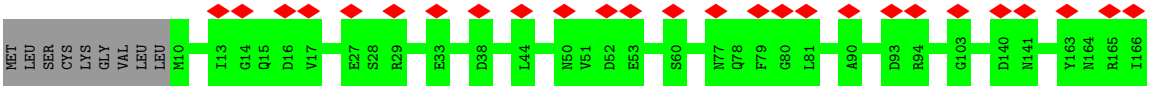






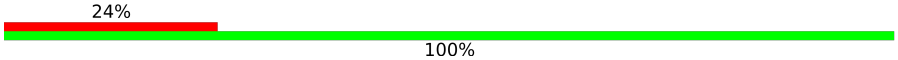
• Molecule 2: uS14m

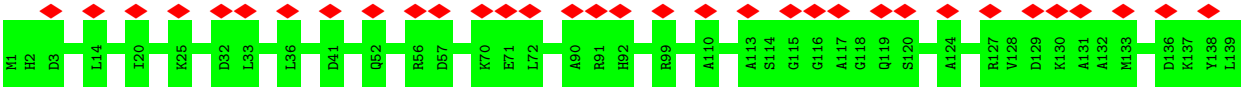
Chain h:



• Molecule 3: mS69

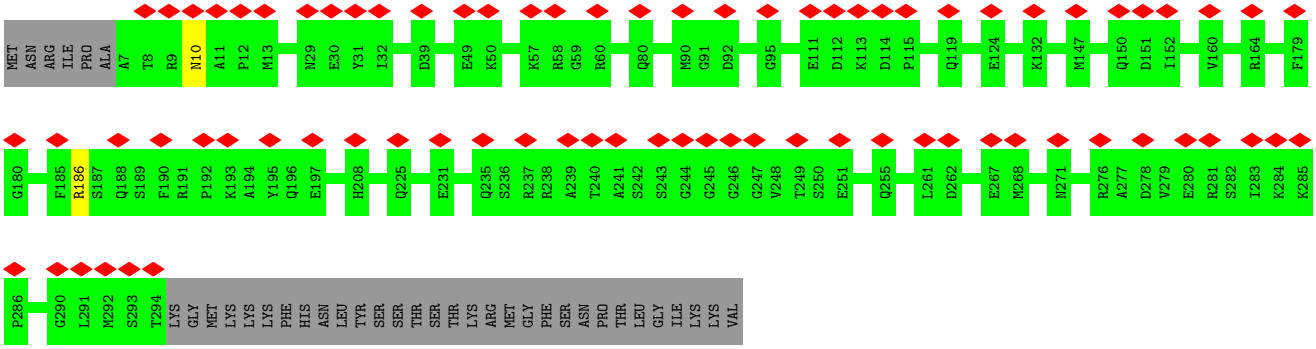
Chain aw:





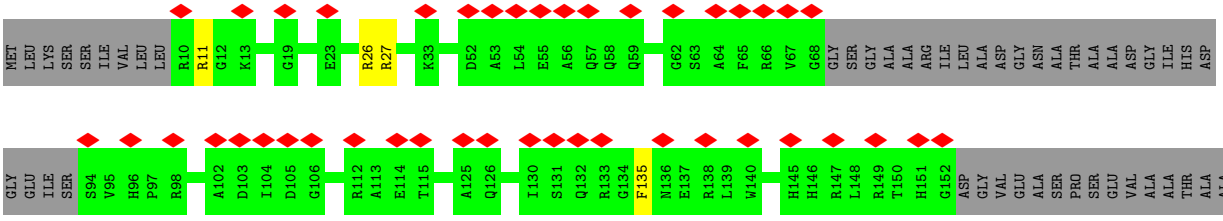
• Molecule 4: bS18m

Chain m:



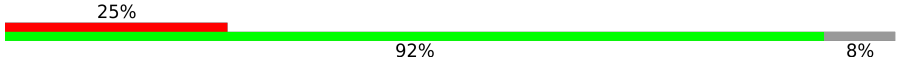
• Molecule 5: uS11m

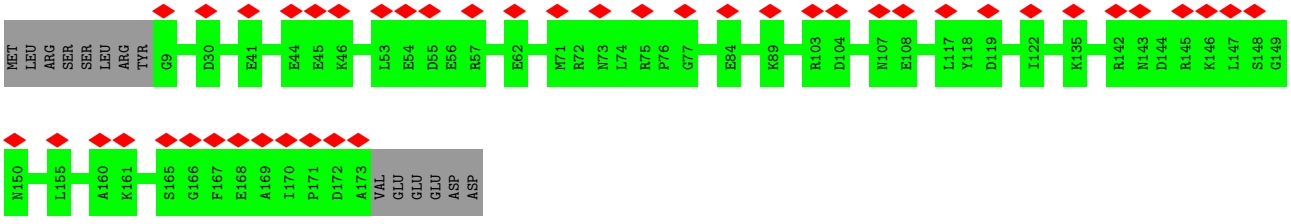
Chain f:



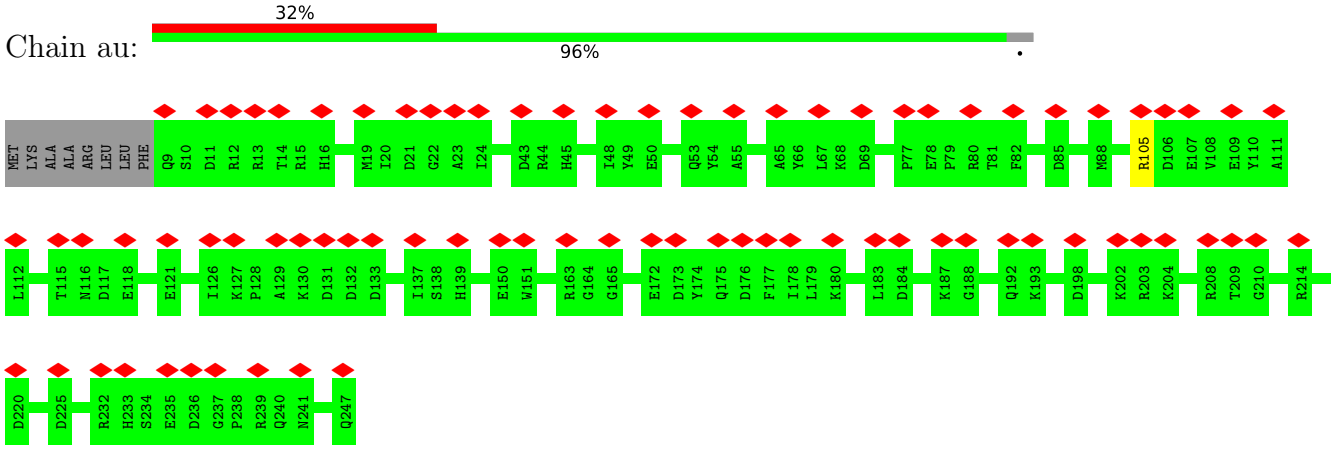
• Molecule 6: mS33

Chain s:

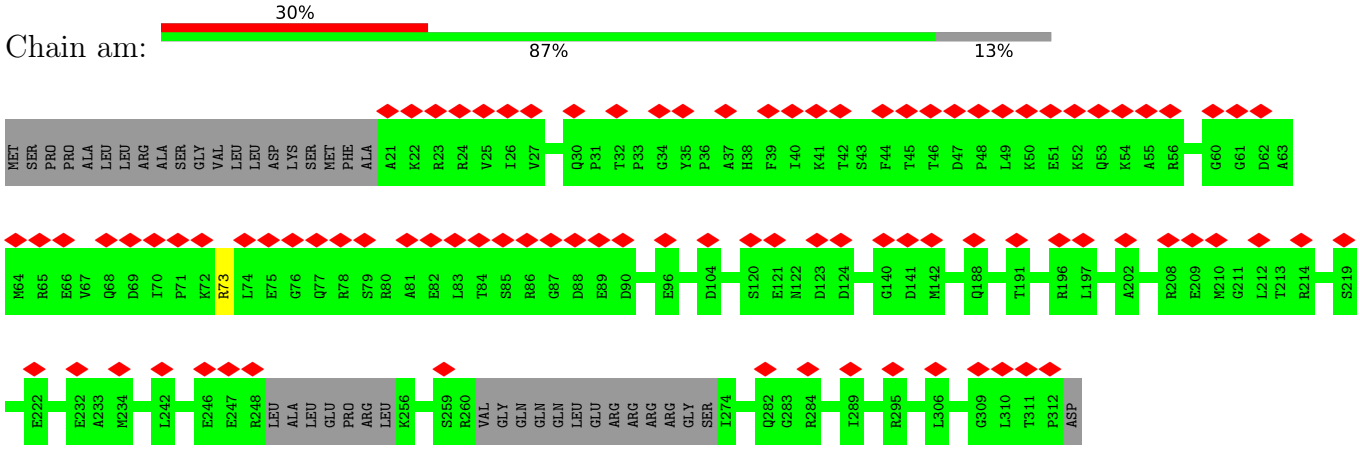




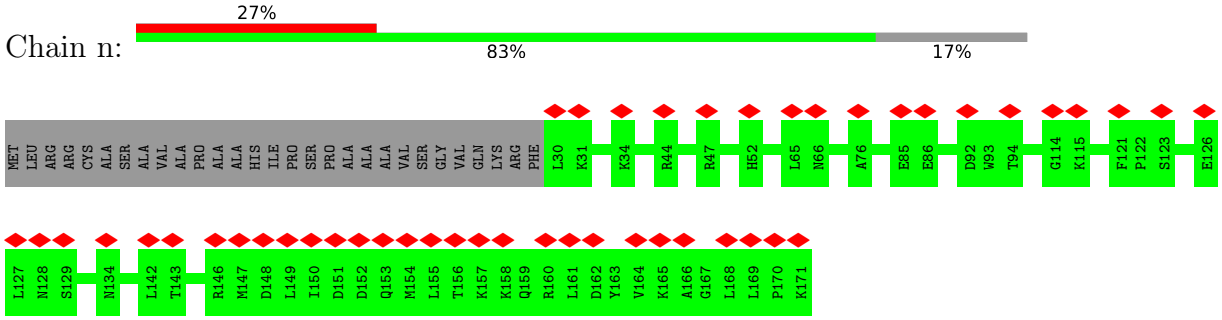
• Molecule 7: Rhodanese domain-containing protein



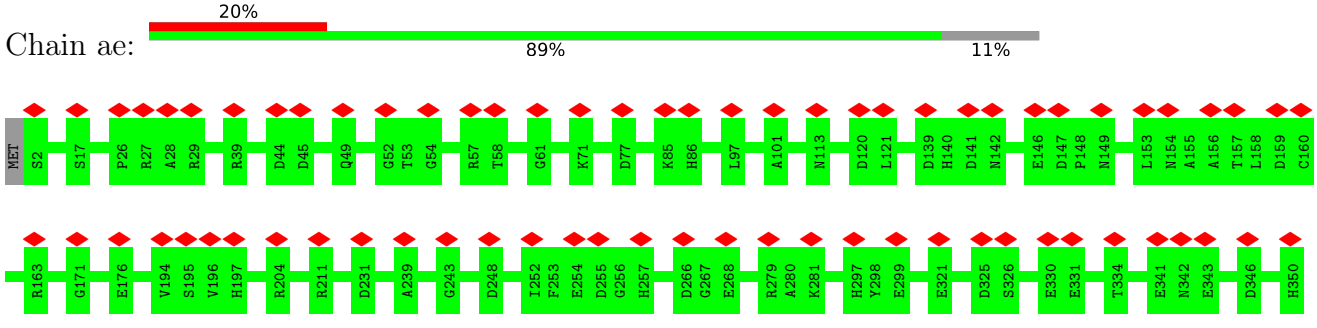
• Molecule 8: mS59

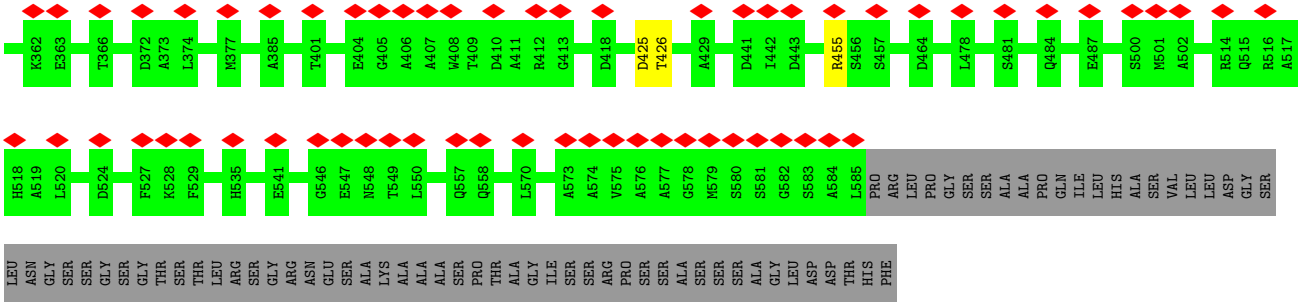


• Molecule 9: uS19m

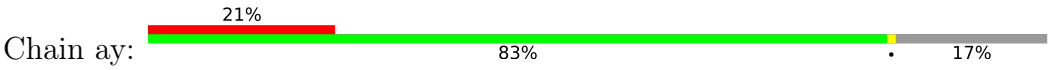


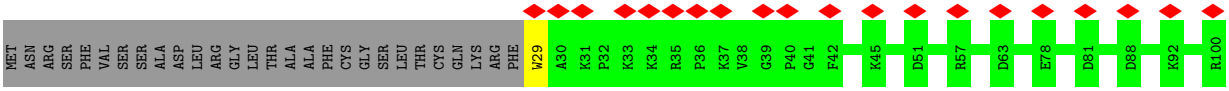
• Molecule 10: mS53

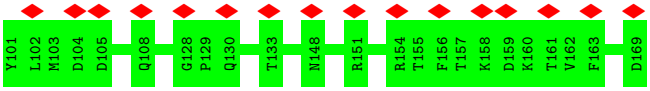




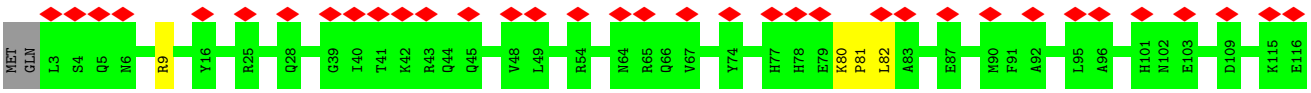
• Molecule 11: mS71

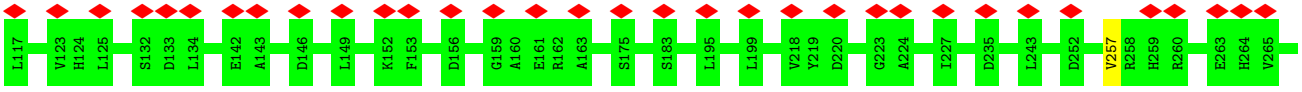


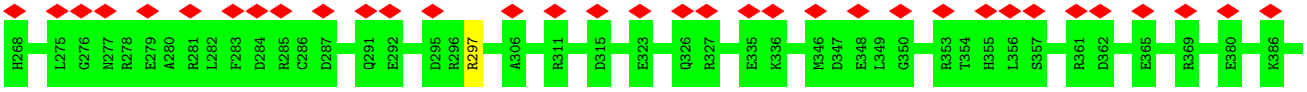


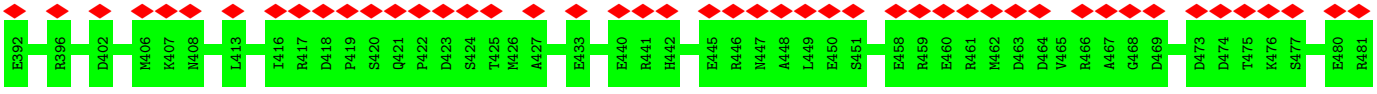


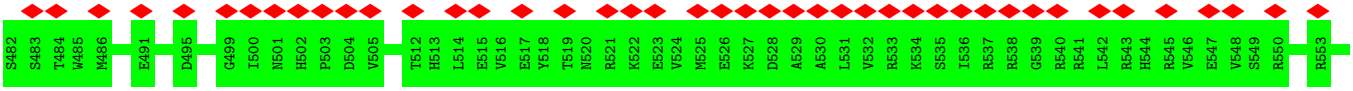
• Molecule 12: mS55

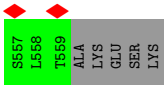




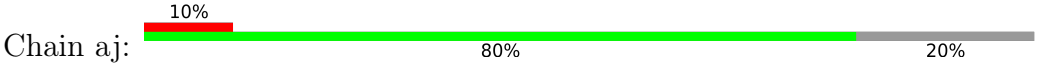


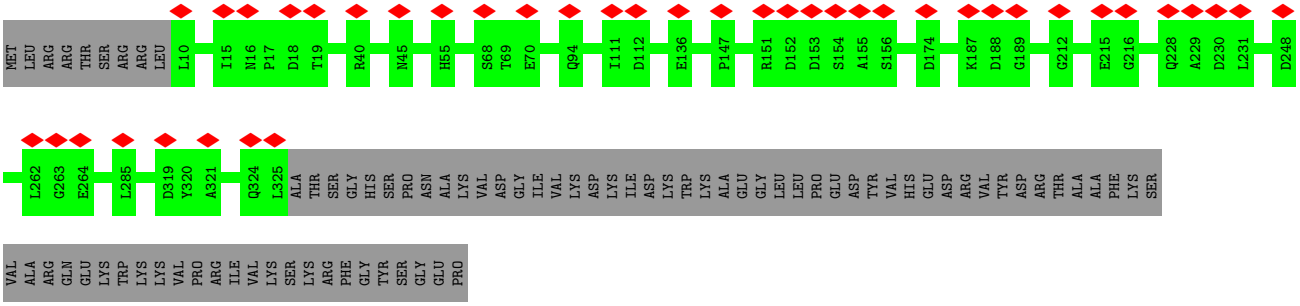






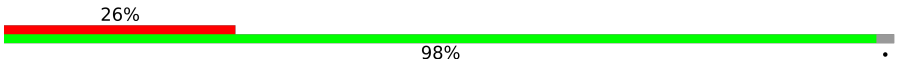
• Molecule 13: mS57





- Molecule 14: uS10m

Chain e:

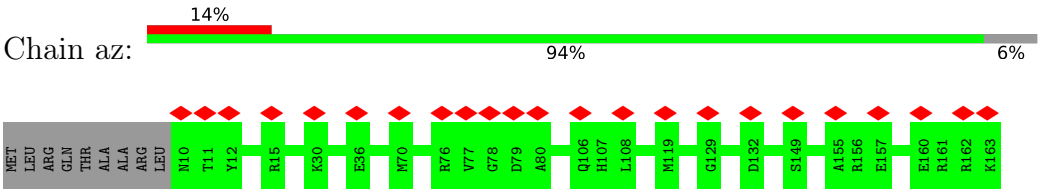


- Molecule 15: uS9m

Chain d:

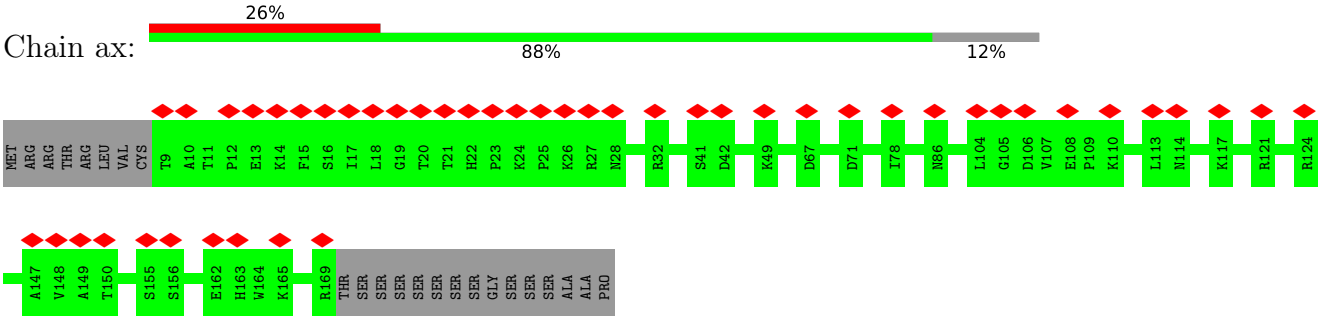
• Molecule 16: mS72

Chain az:



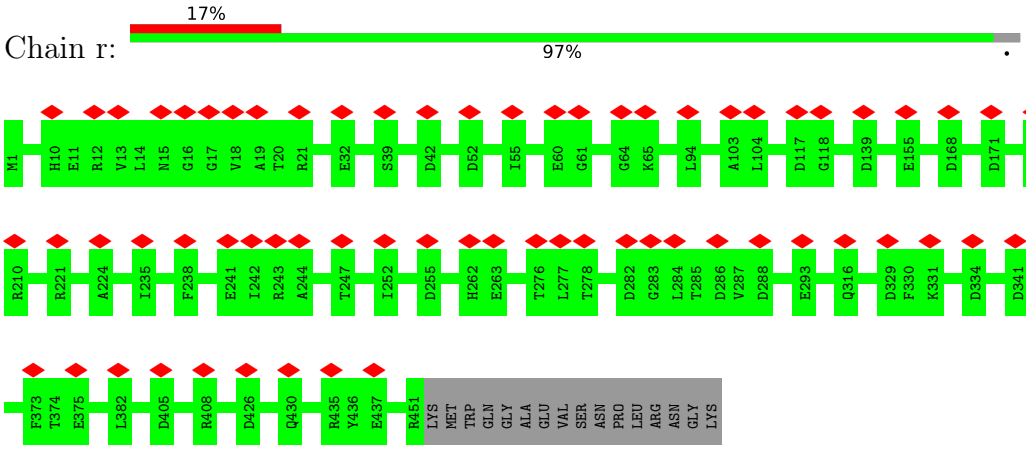
• Molecule 17: mS70

Chain ax:



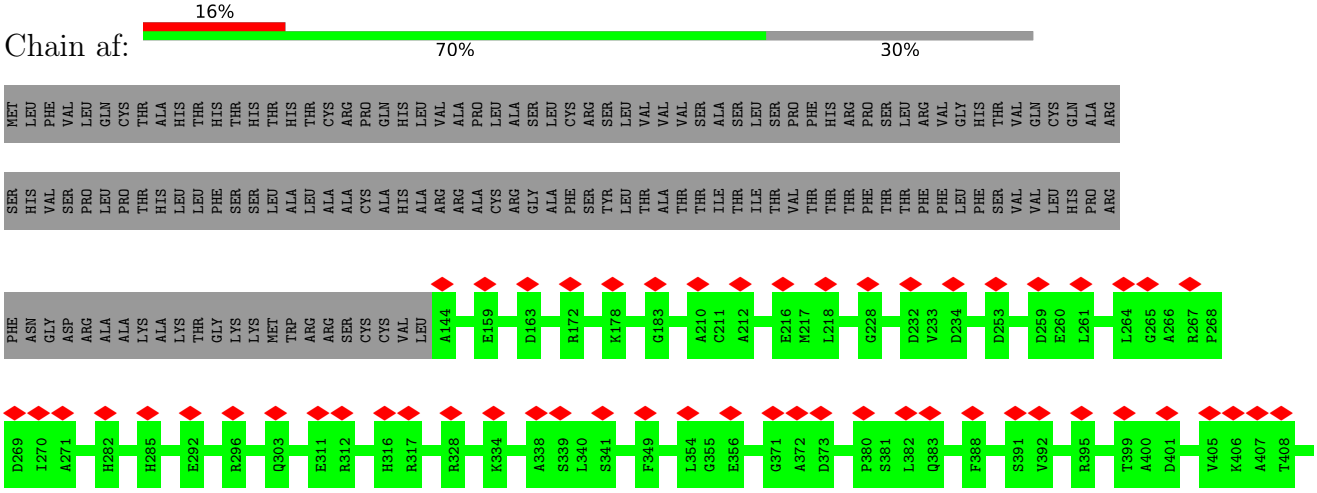
• Molecule 18: mS29

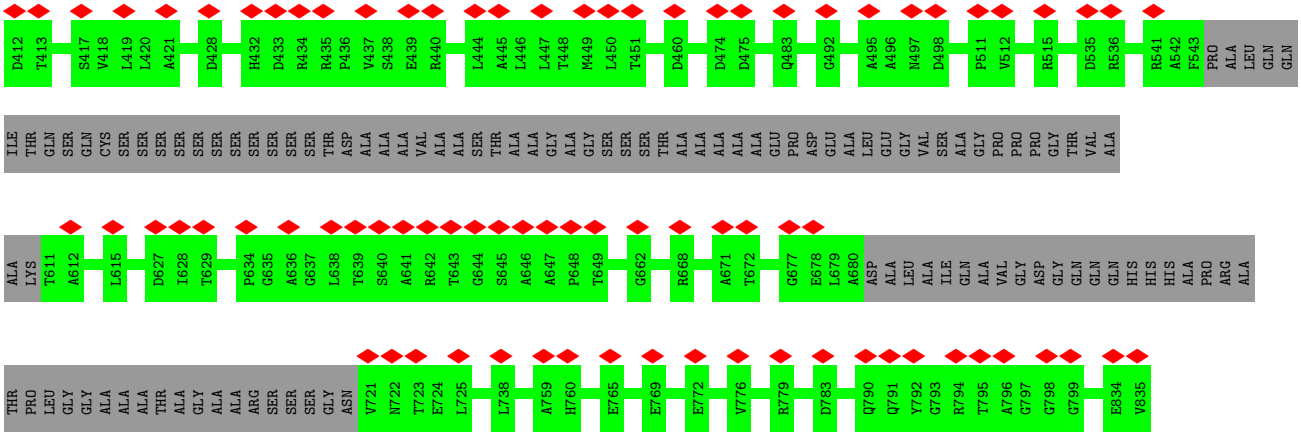
Chain r:



• Molecule 19: Excreted/secreted protein 15

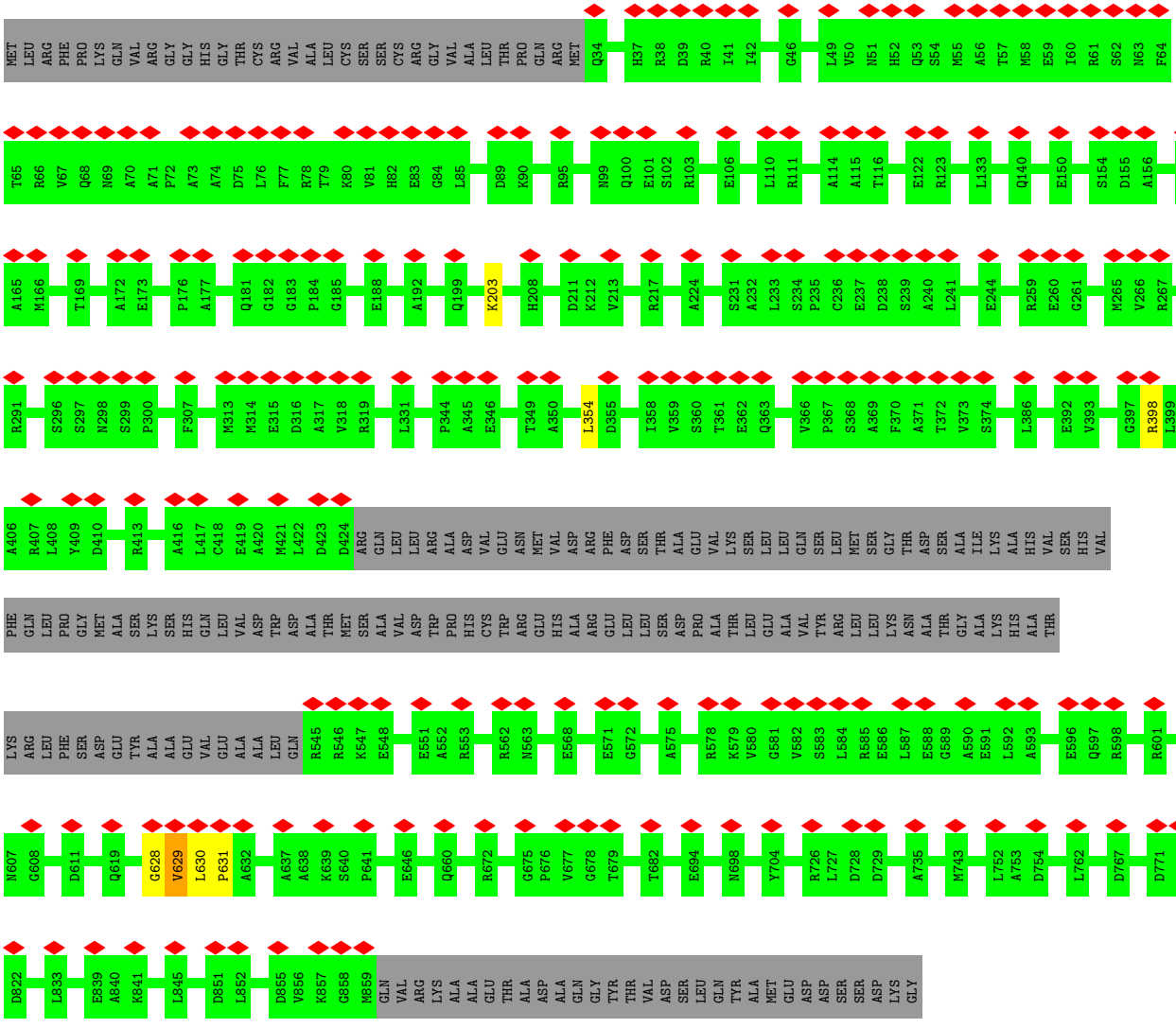
Chain af:





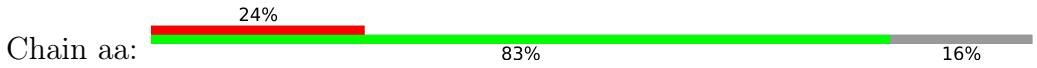
• Molecule 20: mS35

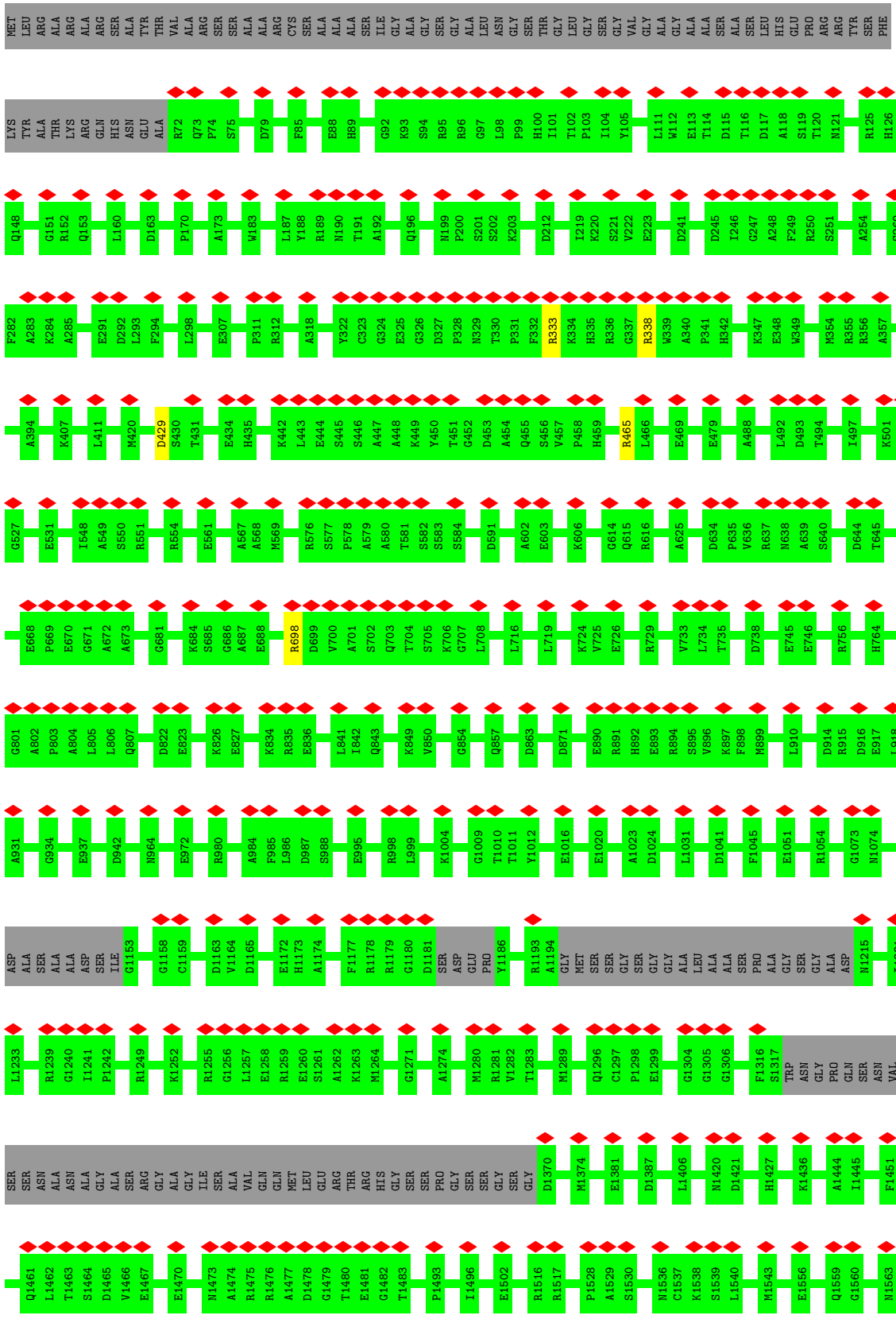
Chain u:

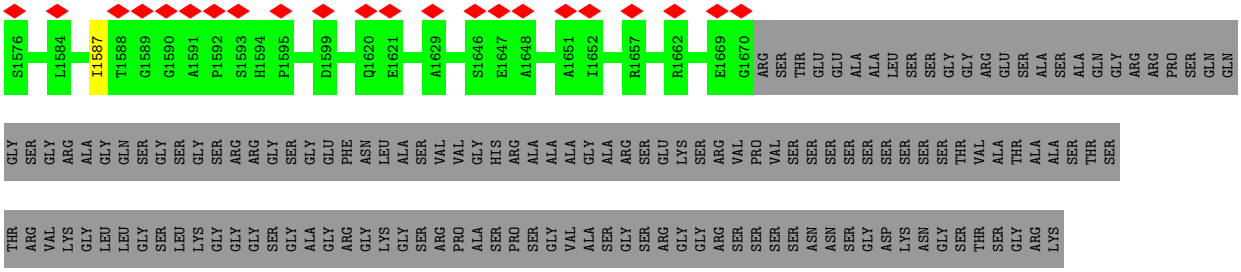


• Molecule 21: mS48

Chain aa:

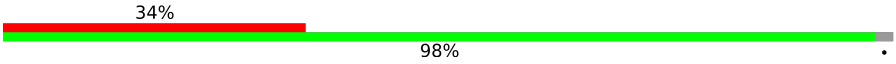

24%
83%
16%

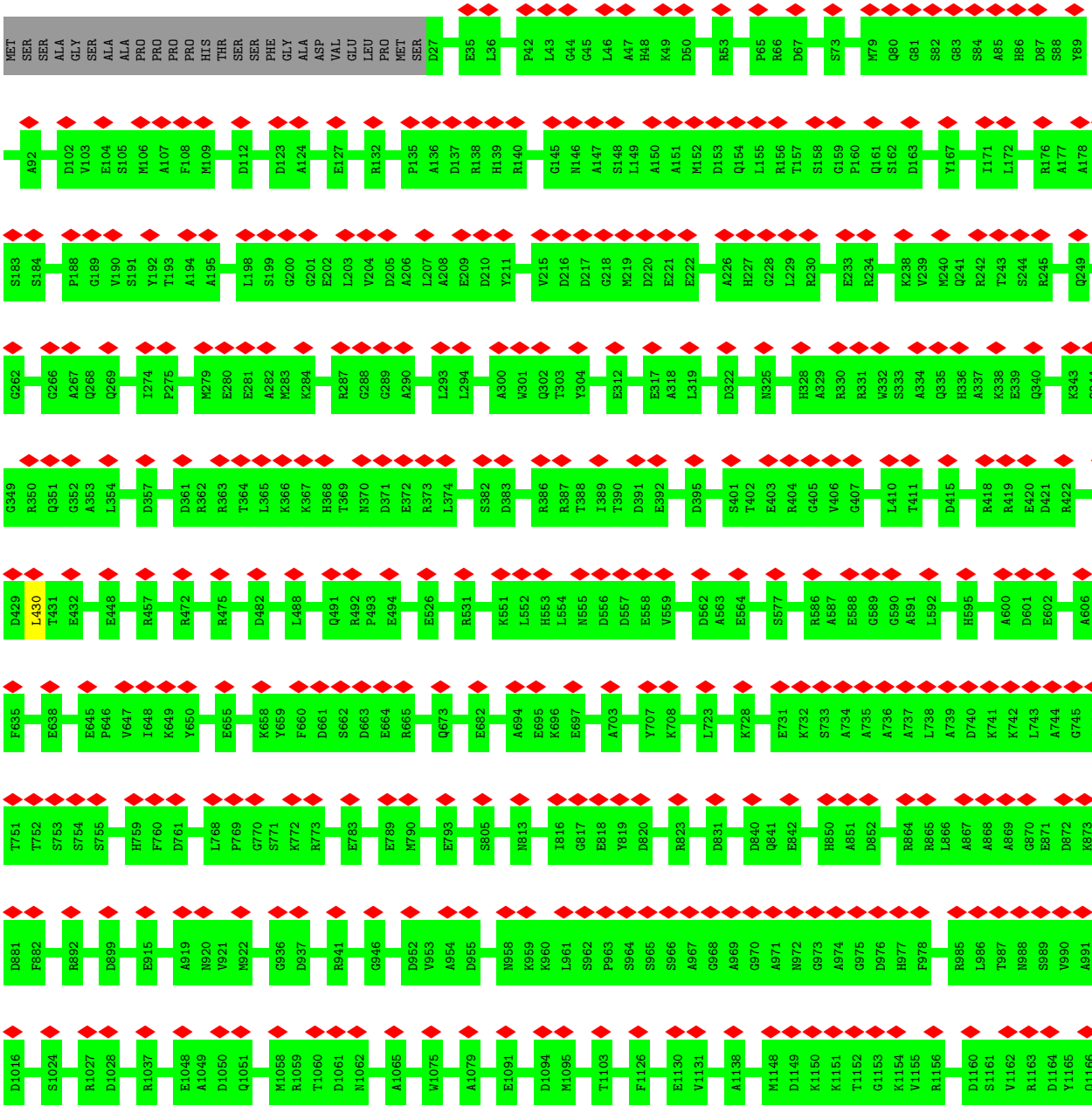

MET LEU ARG ALA ARG ALA ARG SER ALA TYR THR VAL ALA ARG SER SER ALA ALA ALA ARG CYS SER ALA ALA ALA SER ILE GLY ALA GLY SER GLY ALA LEU ASN GLY SER THR GLY LEU GLY SER GLY VAL GLY ALA GLY ALA ALA SER ALA SER LEU HIS GLU PRO ARG ARG TYR SER PHE
LYS TYR ALA THR LYS ARG GLN HIS ASN GLU ALA R72 Q73 P74 S75 D79 F85 E88 H89 G92 K93 S94 R95 R96 G97 L98 P99 H100 I101 T102 P103 I104 Y105 L111 W112 E113 T114 D115 T116 D117 A118 S119 T120 N121 R125 H126 F129 G143 F144 E145 A146 D147
Q148 G151 R152 Q153 L160 D163 P170 A173 W183 L187 Y188 R189 N190 T191 A192 Q196 N199 P200 S201 S202 K203 D212 I219 K220 S221 V222 E223 D241 D245 I246 G247 A248 F249 R250 S251 A254 S269 S270 F271 D272 F273 R276 Q281
F282 A283 K284 A285 E291 D292 L293 F294 L298 E307 P311 R312 A318 Y322 C323 G324 E325 G326 D327 P328 N329 T330 P331 F332 R333 K334 H335 R336 G337 R338 W339 A340 P341 H342 K347 E348 W349 M354 R355 R356 A357 E366 D367 F370 G371 T372 T373 A374 K391
A394 K407 L411 M420 D429 S430 T431 E434 H435 K442 L443 E444 S445 S446 A447 A448 K449 Y450 T451 G452 D453 A454 Q455 S456 V457 P458 H459 R465 L466 E469 E479 A488 L492 D493 T494 I497 K501 V502 D503 P504 Q505 T506 F523 L524
G527 E531 I548 A549 S550 R551 R554 E561 A567 A568 M569 R576 S577 P578 A579 A580 T581 S582 S583 S584 D591 A602 E603 K606 G614 Q615 R616 A625 D634 P635 V636 R637 N638 A639 S640 D644 T645 E648 G654 G655 F656 E657 S658 G659 E660
E668 P669 E670 G671 A672 A673 G681 K684 S685 G686 A687 E688 R698 D699 V700 A701 S702 Q703 T704 S705 K706 G707 L708 L716 L719 K724 V725 E726 R729 V733 L734 T735 D738 E745 E746 R756 H764 S771 E772 Y791 K792 D798 A799 D800
G801 A802 P803 A804 L805 L806 Q807 D822 E823 K826 E827 K834 R835 E836 L841 I842 Q843 K849 V850 G854 Q857 D863 D871 E890 R891 H892 E893 R894 S895 V896 K897 F898 M899 L910 D914 R915 D916 E917 L918 E919 E924 A925 E926 E927 I928 S929 D930
A931 G934 E937 D942 N964 E972 R980 A984 F985 L986 D987 S988 E995 R998 L999 K1004 G1009 T1010 T1011 Y1012 E1016 E1020 A1023 D1024 L1031 D1041 F1045 E1051 R1054 G1073 N1074 E1100 R1114 D1126 C1143 ALA
ASP ALA SER ALA ALA ASP SER ILE G1153 G1158 C1159 D1163 V1164 D1165 E1172 H1173 A1174 F1177 R1178 R1179 G1180 D1181 SER ASP GLU PRO Y1186 R1193 A1194 GLY MET SER SER GLY SER GLY GLY ALA LEU ALA ALA SER PRO ALA GLY SER GLY ALA ASP N1215 I1221 D1224
L1233 R1239 G1240 I1241 P1242 R1249 K1252 R1255 G1256 L1257 E1258 R1259 E1260 S1261 A1262 K1263 M1264 G1271 A1274 M1280 R1281 V1282 T1283 M1289 Q1296 C1297 P1298 E1299 G1304 G1305 G1306 F1316 S1317 TRP ASN GLY PRO GLN SER ASN VAL SER ALA ALA THR SER ASN SER SER
SER SER ASN ALA ASN ALA GLY ALA SER ARG GLY ALA GLY ILE SER ALA VAL GLN GLN MET LEU GLU ARG THR ARG HIS GLY SER SER PRO GLY SER SER GLY SER GLY D1370 M1374 E1381 D1387 L1406 N1420 D1421 H1427 K1436 A1444 I1445 F1451 T1457 H1458
Q1461 L1462 T1463 S1464 D1465 V1466 E1467 E1470 N1473 A1474 R1475 R1476 A1477 D1478 G1479 T1480 E1481 G1482 T1483 P1493 I1496 E1502 R1516 R1517 P1528 A1529 S1530 N1536 C1537 K1538 S1539 L1540 M1543 E1556 Q1559 G1560 N1563 S1567 S1568 A1569 L1570 F1571 K1572 S1573 I1574 A1575



• Molecule 22: mS49

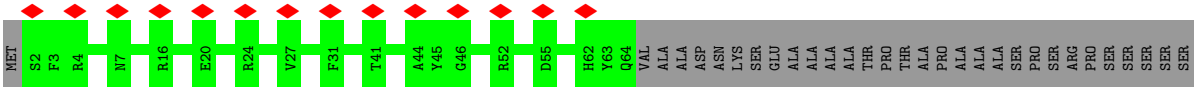
Chain ab:

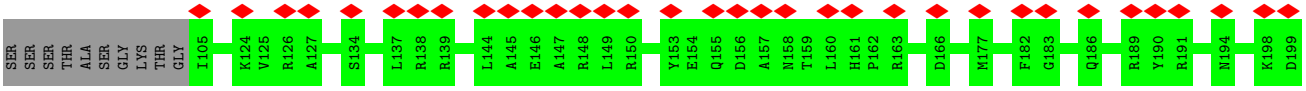


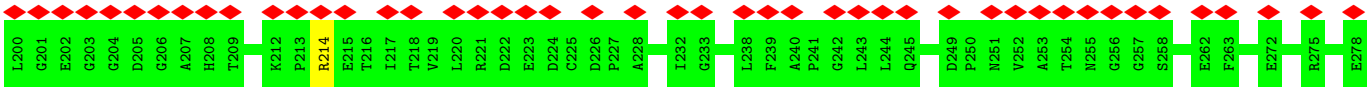


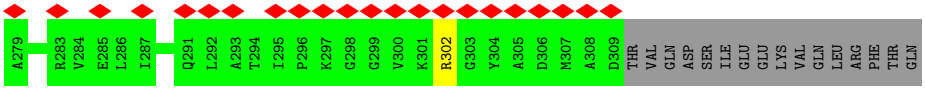
- Molecule 23: mS58

Chain ak:



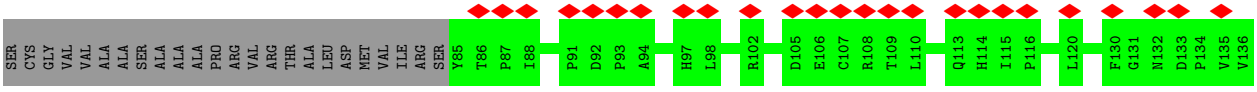


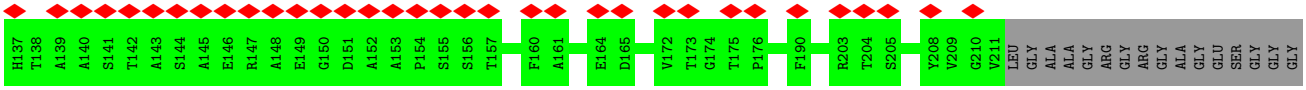


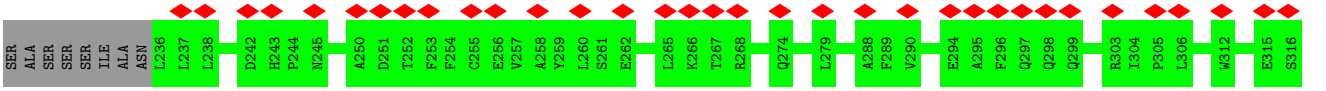


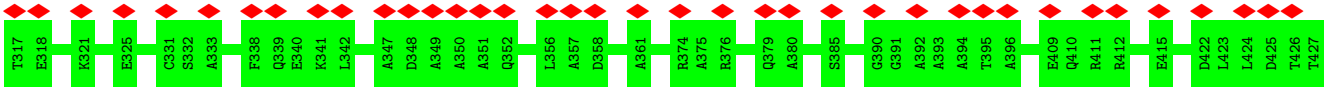
- Molecule 24: mS50

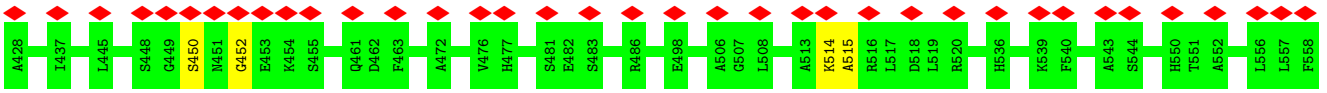
Chain ac:

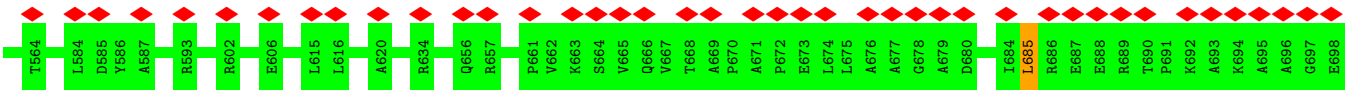


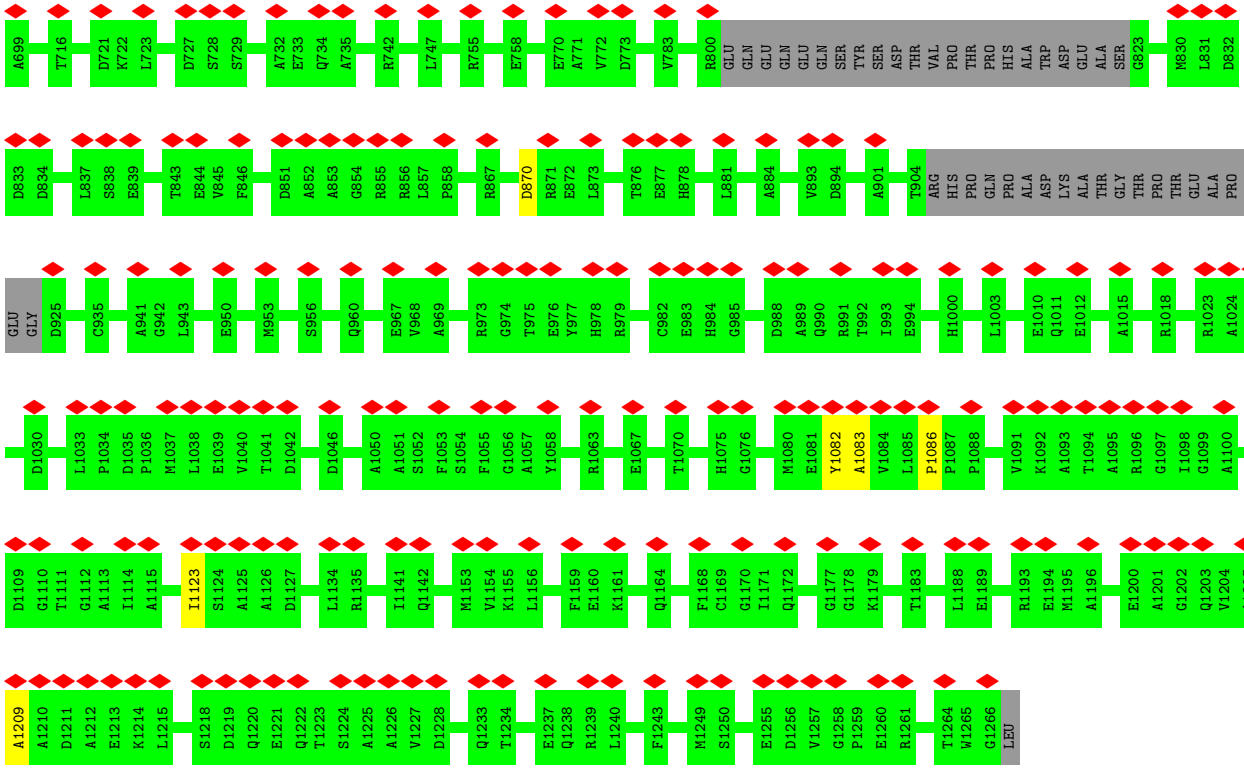






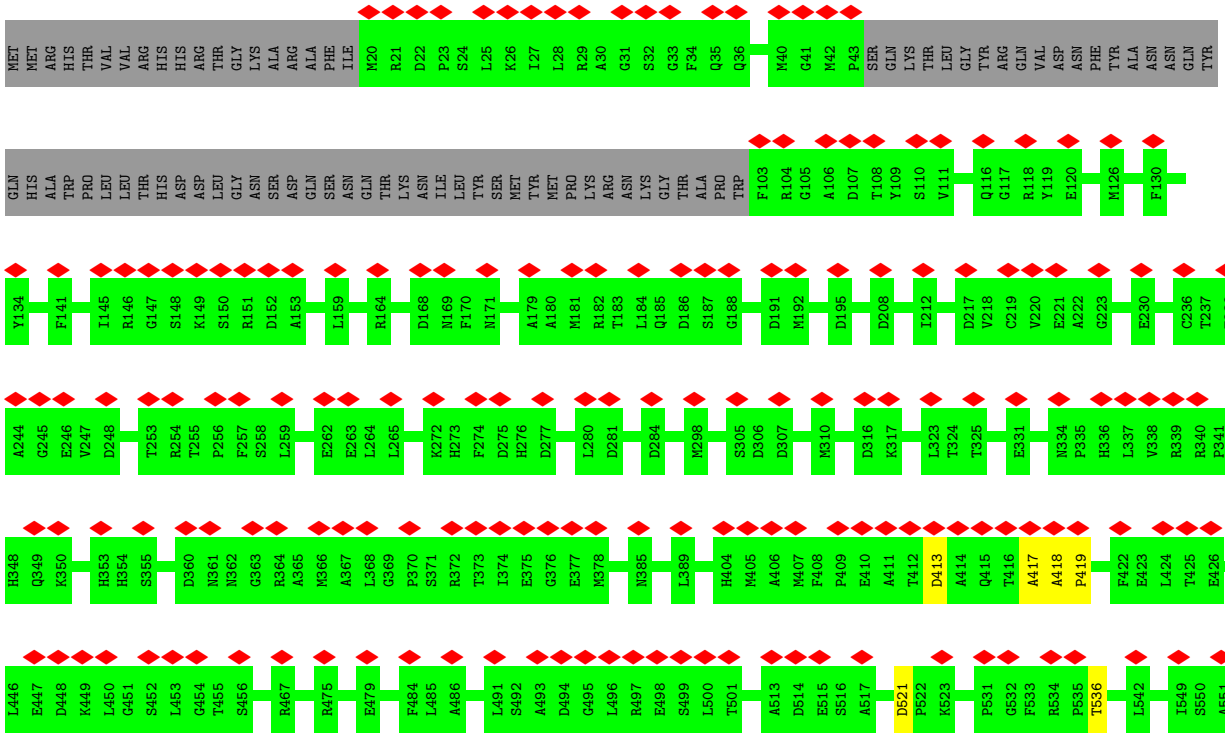


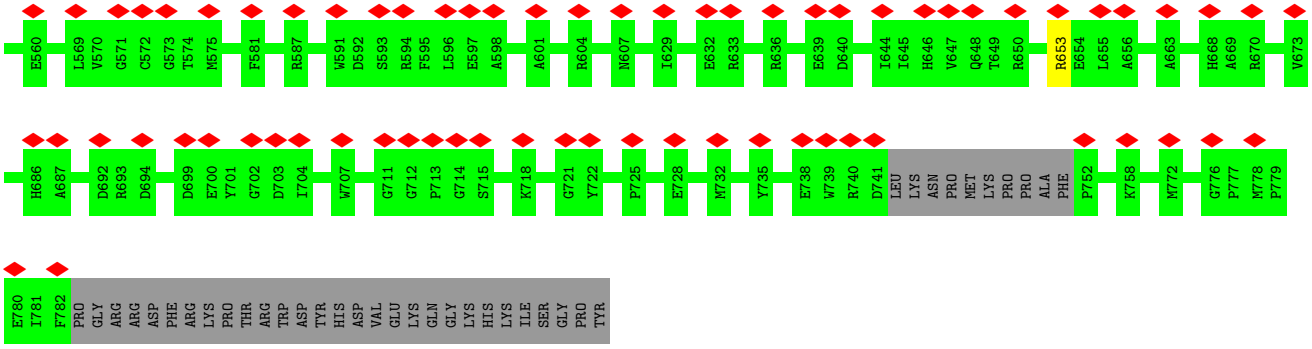




• Molecule 25: mS51

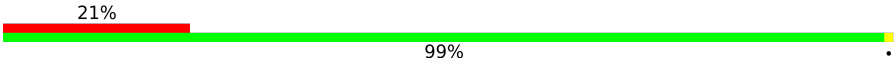
Chain ad:

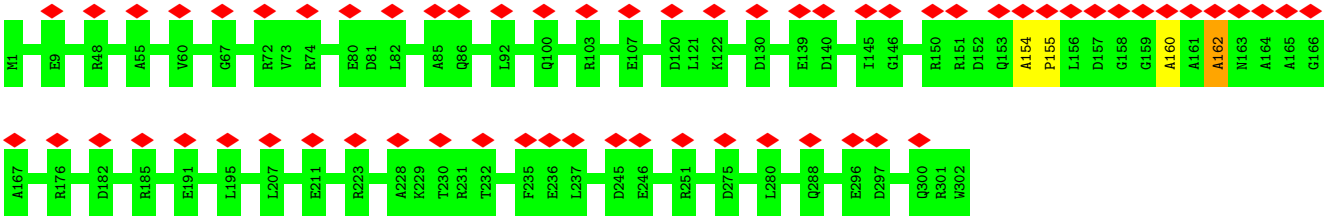




• Molecule 26: mS60

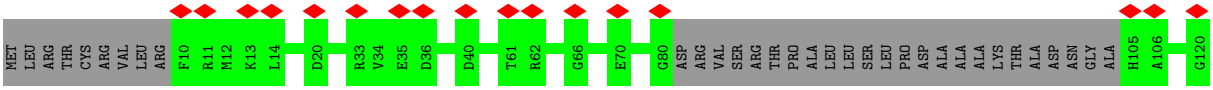
Chain an:

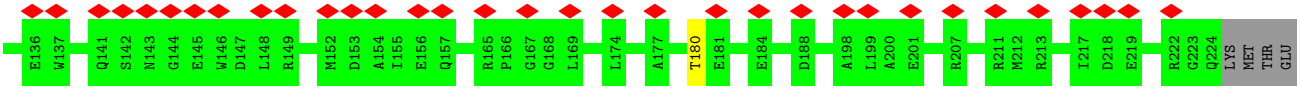




• Molecule 27: mS61

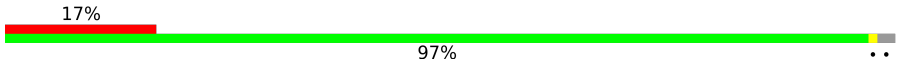
Chain ao:

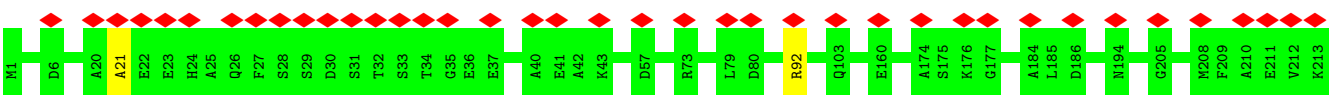




• Molecule 28: mS62

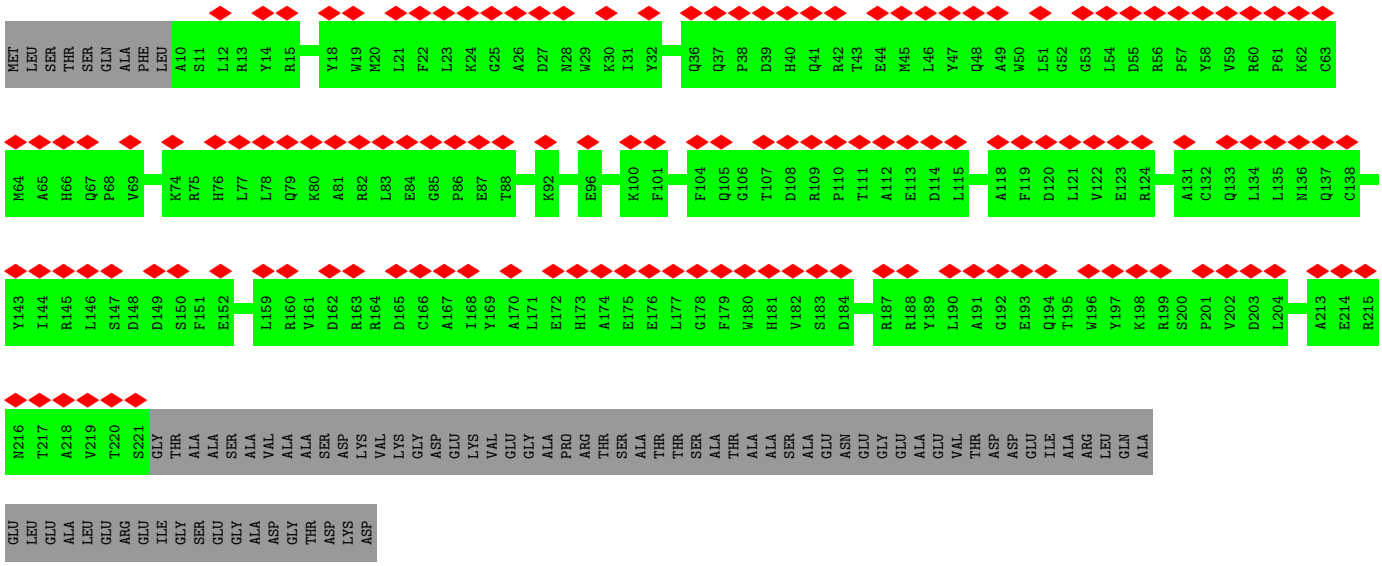
Chain ap:





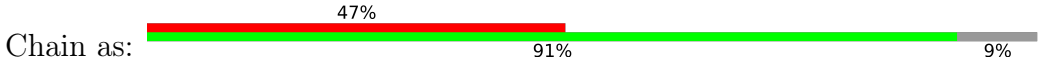
• Molecule 29: mS63

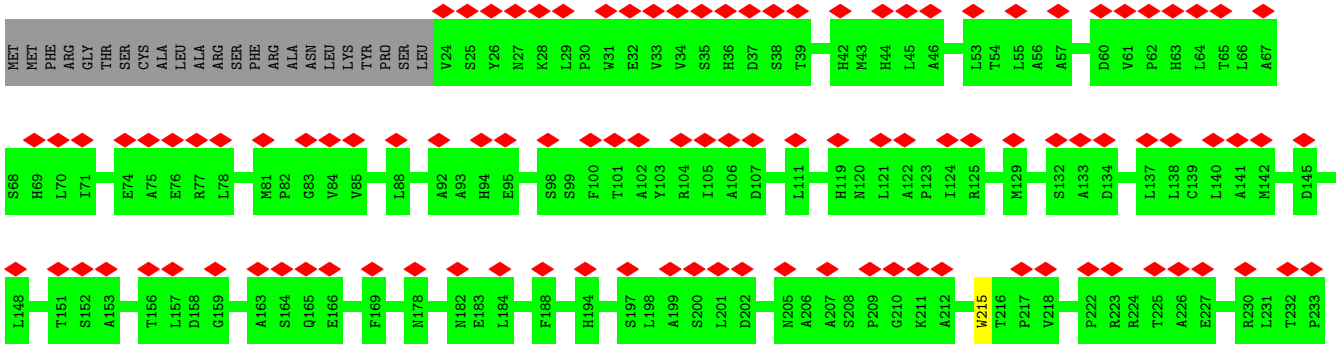
Chain aq:



• Molecule 30: mS65

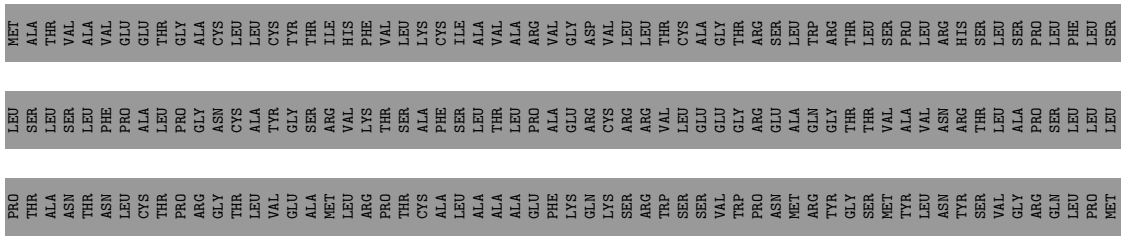
Chain as:

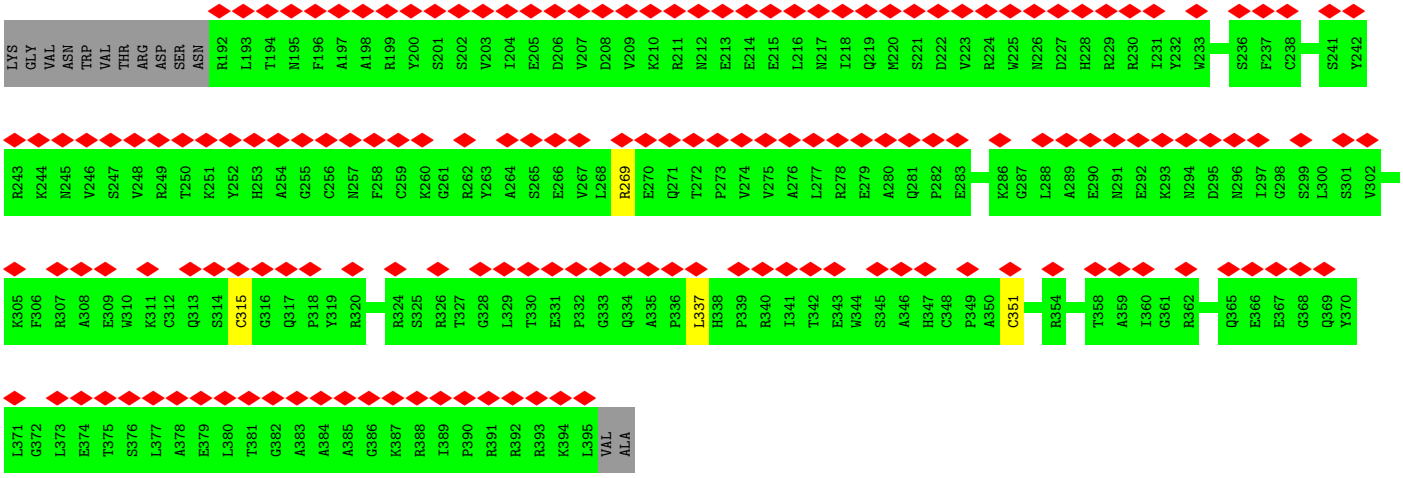




• Molecule 31: mS66

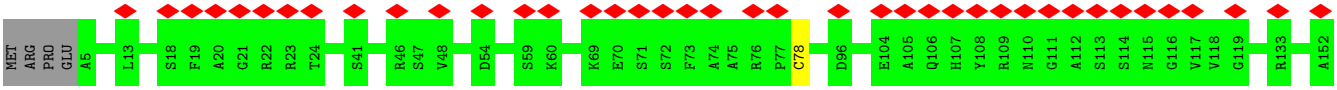
Chain at:

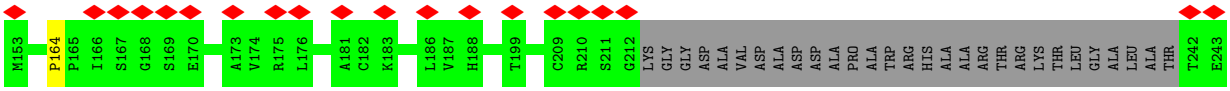


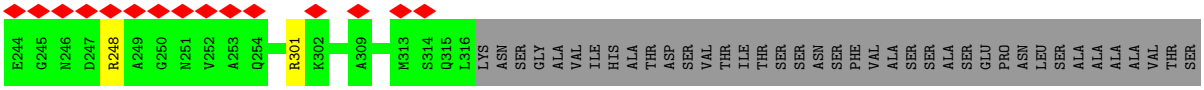


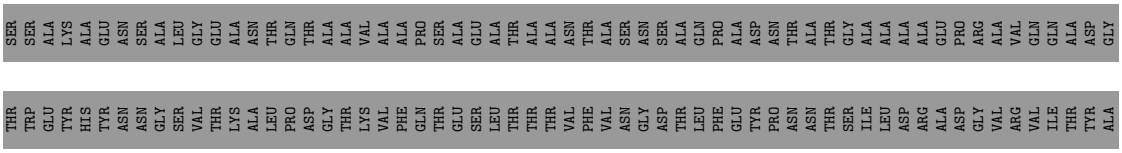
• Molecule 32: mS43

Chain y:



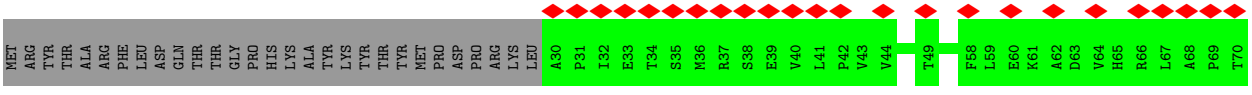


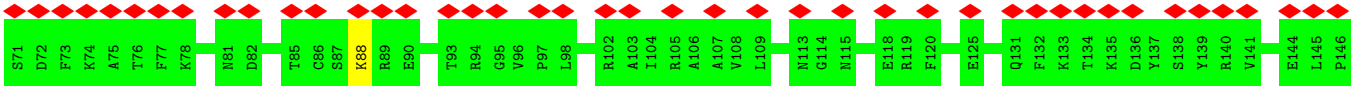


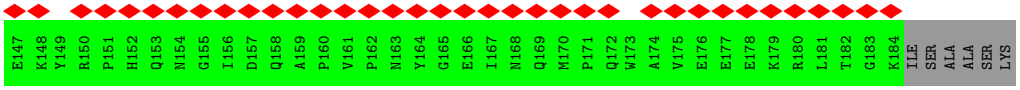


• Molecule 33: Protein FYV4, mitochondrial

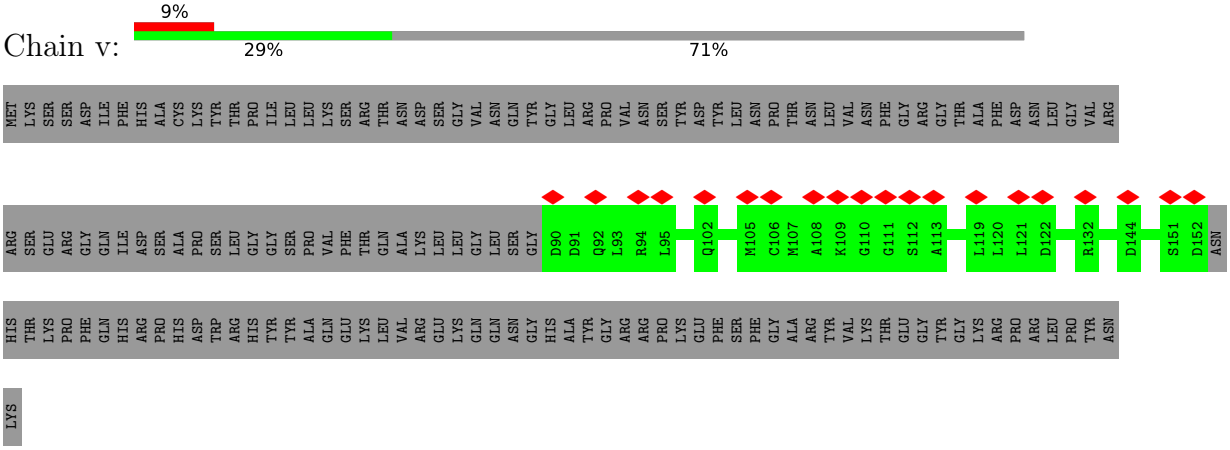
Chain w:



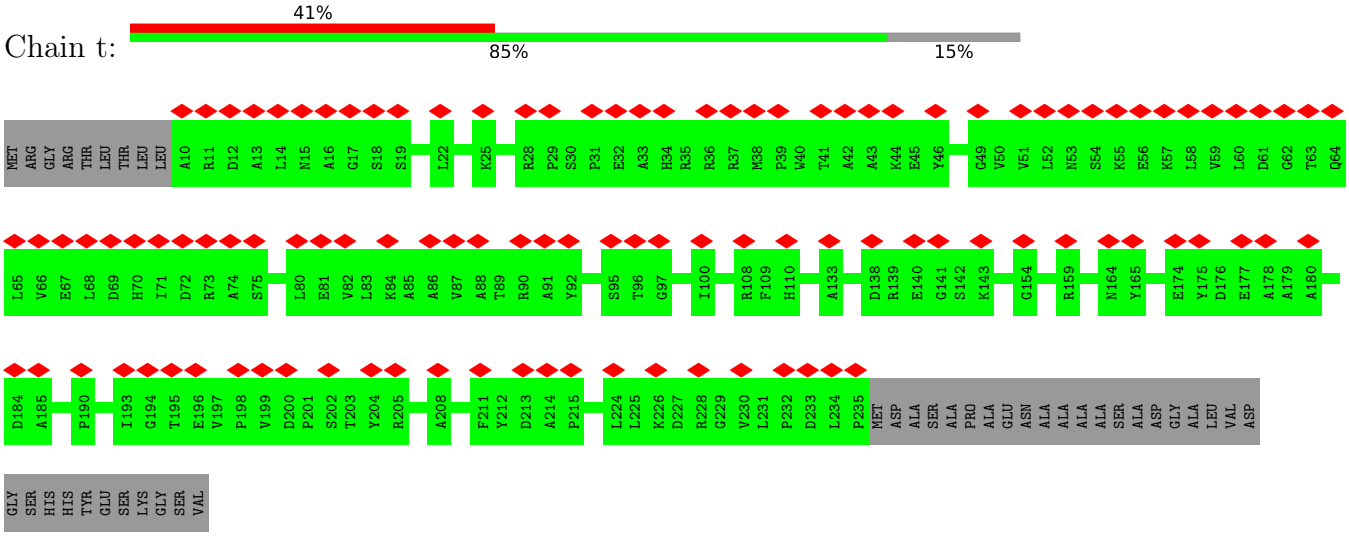




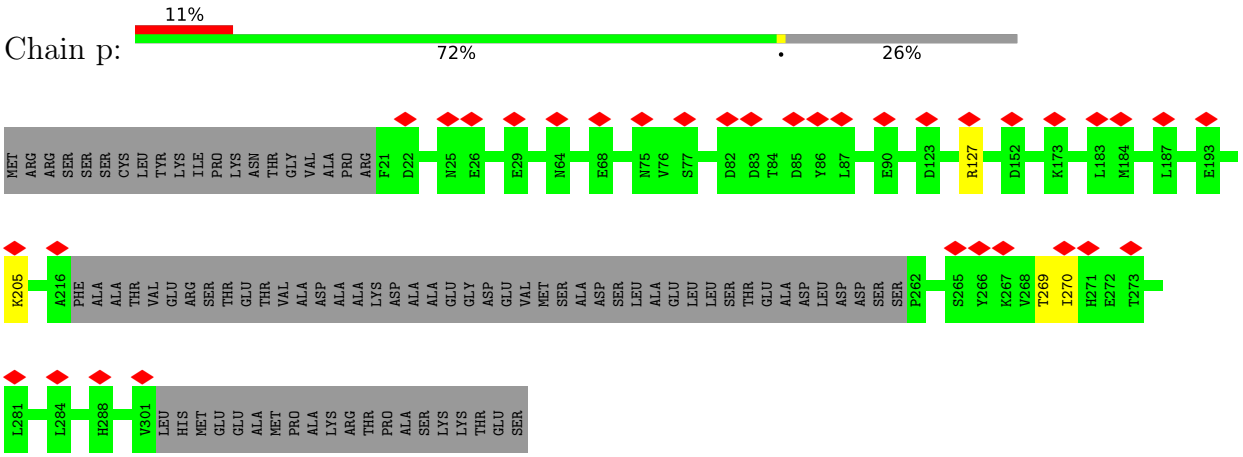
• Molecule 34: mS37



• Molecule 35: mS34

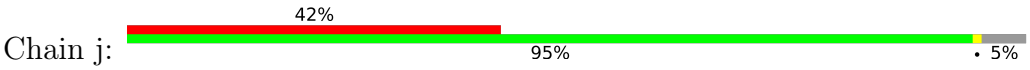


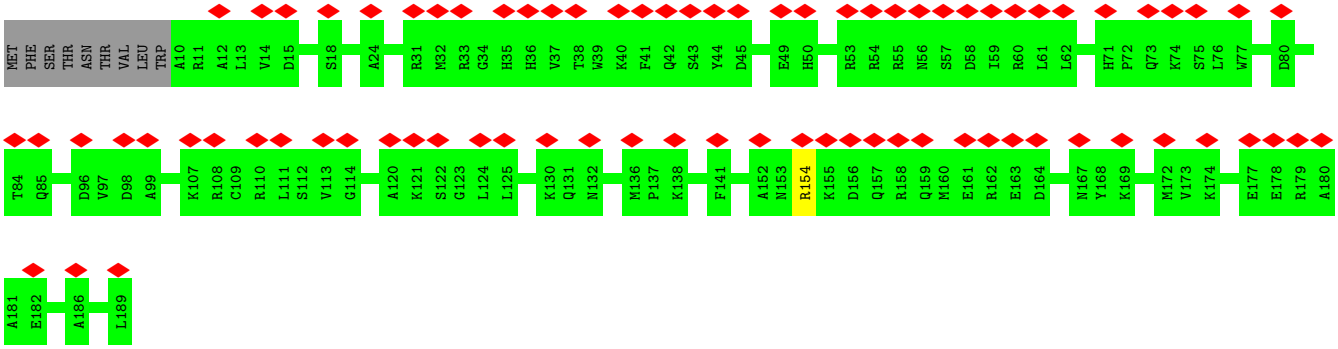
• Molecule 36: mS23



• Molecule 37: bS16m

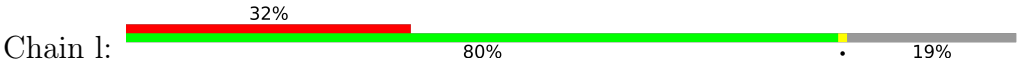
Chain j:

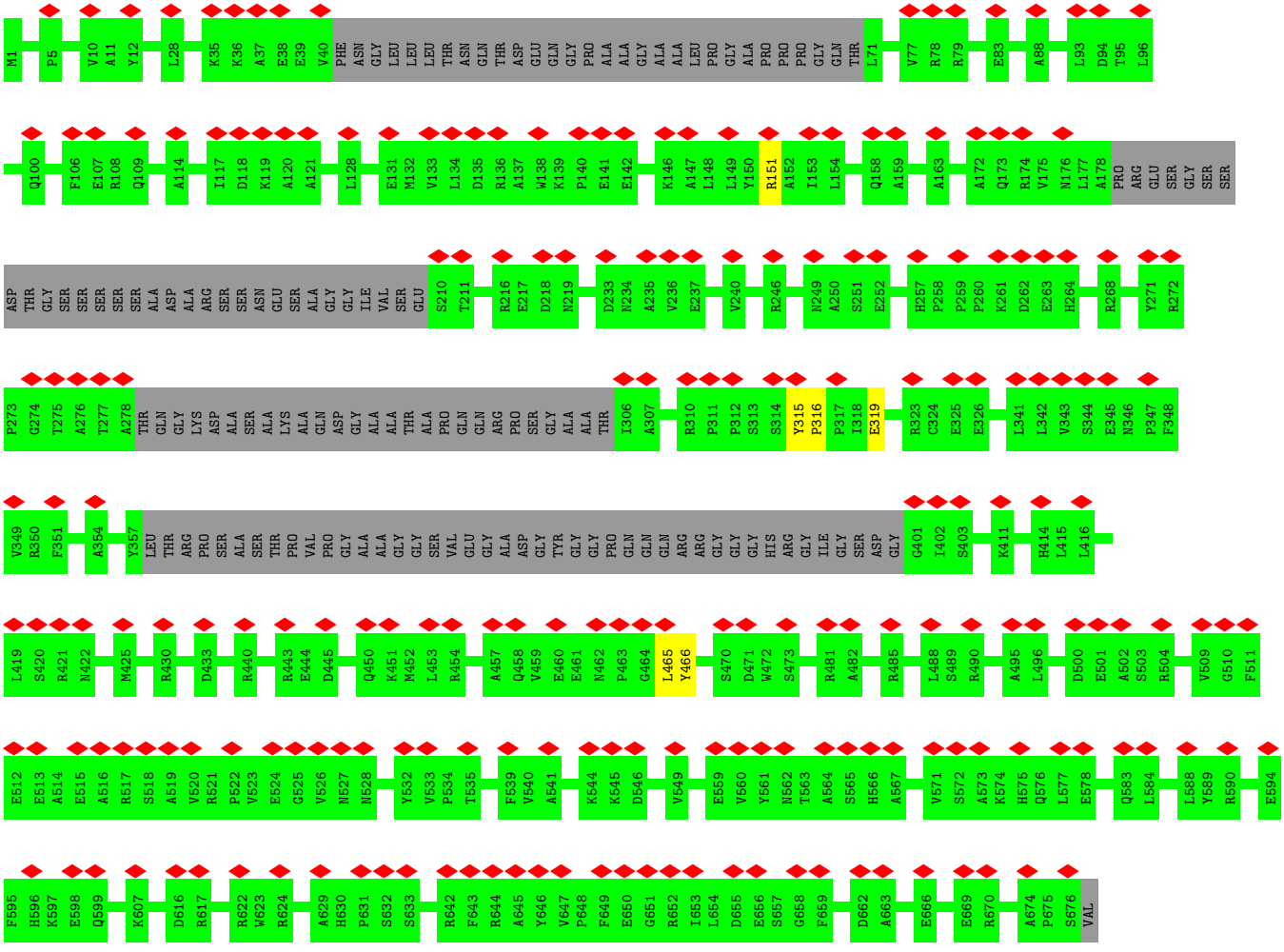




• Molecule 38: mS52

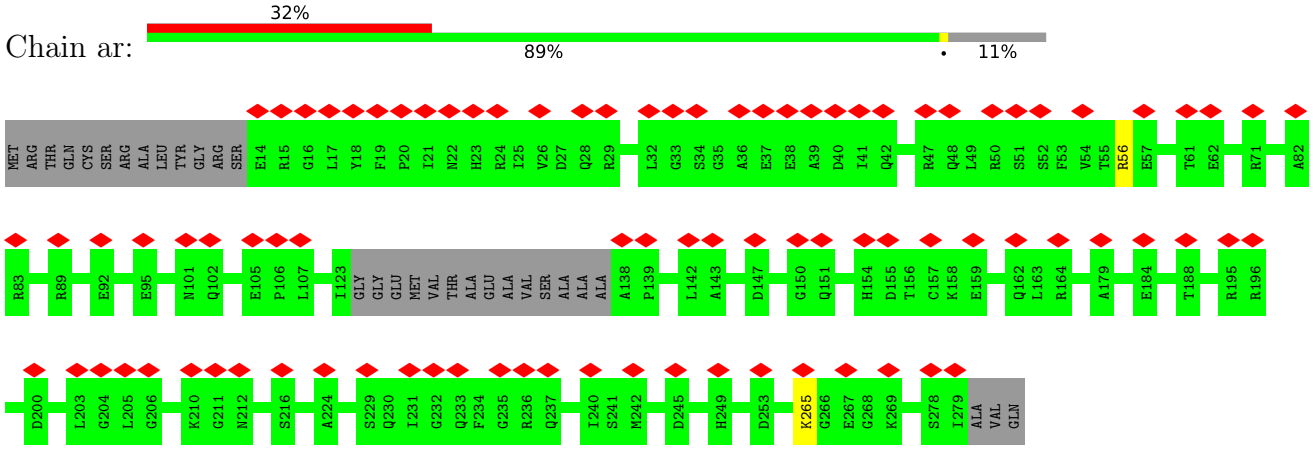
Chain l:





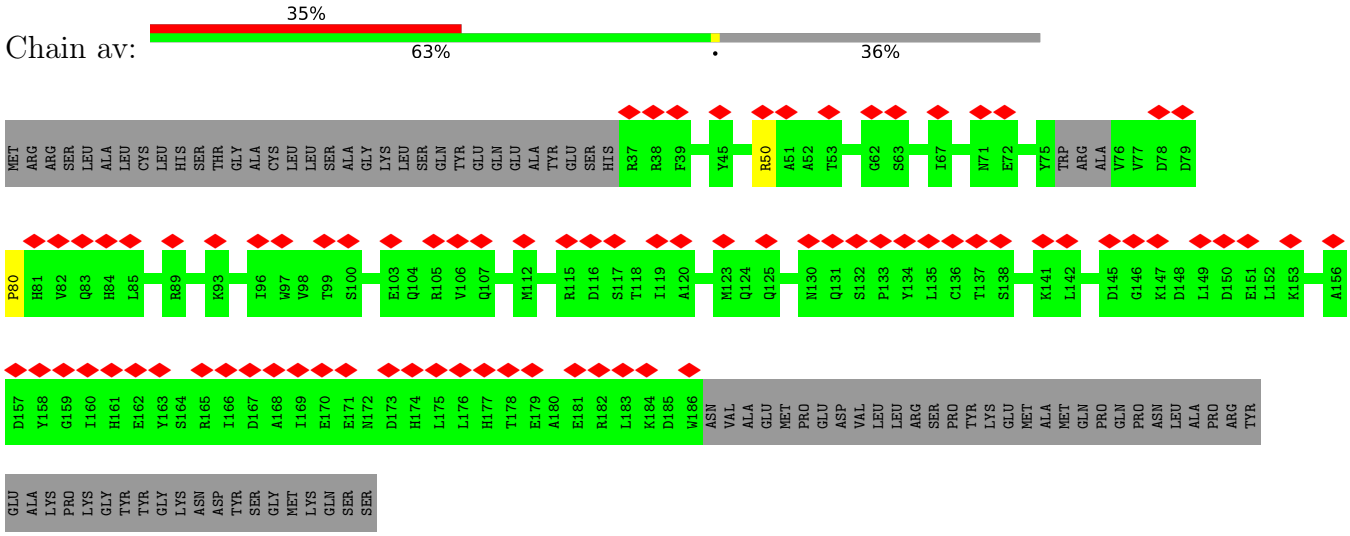
• Molecule 39: AKAP7_NLS domain-containing protein

Chain ar:



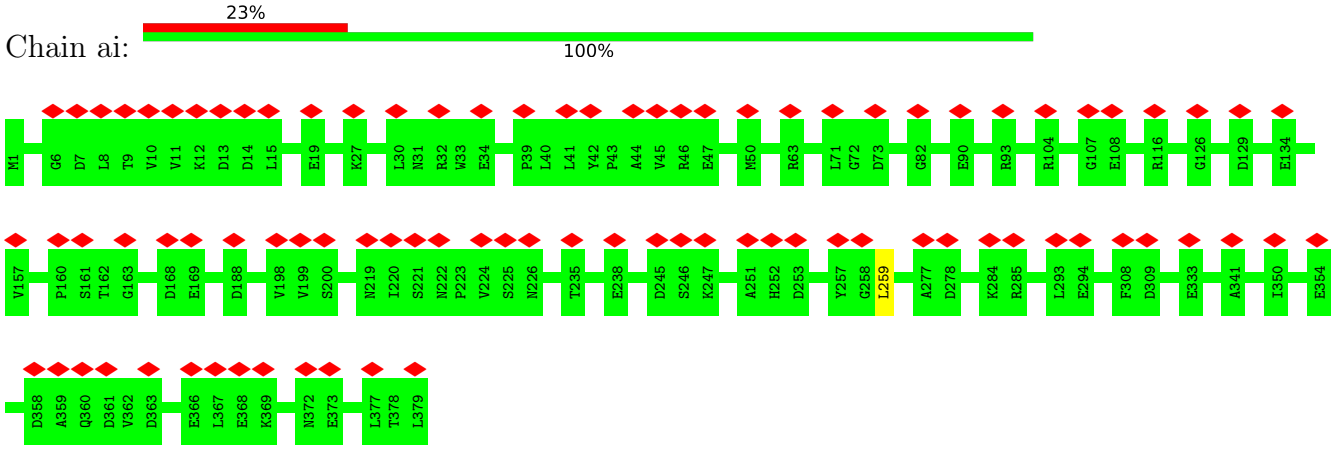
• Molecule 40: Ubiquitin-like domain-containing protein

Chain av:



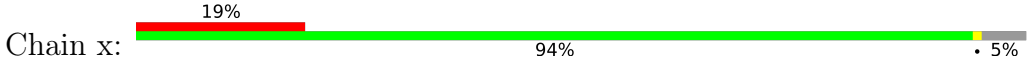
• Molecule 41: mS56

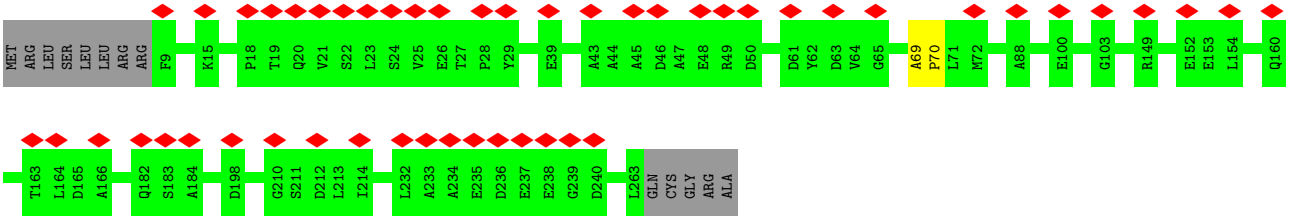
Chain ai:



• Molecule 42: Putative superoxide dismutase

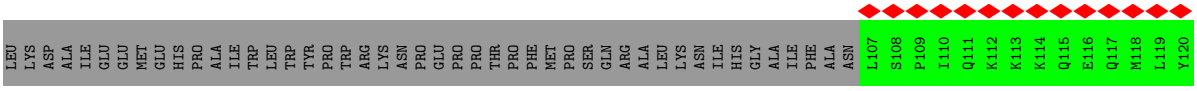
Chain x:

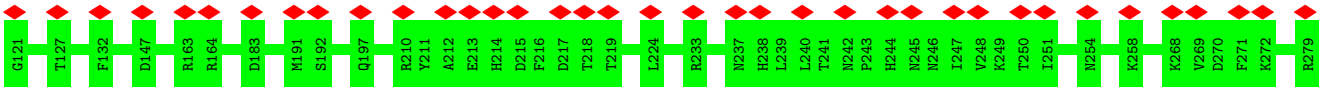


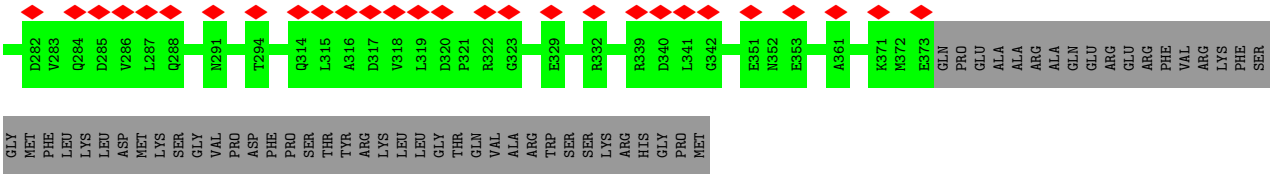


• Molecule 43: uS15m

Chain i:

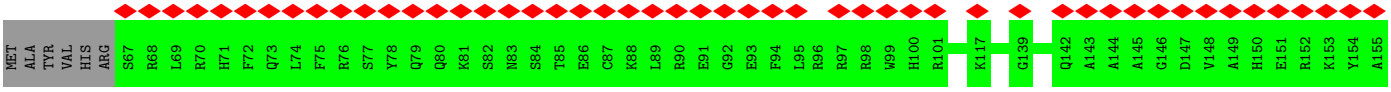


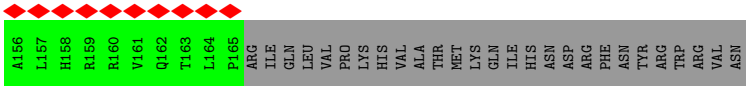




• Molecule 44: bS21m

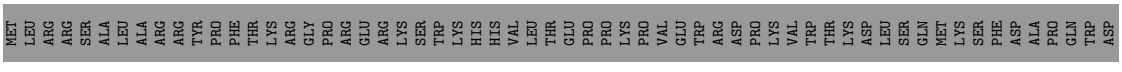
Chain g:

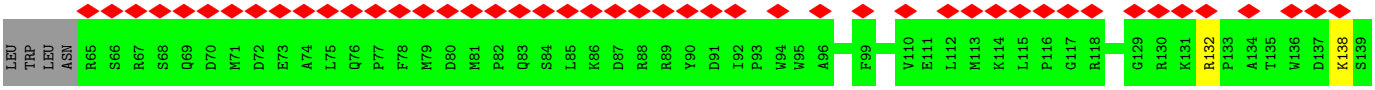


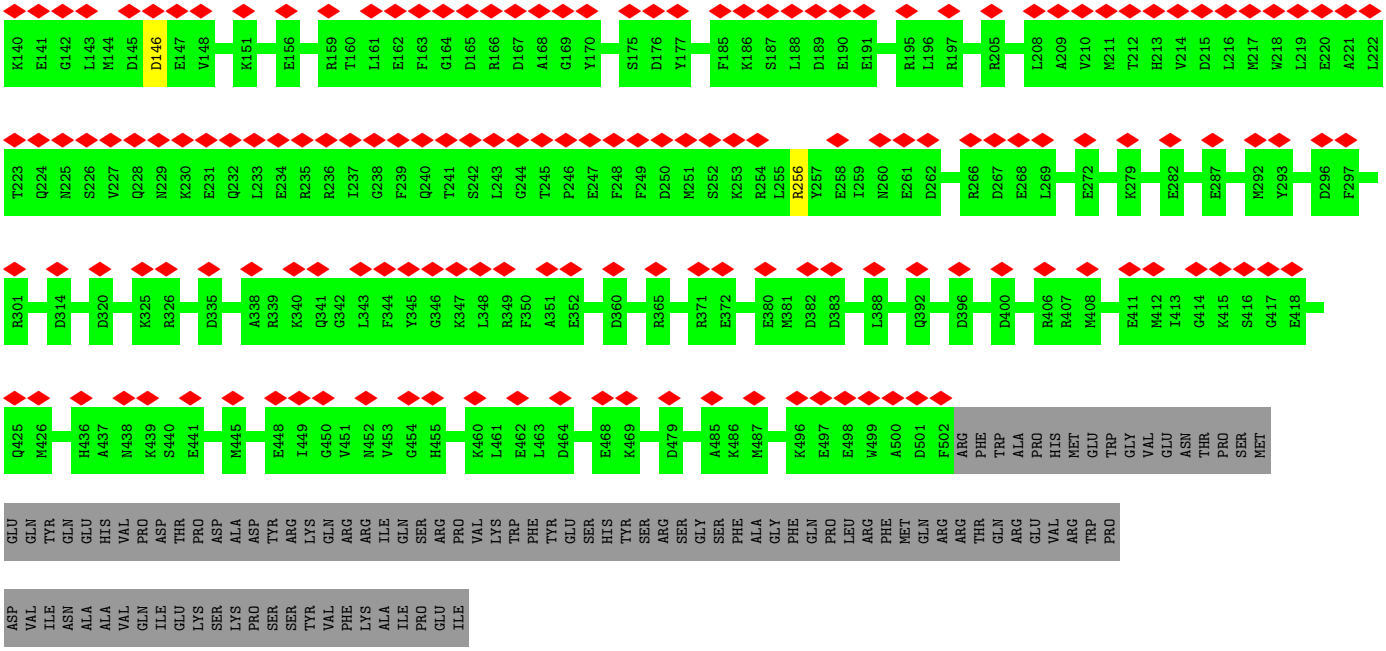


• Molecule 45: mS22

Chain o:

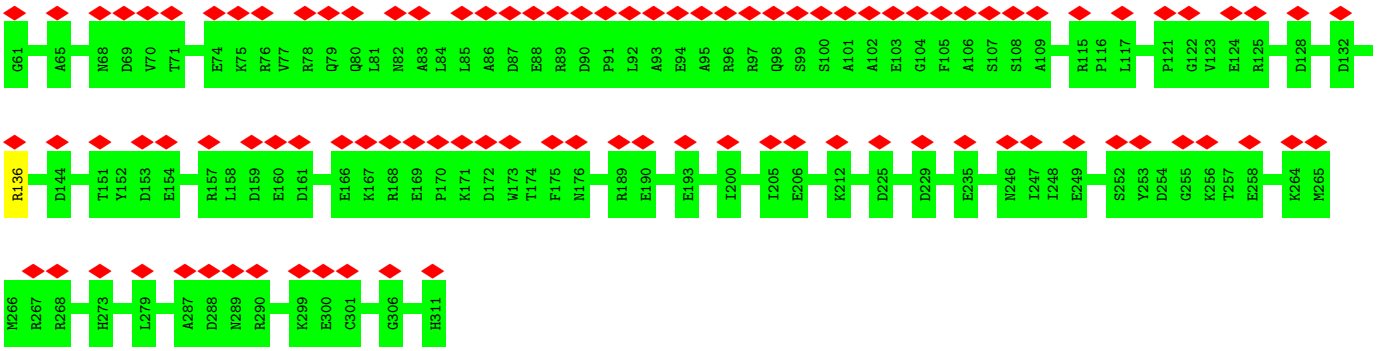






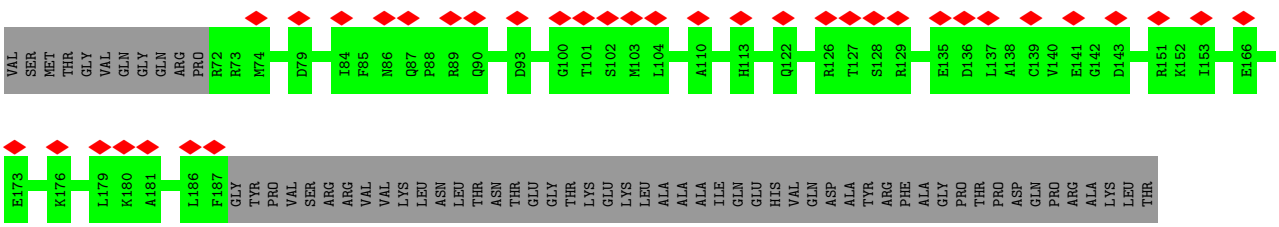
• Molecule 46: uS8m

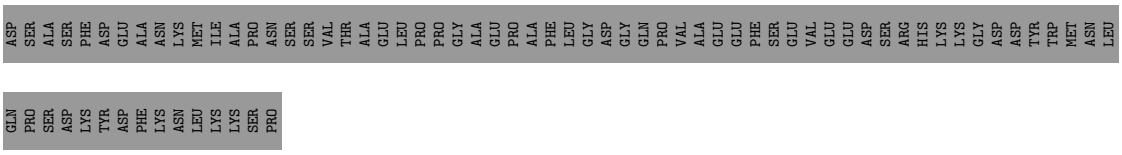
Chain c:



• Molecule 47: 30S Ribosomal protein S17-like protein

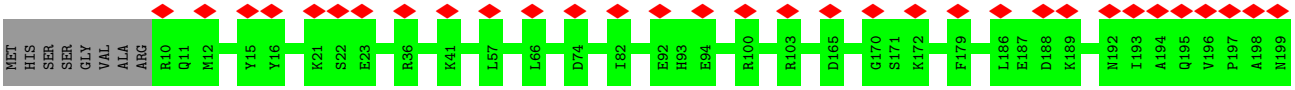
Chain k:

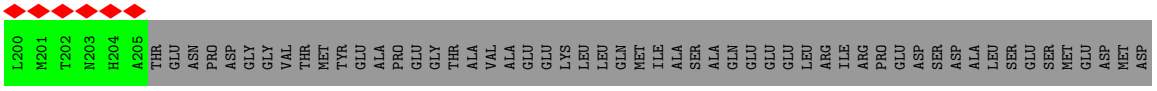


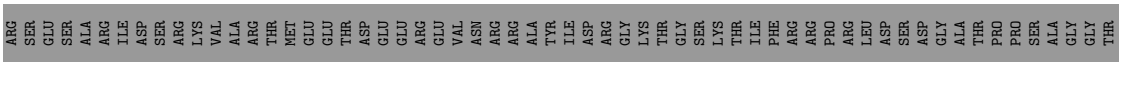


• Molecule 48: mS26

Chain q:

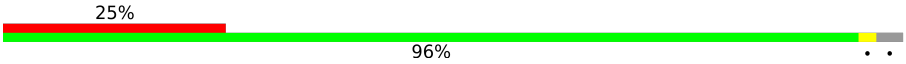


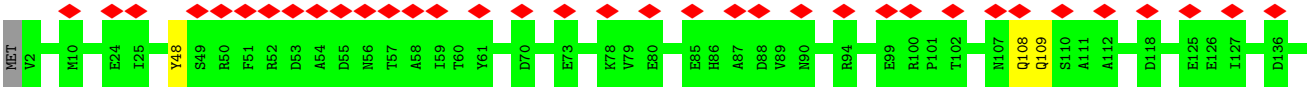


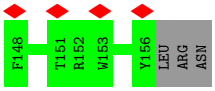


• Molecule 49: bS6m

Chain b:

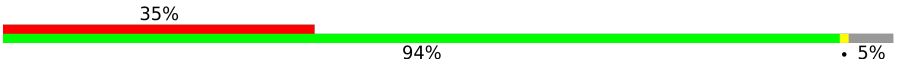


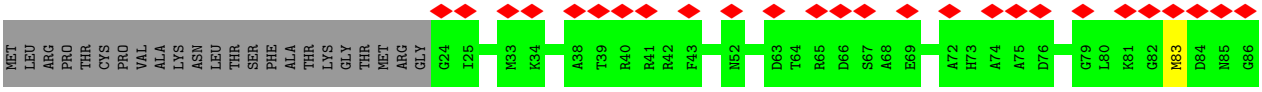


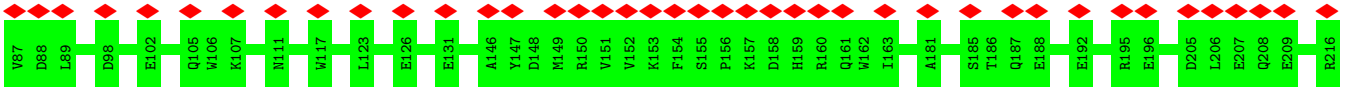


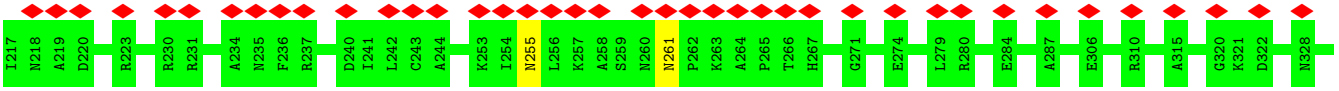
• Molecule 50: Ribosomal_S5_C domain-containing protein

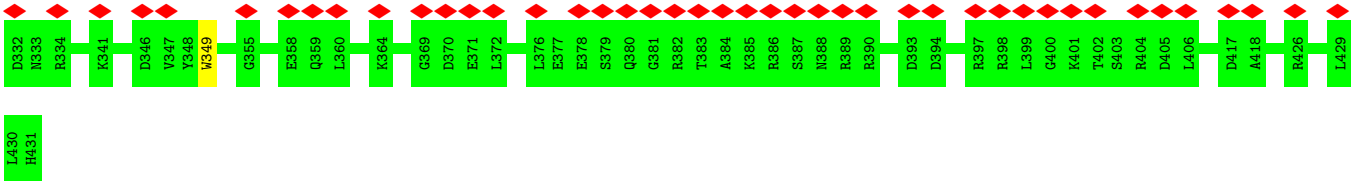
Chain a:





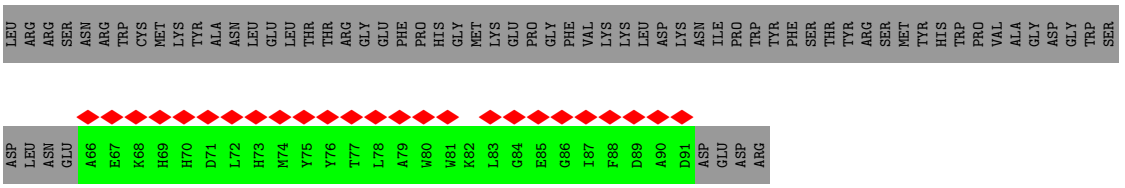






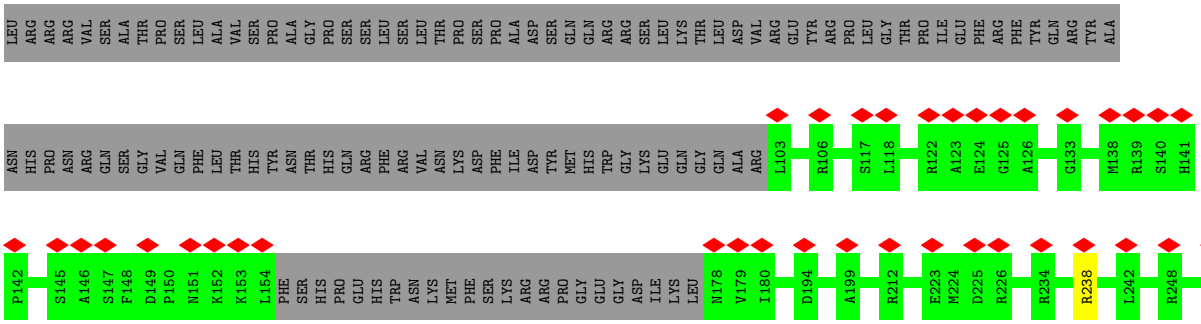
• Molecule 51: mS73

Chain ba:



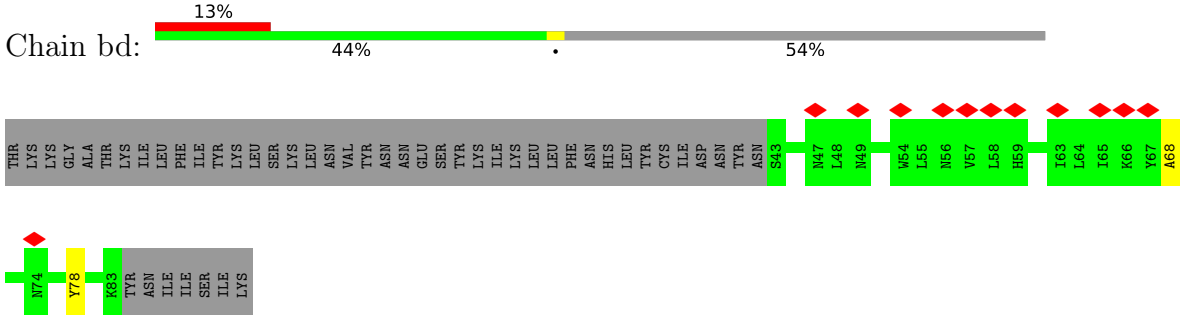
• Molecule 52: mS47

Chain z:



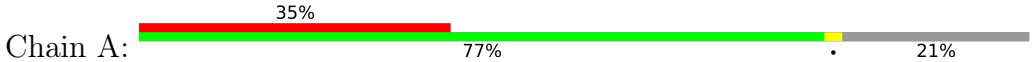
• Molecule 53: uS3m

Chain bd:



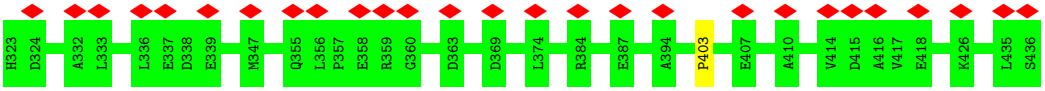
• Molecule 54: Ribosomal protein L3-like protein

Chain A:



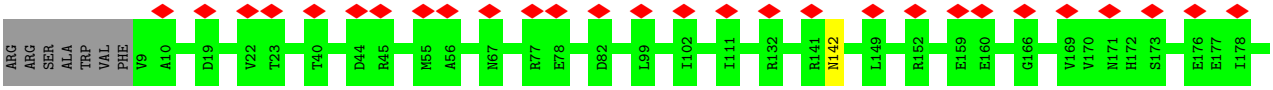
• Molecule 55: uL4m

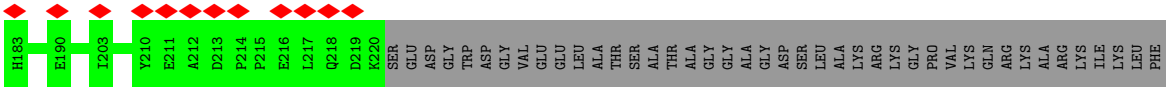
Chain B:



• Molecule 56: RIBOSOMAL_L9 domain-containing protein

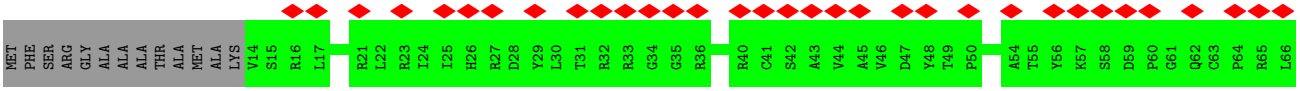
Chain C:

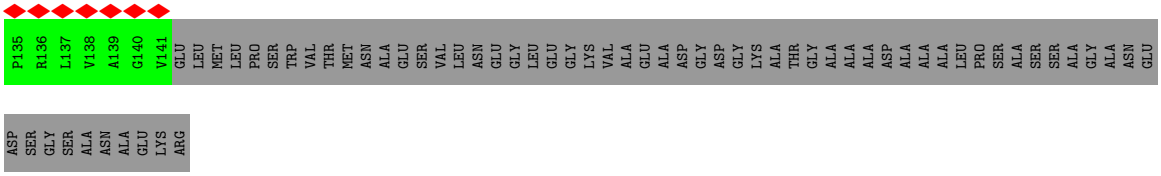




• Molecule 57: uL10m

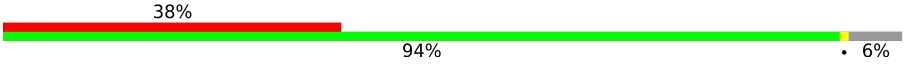
Chain D:

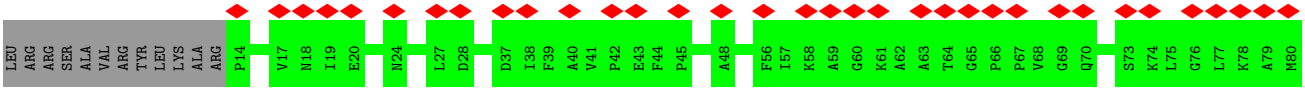


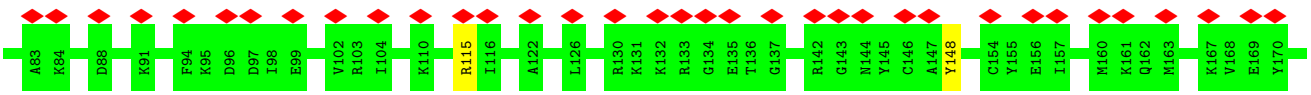


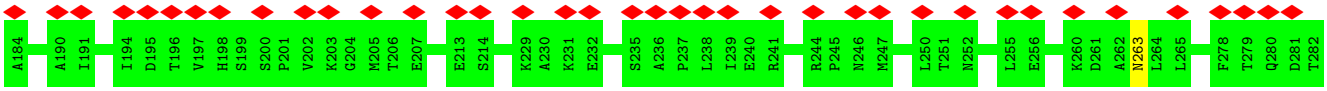
• Molecule 58: Putative ribosomal protein L11

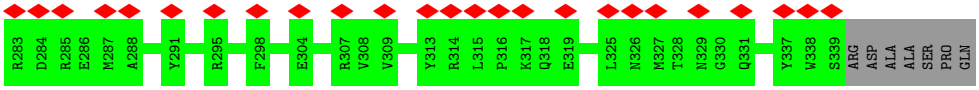
Chain E:





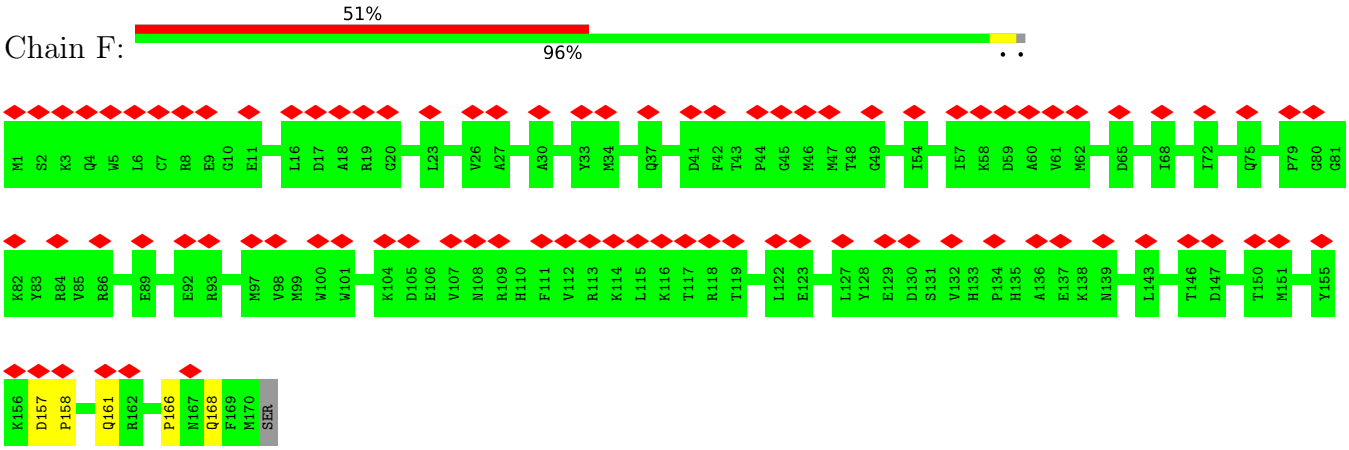






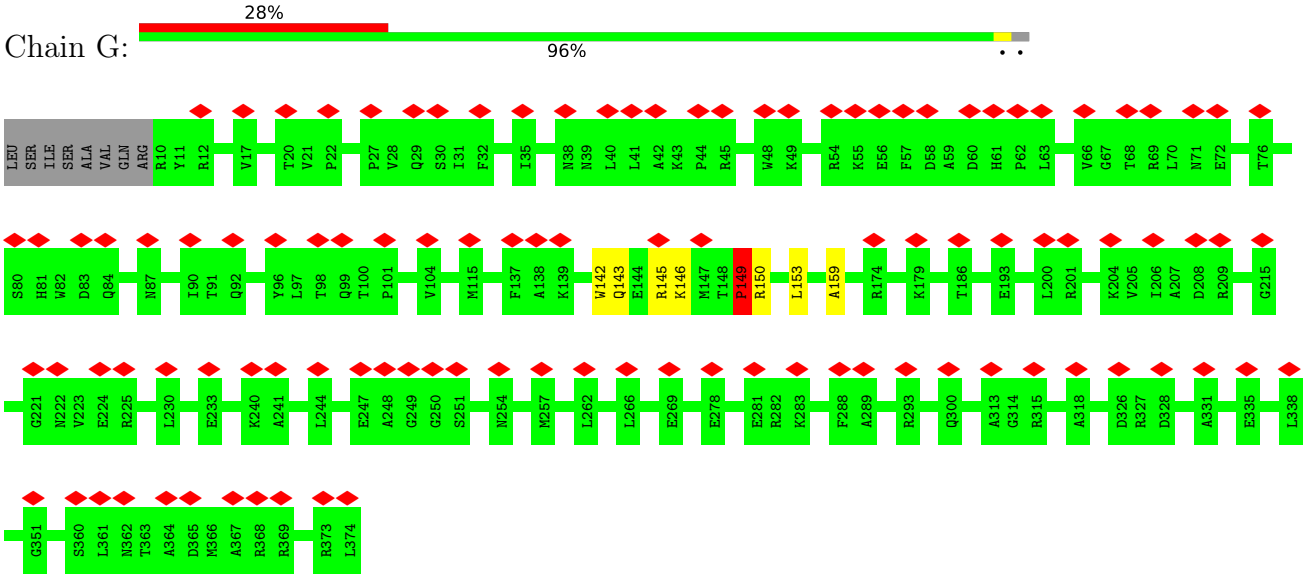
• Molecule 59: 50S ribosomal protein L13-like protein

Chain F:



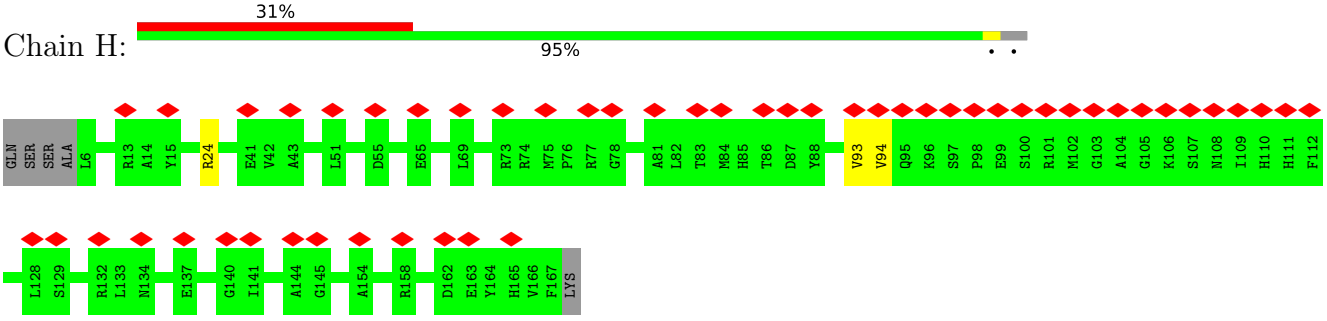
• Molecule 60: Ribosomal_L18e/L15P domain-containing protein

Chain G:



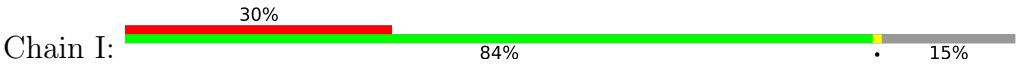
• Molecule 61: Ribosomal_L16 domain-containing protein

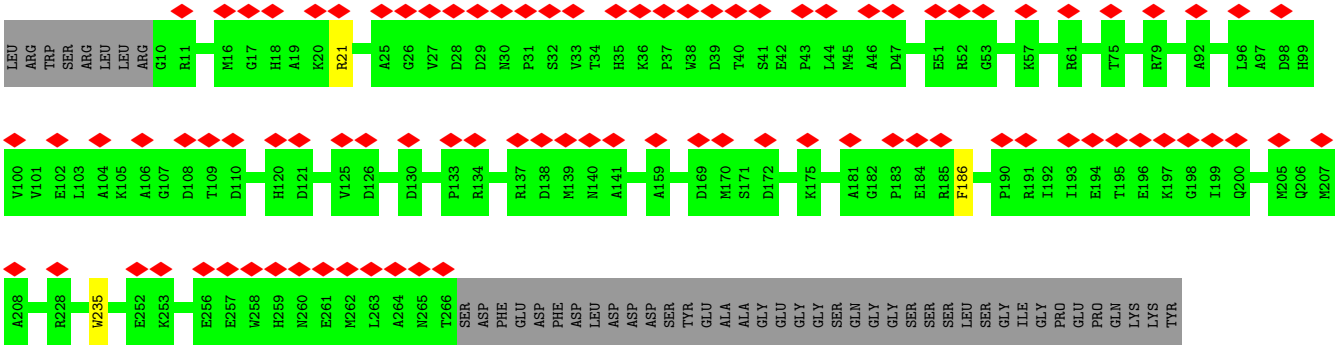
Chain H:



• Molecule 62: Putative 50S ribosomal protein L17

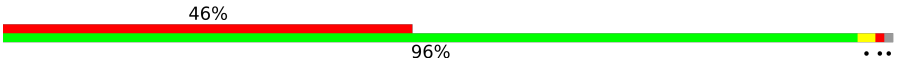
Chain I:

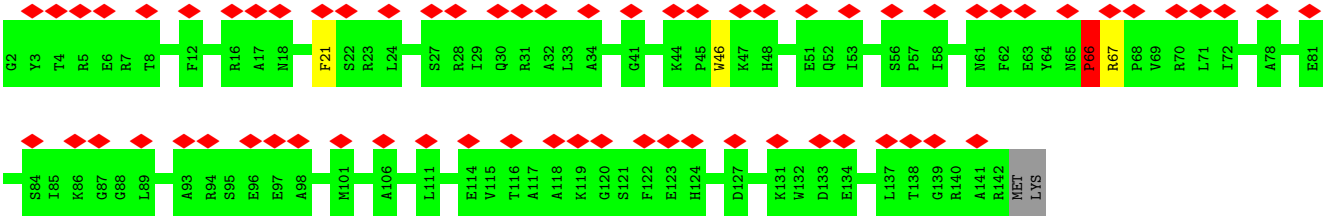




- Molecule 63: bL19m

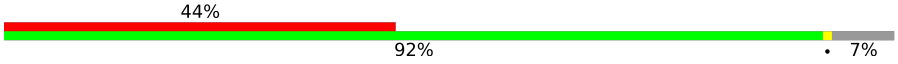
Chain J:

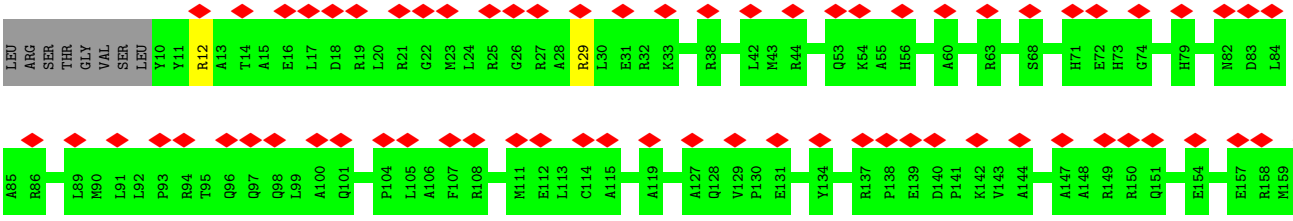


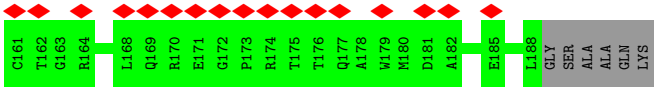


- Molecule 64: bL20m

Chain K:

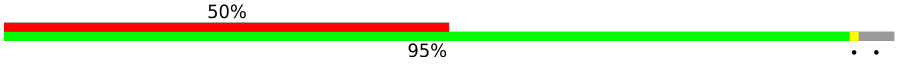


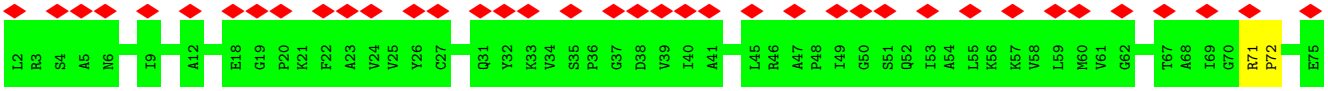


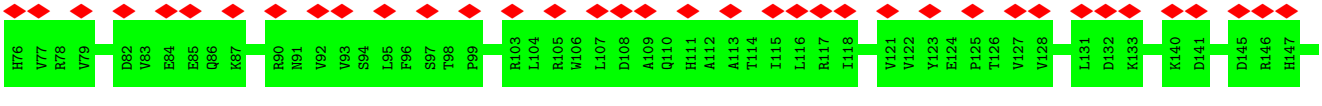


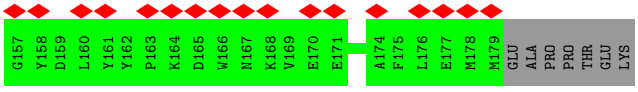
- Molecule 65: bL21m

Chain L:



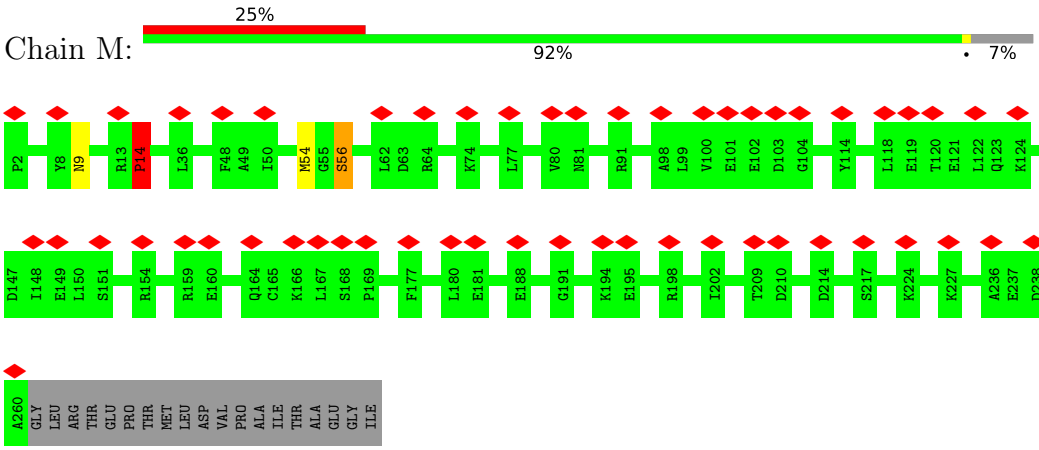






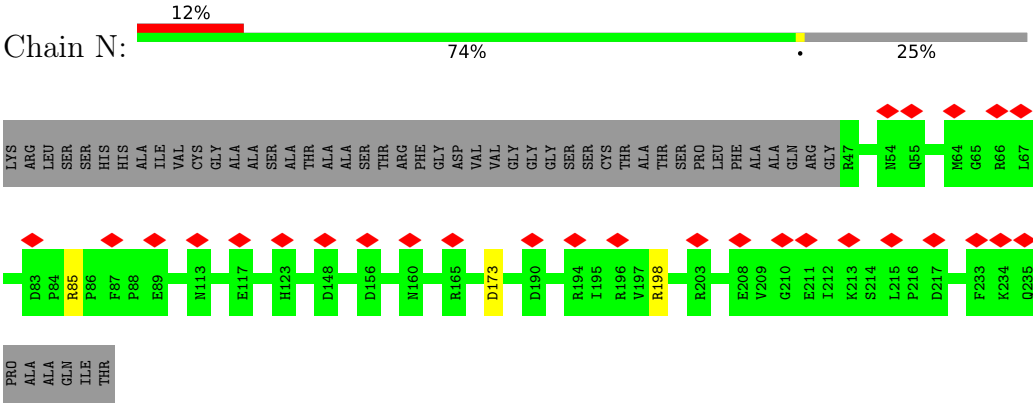
• Molecule 66: uL22m

Chain M:



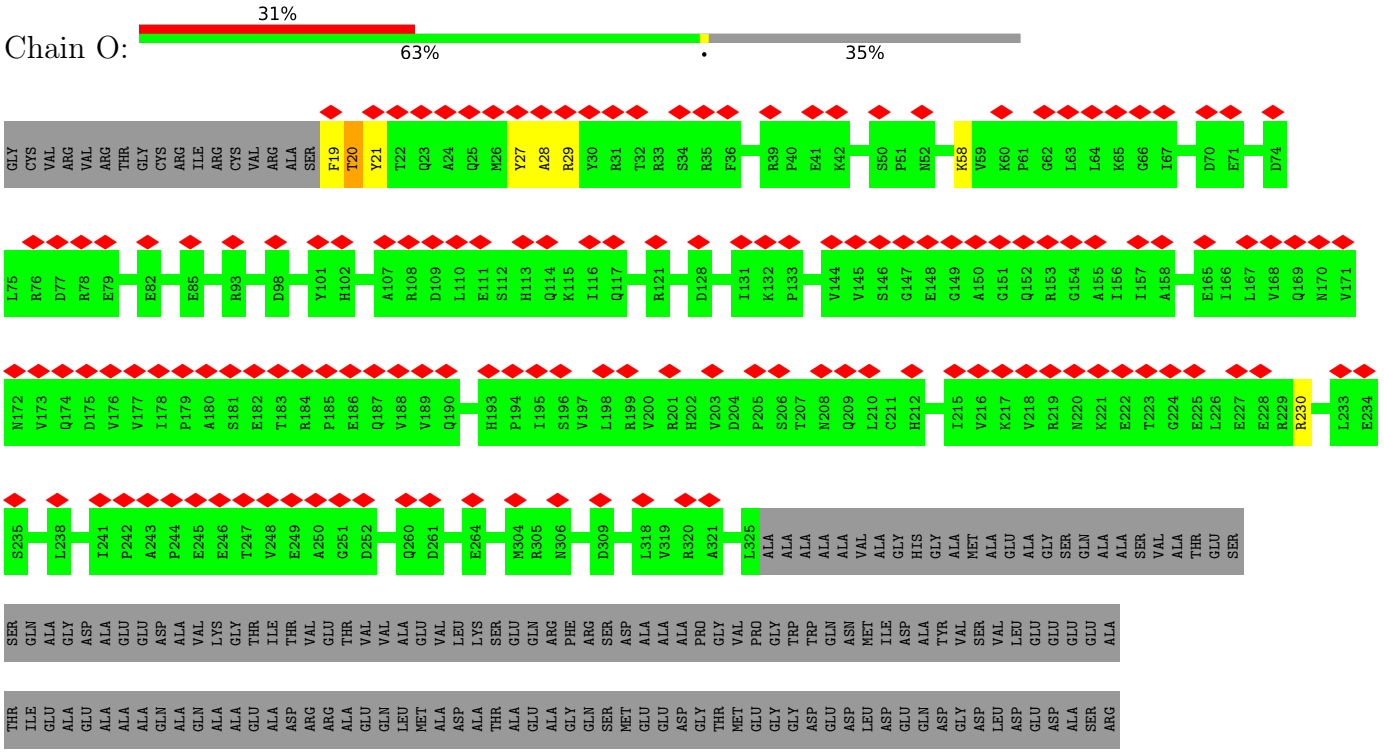
• Molecule 67: uL23m

Chain N:



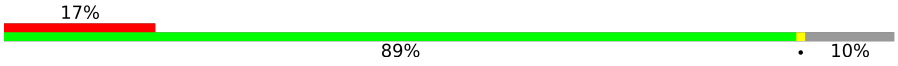
• Molecule 68: uL24m

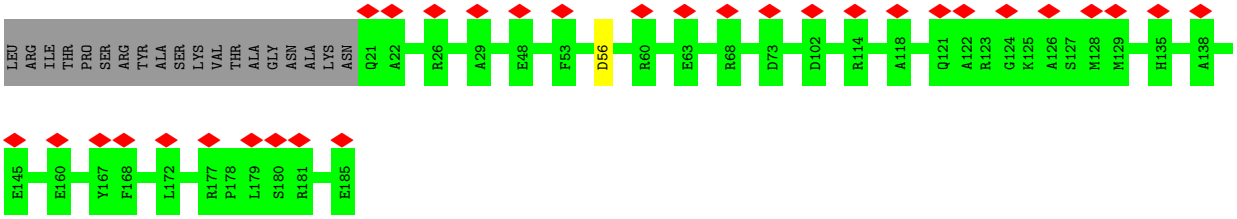
Chain O:



• Molecule 69: bL27m

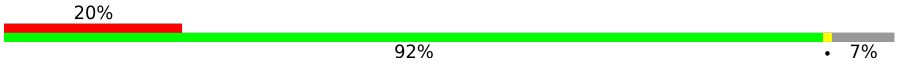
Chain P:

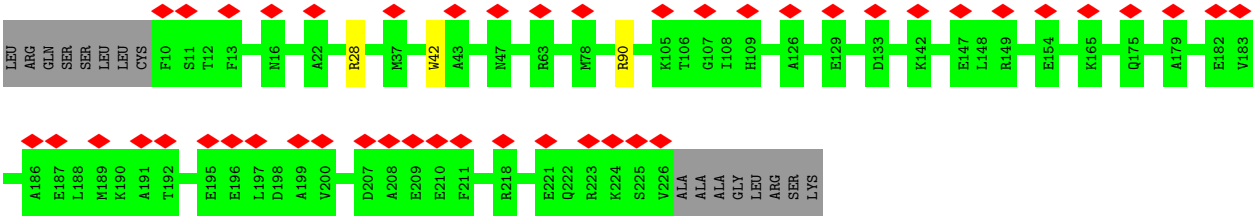




• Molecule 70: bL28m

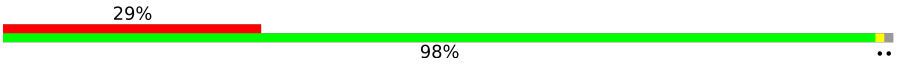
Chain Q:

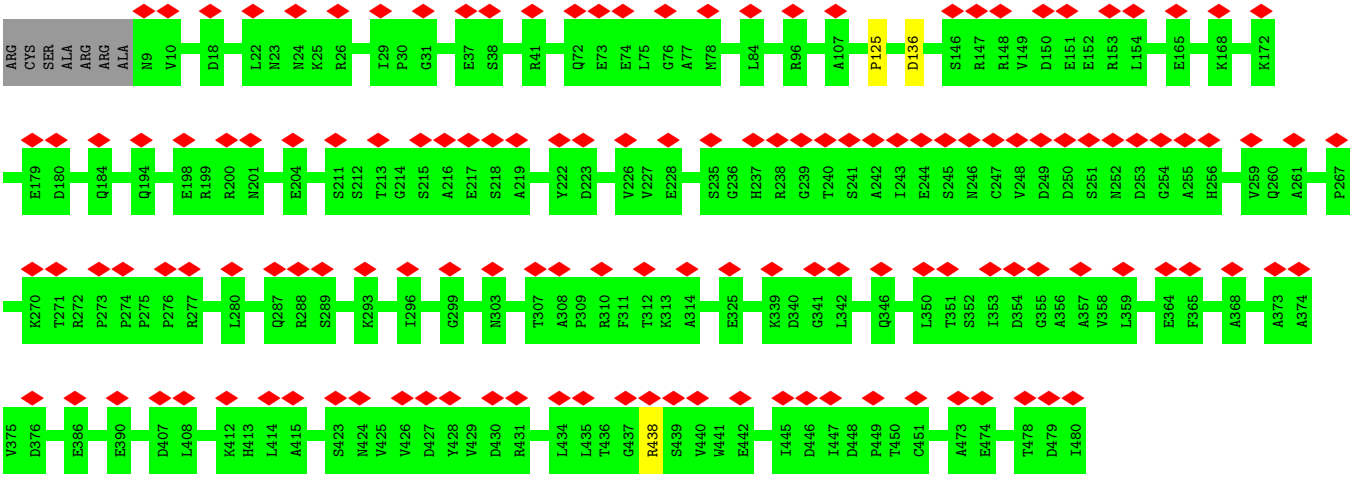




• Molecule 71: uL29m

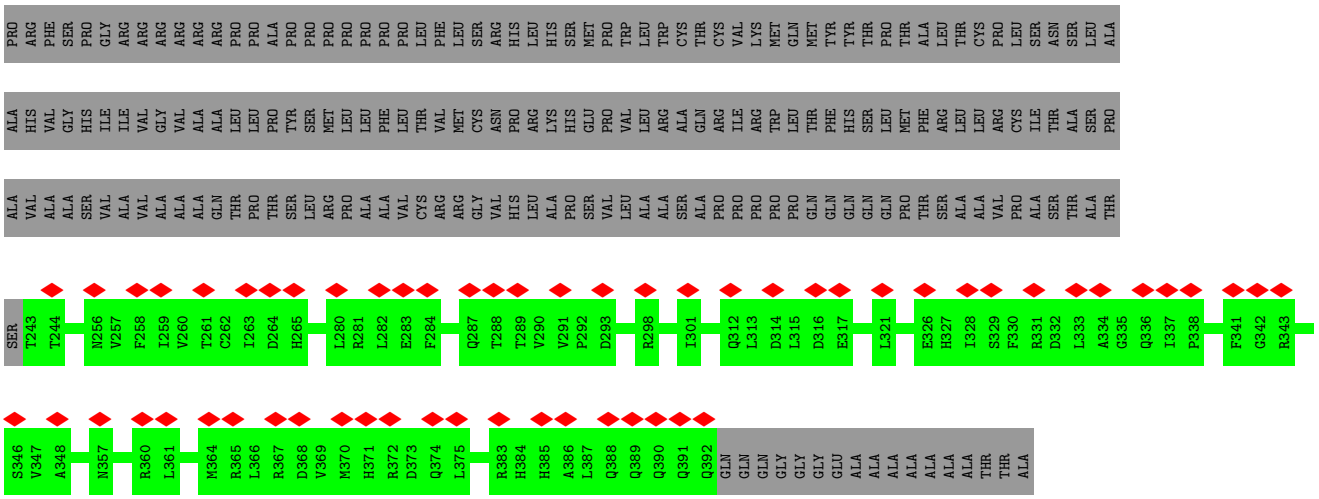
Chain R:





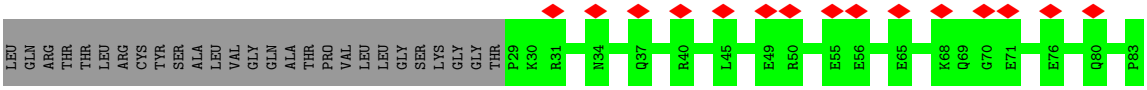
• Molecule 72: uL30m

Chain S:



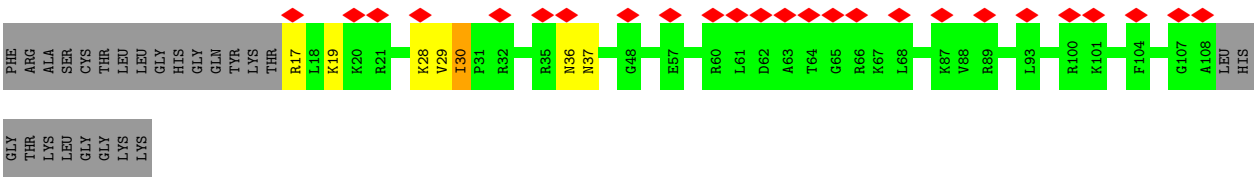
- Molecule 73: bL32m

Chain T:



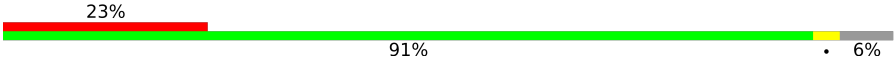
- Molecule 74: bL33m

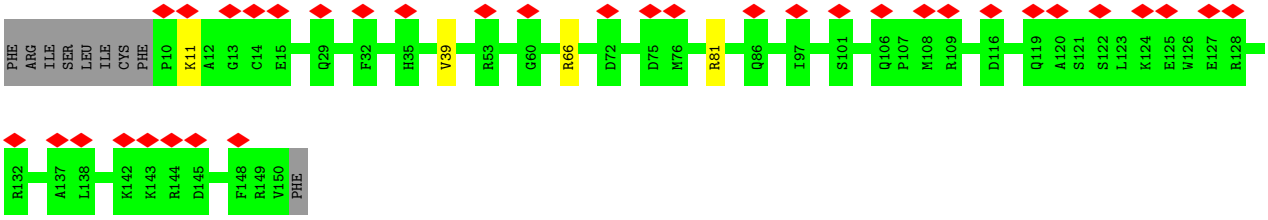
Chain U:



- Molecule 75: bL35m

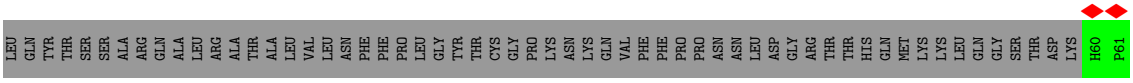
Chain V:

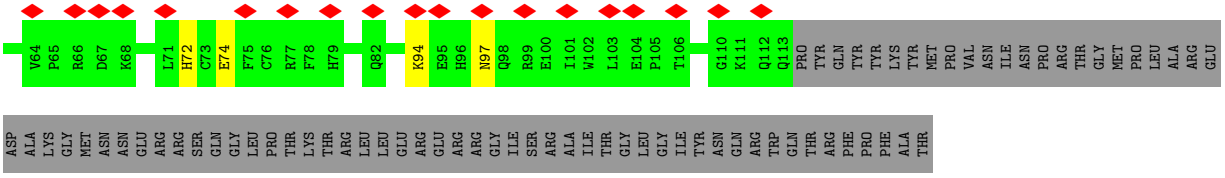




- Molecule 76: bL36m

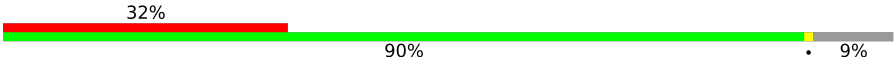
Chain W:

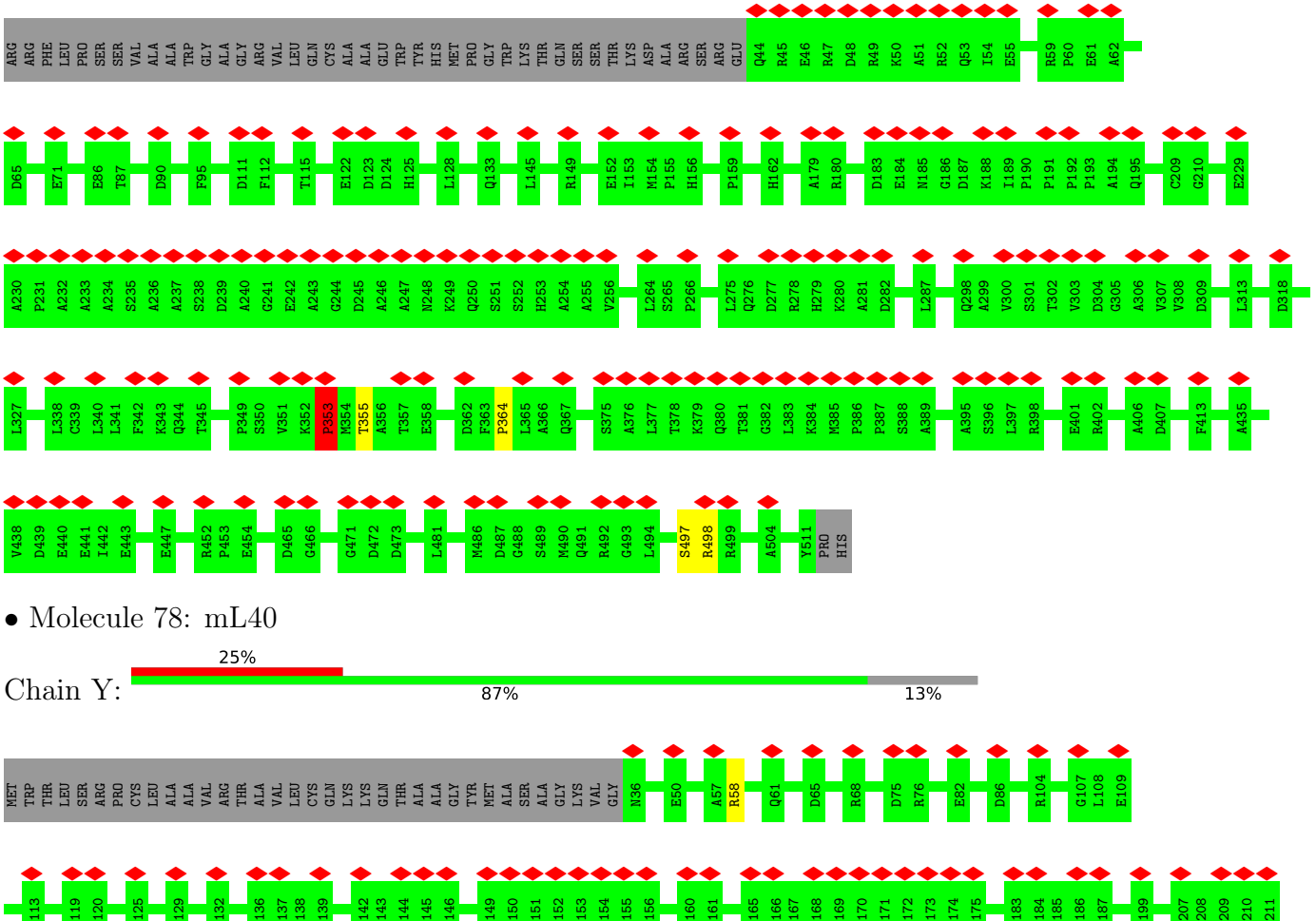




• Molecule 77: mL38

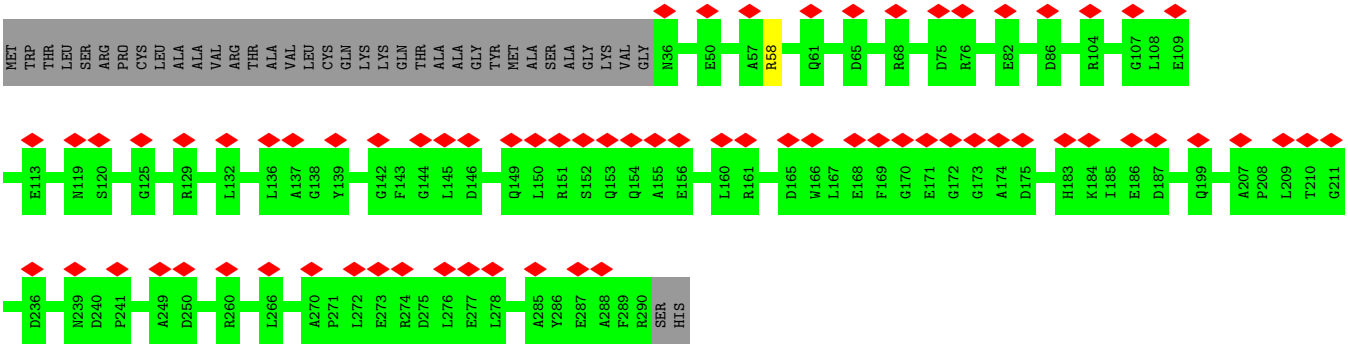
Chain X:





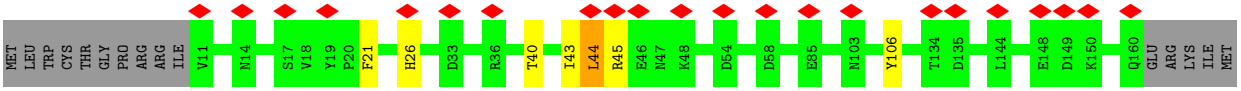
• Molecule 78: mL40

Chain Y:



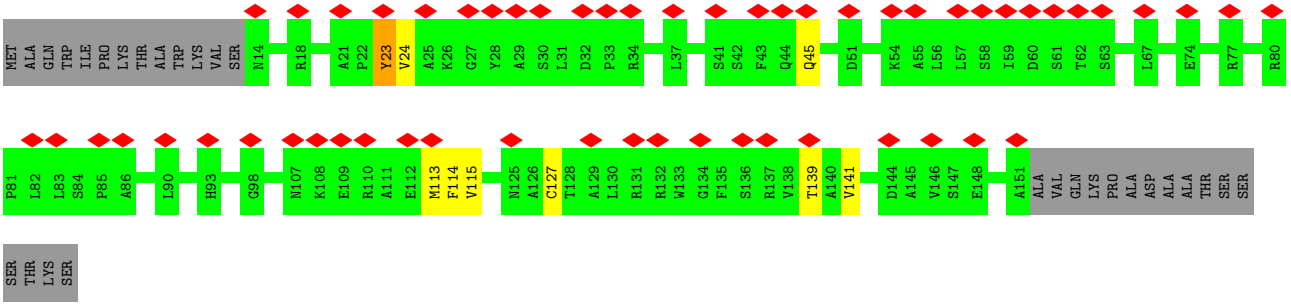
• Molecule 79: mL41

Chain Z:



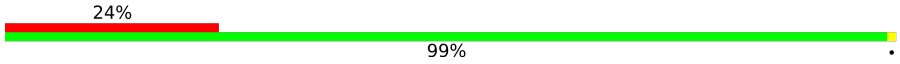
• Molecule 80: mL94

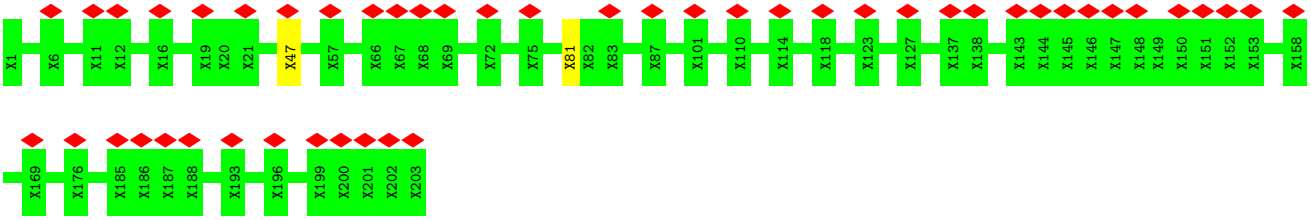
Chain BA:



• Molecule 81: UA

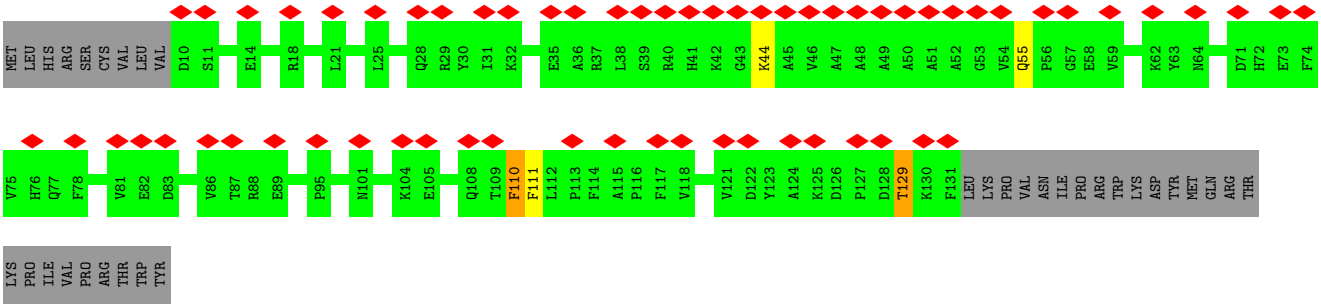
Chain UA:





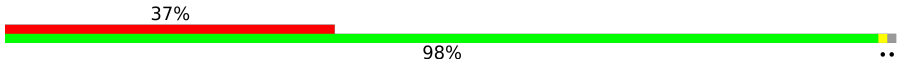
• Molecule 82: mL95

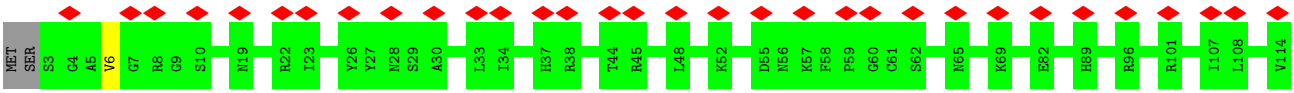
Chain BB:

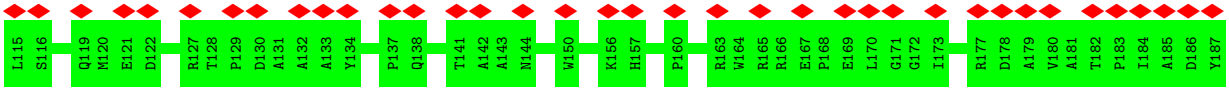


• Molecule 83: mL89

Chain Aw:

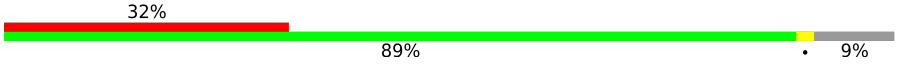


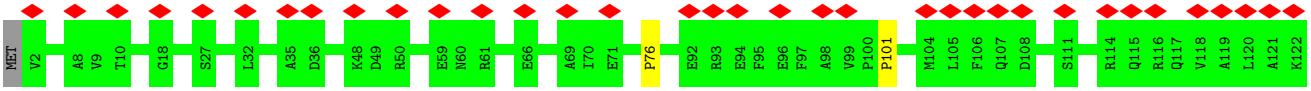


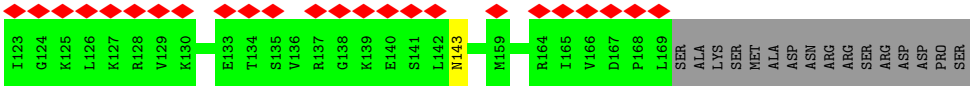


• Molecule 84: bL31m

Chain Bj:

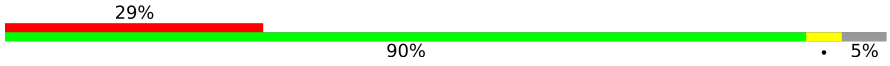


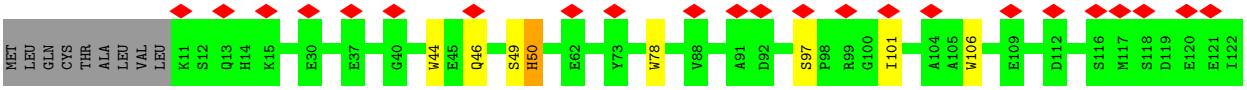


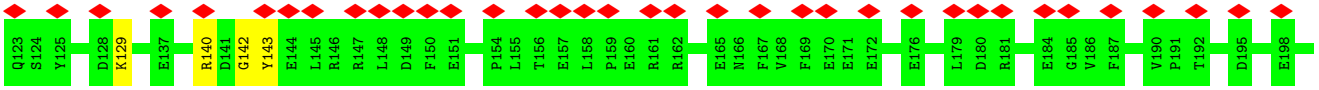


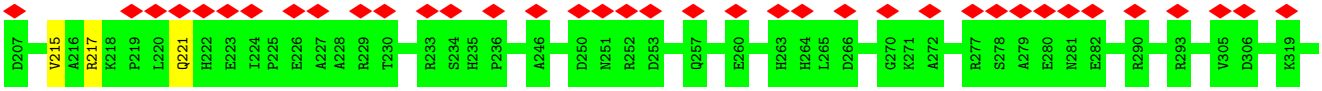
• Molecule 85: mL76

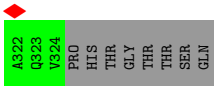
Chain An:





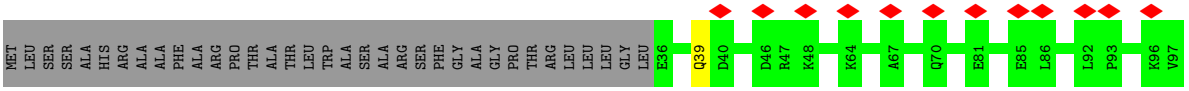


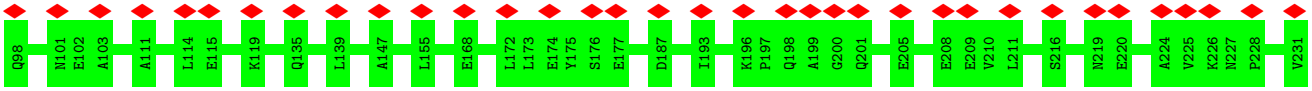


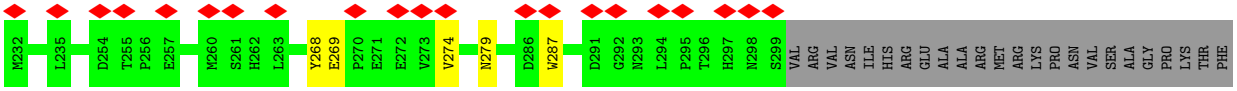


• Molecule 86: mL74

Chain Al:

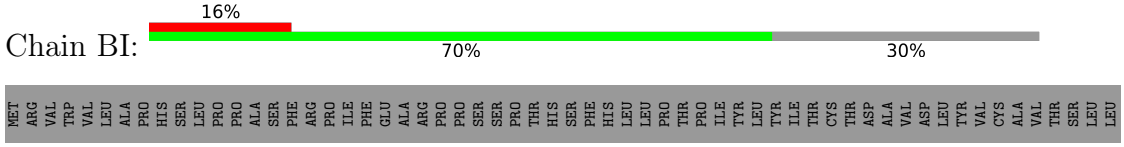


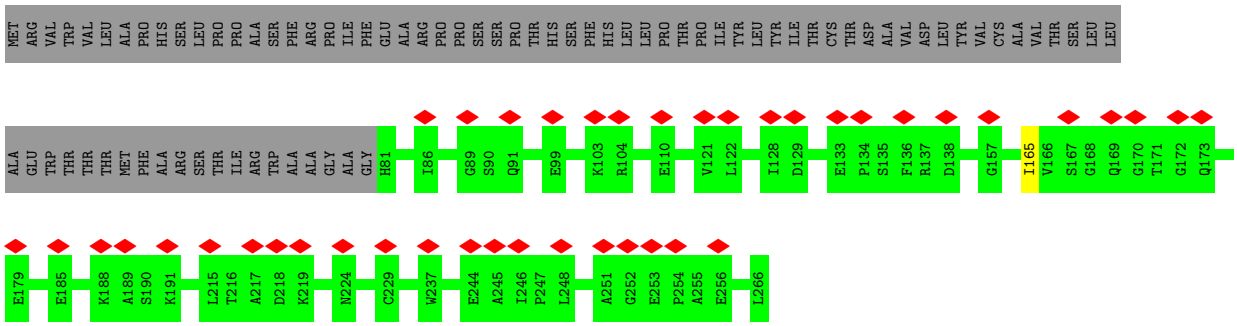




• Molecule 87: Peptidyl-prolyl cis-trans isomerase

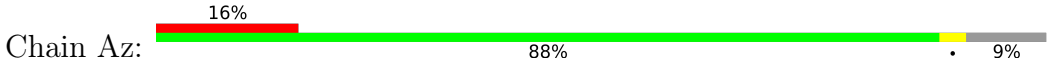
Chain BI:

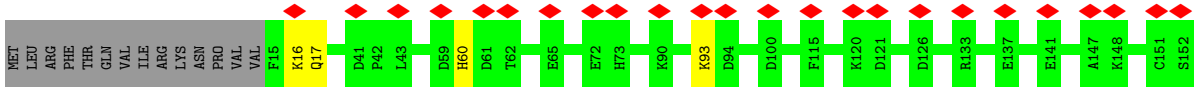




• Molecule 88: mL93

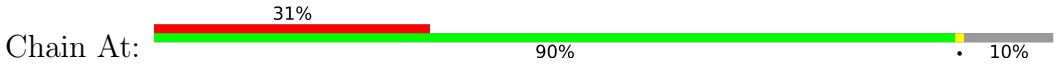
Chain Az:

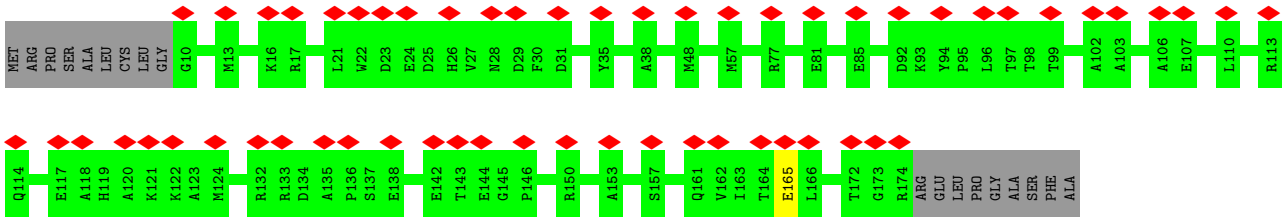




• Molecule 89: mL86

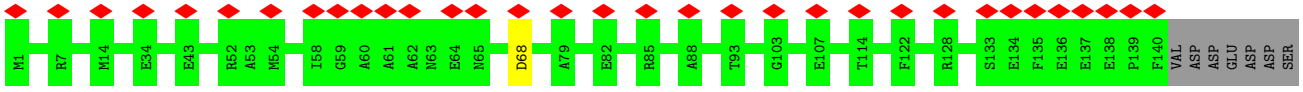
Chain At:





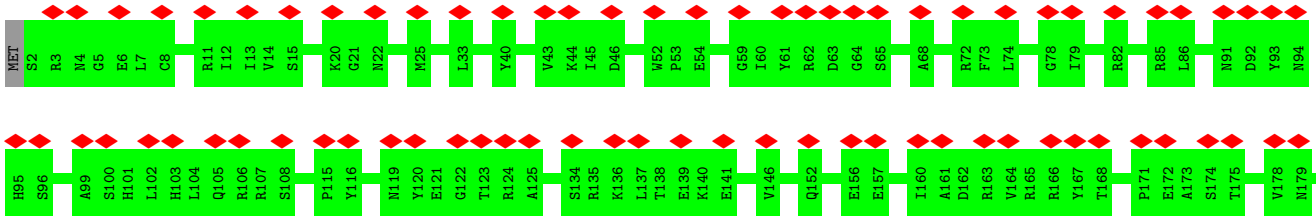
• Molecule 90: mL96

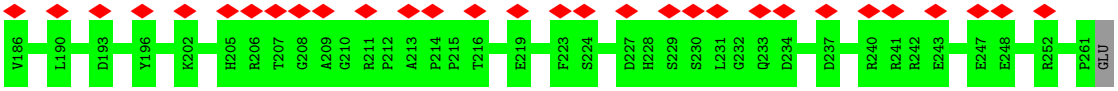
Chain BC:



• Molecule 91: L51_S25_CI-B8 domain-containing protein

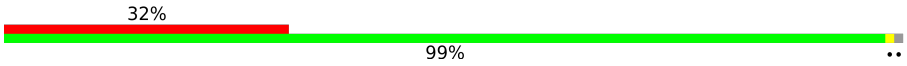
Chain Ab:

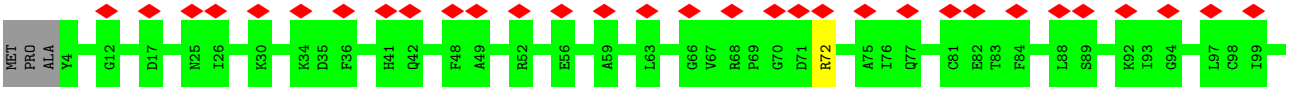


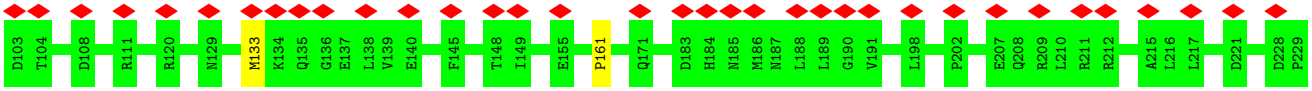


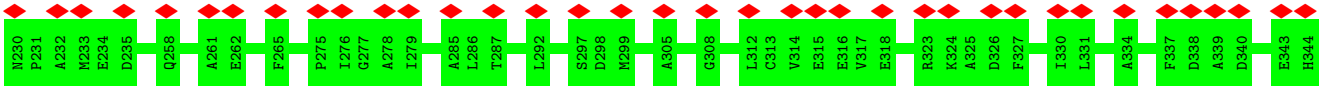
• Molecule 92: mL69

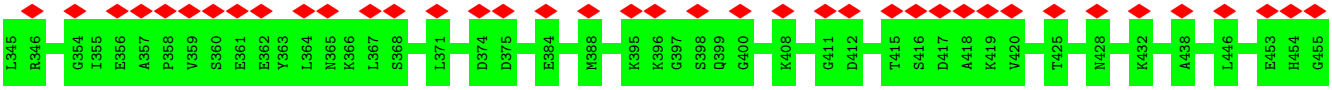
Chain Ai:

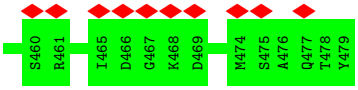






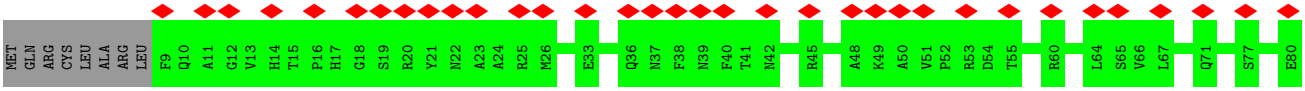


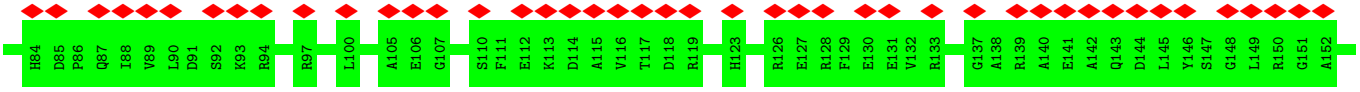


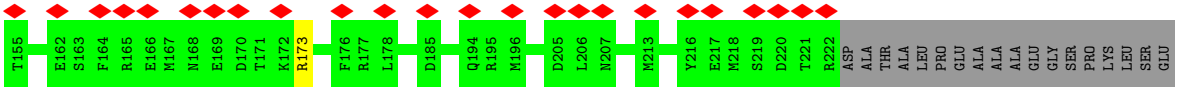


• Molecule 93: mL80

Chain Ap:

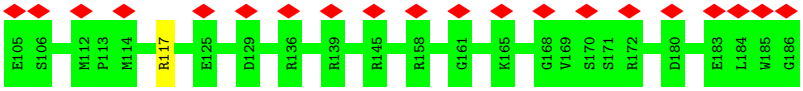






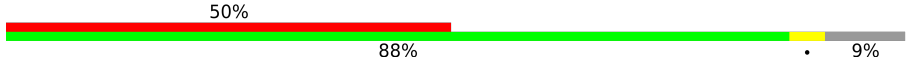
• Molecule 94: mL87

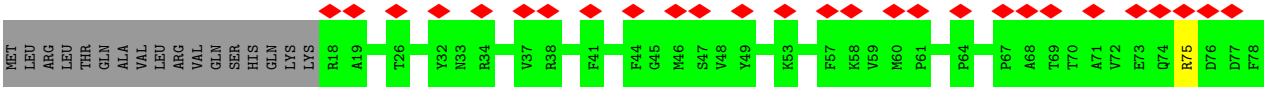
Chain Au:

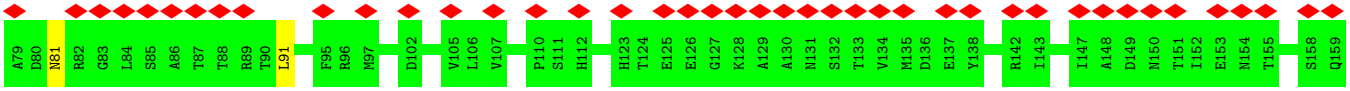


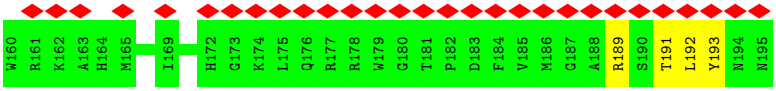
• Molecule 95: mL42

Chain Aa:



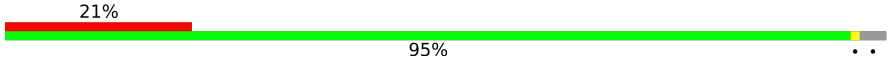


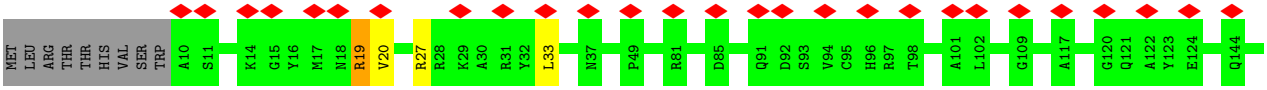


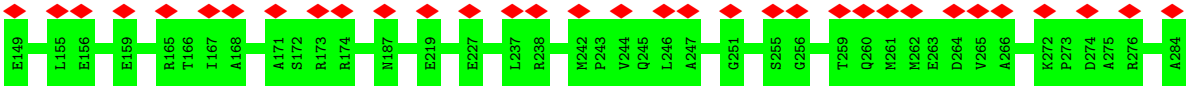


• Molecule 96: mL79

Chain Ao:

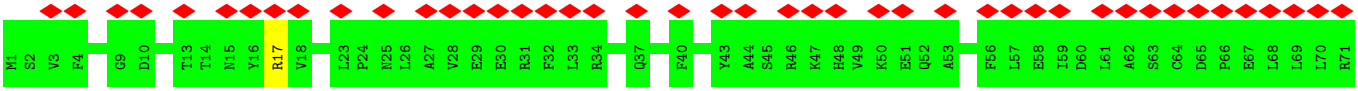


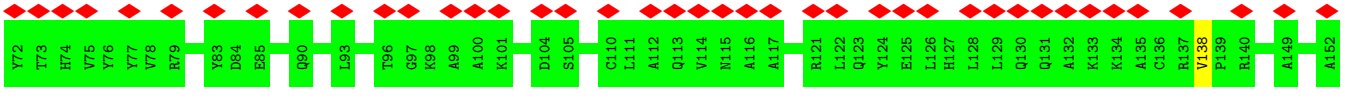


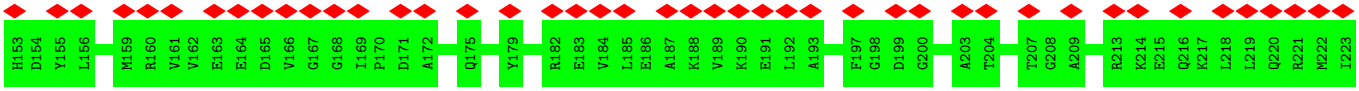


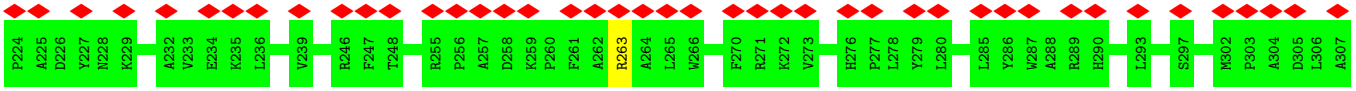
• Molecule 97: mL70

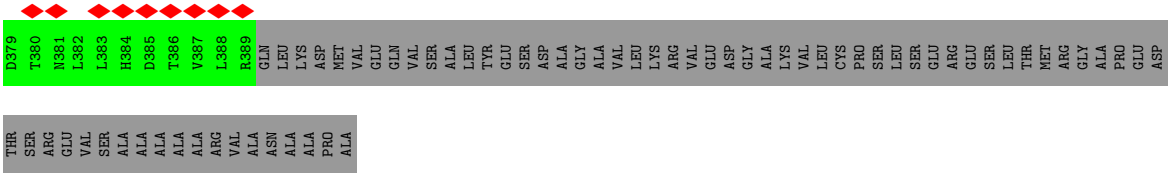
Chain BM:





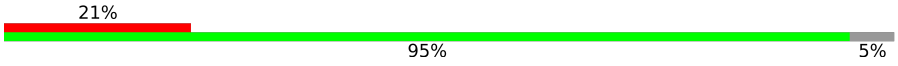


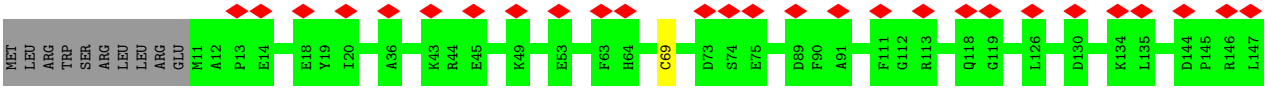


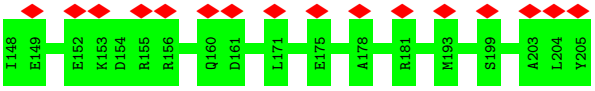


• Molecule 98: mL84

Chain Ar:

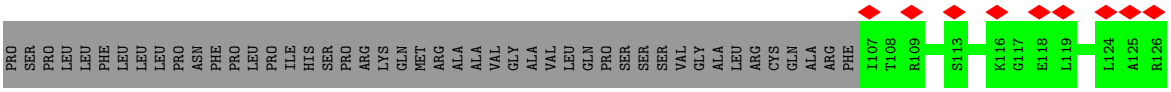


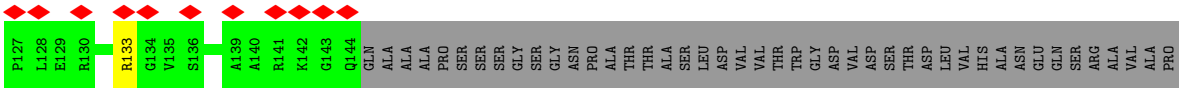


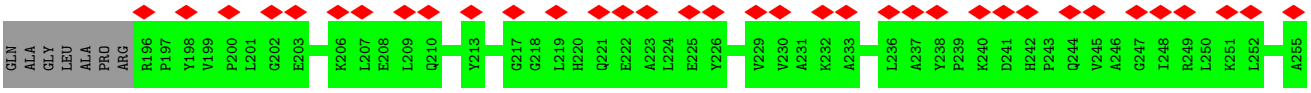


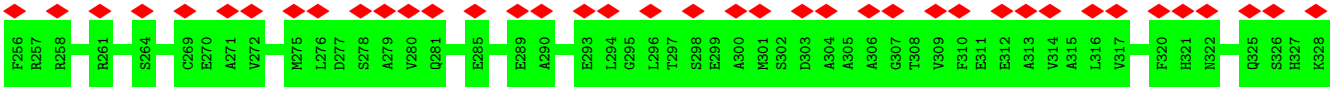
• Molecule 99: mL72

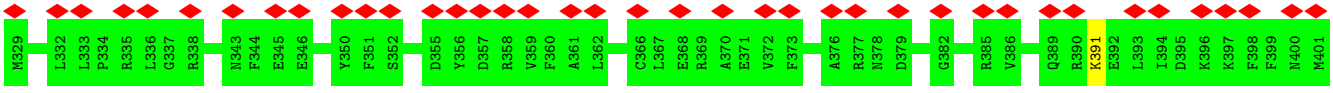
Chain Aj:

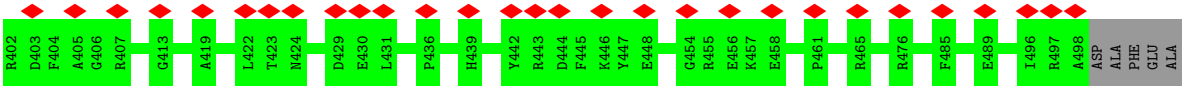






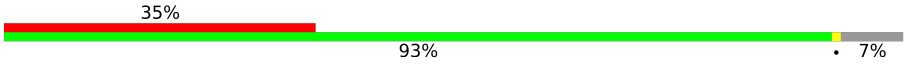


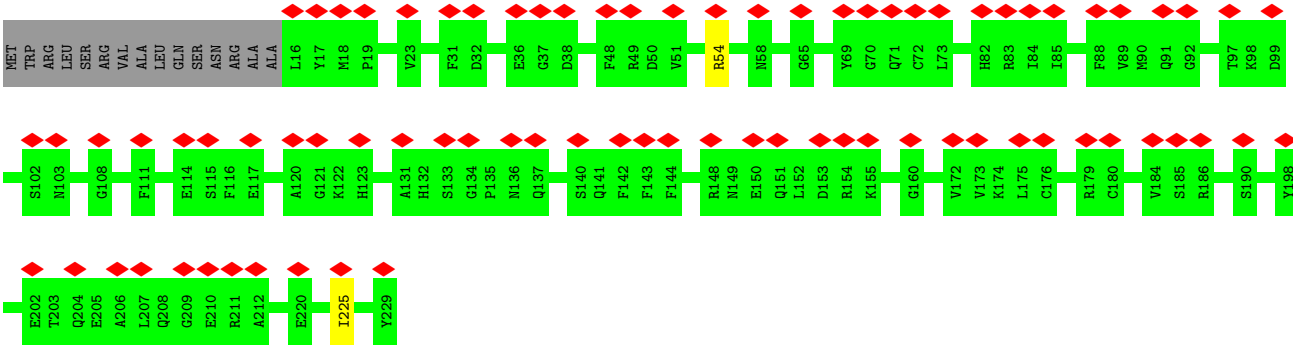




• Molecule 100: Peptidyl-prolyl cis-trans isomerase

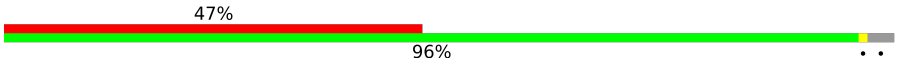
Chain BH:

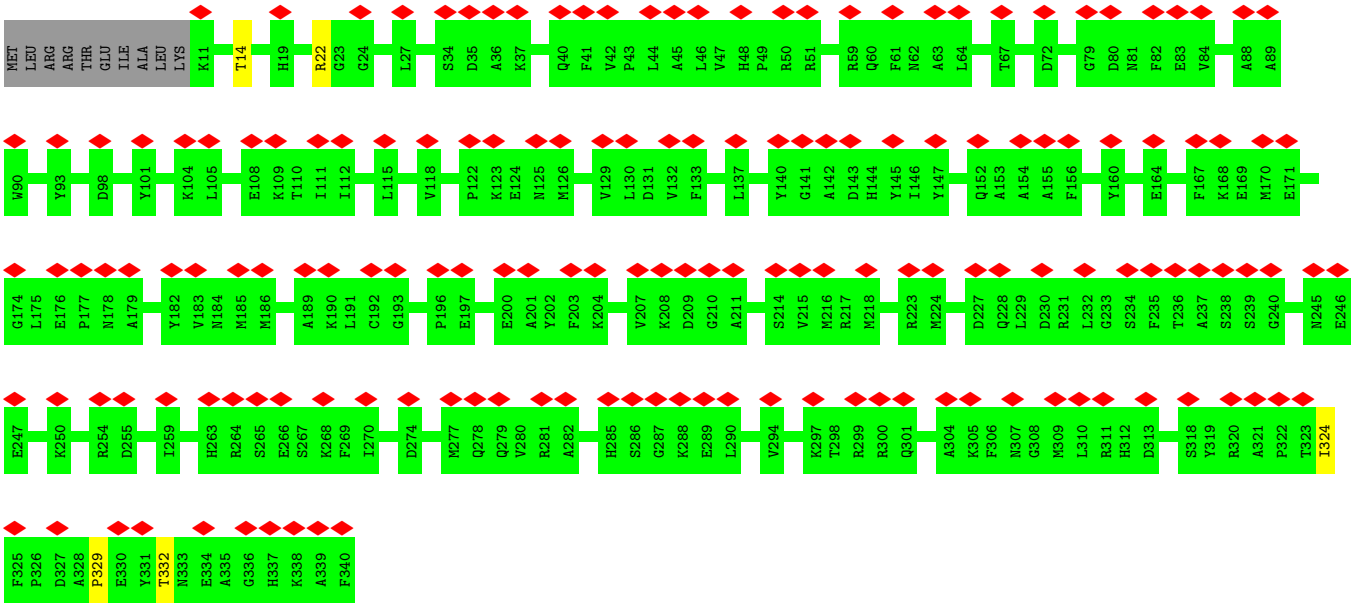




• Molecule 101: mL75

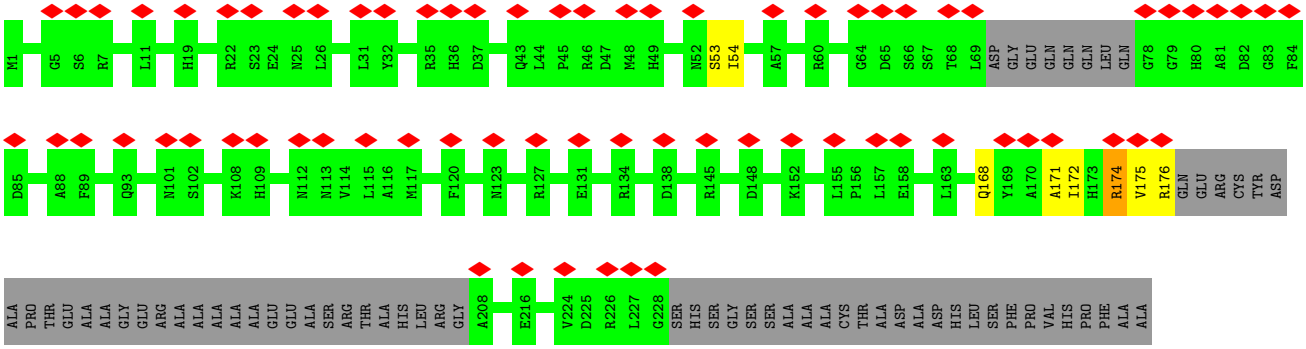
Chain Am:

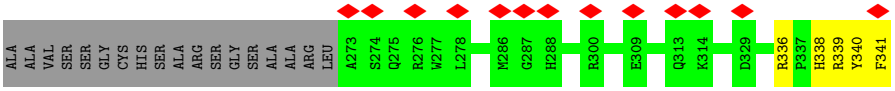




• Molecule 102: mL82

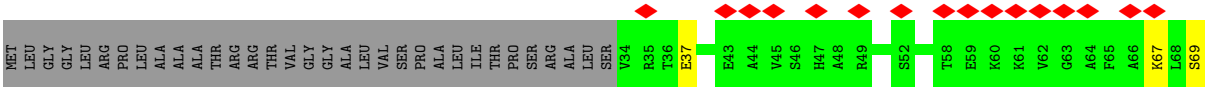
Chain Aq:

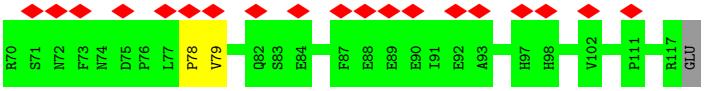




• Molecule 103: mL98

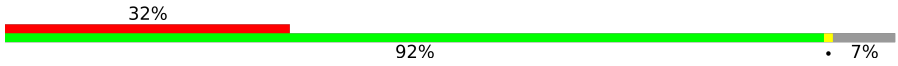
Chain BE:

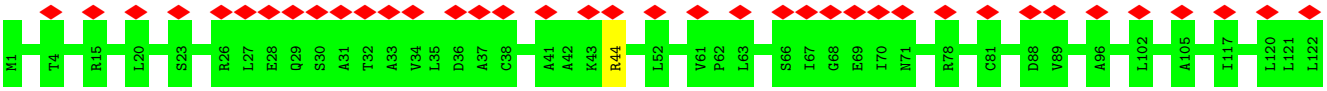


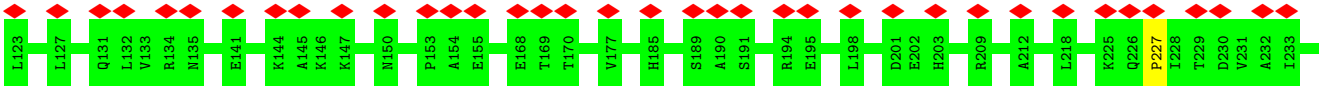


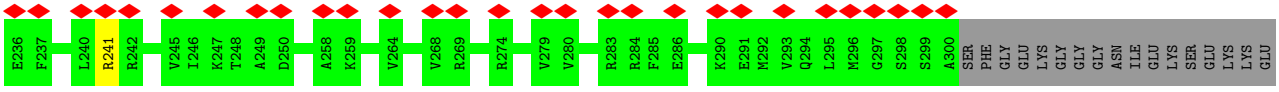
• Molecule 104: mL73

Chain Ak:



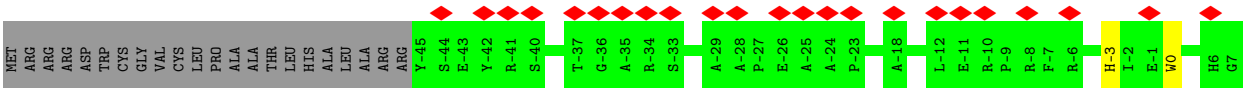


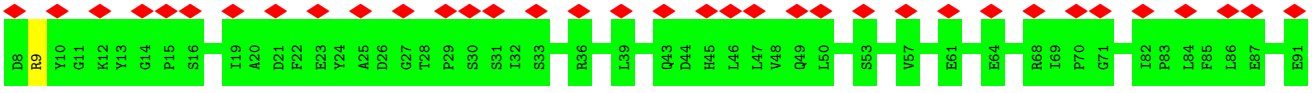


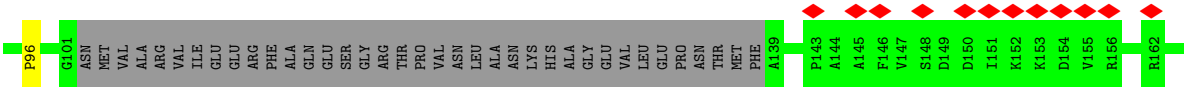


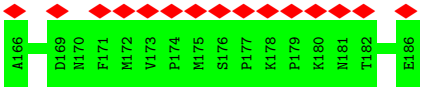
• Molecule 105: mL52

Chain BP:



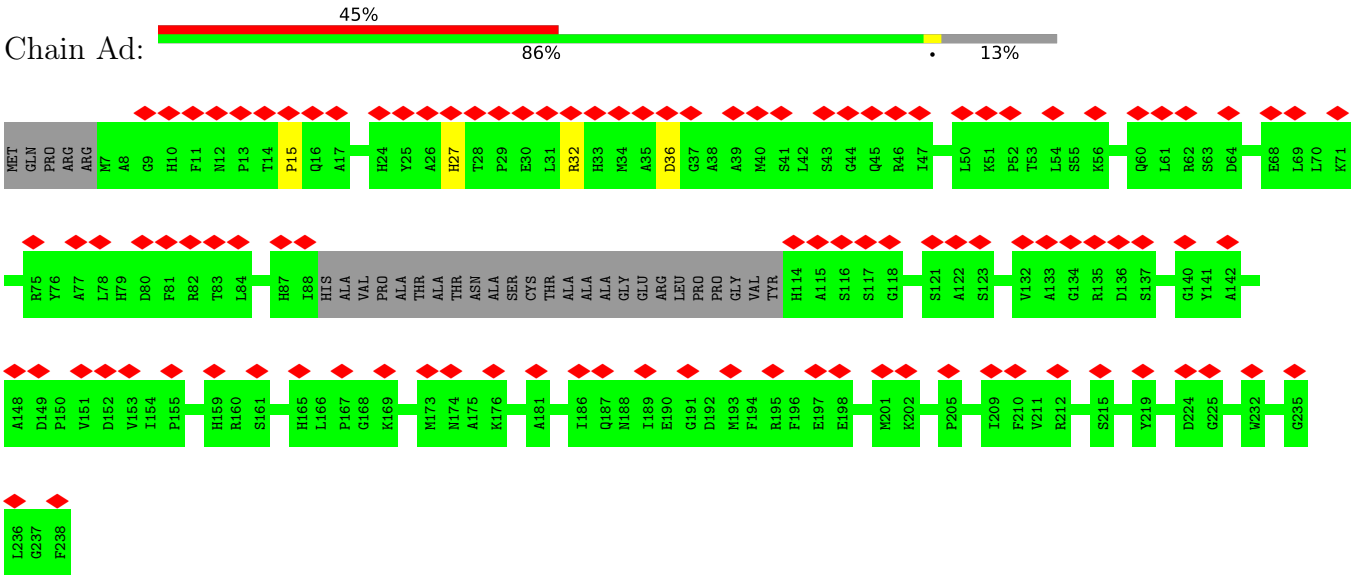






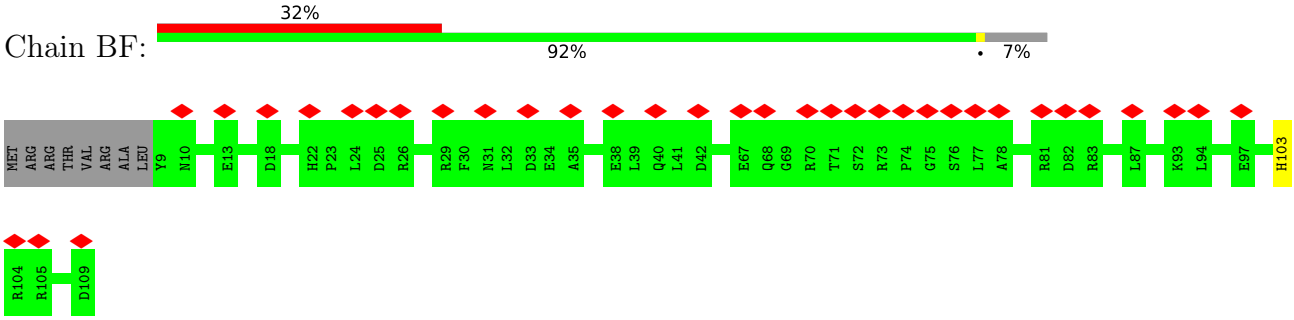
• Molecule 106: mL49

Chain Ad:



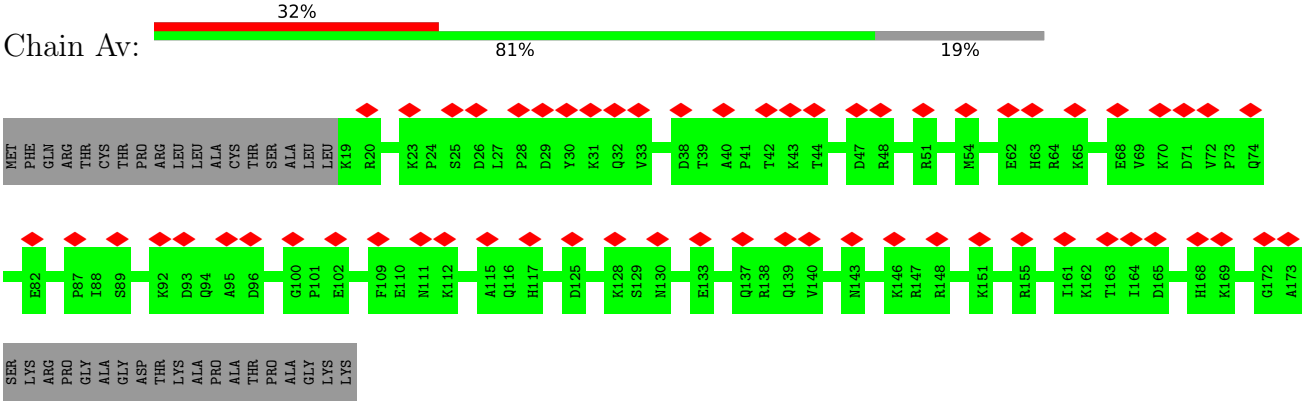
• Molecule 107: mL99

Chain BF:



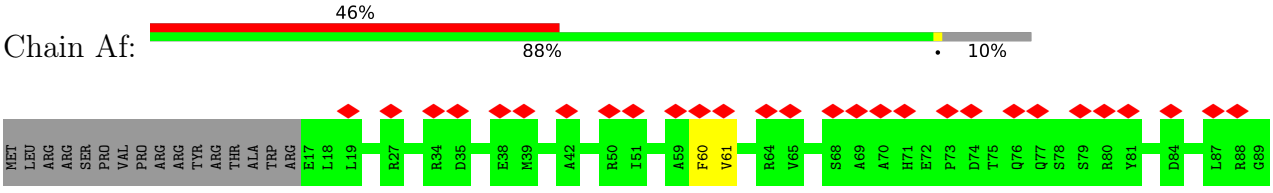
• Molecule 108: mL88

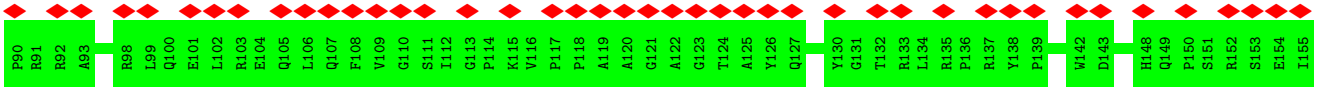
Chain Av:



• Molecule 109: mL63

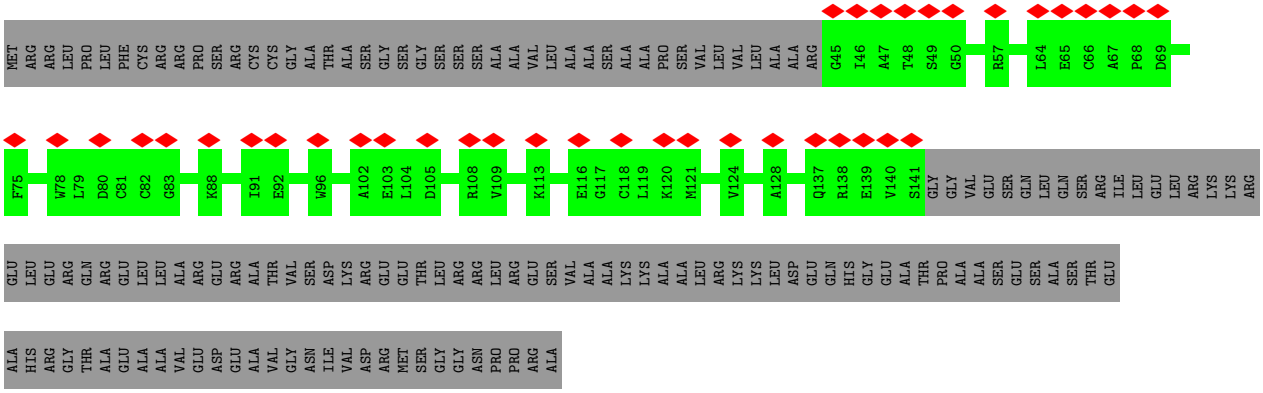
Chain Af:





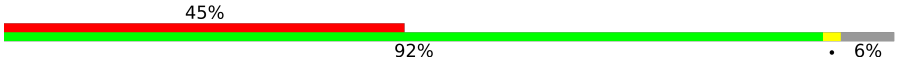
• Molecule 110: mL85

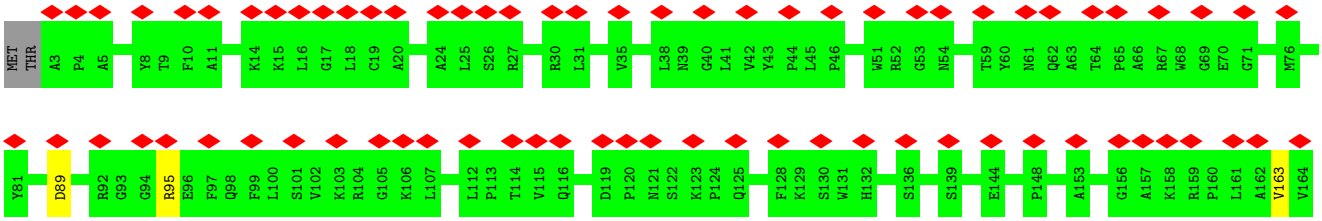
Chain As:



• Molecule 111: mL53

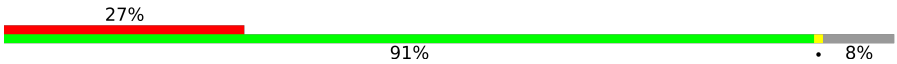
Chain Ae:

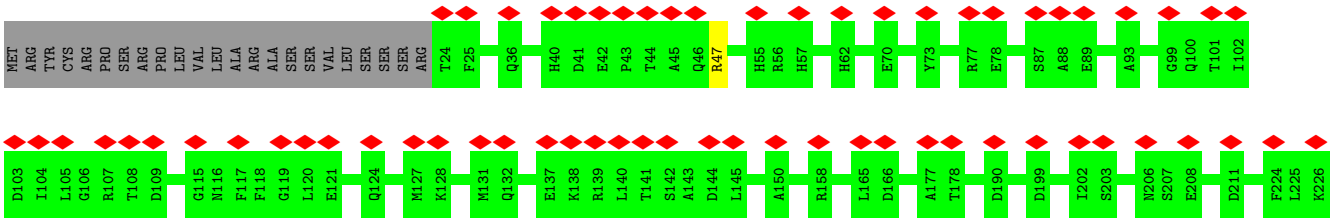


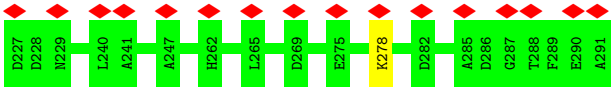


• Molecule 112: MRP-L46 domain-containing protein

Chain Ac:

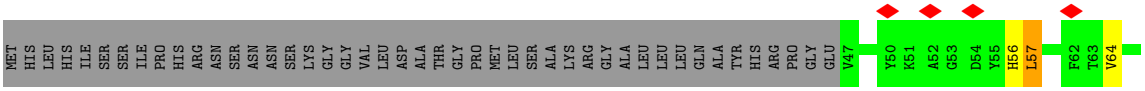


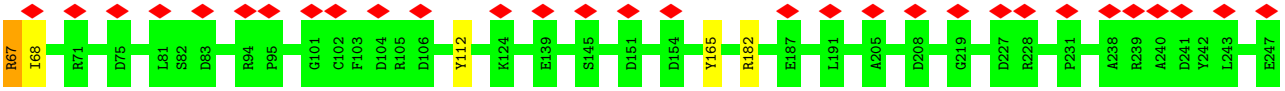


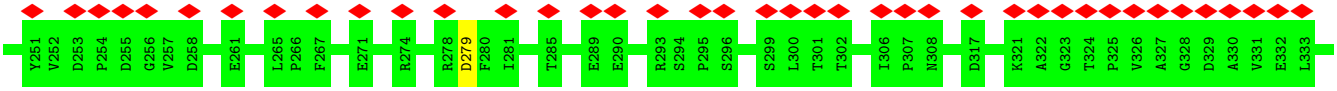


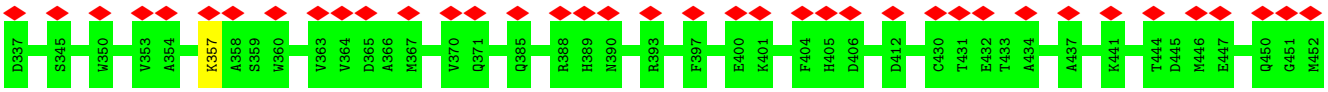
• Molecule 113: mL68

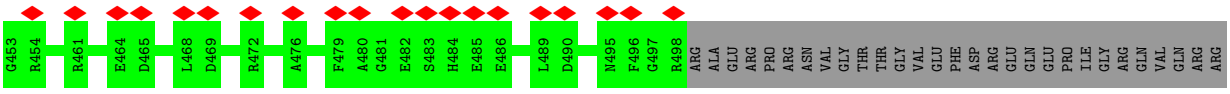
Chain Ah:





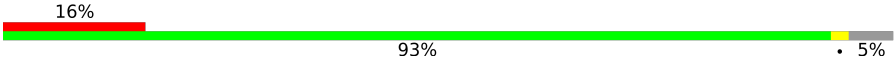






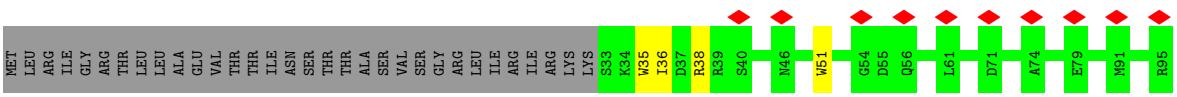
• Molecule 114: mL97

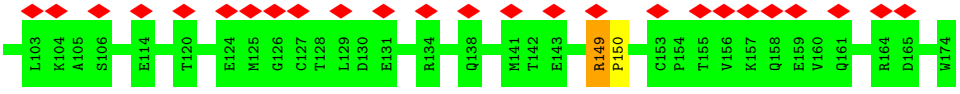
Chain BD:



• Molecule 115: C2H2-type domain-containing protein

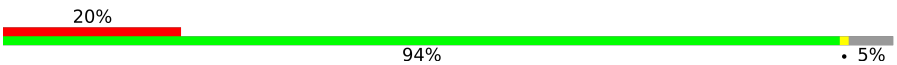
Chain Ay:

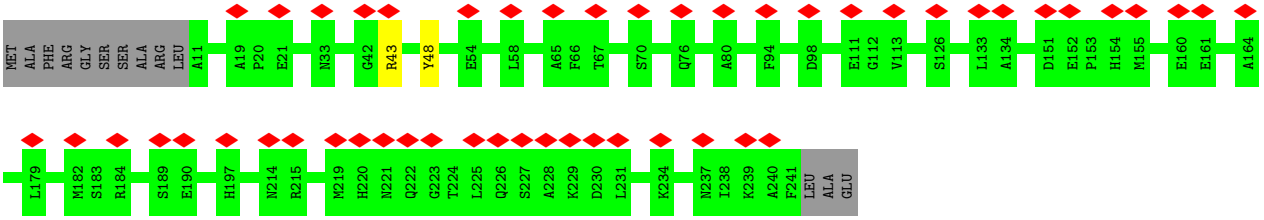




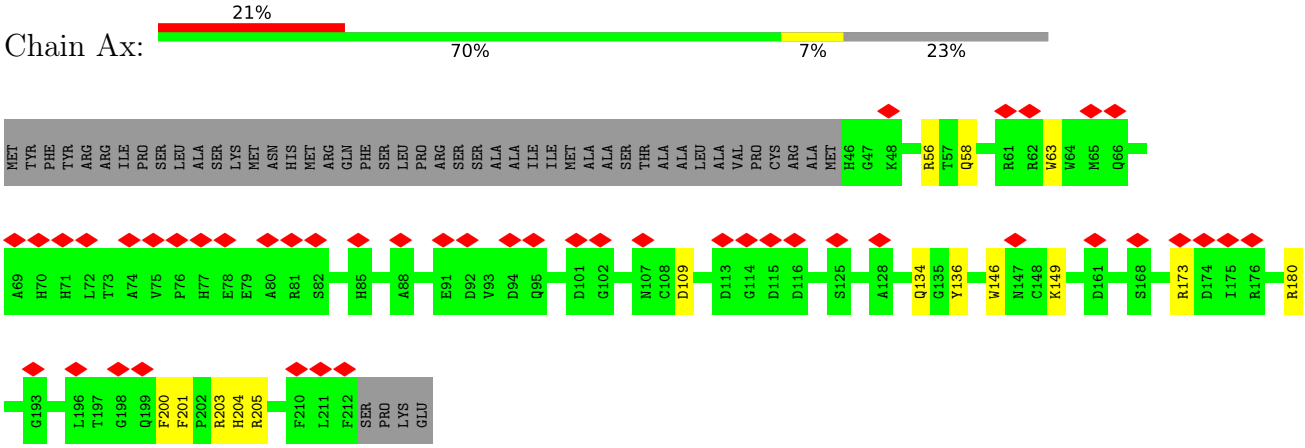
• Molecule 116: mL59/64

Chain Ag:

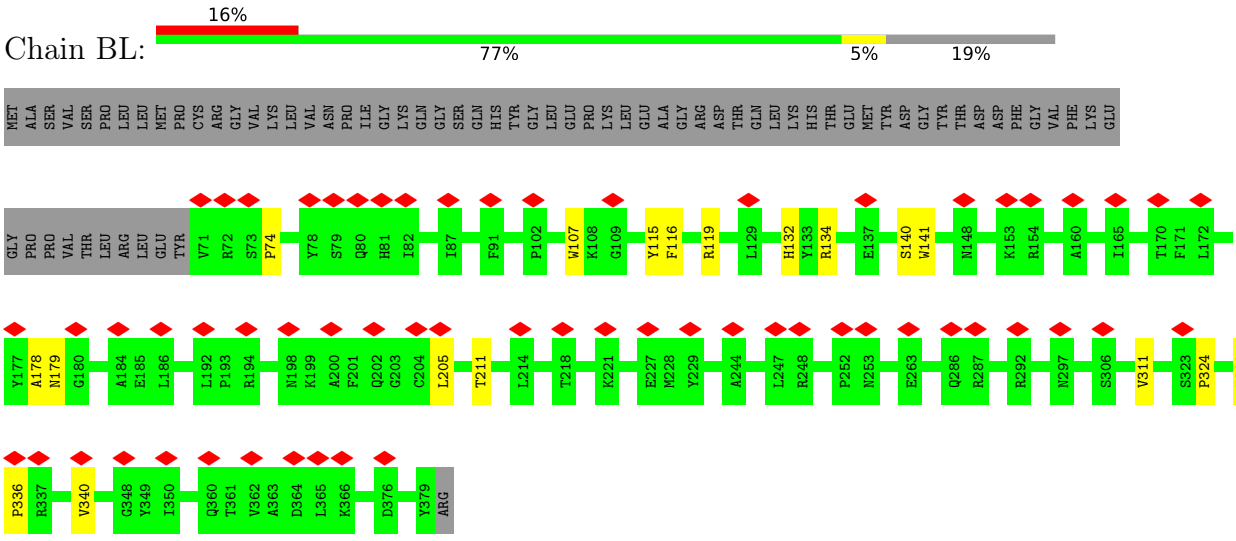




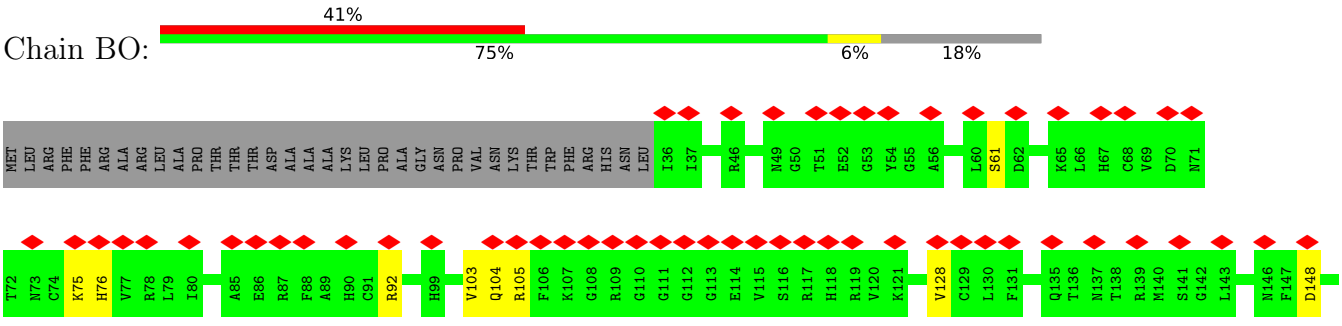
• Molecule 117: LIM zinc-binding domain-containing protein



• Molecule 118: Putative ribosomal protein L2

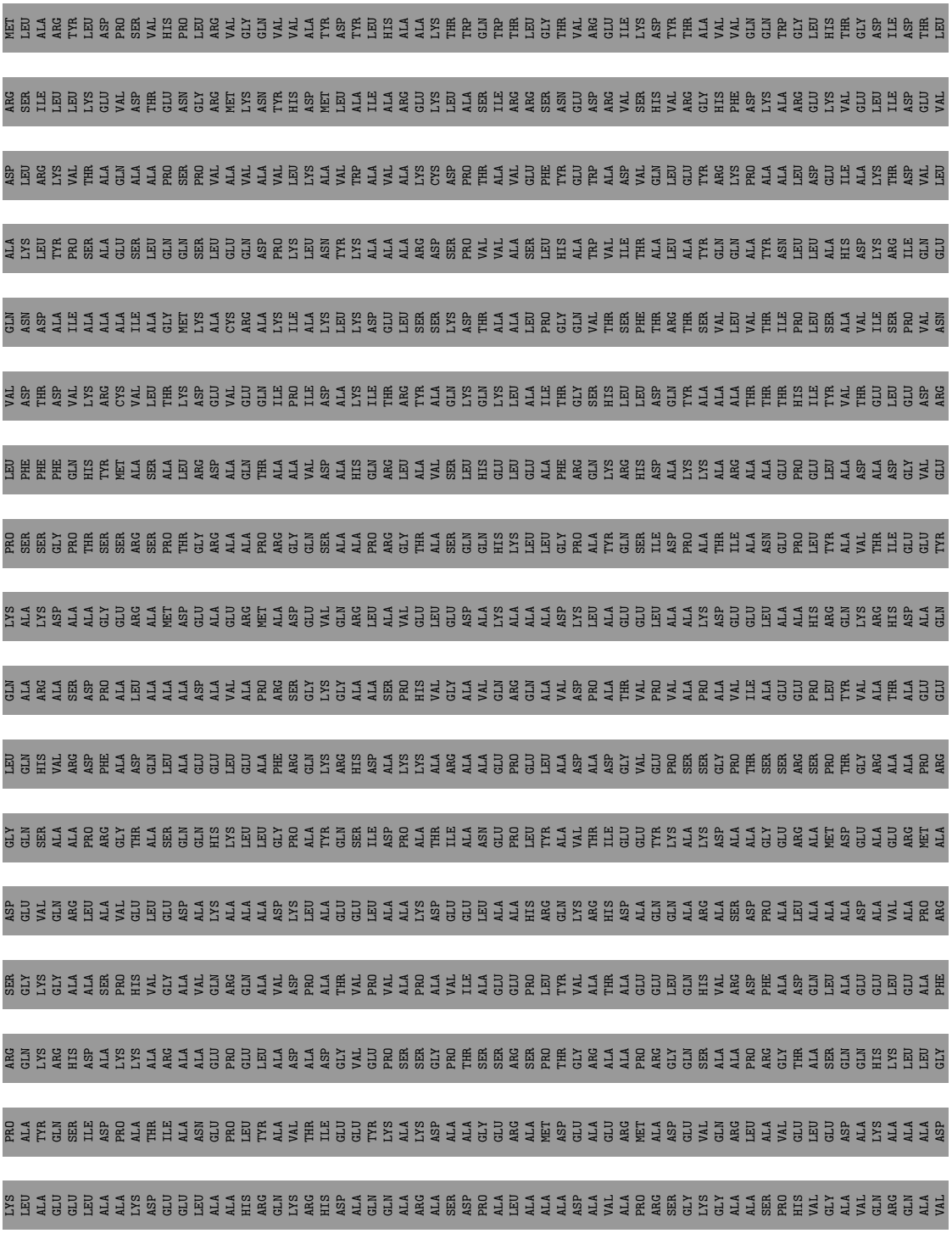


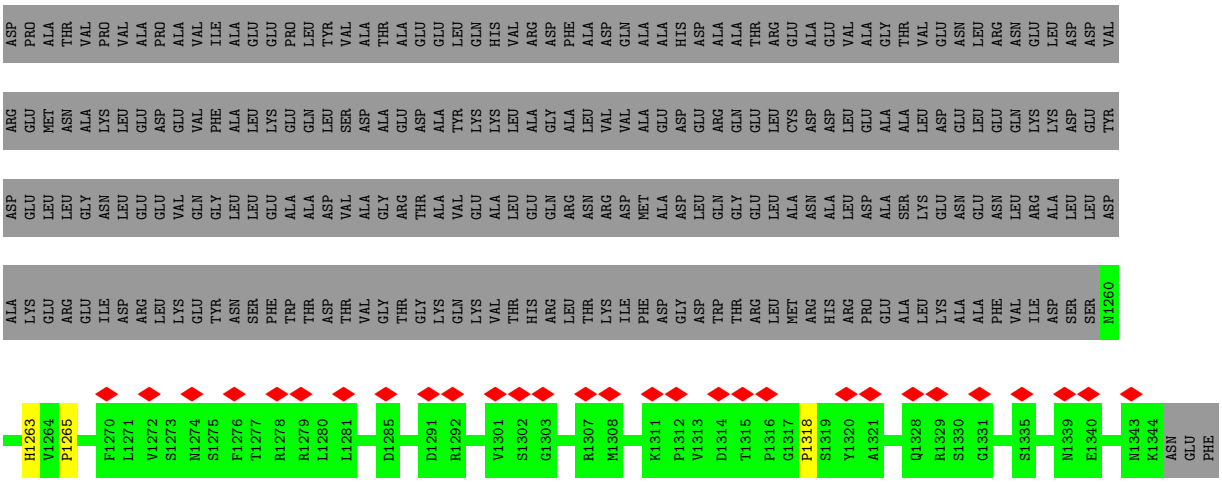
• Molecule 119: Putative ribosomal protein L14



• Molecule 120: mL100

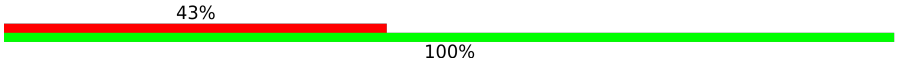
Chain BG:

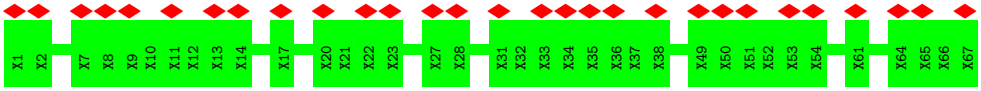

MET LEU ALA ARG TYR LEU ASP PRO SER VAL HIS PRO LEU ARG VAL GLY GLN VAL VAL ALA TYR ASP TYR LEU HIS ALA ALA LYS THR TRP GLN TRP THR LEU GLY THR VAL ARG GLU ILE LYS ASP TYR THR ALA VAL VAL GLN GLN TRP GLY LEU HIS THR GLY ASP ILE ASP THR LEU
ARG SER ILE LEU LEU LYS GLU VAL ASP THR GLU ASN GLY ARG MET LYS ASN TYR HIS ASP MET LEU ALA ILE ALA ARG GLU LYS LEU ALA SER ILE ARG ARG SER ASN GLU ASP ARG VAL SER HIS VAL ARG GLY HIS PHE ASP LYS ALA ALA ARG GLU LYS VAL GLU LEU ILE ASP GLU VAL
ASP LEU ARG LYS VAL THR ALA GLN ALA ALA PRO SER PRO VAL ALA VAL ALA VAL ALA LEU LYS ALA VAL ALA LYS CYS ASP PRO THR ALA VAL GLU PHE TYR GLU TRP ALA ASP VAL GLN LEU GLU TYR ARG LYS PRO ALA ALA LEU ASP GLU ILE ALA LYS THR ASP VAL LEU
ALA LYS LEU TYR PRO SER ALA GLU GLN LEU SER LEU GLU GLN GLN SER LEU ASN TYR LYS ALA ALA ALA ARG ASP SER PRO VAL VAL ALA SER LEU HIS ALA TRP VAL ILE THR ALA LEU ALA TYR GLN GLN ALA TYR ASN LEU LEU LEU ALA HIS ASP LYS ARG ILE GLN GLU
GLN ASN ASP ALA ILE ALA ALA ALA ILE ALA GLY MET LYS ALA CYS ARG ALA ALA LYS ILE ALA LYS LEU LYS ASP GLU LEU SER SER LYS ASP THR ALA ALA LEU PRO GLY GLN VAL THR SER PHE THR ARG THR SER VAL LEU VAL THR ILE PRO LEU SER ALA VAL ILE SER PRO VAL ASN
VAL ASP THR ASP VAL LYS ARG CYS VAL LEU THR LYS ASP GLU VAL GLU GLN ILE PRO ILE ASP ALA LYS ILE LEU THR ARG TYR ALA GLN LYS GLN LYS LEU ALA ILE THR GLY SER HIS LEU LEU LEU ASP GLN TYR ALA ALA ALA THR THR THR HIS ILE TYR VAL THR GLU LEU GLU ASP ARG
LEU PHE PHE PHE GLN HIS TYR MET ALA SER ALA LEU ARG ASP ALA GLN THR ALA ALA VAL ASP ALA HIS GLN ARG LEU ALA VAL SER LEU HIS GLU LEU GLU ALA PHE ARG GLN LYS LYS ALA ARG ALA ALA GLU PRO GLU LEU ALA ASP ALA ASP GLY VAL GLU
PRO SER SER GLY PRO THR SER SER ARG SER PRO THR GLY ARG ALA ALA PRO ARG GLY GLN SER ALA ALA PRO ARG GLY THR ALA SER GLN GLN HIS LYS LEU LEU GLY PRO ALA TYR GLN SER ILE ASP PRO ALA THR ILE ALA ASN GLU PRO LEU TYR ALA VAL THR ILE GLU GLU TYR
LYS ALA LYS ASP ALA ALA GLY GLU ARG ALA MET MET ASP GLU ALA GLU ARG MET ALA ASP GLU VAL GLN ARG LEU ALA VAL GLU LEU GLU ASP ALA LYS ALA LYS LEU ALA GLU GLU LEU ALA ALA ASP ASP LYS LEU ALA ALA ASP ASP LYS LEU ALA GLU GLU



- Molecule 121: UB

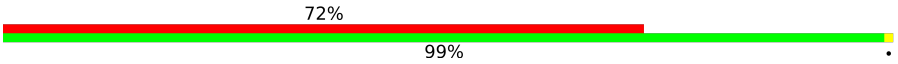
Chain UB:

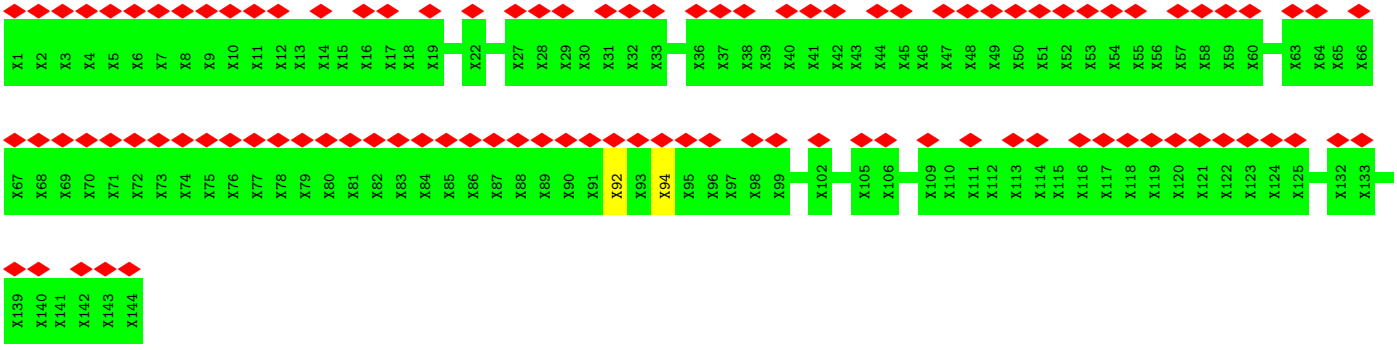




- Molecule 122: UC

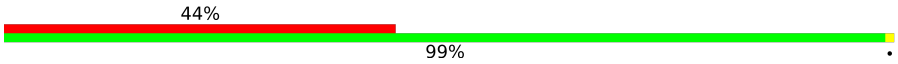
Chain UC:

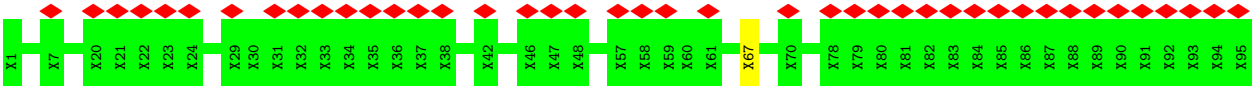




- Molecule 123: UD

Chain UD:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82060	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	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	0.195	Depositor
Minimum map value	-0.108	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	476.00003, 476.00003, 476.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAD, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.91	7/25559 (0.0%)	1.09	102/39736 (0.3%)
1	2	0.89	81/14217 (0.6%)	1.04	51/22099 (0.2%)
2	h	0.32	0/1347	0.42	0/1819
3	aw	0.32	0/1172	0.44	0/1578
4	m	0.31	0/2437	0.44	0/3300
5	f	0.29	0/1239	0.48	0/1660
6	s	0.31	0/1389	0.43	0/1877
7	au	0.30	0/2140	0.41	0/2899
8	am	0.32	0/2252	0.46	0/3035
9	n	0.29	0/1209	0.45	0/1625
10	ae	0.29	0/4698	0.44	0/6385
11	ay	0.31	0/1223	0.42	0/1653
12	ag	0.30	0/4627	0.43	0/6260
13	aj	0.29	0/2641	0.41	0/3591
14	e	0.32	0/6598	0.45	0/8991
15	d	0.31	0/2771	0.42	0/3733
16	az	0.33	0/1343	0.42	0/1815
17	ax	0.29	0/1405	0.42	0/1906
18	r	0.31	0/3818	0.42	0/5177
19	af	0.29	0/4802	0.42	0/6515
20	u	0.29	0/5673	0.44	0/7675
21	aa	0.28	0/12362	0.43	0/16747
22	ab	0.30	0/9432	0.44	0/12775
23	ak	0.28	0/2187	0.43	0/2963
24	ac	0.27	0/8897	0.46	3/12093 (0.0%)
25	ad	0.38	1/5837 (0.0%)	0.46	4/7913 (0.1%)
26	an	0.30	0/2545	0.44	0/3443
27	ao	0.30	0/1574	0.47	0/2141
28	ap	0.29	0/1927	0.45	0/2593
29	aq	0.27	0/1847	0.43	0/2506
30	as	2.26	6/2013 (0.3%)	0.57	4/2745 (0.1%)
31	at	0.27	0/1664	0.52	2/2243 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	y	0.28	0/2191	0.44	0/2965
33	w	0.27	0/1315	0.43	0/1787
34	v	0.26	0/490	0.45	0/656
35	t	0.28	0/1826	0.46	0/2488
36	p	0.32	0/2002	0.43	0/2704
37	j	0.29	0/1553	0.44	0/2098
38	l	0.28	0/4544	0.45	1/6158 (0.0%)
39	ar	0.27	0/2038	0.45	0/2758
40	av	0.28	0/1265	0.50	0/1716
41	ai	0.29	0/3133	0.45	1/4241 (0.0%)
42	x	0.33	0/2091	0.44	0/2844
43	i	0.30	0/2271	0.42	0/3065
44	g	0.26	0/834	0.37	0/1115
45	o	1.17	1/3847 (0.0%)	0.45	2/5196 (0.0%)
46	c	0.31	0/2084	0.44	0/2815
47	k	0.33	0/977	0.45	0/1319
48	q	0.31	0/1748	0.42	0/2354
49	b	0.32	0/1319	0.47	0/1787
50	a	0.90	6/3377 (0.2%)	0.48	0/4558
51	ba	0.24	0/232	0.39	0/314
52	z	0.30	0/7898	0.44	0/10712
53	bd	0.38	0/358	0.62	0/487
54	A	0.58	0/3098	0.53	0/4217
55	B	0.52	0/3623	0.54	1/4931 (0.0%)
56	C	0.52	0/1831	0.53	0/2498
57	D	0.42	0/1062	0.53	0/1438
58	E	0.41	0/2734	0.48	0/3687
59	F	0.52	0/1485	0.56	1/2019 (0.0%)
60	G	0.51	0/3110	0.56	1/4223 (0.0%)
61	H	0.46	0/1338	0.57	0/1808
62	I	0.50	0/2220	0.53	0/2998
63	J	0.48	0/1175	0.61	1/1582 (0.1%)
64	K	0.46	0/1499	0.50	0/2026
65	L	0.52	0/1452	0.55	0/1970
66	M	0.50	0/2168	0.60	1/2928 (0.0%)
67	N	0.55	0/1650	0.51	0/2242
68	O	0.41	0/2591	0.54	1/3507 (0.0%)
69	P	0.51	0/1402	0.52	0/1892
70	Q	0.50	0/1827	0.52	0/2463
71	R	0.44	0/3852	0.49	0/5243
72	S	0.48	0/1271	0.50	0/1712
73	T	0.50	0/501	0.48	0/665
74	U	0.49	0/756	0.73	1/1011 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	V	0.56	0/1231	0.56	0/1645
76	W	0.51	0/483	0.69	0/657
77	X	0.49	0/3846	0.56	3/5250 (0.1%)
78	Y	0.40	0/2116	0.46	0/2866
79	Z	0.53	0/1268	0.66	0/1725
80	BA	0.42	0/1056	0.59	0/1435
82	BB	0.53	0/1061	0.60	0/1438
83	Aw	0.50	0/1552	0.52	0/2107
84	Bj	0.45	0/1389	0.50	0/1878
85	An	0.49	0/2677	0.61	0/3633
86	Al	0.49	0/2212	0.56	0/3013
87	BI	0.42	0/1440	0.53	0/1953
88	Az	0.61	0/1259	0.53	0/1700
89	At	0.45	0/1373	0.51	1/1848 (0.1%)
90	BC	0.38	0/1135	0.49	0/1532
91	Ab	0.48	0/2249	0.49	0/3044
92	Ai	0.48	0/3879	0.51	0/5258
93	Ap	0.40	0/1819	0.47	0/2458
94	Au	0.53	0/1542	0.62	0/2082
95	Aa	0.52	1/1454 (0.1%)	0.63	1/1968 (0.1%)
96	Ao	0.52	0/2351	0.55	0/3196
97	BM	0.30	0/3136	0.51	0/4259
98	Ar	0.55	0/1689	0.54	0/2280
99	Aj	0.47	0/2826	0.50	0/3807
100	BH	0.50	0/1700	0.53	0/2301
101	Am	0.48	0/2791	0.52	1/3775 (0.0%)
102	Aq	0.44	0/2128	0.59	1/2876 (0.0%)
103	BE	0.47	0/723	0.63	0/981
104	Ak	0.38	0/2403	0.50	0/3265
105	BP	0.48	0/1648	0.55	0/2238
106	Ad	0.52	0/1682	0.60	0/2283
107	BF	0.47	0/871	0.52	0/1170
108	Av	0.40	0/1335	0.48	0/1797
109	Af	0.48	0/1165	0.55	0/1585
110	As	0.42	0/804	0.53	0/1093
111	Ae	0.48	0/2441	0.51	0/3324
112	Ac	0.41	0/2236	0.49	0/3038
113	Ah	0.44	0/3780	0.55	1/5125 (0.0%)
114	BD	0.49	0/826	0.47	0/1109
115	Ay	0.49	0/1269	0.52	0/1724
116	Ag	0.52	0/1968	0.50	0/2661
117	Ax	0.56	0/1439	0.79	3/1952 (0.2%)
118	BL	0.53	0/2572	0.65	1/3482 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
119	BO	0.51	0/1266	0.67	0/1702
120	BG	0.46	0/657	0.68	0/888
All	All	0.54	103/311630 (0.0%)	0.61	189/430089 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	2	0
1	2	1	1
4	m	0	1
10	ae	0	1
12	ag	0	1
14	e	0	1
20	u	0	2
24	ac	0	6
25	ad	0	3
26	an	0	3
27	ao	0	1
28	ap	0	1
32	y	0	1
36	p	0	1
38	l	0	1
42	x	0	1
49	b	0	1
50	a	0	1
52	z	0	2
53	bd	0	1
54	A	0	1
56	C	0	1
59	F	0	1
62	I	0	1
65	L	0	1
71	R	0	2
79	Z	0	1
80	BA	0	2
81	UA	0	2
82	BB	0	2
84	Bj	0	1
85	An	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
94	Au	0	3
96	Ao	0	1
101	Am	0	1
102	Aq	0	2
103	BE	0	3
104	Ak	0	1
106	Ad	0	1
109	Af	0	1
115	Ay	0	1
118	BL	0	3
119	BO	0	5
122	UC	0	2
123	UD	0	1
All	All	3	72

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	as	215	TRP	CE3-CZ3	72.01	2.60	1.38
45	o	132	ARG	CB-CG	70.18	3.42	1.52
30	as	215	TRP	CZ3-CH2	45.96	2.13	1.40
30	as	215	TRP	CE2-CZ2	32.69	1.95	1.39
50	a	349	TRP	CE3-CZ3	32.57	1.93	1.38
30	as	215	TRP	CD2-CE2	29.79	1.77	1.41
50	a	349	TRP	CZ3-CH2	22.17	1.75	1.40
30	as	215	TRP	CZ2-CH2	21.23	1.77	1.37
30	as	215	TRP	CD2-CE3	20.28	1.70	1.40
25	ad	536	THR	CA-C	18.69	2.01	1.52
50	a	349	TRP	CE2-CZ2	18.11	1.70	1.39
50	a	349	TRP	CD2-CE2	16.21	1.60	1.41
50	a	349	TRP	CZ2-CH2	11.24	1.58	1.37
1	2	144	C	O3'-P	-11.23	1.47	1.61
50	a	349	TRP	CD2-CE3	10.82	1.56	1.40
95	Aa	193	TYR	N-CA	10.02	1.66	1.46
1	2	536	A	O3'-P	-9.08	1.50	1.61
1	2	438	G	O3'-P	7.99	1.70	1.61
1	2	147	U	O3'-P	-7.95	1.51	1.61
1	2	369	G	C1'-N9	-7.47	1.36	1.46
1	1	654	A	N9-C4	-7.40	1.33	1.37
1	2	89	U	O3'-P	-7.36	1.52	1.61
1	2	166	G	C1'-N9	-7.29	1.36	1.46
1	2	168	G	C1'-N9	-7.24	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	95	G	O3'-P	-7.21	1.52	1.61
1	2	63	G	C1'-N9	-7.19	1.36	1.46
1	2	105	A	O3'-P	-6.74	1.53	1.61
1	2	480	A	O3'-P	-6.70	1.53	1.61
1	2	90	A	C1'-N9	-6.64	1.37	1.46
1	2	50	U	O3'-P	6.63	1.69	1.61
1	2	582	A	O3'-P	-6.57	1.53	1.61
1	1	886	A	N9-C4	-6.49	1.33	1.37
1	2	201	A	C1'-N9	-6.40	1.37	1.46
1	2	108	A	O3'-P	-6.38	1.53	1.61
1	2	164	A	C1'-N9	-6.21	1.38	1.46
1	2	180	A	C1'-N9	-6.21	1.38	1.46
1	2	382	A	C1'-N9	-6.17	1.38	1.46
1	2	160	G	O3'-P	-6.15	1.53	1.61
1	2	499	A	O3'-P	-6.15	1.53	1.61
1	2	199	A	C1'-N9	-6.13	1.38	1.46
1	2	326	U	O3'-P	-6.11	1.53	1.61
1	2	121	C	O3'-P	-6.08	1.53	1.61
1	2	204	A	C1'-N9	-6.01	1.38	1.46
1	2	292	A	C1'-N9	-6.01	1.38	1.46
1	2	218	A	O3'-P	-6.00	1.53	1.61
1	2	89	U	C1'-N1	5.95	1.57	1.48
1	2	90	A	O3'-P	-5.93	1.54	1.61
1	2	369	G	O3'-P	-5.89	1.54	1.61
1	2	368	U	O3'-P	-5.87	1.54	1.61
1	2	172	A	O3'-P	-5.85	1.54	1.61
1	2	4	A	C1'-N9	-5.84	1.38	1.46
1	2	327	U	O3'-P	-5.83	1.54	1.61
1	2	596	U	O3'-P	-5.80	1.54	1.61
1	2	145	U	O3'-P	-5.79	1.54	1.61
1	2	322	A	C1'-N9	-5.78	1.38	1.46
1	2	447	A	C1'-N9	-5.78	1.38	1.46
1	2	82	A	C1'-N9	-5.78	1.38	1.46
1	1	799	A	N9-C4	-5.76	1.34	1.37
1	2	460	A	C1'-N9	-5.75	1.38	1.46
1	2	68	A	C1'-N9	-5.75	1.38	1.46
1	2	363	A	C1'-N9	-5.72	1.38	1.46
1	1	814	A	N9-C4	-5.70	1.34	1.37
1	2	309	A	O3'-P	-5.69	1.54	1.61
1	2	439	A	O3'-P	-5.67	1.54	1.61
1	1	898	A	N9-C4	-5.67	1.34	1.37
1	2	118	A	O3'-P	-5.65	1.54	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	69	A	C1'-N9	-5.62	1.39	1.46
1	2	319	A	C1'-N9	-5.60	1.39	1.46
1	2	69	A	O3'-P	-5.59	1.54	1.61
1	2	207	A	C1'-N9	-5.58	1.39	1.46
1	2	149	A	C1'-N9	-5.55	1.39	1.46
1	2	189	A	C1'-N9	-5.55	1.39	1.46
1	2	384	U	O3'-P	-5.54	1.54	1.61
1	2	608	U	O3'-P	-5.46	1.54	1.61
1	2	178	U	O3'-P	-5.40	1.54	1.61
1	1	880	A	N9-C4	-5.39	1.34	1.37
1	2	442	A	C1'-N9	-5.36	1.39	1.46
1	2	329	U	O3'-P	-5.33	1.54	1.61
1	2	209	U	C1'-N1	5.31	1.56	1.48
1	2	552	C	O3'-P	-5.31	1.54	1.61
1	2	230	C	O3'-P	-5.30	1.54	1.61
1	2	96	G	O3'-P	-5.29	1.54	1.61
1	1	863	A	N9-C4	-5.26	1.34	1.37
1	2	42	U	C1'-N1	5.25	1.56	1.48
1	2	272	U	O3'-P	-5.25	1.54	1.61
1	2	254	U	O3'-P	-5.24	1.54	1.61
1	2	299	U	O3'-P	-5.24	1.54	1.61
1	2	169	U	C1'-N1	5.22	1.56	1.48
1	2	68	A	O3'-P	-5.18	1.54	1.61
1	2	375	A	O3'-P	-5.16	1.54	1.61
1	2	320	U	C1'-N1	5.15	1.56	1.48
1	2	88	U	O3'-P	-5.14	1.54	1.61
1	2	323	U	C1'-N1	5.13	1.56	1.48
1	2	321	U	C1'-N1	5.12	1.56	1.48
1	2	294	A	C1'-N9	-5.12	1.39	1.46
1	2	164	A	O3'-P	-5.11	1.55	1.61
1	2	551	A	O3'-P	-5.08	1.55	1.61
1	2	298	U	O3'-P	-5.08	1.55	1.61
1	2	197	A	O3'-P	-5.05	1.55	1.61
1	2	116	U	O3'-P	-5.05	1.55	1.61
1	2	474	U	O3'-P	-5.04	1.55	1.61
1	2	94	A	O3'-P	-5.02	1.55	1.61
1	2	472	A	O3'-P	-5.01	1.55	1.61

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	438	G	N9-C1'-C2'	-17.25	91.57	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	136	A	C2'-C3'-O3'	-17.05	71.99	109.50
1	2	438	G	C4'-C3'-O3'	12.40	137.80	113.00
1	1	146	U	N1-C1'-C2'	-11.88	98.56	114.00
1	2	529	A	N9-C1'-C2'	11.32	128.72	114.00
30	as	215	TRP	CE3-CZ3-CH2	-11.15	108.94	121.20
25	ad	536	THR	O-C-N	-9.75	107.11	122.70
1	1	359	C	C2-N1-C1'	9.27	129.00	118.80
1	1	347	A	N1-C6-N6	8.81	123.89	118.60
1	2	438	G	C8-N9-C1'	-8.55	115.89	127.00
1	1	359	C	N1-C2-O2	8.38	123.93	118.90
31	at	315	CYS	CA-CB-SG	8.37	129.07	114.00
1	2	166	G	O5'-P-OP2	-8.25	98.28	105.70
1	2	166	G	O5'-P-OP1	8.23	120.57	110.70
1	2	106	U	C2'-C3'-O3'	8.11	127.34	109.50
1	1	42	A	C4'-C3'-O3'	8.02	129.03	113.00
1	2	93	U	P-O3'-C3'	-7.98	110.12	119.70
1	1	411	U	C2-N1-C1'	7.86	127.13	117.70
1	1	136	A	C5'-C4'-O4'	-7.69	99.88	109.10
45	o	132	ARG	CA-CB-CG	7.66	130.26	113.40
117	Ax	200	PHE	CB-CA-C	7.66	125.72	110.40
25	ad	536	THR	N-CA-CB	-7.58	95.90	110.30
1	2	529	A	O4'-C1'-N9	7.52	114.22	108.20
1	2	144	C	P-O3'-C3'	-7.42	110.80	119.70
1	2	450	A	C4'-C3'-O3'	7.42	127.84	113.00
1	1	286	G	N3-C4-C5	7.37	132.29	128.60
45	o	132	ARG	CB-CG-CD	7.33	130.66	111.60
1	2	529	A	C3'-C2'-C1'	7.32	107.36	101.50
1	1	1105	G	C6-C5-N7	-7.30	126.02	130.40
66	M	14	PRO	N-CA-CB	-7.26	94.59	103.30
1	1	347	A	C6-C5-N7	-7.21	127.26	132.30
30	as	215	TRP	CH2-CZ2-CE2	7.14	124.54	117.40
1	1	359	C	C6-N1-C1'	-7.10	112.28	120.80
1	1	282	U	C4'-C3'-O3'	-7.09	94.52	109.40
1	2	165	A	C4'-C3'-O3'	-7.07	94.56	109.40
1	1	112	U	C2-N1-C1'	7.04	126.15	117.70
1	1	286	G	N3-C4-N9	-7.03	121.78	126.00
59	F	158	PRO	N-CA-C	-7.02	93.84	112.10
1	2	325	U	C2'-C3'-O3'	-7.01	94.07	109.50
1	2	559	U	C2'-C3'-O3'	7.01	124.92	109.50
1	2	94	A	O5'-P-OP2	-6.98	99.42	105.70
77	X	353	PRO	CA-N-CD	-6.97	101.74	111.50
1	1	921	G	N3-C4-N9	-6.95	121.83	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	ac	685	LEU	N-CA-C	6.92	129.69	111.00
1	1	1045	U	N3-C2-O2	-6.89	117.38	122.20
1	1	41	A	N9-C1'-C2'	-6.83	104.49	112.00
1	2	167	U	N1-C1'-C2'	6.79	122.83	114.00
1	2	520	A	N9-C1'-C2'	-6.71	104.62	112.00
1	2	529	A	C3'-C2'-O2'	6.70	132.73	113.30
1	2	255	U	C2'-C3'-O3'	6.66	124.36	113.70
1	1	974	U	C2-N1-C1'	6.66	125.69	117.70
1	2	529	A	C4'-C3'-O3'	-6.64	95.46	109.40
1	1	286	G	C2-N3-C4	-6.63	108.58	111.90
77	X	353	PRO	N-CA-CB	-6.60	95.34	102.60
60	G	149	PRO	N-CA-CB	-6.56	95.39	102.60
1	2	82	A	C4'-C3'-O3'	6.54	126.07	113.00
101	Am	324	ILE	C-N-CA	6.53	138.01	121.70
1	1	782	U	N1-C2-O2	6.51	127.36	122.80
1	1	359	C	C5-C6-N1	6.48	124.24	121.00
63	J	66	PRO	N-CA-CB	-6.43	95.52	102.60
1	1	347	A	O4'-C1'-N9	-6.39	103.09	108.20
1	2	308	U	C2'-C3'-O3'	-6.34	95.55	109.50
1	1	347	A	C4-C5-N7	6.34	113.87	110.70
25	ad	536	THR	CB-CA-C	6.33	128.70	111.60
1	2	490	A	N9-C1'-C2'	-6.29	105.08	112.00
95	Aa	192	LEU	C-N-CA	6.29	137.43	121.70
1	1	925	G	N7-C8-N9	6.27	116.24	113.10
1	1	554	G	O4'-C1'-N9	6.26	113.21	108.20
1	1	411	U	N1-C2-O2	6.25	127.17	122.80
1	1	1045	U	N1-C2-O2	6.22	127.15	122.80
1	1	816	C	N1-C2-O2	6.22	122.63	118.90
1	2	166	G	C5'-C4'-O4'	6.21	116.56	109.10
1	1	1105	G	N1-C2-N2	-6.19	110.63	116.20
1	2	438	G	C4-N9-C1'	6.13	134.47	126.50
1	1	1045	U	C2-N1-C1'	6.13	125.05	117.70
1	2	450	A	N9-C1'-C2'	-6.12	105.26	112.00
1	1	974	U	N3-C2-O2	-6.12	117.92	122.20
1	2	390	U	C2'-C3'-O3'	6.11	123.48	113.70
117	Ax	201	PHE	CB-CA-C	-6.11	98.18	110.40
1	1	136	A	C4'-C3'-O3'	6.07	125.14	113.00
68	O	27	TYR	CB-CA-C	6.05	122.51	110.40
1	1	782	U	C2-N1-C1'	6.04	124.95	117.70
1	1	284	A	OP1-P-O3'	6.00	118.40	105.20
1	2	402	A	N9-C1'-C2'	-5.96	105.45	112.00
1	1	1105	G	C2-N3-C4	-5.92	108.94	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1105	G	C4-N9-C1'	5.92	134.19	126.50
1	1	179	U	N1-C2-O2	5.91	126.94	122.80
1	2	418	A	N9-C1'-C2'	5.91	121.69	114.00
1	2	438	G	C2'-C3'-O3'	-5.90	96.52	109.50
1	1	654	A	C2-N3-C4	-5.87	107.67	110.60
1	2	164	A	C3'-C2'-O2'	-5.85	96.33	113.30
1	1	411	U	N3-C2-O2	-5.85	118.10	122.20
1	2	413	U	O5'-P-OP1	-5.85	100.44	105.70
1	1	179	U	C2-N1-C1'	5.83	124.70	117.70
1	1	50	A	P-O3'-C3'	5.82	126.69	119.70
1	1	433	G	N9-C4-C5	-5.82	103.07	105.40
1	1	974	U	N1-C2-O2	5.82	126.87	122.80
1	1	921	G	N3-C4-C5	5.81	131.50	128.60
1	1	433	G	C4-C5-N7	5.81	113.12	110.80
1	1	458	A	N7-C8-N9	5.80	116.70	113.80
1	1	1105	G	N7-C8-N9	5.79	116.00	113.10
1	1	347	A	C5-C6-N6	-5.79	119.07	123.70
1	1	1105	G	N1-C2-N3	5.77	127.36	123.90
1	1	928	U	P-O3'-C3'	5.76	126.61	119.70
1	1	347	A	N9-C4-C5	-5.75	103.50	105.80
1	2	437	U	N1-C1'-C2'	-5.72	105.71	112.00
1	1	855	A	N1-C2-N3	5.70	132.15	129.30
1	1	816	C	N3-C2-O2	-5.68	117.92	121.90
1	1	558	C	C2-N1-C1'	5.67	125.04	118.80
1	1	782	U	N3-C2-O2	-5.66	118.24	122.20
24	ac	685	LEU	CB-CA-C	-5.66	99.45	110.20
1	1	906	C	C4'-C3'-O3'	-5.66	97.52	109.40
1	1	781	A	P-O3'-C3'	5.65	126.48	119.70
1	1	814	A	C2-N3-C4	-5.65	107.78	110.60
1	1	650	U	C2-N1-C1'	5.63	124.46	117.70
74	U	37	ASN	CB-CA-C	5.59	121.59	110.40
1	1	1126	A	P-O3'-C3'	5.59	126.41	119.70
1	1	130	U	N1-C2-O2	5.55	126.68	122.80
102	Aq	340	TYR	CB-CA-C	5.54	121.47	110.40
1	1	347	A	C5-N7-C8	-5.53	101.13	103.90
1	1	916	U	OP1-P-O3'	5.52	117.35	105.20
1	1	916	U	P-O3'-C3'	5.52	126.32	119.70
1	2	144	C	C1'-C2'-O2'	-5.52	94.05	110.60
1	2	218	A	C2'-C3'-O3'	-5.51	97.38	109.50
1	1	1128	U	P-O3'-C3'	5.51	126.31	119.70
55	B	3	ASP	CB-CG-OD1	5.47	123.23	118.30
1	2	243	A	C2'-C3'-O3'	-5.45	97.51	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	50	A	OP1-P-O3'	5.45	117.19	105.20
1	2	166	G	C2'-C3'-O3'	5.45	122.41	113.70
113	Ah	57	LEU	CA-CB-CG	5.45	127.82	115.30
30	as	215	TRP	CE2-CD2-CG	-5.44	102.95	107.30
1	2	529	A	C1'-C2'-O2'	-5.43	94.31	110.60
1	1	1128	U	OP2-P-O3'	5.42	117.12	105.20
1	1	112	U	N1-C2-O2	5.42	126.59	122.80
1	2	449	A	O4'-C4'-C3'	-5.42	98.58	104.00
77	X	353	PRO	CB-CA-C	5.40	125.50	112.00
1	2	69	A	O5'-P-OP1	-5.38	100.86	105.70
1	1	554	G	C6-C5-N7	-5.38	127.17	130.40
1	1	554	G	C4-N9-C1'	5.38	133.49	126.50
1	1	130	U	N3-C2-O2	-5.37	118.44	122.20
30	as	215	TRP	CD2-CE2-CZ2	5.36	128.73	122.30
24	ac	685	LEU	CA-CB-CG	5.34	127.58	115.30
25	ad	536	THR	CA-C-N	5.32	128.89	117.20
1	1	925	G	C8-N9-C4	-5.31	104.27	106.40
1	1	115	U	N1-C2-O2	5.31	126.52	122.80
1	1	131	U	P-O3'-C3'	5.30	126.06	119.70
1	1	1114	A	N1-C2-N3	5.30	131.95	129.30
1	1	943	U	C2-N1-C1'	5.29	124.05	117.70
1	1	1044	U	N3-C2-O2	-5.29	118.50	122.20
1	2	505	U	O4'-C1'-N1	5.28	112.42	108.20
1	1	949	U	N3-C2-O2	-5.28	118.50	122.20
1	1	691	G	N3-C4-C5	5.28	131.24	128.60
89	At	165	GLU	C-N-CA	5.28	134.89	121.70
1	2	136	U	P-O3'-C3'	-5.27	113.38	119.70
1	2	371	C	N1-C1'-C2'	5.27	120.85	114.00
1	1	855	A	C2-N3-C4	-5.25	107.98	110.60
1	2	448	U	N1-C1'-C2'	5.25	120.82	114.00
1	1	433	G	O4'-C1'-N9	5.23	112.39	108.20
1	1	284	A	P-O3'-C3'	5.23	125.98	119.70
1	1	812	A	OP2-P-O3'	5.22	116.70	105.20
1	1	850	U	O4'-C1'-N1	5.21	112.37	108.20
38	l	465	LEU	CA-CB-CG	5.21	127.28	115.30
1	1	596	U	P-O3'-C3'	5.20	125.94	119.70
1	1	520	A	O5'-P-OP1	-5.19	101.03	105.70
1	1	1131	A	C2-N3-C4	-5.18	108.01	110.60
1	2	438	G	C3'-C2'-C1'	5.18	105.64	101.50
1	1	112	U	N3-C2-O2	-5.18	118.58	122.20
1	1	286	G	N3-C2-N2	-5.17	116.28	119.90
1	1	654	A	N3-C4-C5	5.17	130.42	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	907	G	C4-C5-N7	5.16	112.86	110.80
1	1	390	A	N1-C2-N3	5.13	131.86	129.30
1	1	596	U	OP1-P-O3'	5.12	116.46	105.20
1	1	411	U	C6-N1-C1'	-5.11	114.04	121.20
1	1	617	G	N3-C4-C5	-5.11	126.04	128.60
1	1	759	C	P-O3'-C3'	5.11	125.83	119.70
1	1	359	C	N3-C2-O2	-5.09	118.33	121.90
1	1	816	C	C2-N1-C1'	5.09	124.40	118.80
117	Ax	149	LYS	CB-CA-C	5.09	120.58	110.40
1	1	1088	G	N3-C4-C5	5.08	131.14	128.60
31	at	337	LEU	CA-CB-CG	5.06	126.94	115.30
1	2	313	C	O4'-C1'-N1	5.05	112.24	108.20
1	2	83	A	C2'-C3'-O3'	5.05	121.77	113.70
41	ai	259	LEU	CA-CB-CG	5.05	126.91	115.30
1	2	520	A	C4'-C3'-O3'	5.04	123.08	113.00
1	1	1114	A	C2-N3-C4	-5.04	108.08	110.60
1	1	511	A	C4'-C3'-O3'	-5.03	98.83	109.40
118	BL	205	LEU	CA-CB-CG	5.02	126.85	115.30
1	2	528	A	O5'-P-OP1	-5.01	101.19	105.70
1	2	70	A	C2'-C3'-O3'	5.00	121.71	113.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	2	529	A	C2'
1	1	136	A	C4',C3'

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	438	G	Sidechain
54	A	288	HIS	Peptide
106	Ad	36	ASP	Peptide
109	Af	60	PHE	Peptide
104	Ak	227	PRO	Peptide
101	Am	329	PRO	Peptide
85	An	49	SER	Peptide
85	An	50	HIS	Peptide
96	Ao	19	ARG	Peptide
102	Aq	171	ALA	Peptide
102	Aq	174	ARG	Peptide
94	Au	26	TYR	Peptide

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Mol	Chain	Res	Type	Group
94	Au	55	SER	Peptide
94	Au	61	PHE	Peptide
115	Ay	149	ARG	Peptide
80	BA	139	THR	Peptide
80	BA	141	VAL	Peptide
82	BB	129	THR	Peptide
82	BB	55	GLN	Peptide
103	BE	69	SER	Peptide
103	BE	78	PRO	Peptide
103	BE	79	VAL	Peptide
118	BL	178	ALA	Peptide
118	BL	179	ASN	Peptide
118	BL	336	PRO	Peptide
119	BO	103	VAL	Peptide
119	BO	104	GLN	Peptide
119	BO	183	VAL	Peptide
119	BO	75	LYS	Peptide
119	BO	76	HIS	Peptide
84	Bj	101	PRO	Peptide
56	C	142	ASN	Peptide
59	F	166	PRO	Peptide
62	I	235	TRP	Peptide
65	L	71	ARG	Peptide
71	R	125	PRO	Peptide
71	R	136	ASP	Peptide
81	UA	47	UNK	Peptide
81	UA	81	UNK	Peptide
122	UC	92	UNK	Peptide
122	UC	94	UNK	Peptide
123	UD	67	UNK	Peptide
79	Z	21	PHE	Peptide
50	a	261	ASN	Peptide
24	ac	1082	TYR	Peptide
24	ac	1086	PRO	Peptide
24	ac	1208	GLN	Peptide
24	ac	450	SER	Peptide
24	ac	514	LYS	Peptide
24	ac	515	ALA	Peptide
25	ad	413	ASP	Peptide
25	ad	418	ALA	Peptide
25	ad	521	ASP	Peptide
10	ae	425	ASP	Peptide

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Mol	Chain	Res	Type	Group
12	ag	257	VAL	Peptide
26	an	154	ALA	Peptide
26	an	160	ALA	Peptide
26	an	162	ALA	Peptide
27	ao	180	THR	Peptide
28	ap	21	ALA	Peptide
49	b	108	GLN	Peptide
53	bd	68	ALA	Peptide
14	e	291	SER	Peptide
38	l	315	TYR	Peptide
4	m	10	ASN	Peptide
36	p	269	THR	Peptide
20	u	628	GLY	Peptide
20	u	629	VAL	Peptide
42	x	69	ALA	Peptide
32	y	164	PRO	Peptide
52	z	673	ASP	Peptide
52	z	926	VAL	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	h	155/166 (93%)	148 (96%)	7 (4%)	0	100	100
3	aw	137/139 (99%)	123 (90%)	14 (10%)	0	100	100
4	m	286/325 (88%)	267 (93%)	19 (7%)	0	100	100
5	f	140/371 (38%)	118 (84%)	22 (16%)	0	100	100
6	s	163/179 (91%)	148 (91%)	15 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	au	237/247 (96%)	225 (95%)	12 (5%)	0	100	100
8	am	264/313 (84%)	242 (92%)	22 (8%)	0	100	100
9	n	140/171 (82%)	129 (92%)	11 (8%)	0	100	100
10	ae	582/655 (89%)	542 (93%)	39 (7%)	1 (0%)	44	75
11	ay	139/169 (82%)	129 (93%)	10 (7%)	0	100	100
12	ag	555/564 (98%)	520 (94%)	33 (6%)	2 (0%)	30	65
13	aj	314/397 (79%)	297 (95%)	17 (5%)	0	100	100
14	e	805/822 (98%)	736 (91%)	67 (8%)	2 (0%)	44	75
15	d	339/351 (97%)	317 (94%)	22 (6%)	0	100	100
16	az	152/163 (93%)	148 (97%)	4 (3%)	0	100	100
17	ax	159/184 (86%)	147 (92%)	12 (8%)	0	100	100
18	r	449/467 (96%)	423 (94%)	26 (6%)	0	100	100
19	af	579/835 (69%)	541 (93%)	38 (7%)	0	100	100
20	u	702/890 (79%)	652 (93%)	47 (7%)	3 (0%)	30	65
21	aa	1504/1813 (83%)	1411 (94%)	92 (6%)	1 (0%)	48	80
22	ab	1149/1177 (98%)	1070 (93%)	79 (7%)	0	100	100
23	ak	264/325 (81%)	244 (92%)	20 (8%)	0	100	100
24	ac	1108/1267 (88%)	1014 (92%)	89 (8%)	5 (0%)	25	60
25	ad	688/811 (85%)	643 (94%)	43 (6%)	2 (0%)	37	70
26	an	300/302 (99%)	272 (91%)	26 (9%)	2 (1%)	19	54
27	ao	187/291 (64%)	170 (91%)	17 (9%)	0	100	100
28	ap	238/245 (97%)	213 (90%)	25 (10%)	0	100	100
29	aq	210/295 (71%)	202 (96%)	8 (4%)	0	100	100
30	as	245/270 (91%)	213 (87%)	32 (13%)	0	100	100
31	at	202/397 (51%)	185 (92%)	17 (8%)	0	100	100
32	y	279/485 (58%)	250 (90%)	29 (10%)	0	100	100
33	w	153/190 (80%)	143 (94%)	10 (6%)	0	100	100
34	v	61/214 (28%)	55 (90%)	6 (10%)	0	100	100
35	t	224/267 (84%)	210 (94%)	14 (6%)	0	100	100
36	p	232/321 (72%)	210 (90%)	21 (9%)	1 (0%)	30	65
37	j	178/189 (94%)	158 (89%)	20 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
38	l	535/677 (79%)	489 (91%)	44 (8%)	2 (0%)	30 65
39	ar	248/282 (88%)	235 (95%)	13 (5%)	0	100 100
40	av	148/236 (63%)	124 (84%)	23 (16%)	1 (1%)	19 54
41	ai	377/379 (100%)	346 (92%)	31 (8%)	0	100 100
42	x	253/268 (94%)	236 (93%)	16 (6%)	1 (0%)	30 65
43	i	265/429 (62%)	248 (94%)	17 (6%)	0	100 100
44	g	97/192 (50%)	94 (97%)	3 (3%)	0	100 100
45	o	436/604 (72%)	412 (94%)	23 (5%)	1 (0%)	44 75
46	c	249/311 (80%)	223 (90%)	26 (10%)	0	100 100
47	k	114/312 (36%)	107 (94%)	7 (6%)	0	100 100
48	q	194/425 (46%)	189 (97%)	5 (3%)	0	100 100
49	b	153/159 (96%)	127 (83%)	25 (16%)	1 (1%)	19 54
50	a	406/431 (94%)	373 (92%)	32 (8%)	1 (0%)	44 75
51	ba	24/94 (26%)	23 (96%)	1 (4%)	0	100 100
52	z	965/1169 (82%)	891 (92%)	73 (8%)	1 (0%)	48 80
53	bd	39/89 (44%)	30 (77%)	9 (23%)	0	100 100
54	A	366/466 (78%)	311 (85%)	50 (14%)	5 (1%)	9 39
55	B	433/435 (100%)	380 (88%)	52 (12%)	1 (0%)	44 75
56	C	210/261 (80%)	179 (85%)	31 (15%)	0	100 100
57	D	126/204 (62%)	109 (86%)	17 (14%)	0	100 100
58	E	324/345 (94%)	293 (90%)	31 (10%)	0	100 100
59	F	168/171 (98%)	153 (91%)	14 (8%)	1 (1%)	22 57
60	G	363/373 (97%)	314 (86%)	47 (13%)	2 (1%)	22 57
61	H	160/167 (96%)	144 (90%)	14 (9%)	2 (1%)	10 41
62	I	255/304 (84%)	224 (88%)	31 (12%)	0	100 100
63	J	139/143 (97%)	102 (73%)	36 (26%)	1 (1%)	19 54
64	K	177/193 (92%)	158 (89%)	19 (11%)	0	100 100
65	L	176/185 (95%)	157 (89%)	18 (10%)	1 (1%)	22 57
66	M	257/278 (92%)	217 (84%)	38 (15%)	2 (1%)	16 51
67	N	187/251 (74%)	163 (87%)	24 (13%)	0	100 100
68	O	305/475 (64%)	273 (90%)	29 (10%)	3 (1%)	13 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
69	P	163/184 (89%)	145 (89%)	17 (10%)	1 (1%)	22 57
70	Q	215/233 (92%)	192 (89%)	22 (10%)	1 (0%)	25 60
71	R	470/479 (98%)	405 (86%)	65 (14%)	0	100 100
72	S	148/408 (36%)	132 (89%)	16 (11%)	0	100 100
73	T	53/82 (65%)	50 (94%)	3 (6%)	0	100 100
74	U	90/117 (77%)	76 (84%)	12 (13%)	2 (2%)	5 32
75	V	139/150 (93%)	120 (86%)	19 (14%)	0	100 100
76	W	52/185 (28%)	46 (88%)	6 (12%)	0	100 100
77	X	466/512 (91%)	417 (90%)	46 (10%)	3 (1%)	22 57
78	Y	253/292 (87%)	233 (92%)	20 (8%)	0	100 100
79	Z	148/197 (75%)	114 (77%)	31 (21%)	3 (2%)	6 33
80	BA	136/167 (81%)	103 (76%)	29 (21%)	4 (3%)	3 27
82	BB	120/156 (77%)	95 (79%)	23 (19%)	2 (2%)	7 36
83	Aw	183/187 (98%)	161 (88%)	22 (12%)	0	100 100
84	Bj	166/185 (90%)	143 (86%)	22 (13%)	1 (1%)	22 57
85	An	312/331 (94%)	253 (81%)	52 (17%)	7 (2%)	5 32
86	Al	262/346 (76%)	219 (84%)	43 (16%)	0	100 100
87	BI	184/266 (69%)	155 (84%)	29 (16%)	0	100 100
88	Az	136/152 (90%)	110 (81%)	24 (18%)	2 (2%)	8 39
89	At	163/183 (89%)	145 (89%)	18 (11%)	0	100 100
90	BC	138/147 (94%)	129 (94%)	9 (6%)	0	100 100
91	Ab	258/262 (98%)	226 (88%)	32 (12%)	0	100 100
92	Ai	474/479 (99%)	413 (87%)	60 (13%)	1 (0%)	44 75
93	Ap	212/240 (88%)	188 (89%)	24 (11%)	0	100 100
94	Au	174/186 (94%)	131 (75%)	37 (21%)	6 (3%)	3 25
95	Aa	176/195 (90%)	142 (81%)	31 (18%)	3 (2%)	7 36
96	Ao	273/284 (96%)	232 (85%)	39 (14%)	2 (1%)	19 54
97	BM	387/457 (85%)	326 (84%)	61 (16%)	0	100 100
98	Ar	193/205 (94%)	168 (87%)	25 (13%)	0	100 100
99	Aj	337/503 (67%)	292 (87%)	45 (13%)	0	100 100
100	BH	212/229 (93%)	185 (87%)	27 (13%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
101	Am	328/340 (96%)	275 (84%)	53 (16%)	0	100 100
102	Aq	250/341 (73%)	201 (80%)	43 (17%)	6 (2%)	5 30
103	BE	82/118 (70%)	56 (68%)	25 (30%)	1 (1%)	11 43
104	Ak	298/323 (92%)	254 (85%)	44 (15%)	0	100 100
105	BP	191/254 (75%)	161 (84%)	28 (15%)	2 (1%)	13 46
106	Ad	203/237 (86%)	163 (80%)	38 (19%)	2 (1%)	13 46
107	BF	99/109 (91%)	79 (80%)	20 (20%)	0	100 100
108	Av	153/192 (80%)	128 (84%)	25 (16%)	0	100 100
109	Af	137/155 (88%)	117 (85%)	19 (14%)	1 (1%)	19 54
110	As	95/249 (38%)	87 (92%)	8 (8%)	0	100 100
111	Ae	289/311 (93%)	253 (88%)	36 (12%)	0	100 100
112	Ac	266/291 (91%)	234 (88%)	32 (12%)	0	100 100
113	Ah	450/570 (79%)	386 (86%)	60 (13%)	4 (1%)	14 48
114	BD	95/102 (93%)	85 (90%)	10 (10%)	0	100 100
115	Ay	140/174 (80%)	118 (84%)	18 (13%)	4 (3%)	3 27
116	Ag	229/244 (94%)	204 (89%)	25 (11%)	0	100 100
117	Ax	165/216 (76%)	129 (78%)	33 (20%)	3 (2%)	7 35
118	BL	307/380 (81%)	233 (76%)	67 (22%)	7 (2%)	5 31
119	BO	153/190 (80%)	104 (68%)	46 (30%)	3 (2%)	6 33
120	BG	83/1347 (6%)	57 (69%)	23 (28%)	3 (4%)	3 24
All	All	32374/40717 (80%)	28909 (89%)	3346 (10%)	119 (0%)	32 65

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	ac	685	LEU
54	A	289	ARG
54	A	290	MET
61	H	94	VAL
63	J	66	PRO
68	O	28	ALA
74	U	30	ILE
77	X	353	PRO
79	Z	26	HIS
80	BA	24	VAL

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Mol	Chain	Res	Type
82	BB	110	PHE
85	An	46	GLN
85	An	50	HIS
85	An	78	TRP
85	An	97	SER
94	Au	54	PRO
95	Aa	91	LEU
95	Aa	191	THR
102	Aq	172	ILE
102	Aq	175	VAL
105	BP	-3	HIS
115	Ay	36	ILE
117	Ax	204	HIS
118	BL	115	TYR
119	BO	184	VAL
120	BG	1265	PRO
21	aa	1587	ILE
24	ac	1083	ALA
59	F	168	GLN
60	G	149	PRO
60	G	159	ALA
66	M	56	SER
68	O	20	THR
68	O	21	TYR
77	X	355	THR
79	Z	44	LEU
79	Z	106	TYR
88	Az	16	LYS
94	Au	27	GLU
94	Au	92	VAL
94	Au	93	HIS
95	Aa	189	ARG
96	Ao	20	VAL
102	Aq	338	HIS
103	BE	37	GLU
105	BP	96	PRO
109	Af	61	VAL
113	Ah	67	ARG
119	BO	92	ARG
12	ag	81	PRO
20	u	354	LEU
20	u	631	PRO

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Mol	Chain	Res	Type
24	ac	1209	ALA
26	an	155	PRO
26	an	162	ALA
45	o	146	ASP
49	b	109	GLN
80	BA	114	PHE
82	BB	129	THR
88	Az	17	GLN
94	Au	96	LEU
102	Aq	53	SER
102	Aq	168	GLN
106	Ad	15	PRO
106	Ad	27	HIS
115	Ay	35	TRP
117	Ax	56	ARG
117	Ax	58	GLN
120	BG	1263	HIS
10	ae	426	THR
24	ac	1123	ILE
38	l	316	PRO
38	l	319	GLU
40	av	80	PRO
42	x	70	PRO
50	a	255	ASN
74	U	29	VAL
84	Bj	76	PRO
85	An	44	TRP
94	Au	45	THR
96	Ao	19	ARG
113	Ah	56	HIS
12	ag	82	LEU
14	e	292	GLY
14	e	310	PRO
25	ad	417	ALA
25	ad	419	PRO
54	A	284	ILE
69	P	56	ASP
70	Q	90	ARG
80	BA	23	TYR
85	An	215	VAL
113	Ah	57	LEU
115	Ay	149	ARG

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Mol	Chain	Res	Type
118	BL	116	PHE
119	BO	61	SER
20	u	630	LEU
24	ac	452	GLY
65	L	72	PRO
80	BA	45	GLN
85	An	142	GLY
118	BL	140	SER
54	A	159	PRO
52	z	674	PRO
54	A	377	PRO
113	Ah	64	VAL
115	Ay	150	PRO
61	H	93	VAL
77	X	364	PRO
92	Ai	161	PRO
118	BL	74	PRO
118	BL	324	PRO
118	BL	340	VAL
120	BG	1318	PRO
36	p	270	ILE
55	B	302	GLY
66	M	14	PRO
118	BL	311	VAL
102	Aq	54	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	h	138/146 (94%)	138 (100%)	0	100 100
3	aw	120/120 (100%)	120 (100%)	0	100 100
4	m	250/283 (88%)	249 (100%)	1 (0%)	89 91
5	f	122/292 (42%)	118 (97%)	4 (3%)	33 56
6	s	143/157 (91%)	143 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	au	217/223 (97%)	216 (100%)	1 (0%)	86 90
8	am	228/262 (87%)	227 (100%)	1 (0%)	89 91
9	n	127/147 (86%)	127 (100%)	0	100 100
10	ae	479/532 (90%)	478 (100%)	1 (0%)	92 94
11	ay	126/149 (85%)	125 (99%)	1 (1%)	79 84
12	ag	478/484 (99%)	475 (99%)	3 (1%)	84 88
13	aj	275/345 (80%)	275 (100%)	0	100 100
14	e	688/700 (98%)	687 (100%)	1 (0%)	92 95
15	d	289/296 (98%)	287 (99%)	2 (1%)	81 86
16	az	137/144 (95%)	137 (100%)	0	100 100
17	ax	146/166 (88%)	146 (100%)	0	100 100
18	r	396/409 (97%)	396 (100%)	0	100 100
19	af	486/676 (72%)	486 (100%)	0	100 100
20	u	582/733 (79%)	579 (100%)	3 (0%)	86 90
21	aa	1266/1465 (86%)	1261 (100%)	5 (0%)	89 91
22	ab	951/971 (98%)	950 (100%)	1 (0%)	92 95
23	ak	224/268 (84%)	222 (99%)	2 (1%)	75 83
24	ac	889/1002 (89%)	888 (100%)	1 (0%)	92 95
25	ad	595/699 (85%)	593 (100%)	2 (0%)	91 92
26	an	248/248 (100%)	248 (100%)	0	100 100
27	ao	167/253 (66%)	167 (100%)	0	100 100
28	ap	191/194 (98%)	190 (100%)	1 (0%)	86 90
29	aq	190/249 (76%)	190 (100%)	0	100 100
30	as	207/226 (92%)	207 (100%)	0	100 100
31	at	172/334 (52%)	170 (99%)	2 (1%)	67 78
32	y	230/379 (61%)	227 (99%)	3 (1%)	65 76
33	w	140/170 (82%)	139 (99%)	1 (1%)	81 86
34	v	53/182 (29%)	53 (100%)	0	100 100
35	t	186/214 (87%)	186 (100%)	0	100 100
36	p	209/278 (75%)	207 (99%)	2 (1%)	73 81
37	j	163/172 (95%)	162 (99%)	1 (1%)	84 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	l	465/552 (84%)	463 (100%)	2 (0%)	89 91
39	ar	217/237 (92%)	215 (99%)	2 (1%)	75 83
40	av	136/208 (65%)	135 (99%)	1 (1%)	81 86
41	ai	338/338 (100%)	338 (100%)	0	100 100
42	x	211/222 (95%)	211 (100%)	0	100 100
43	i	241/383 (63%)	241 (100%)	0	100 100
44	g	84/168 (50%)	84 (100%)	0	100 100
45	o	393/546 (72%)	391 (100%)	2 (0%)	86 90
46	c	217/260 (84%)	216 (100%)	1 (0%)	86 90
47	k	104/272 (38%)	104 (100%)	0	100 100
48	q	177/363 (49%)	177 (100%)	0	100 100
49	b	140/144 (97%)	139 (99%)	1 (1%)	81 86
50	a	346/365 (95%)	345 (100%)	1 (0%)	91 92
51	ba	21/82 (26%)	21 (100%)	0	100 100
52	z	817/979 (84%)	814 (100%)	3 (0%)	89 91
53	bd	39/85 (46%)	38 (97%)	1 (3%)	41 61
54	A	314/393 (80%)	313 (100%)	1 (0%)	91 92
55	B	380/380 (100%)	375 (99%)	5 (1%)	65 76
56	C	190/226 (84%)	190 (100%)	0	100 100
57	D	106/154 (69%)	103 (97%)	3 (3%)	38 59
58	E	285/300 (95%)	282 (99%)	3 (1%)	70 79
59	F	151/152 (99%)	149 (99%)	2 (1%)	65 76
60	G	315/322 (98%)	308 (98%)	7 (2%)	47 65
61	H	138/142 (97%)	137 (99%)	1 (1%)	81 86
62	I	223/261 (85%)	221 (99%)	2 (1%)	75 83
63	J	119/121 (98%)	115 (97%)	4 (3%)	32 55
64	K	151/161 (94%)	149 (99%)	2 (1%)	65 76
65	L	151/157 (96%)	151 (100%)	0	100 100
66	M	226/241 (94%)	222 (98%)	4 (2%)	54 71
67	N	175/219 (80%)	172 (98%)	3 (2%)	56 72
68	O	278/396 (70%)	273 (98%)	5 (2%)	54 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
69	P	147/162 (91%)	147 (100%)	0	100 100
70	Q	191/203 (94%)	189 (99%)	2 (1%)	73 81
71	R	406/411 (99%)	405 (100%)	1 (0%)	92 94
72	S	135/335 (40%)	135 (100%)	0	100 100
73	T	52/73 (71%)	52 (100%)	0	100 100
74	U	80/99 (81%)	75 (94%)	5 (6%)	15 40
75	V	125/134 (93%)	121 (97%)	4 (3%)	34 56
76	W	50/163 (31%)	46 (92%)	4 (8%)	10 33
77	X	402/437 (92%)	399 (99%)	3 (1%)	81 86
78	Y	209/236 (89%)	208 (100%)	1 (0%)	86 90
79	Z	132/172 (77%)	128 (97%)	4 (3%)	36 58
80	BA	112/135 (83%)	108 (96%)	4 (4%)	30 54
82	BB	106/140 (76%)	103 (97%)	3 (3%)	38 59
83	Aw	157/159 (99%)	156 (99%)	1 (1%)	84 88
84	Bj	150/165 (91%)	149 (99%)	1 (1%)	81 86
85	An	274/289 (95%)	267 (97%)	7 (3%)	41 61
86	Al	236/299 (79%)	230 (98%)	6 (2%)	42 62
87	BI	153/221 (69%)	152 (99%)	1 (1%)	81 86
88	Az	129/143 (90%)	127 (98%)	2 (2%)	58 73
89	At	140/153 (92%)	140 (100%)	0	100 100
90	BC	117/124 (94%)	116 (99%)	1 (1%)	75 83
91	Ab	233/235 (99%)	233 (100%)	0	100 100
92	Ai	408/410 (100%)	406 (100%)	2 (0%)	86 90
93	Ap	189/208 (91%)	188 (100%)	1 (0%)	86 90
94	Au	154/164 (94%)	145 (94%)	9 (6%)	17 42
95	Aa	150/166 (90%)	148 (99%)	2 (1%)	65 76
96	Ao	236/245 (96%)	234 (99%)	2 (1%)	79 84
97	BM	319/370 (86%)	316 (99%)	3 (1%)	75 83
98	Ar	169/179 (94%)	168 (99%)	1 (1%)	84 88
99	Aj	286/420 (68%)	284 (99%)	2 (1%)	81 86
100	BH	177/189 (94%)	175 (99%)	2 (1%)	70 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
101	Am	278/287 (97%)	275 (99%)	3 (1%)	70	79
102	Aq	221/276 (80%)	216 (98%)	5 (2%)	45	64
103	BE	76/100 (76%)	75 (99%)	1 (1%)	65	76
104	Ak	254/272 (93%)	252 (99%)	2 (1%)	79	84
105	BP	167/215 (78%)	165 (99%)	2 (1%)	67	78
106	Ad	172/193 (89%)	171 (99%)	1 (1%)	84	88
107	BF	88/95 (93%)	87 (99%)	1 (1%)	70	79
108	Av	141/169 (83%)	141 (100%)	0	100	100
109	Af	120/135 (89%)	120 (100%)	0	100	100
110	As	88/204 (43%)	88 (100%)	0	100	100
111	Ae	249/261 (95%)	244 (98%)	5 (2%)	50	68
112	Ac	232/253 (92%)	230 (99%)	2 (1%)	75	83
113	Ah	385/485 (79%)	378 (98%)	7 (2%)	54	71
114	BD	85/90 (94%)	83 (98%)	2 (2%)	44	63
115	Ay	130/158 (82%)	128 (98%)	2 (2%)	60	74
116	Ag	202/211 (96%)	200 (99%)	2 (1%)	73	81
117	Ax	150/190 (79%)	141 (94%)	9 (6%)	16	41
118	BL	268/329 (82%)	261 (97%)	7 (3%)	41	61
119	BO	130/158 (82%)	126 (97%)	4 (3%)	35	56
120	BG	67/1047 (6%)	67 (100%)	0	100	100
All	All	27983/34364 (81%)	27759 (99%)	224 (1%)	77	84

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	m	186	ARG
5	f	11	ARG
5	f	26	ARG
5	f	27	ARG
5	f	135	PHE
7	au	105	ARG
8	am	73	ARG
10	ae	455	ARG
11	ay	29	TRP
12	ag	9	ARG

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Mol	Chain	Res	Type
12	ag	80	LYS
12	ag	297	ARG
14	e	39	LYS
15	d	36	ARG
15	d	73	ARG
20	u	203	LYS
20	u	398	ARG
20	u	629	VAL
21	aa	333	ARG
21	aa	338	ARG
21	aa	429	ASP
21	aa	465	ARG
21	aa	698	ARG
22	ab	430	LEU
23	ak	214	ARG
23	ak	302	ARG
24	ac	870	ASP
25	ad	434	PHE
25	ad	653	ARG
28	ap	92	ARG
31	at	269	ARG
31	at	351	CYS
32	y	78	CYS
32	y	248	ARG
32	y	301	ARG
33	w	88	LYS
36	p	127	ARG
36	p	205	LYS
37	j	154	ARG
38	l	151	ARG
38	l	466	TYR
39	ar	56	ARG
39	ar	265	LYS
40	av	50	ARG
45	o	138	LYS
45	o	256	ARG
46	c	136	ARG
49	b	48	TYR
50	a	83	MET
52	z	238	ARG
52	z	600	ARG
52	z	975	VAL

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Mol	Chain	Res	Type
53	bd	78	TYR
54	A	47	ARG
55	B	131	ARG
55	B	192	ASP
55	B	193	VAL
55	B	194	LYS
55	B	403	PRO
57	D	68	ASP
57	D	88	ARG
57	D	93	ARG
58	E	115	ARG
58	E	148	TYR
58	E	263	ASN
59	F	157	ASP
59	F	161	GLN
60	G	142	TRP
60	G	143	GLN
60	G	145	ARG
60	G	146	LYS
60	G	149	PRO
60	G	150	ARG
60	G	153	LEU
61	H	24	ARG
62	I	21	ARG
62	I	186	PHE
63	J	21	PHE
63	J	46	TRP
63	J	66	PRO
63	J	67	ARG
64	K	12	ARG
64	K	29	ARG
66	M	9	ASN
66	M	14	PRO
66	M	54	MET
66	M	56	SER
67	N	85	ARG
67	N	173	ASP
67	N	198	ARG
68	O	19	PHE
68	O	20	THR
68	O	29	ARG
68	O	58	LYS

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Mol	Chain	Res	Type
68	O	230	ARG
70	Q	28	ARG
70	Q	42	TRP
71	R	438	ARG
74	U	17	ARG
74	U	19	LYS
74	U	28	LYS
74	U	30	ILE
74	U	36	ASN
75	V	11	LYS
75	V	39	VAL
75	V	66	ARG
75	V	81	ARG
76	W	72	HIS
76	W	74	GLU
76	W	94	LYS
76	W	97	ASN
77	X	353	PRO
77	X	497	SER
77	X	498	ARG
78	Y	58	ARG
79	Z	40	THR
79	Z	43	ILE
79	Z	44	LEU
79	Z	45	ARG
80	BA	23	TYR
80	BA	113	MET
80	BA	115	VAL
80	BA	127	CYS
82	BB	44	LYS
82	BB	110	PHE
82	BB	111	PHE
83	Aw	6	VAL
84	Bj	143	ASN
85	An	101	ILE
85	An	106	TRP
85	An	129	LYS
85	An	140	ARG
85	An	143	TYR
85	An	217	ARG
85	An	221	GLN
86	Al	39	GLN

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Mol	Chain	Res	Type
86	Al	268	TYR
86	Al	269	GLU
86	Al	274	VAL
86	Al	279	ASN
86	Al	287	TRP
87	BI	165	ILE
88	Az	60	HIS
88	Az	93	LYS
90	BC	68	ASP
92	Ai	72	ARG
92	Ai	133	MET
93	Ap	173	ARG
94	Au	44	ARG
94	Au	46	VAL
94	Au	47	LEU
94	Au	51	PHE
94	Au	71	MET
94	Au	72	ASP
94	Au	77	VAL
94	Au	93	HIS
94	Au	117	ARG
95	Aa	75	ARG
95	Aa	81	ASN
96	Ao	27	ARG
96	Ao	33	LEU
97	BM	17	ARG
97	BM	138	VAL
97	BM	263	ARG
98	Ar	69	CYS
99	Aj	133	ARG
99	Aj	391	LYS
100	BH	54	ARG
100	BH	225	ILE
101	Am	14	THR
101	Am	22	ARG
101	Am	332	THR
102	Aq	174	ARG
102	Aq	176	ARG
102	Aq	336	ARG
102	Aq	339	ARG
102	Aq	341	PHE
103	BE	67	LYS

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Mol	Chain	Res	Type
104	Ak	44	ARG
104	Ak	241	ARG
105	BP	0	TRP
105	BP	9	ARG
106	Ad	32	ARG
107	BF	103	HIS
111	Ae	89	ASP
111	Ae	95	ARG
111	Ae	163	VAL
111	Ae	254	ASP
111	Ae	286	LYS
112	Ac	47	ARG
112	Ac	278	LYS
113	Ah	67	ARG
113	Ah	68	ILE
113	Ah	112	TYR
113	Ah	165	TYR
113	Ah	182	ARG
113	Ah	279	ASP
113	Ah	357	LYS
114	BD	21	ARG
114	BD	62	ARG
115	Ay	38	ARG
115	Ay	51	TRP
116	Ag	43	ARG
116	Ag	48	TYR
117	Ax	63	TRP
117	Ax	109	ASP
117	Ax	134	GLN
117	Ax	136	TYR
117	Ax	146	TRP
117	Ax	173	ARG
117	Ax	180	ARG
117	Ax	203	ARG
117	Ax	205	ARG
118	BL	107	TRP
118	BL	119	ARG
118	BL	132	HIS
118	BL	134	ARG
118	BL	141	TRP
118	BL	211	THR
118	BL	328	THR

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Mol	Chain	Res	Type
119	BO	105	ARG
119	BO	128	VAL
119	BO	148	ASP
119	BO	172	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (648) such sidechains are listed below:

Mol	Chain	Res	Type
2	h	15	GLN
2	h	68	GLN
2	h	77	ASN
2	h	112	ASN
2	h	133	HIS
3	aw	22	HIS
3	aw	108	GLN
4	m	20	GLN
4	m	29	ASN
4	m	68	GLN
4	m	72	HIS
4	m	156	ASN
4	m	208	HIS
4	m	219	GLN
4	m	225	GLN
4	m	252	HIS
4	m	255	GLN
5	f	35	GLN
5	f	126	GLN
6	s	81	ASN
6	s	94	ASN
6	s	134	HIS
6	s	138	ASN
6	s	141	GLN
7	au	45	HIS
7	au	58	ASN
7	au	72	HIS
7	au	113	GLN
7	au	139	HIS
7	au	146	GLN
7	au	154	GLN
7	au	167	ASN
7	au	247	GLN
9	n	66	ASN

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Mol	Chain	Res	Type
9	n	103	GLN
9	n	109	HIS
10	ae	33	GLN
10	ae	41	ASN
10	ae	73	HIS
10	ae	178	ASN
10	ae	203	GLN
10	ae	213	HIS
10	ae	272	ASN
10	ae	291	ASN
10	ae	297	HIS
10	ae	370	GLN
10	ae	371	GLN
10	ae	382	ASN
11	ay	58	HIS
11	ay	108	GLN
11	ay	114	HIS
11	ay	130	GLN
12	ag	5	GLN
12	ag	6	ASN
12	ag	51	GLN
12	ag	66	GLN
12	ag	197	ASN
12	ag	264	HIS
12	ag	291	GLN
12	ag	316	HIS
12	ag	408	ASN
12	ag	501	ASN
12	ag	552	HIS
13	aj	60	ASN
13	aj	72	HIS
13	aj	127	HIS
13	aj	253	ASN
13	aj	307	GLN
13	aj	310	GLN
14	e	33	GLN
14	e	82	HIS
14	e	116	HIS
14	e	224	ASN
14	e	231	ASN
14	e	233	ASN
14	e	394	HIS

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Mol	Chain	Res	Type
14	e	417	GLN
14	e	463	HIS
14	e	464	HIS
14	e	571	GLN
14	e	693	GLN
14	e	716	HIS
14	e	758	ASN
14	e	766	GLN
14	e	774	GLN
14	e	795	GLN
14	e	797	HIS
14	e	809	ASN
14	e	810	HIS
15	d	58	GLN
15	d	116	HIS
15	d	119	ASN
15	d	223	GLN
15	d	238	ASN
15	d	344	ASN
16	az	112	HIS
16	az	142	HIS
17	ax	86	ASN
17	ax	92	HIS
17	ax	98	HIS
17	ax	120	HIS
17	ax	131	HIS
17	ax	153	HIS
17	ax	163	HIS
18	r	130	GLN
18	r	184	ASN
18	r	189	GLN
18	r	270	HIS
18	r	401	HIS
18	r	427	HIS
18	r	443	GLN
19	af	199	ASN
19	af	205	ASN
19	af	332	ASN
19	af	531	HIS
19	af	655	GLN
19	af	751	GLN
19	af	763	GLN

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Mol	Chain	Res	Type
20	u	140	GLN
20	u	208	HIS
20	u	298	ASN
20	u	569	GLN
20	u	621	HIS
20	u	668	GLN
20	u	695	GLN
20	u	707	GLN
20	u	744	GLN
20	u	773	HIS
21	aa	100	HIS
21	aa	142	HIS
21	aa	148	GLN
21	aa	161	ASN
21	aa	164	GLN
21	aa	185	GLN
21	aa	239	HIS
21	aa	343	GLN
21	aa	392	HIS
21	aa	401	HIS
21	aa	433	HIS
21	aa	508	HIS
21	aa	575	GLN
21	aa	622	GLN
21	aa	717	GLN
21	aa	762	GLN
21	aa	794	GLN
21	aa	843	GLN
21	aa	880	HIS
21	aa	905	GLN
21	aa	950	ASN
21	aa	964	ASN
21	aa	978	HIS
21	aa	982	GLN
21	aa	1034	HIS
21	aa	1040	HIS
21	aa	1084	GLN
21	aa	1400	ASN
21	aa	1503	ASN
21	aa	1616	GLN
21	aa	1634	GLN
21	aa	1637	ASN

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Mol	Chain	Res	Type
22	ab	48	HIS
22	ab	78	HIS
22	ab	80	GLN
22	ab	265	HIS
22	ab	325	ASN
22	ab	344	GLN
22	ab	356	GLN
22	ab	425	HIS
22	ab	434	ASN
22	ab	444	GLN
22	ab	510	GLN
22	ab	670	GLN
22	ab	698	GLN
22	ab	716	HIS
22	ab	717	GLN
22	ab	763	GLN
22	ab	1025	HIS
22	ab	1032	GLN
22	ab	1047	GLN
22	ab	1051	GLN
22	ab	1072	ASN
22	ab	1107	GLN
22	ab	1120	HIS
22	ab	1144	HIS
23	ak	23	HIS
23	ak	36	ASN
23	ak	133	HIS
23	ak	142	GLN
23	ak	158	ASN
24	ac	132	ASN
24	ac	245	ASN
24	ac	271	ASN
24	ac	299	GLN
24	ac	367	HIS
24	ac	410	GLN
24	ac	438	GLN
24	ac	443	GLN
24	ac	527	HIS
24	ac	547	GLN
24	ac	550	HIS
24	ac	565	GLN
24	ac	612	GLN

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Mol	Chain	Res	Type
24	ac	613	GLN
24	ac	652	GLN
24	ac	775	GLN
24	ac	841	GLN
24	ac	978	HIS
24	ac	990	GLN
24	ac	1005	HIS
24	ac	1101	GLN
24	ac	1103	GLN
24	ac	1172	GLN
24	ac	1208	GLN
25	ad	156	GLN
25	ad	173	GLN
25	ad	233	ASN
25	ad	276	HIS
25	ad	313	HIS
25	ad	336	HIS
25	ad	348	HIS
25	ad	349	GLN
25	ad	387	GLN
25	ad	507	GLN
25	ad	606	HIS
25	ad	646	HIS
25	ad	706	GLN
26	an	153	GLN
26	an	188	HIS
26	an	216	HIS
26	an	282	GLN
26	an	284	GLN
26	an	291	HIS
26	an	300	GLN
27	ao	27	ASN
27	ao	78	ASN
28	ap	26	GLN
28	ap	118	GLN
28	ap	200	ASN
28	ap	221	GLN
29	aq	41	GLN
29	aq	136	ASN
29	aq	140	ASN
29	aq	141	HIS
30	as	48	ASN

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Mol	Chain	Res	Type
30	as	96	ASN
34	v	102	GLN
35	t	64	GLN
35	t	102	GLN
35	t	153	HIS
36	p	33	HIS
36	p	67	GLN
36	p	75	ASN
36	p	114	ASN
36	p	139	HIS
36	p	194	GLN
36	p	280	GLN
37	j	50	HIS
37	j	88	HIS
37	j	117	ASN
37	j	131	GLN
37	j	157	GLN
38	l	249	ASN
38	l	257	HIS
38	l	355	GLN
38	l	438	GLN
38	l	583	GLN
39	ar	42	GLN
39	ar	74	HIS
39	ar	220	HIS
39	ar	230	GLN
39	ar	246	HIS
39	ar	248	HIS
40	av	84	HIS
40	av	124	GLN
40	av	177	HIS
41	ai	52	GLN
41	ai	53	GLN
41	ai	97	GLN
41	ai	177	GLN
41	ai	222	ASN
41	ai	279	ASN
41	ai	289	HIS
42	x	95	HIS
42	x	123	HIS
42	x	129	HIS
42	x	155	GLN

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Mol	Chain	Res	Type
43	i	136	HIS
43	i	260	ASN
44	g	83	ASN
44	g	100	HIS
44	g	104	GLN
44	g	122	GLN
44	g	131	GLN
44	g	135	ASN
45	o	76	GLN
45	o	105	GLN
45	o	106	ASN
45	o	199	HIS
45	o	224	GLN
45	o	392	GLN
45	o	438	ASN
45	o	452	ASN
45	o	477	GLN
46	c	79	GLN
46	c	276	HIS
46	c	277	ASN
46	c	311	HIS
47	k	133	HIS
48	q	72	ASN
48	q	81	ASN
48	q	106	GLN
48	q	119	HIS
48	q	203	ASN
49	b	106	HIS
49	b	108	GLN
50	a	85	ASN
50	a	91	ASN
50	a	105	GLN
50	a	132	HIS
50	a	191	ASN
50	a	208	GLN
50	a	248	GLN
50	a	255	ASN
50	a	338	HIS
50	a	410	GLN
50	a	427	ASN
50	a	431	HIS
51	ba	69	HIS

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Mol	Chain	Res	Type
52	z	141	HIS
52	z	151	ASN
52	z	217	ASN
52	z	246	ASN
52	z	318	GLN
52	z	772	HIS
52	z	836	GLN
52	z	860	HIS
53	bd	56	ASN
53	bd	74	ASN
54	A	81	GLN
54	A	162	GLN
54	A	184	ASN
54	A	207	HIS
54	A	337	ASN
55	B	74	GLN
55	B	88	GLN
55	B	133	GLN
55	B	153	ASN
55	B	170	HIS
55	B	172	HIS
55	B	177	HIS
55	B	200	ASN
55	B	273	ASN
55	B	276	ASN
55	B	306	GLN
55	B	323	HIS
56	C	67	ASN
56	C	120	ASN
56	C	142	ASN
57	D	26	HIS
57	D	38	HIS
58	E	52	ASN
58	E	221	HIS
58	E	224	GLN
58	E	246	ASN
58	E	273	HIS
58	E	280	GLN
59	F	25	HIS
59	F	135	HIS
59	F	161	GLN
60	G	15	HIS

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Mol	Chain	Res	Type
60	G	19	GLN
60	G	29	GLN
60	G	38	ASN
60	G	89	GLN
60	G	143	GLN
60	G	202	ASN
60	G	277	GLN
60	G	300	GLN
60	G	310	HIS
60	G	319	HIS
60	G	346	HIS
61	H	19	HIS
61	H	61	GLN
61	H	108	ASN
61	H	134	ASN
61	H	152	GLN
62	I	65	HIS
62	I	99	HIS
62	I	223	HIS
62	I	242	HIS
62	I	259	HIS
63	J	52	GLN
63	J	99	ASN
64	K	65	ASN
64	K	73	HIS
64	K	78	GLN
64	K	79	HIS
64	K	98	GLN
64	K	101	GLN
64	K	145	HIS
65	L	14	GLN
65	L	29	ASN
65	L	30	HIS
65	L	52	GLN
66	M	19	GLN
66	M	24	GLN
66	M	31	HIS
66	M	76	ASN
66	M	131	GLN
66	M	173	HIS
66	M	230	HIS
67	N	58	ASN

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Mol	Chain	Res	Type
67	N	77	ASN
68	O	23	GLN
68	O	89	HIS
68	O	104	GLN
68	O	187	GLN
68	O	212	HIS
68	O	296	HIS
68	O	303	GLN
68	O	306	ASN
68	O	314	GLN
69	P	61	GLN
70	Q	24	HIS
70	Q	170	ASN
71	R	23	ASN
71	R	67	HIS
71	R	71	HIS
71	R	167	HIS
71	R	194	GLN
71	R	246	ASN
71	R	286	GLN
71	R	419	GLN
71	R	421	ASN
71	R	470	HIS
72	S	256	ASN
72	S	312	GLN
72	S	327	HIS
72	S	336	GLN
72	S	371	HIS
72	S	384	HIS
72	S	385	HIS
72	S	388	GLN
73	T	46	HIS
74	U	37	ASN
74	U	78	GLN
75	V	29	GLN
75	V	88	GLN
75	V	119	GLN
76	W	60	HIS
76	W	72	HIS
76	W	79	HIS
76	W	97	ASN
77	X	64	HIS

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Mol	Chain	Res	Type
77	X	257	ASN
77	X	344	GLN
77	X	479	GLN
77	X	491	GLN
78	Y	149	GLN
78	Y	153	GLN
78	Y	231	GLN
78	Y	279	HIS
78	Y	282	GLN
79	Z	13	HIS
79	Z	14	ASN
79	Z	67	ASN
79	Z	91	ASN
79	Z	146	GLN
80	BA	91	HIS
82	BB	41	HIS
82	BB	55	GLN
82	BB	108	GLN
83	Aw	79	HIS
83	Aw	89	HIS
84	Bj	4	ASN
84	Bj	91	ASN
85	An	24	HIS
85	An	48	HIS
85	An	60	ASN
85	An	123	GLN
85	An	166	ASN
85	An	212	HIS
85	An	221	GLN
85	An	238	GLN
85	An	240	GLN
85	An	264	HIS
85	An	295	HIS
85	An	314	HIS
86	Al	133	GLN
86	Al	250	GLN
86	Al	276	GLN
86	Al	279	ASN
86	Al	298	ASN
87	BI	81	HIS
87	BI	148	ASN
88	Az	19	GLN

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Mol	Chain	Res	Type
88	Az	31	ASN
88	Az	73	HIS
88	Az	128	GLN
89	At	28	ASN
89	At	33	ASN
89	At	56	ASN
89	At	73	HIS
89	At	90	GLN
90	BC	22	HIS
90	BC	63	ASN
90	BC	67	ASN
90	BC	90	GLN
90	BC	119	GLN
90	BC	123	ASN
90	BC	125	HIS
91	Ab	10	GLN
91	Ab	27	GLN
91	Ab	37	HIS
91	Ab	84	HIS
91	Ab	94	ASN
91	Ab	205	HIS
91	Ab	245	GLN
91	Ab	257	GLN
92	Ai	64	GLN
92	Ai	142	ASN
92	Ai	151	ASN
92	Ai	184	HIS
92	Ai	245	ASN
92	Ai	248	ASN
92	Ai	470	ASN
93	Ap	17	HIS
93	Ap	81	HIS
93	Ap	123	HIS
94	Au	74	GLN
94	Au	93	HIS
94	Au	99	HIS
94	Au	135	HIS
94	Au	157	GLN
94	Au	167	HIS
95	Aa	20	GLN
95	Aa	109	HIS
95	Aa	112	HIS

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Mol	Chain	Res	Type
95	Aa	159	GLN
95	Aa	194	ASN
96	Ao	90	HIS
96	Ao	248	GLN
96	Ao	271	GLN
96	Ao	280	ASN
97	BM	35	GLN
97	BM	113	GLN
97	BM	130	GLN
97	BM	228	ASN
97	BM	314	GLN
97	BM	325	GLN
97	BM	381	ASN
98	Ar	48	GLN
98	Ar	114	GLN
98	Ar	164	HIS
98	Ar	186	ASN
98	Ar	194	HIS
99	Aj	122	ASN
99	Aj	242	HIS
99	Aj	281	GLN
99	Aj	375	GLN
99	Aj	409	HIS
99	Aj	440	GLN
99	Aj	450	ASN
99	Aj	468	HIS
100	BH	82	HIS
100	BH	132	HIS
100	BH	137	GLN
100	BH	149	ASN
100	BH	214	HIS
101	Am	15	HIS
101	Am	106	HIS
101	Am	144	HIS
101	Am	148	ASN
101	Am	152	GLN
101	Am	184	ASN
101	Am	228	GLN
101	Am	263	HIS
101	Am	278	GLN
101	Am	307	ASN
101	Am	315	ASN

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Mol	Chain	Res	Type
102	Aq	19	HIS
102	Aq	36	HIS
102	Aq	55	ASN
102	Aq	109	HIS
102	Aq	159	HIS
102	Aq	211	HIS
102	Aq	281	GLN
102	Aq	308	GLN
104	Ak	22	HIS
104	Ak	64	GLN
104	Ak	93	HIS
104	Ak	216	HIS
104	Ak	294	GLN
105	BP	6	HIS
105	BP	49	GLN
106	Ad	85	GLN
106	Ad	187	GLN
106	Ad	220	ASN
106	Ad	230	HIS
108	Av	137	GLN
108	Av	168	HIS
109	Af	20	HIS
109	Af	100	GLN
109	Af	105	GLN
111	Ae	54	ASN
111	Ae	79	GLN
111	Ae	83	HIS
112	Ac	55	HIS
112	Ac	57	HIS
112	Ac	124	GLN
112	Ac	132	GLN
112	Ac	147	GLN
112	Ac	245	GLN
113	Ah	56	HIS
113	Ah	107	HIS
113	Ah	184	HIS
113	Ah	200	GLN
113	Ah	272	GLN
113	Ah	347	ASN
113	Ah	385	GLN
114	BD	48	GLN
114	BD	80	GLN

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Mol	Chain	Res	Type
115	Ay	83	ASN
115	Ay	158	GLN
116	Ag	197	HIS
116	Ag	226	GLN
117	Ax	66	GLN
117	Ax	85	HIS
117	Ax	183	HIS
117	Ax	188	ASN
117	Ax	204	HIS
118	BL	84	GLN
118	BL	92	GLN
118	BL	118	HIS
118	BL	152	GLN
118	BL	224	HIS
118	BL	232	HIS
118	BL	284	ASN
118	BL	305	HIS
118	BL	335	HIS
118	BL	374	ASN
119	BO	118	HIS
119	BO	137	ASN
119	BO	144	GLN
119	BO	176	HIS
120	BG	1274	ASN
120	BG	1328	GLN
120	BG	1336	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1082/18998 (5%)	638 (58%)	129 (11%)
1	2	602/18998 (3%)	481 (79%)	200 (33%)
All	All	1684/37996 (4%)	1119 (66%)	329 (19%)

All (1119) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	U
1	2	3	C
1	2	6	U
1	2	7	U

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Mol	Chain	Res	Type
1	2	9	U
1	2	10	U
1	2	11	A
1	2	12	U
1	2	13	U
1	2	15	U
1	2	16	U
1	2	17	C
1	2	18	A
1	2	24	A
1	2	25	U
1	2	26	U
1	2	27	U
1	2	28	U
1	2	29	U
1	2	32	A
1	2	33	A
1	2	34	A
1	2	35	A
1	2	36	G
1	2	37	U
1	2	41	U
1	2	42	U
1	2	43	A
1	2	44	A
1	2	46	U
1	2	47	U
1	2	48	U
1	2	49	A
1	2	50	U
1	2	51	A
1	2	52	U
1	2	53	U
1	2	54	A
1	2	55	G
1	2	56	U
1	2	57	U
1	2	58	U
1	2	60	U
1	2	61	U
1	2	64	U
1	2	65	U

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Mol	Chain	Res	Type
1	2	66	U
1	2	67	A
1	2	68	A
1	2	69	A
1	2	70	A
1	2	83	A
1	2	84	U
1	2	86	C
1	2	87	A
1	2	88	U
1	2	90	A
1	2	91	U
1	2	92	U
1	2	93	U
1	2	94	A
1	2	95	G
1	2	96	G
1	2	97	A
1	2	98	A
1	2	99	U
1	2	100	A
1	2	101	G
1	2	102	U
1	2	103	U
1	2	107	A
1	2	108	A
1	2	109	U
1	2	110	A
1	2	111	A
1	2	112	U
1	2	113	U
1	2	114	U
1	2	116	U
1	2	117	A
1	2	120	U
1	2	123	G
1	2	125	U
1	2	127	A
1	2	131	U
1	2	132	U
1	2	133	G
1	2	134	U

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Mol	Chain	Res	Type
1	2	136	U
1	2	138	U
1	2	139	U
1	2	140	A
1	2	141	A
1	2	142	U
1	2	148	U
1	2	149	A
1	2	150	A
1	2	151	A
1	2	152	G
1	2	155	G
1	2	156	U
1	2	161	A
1	2	163	A
1	2	165	A
1	2	166	G
1	2	167	U
1	2	168	G
1	2	169	U
1	2	170	U
1	2	171	A
1	2	172	A
1	2	173	A
1	2	174	U
1	2	175	U
1	2	176	U
1	2	177	U
1	2	178	U
1	2	179	G
1	2	180	A
1	2	182	A
1	2	183	U
1	2	184	A
1	2	185	U
1	2	186	U
1	2	189	A
1	2	191	U
1	2	192	A
1	2	193	A
1	2	194	U
1	2	195	A

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Mol	Chain	Res	Type
1	2	197	A
1	2	198	U
1	2	199	A
1	2	200	A
1	2	201	A
1	2	202	A
1	2	203	U
1	2	204	A
1	2	205	U
1	2	206	A
1	2	208	C
1	2	209	U
1	2	210	U
1	2	211	A
1	2	212	U
1	2	213	U
1	2	214	A
1	2	215	G
1	2	217	C
1	2	218	A
1	2	219	G
1	2	220	A
1	2	221	A
1	2	222	A
1	2	223	U
1	2	225	G
1	2	227	U
1	2	228	G
1	2	229	C
1	2	230	C
1	2	232	G
1	2	234	C
1	2	235	G
1	2	237	U
1	2	238	G
1	2	239	C
1	2	240	G
1	2	241	G
1	2	242	U
1	2	243	A
1	2	244	A
1	2	245	U

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Mol	Chain	Res	Type
1	2	246	U
1	2	247	U
1	2	248	C
1	2	249	U
1	2	250	A
1	2	251	U
1	2	254	U
1	2	255	U
1	2	257	U
1	2	258	A
1	2	259	A
1	2	260	A
1	2	262	A
1	2	264	U
1	2	266	U
1	2	267	A
1	2	268	C
1	2	269	A
1	2	270	U
1	2	271	U
1	2	272	U
1	2	273	A
1	2	274	U
1	2	275	U
1	2	276	U
1	2	277	U
1	2	279	U
1	2	280	A
1	2	281	A
1	2	282	A
1	2	286	G
1	2	287	U
1	2	290	C
1	2	291	U
1	2	292	A
1	2	293	U
1	2	294	A
1	2	295	U
1	2	296	A
1	2	297	U
1	2	300	U
1	2	301	U

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Mol	Chain	Res	Type
1	2	302	A
1	2	303	G
1	2	304	U
1	2	305	C
1	2	306	A
1	2	307	A
1	2	308	U
1	2	310	A
1	2	311	A
1	2	312	A
1	2	313	C
1	2	314	U
1	2	315	A
1	2	317	U
1	2	318	A
1	2	319	A
1	2	320	U
1	2	321	U
1	2	322	A
1	2	323	U
1	2	324	U
1	2	325	U
1	2	326	U
1	2	327	U
1	2	328	A
1	2	330	U
1	2	331	U
1	2	332	G
1	2	335	U
1	2	336	U
1	2	337	U
1	2	338	A
1	2	339	A
1	2	340	A
1	2	342	A
1	2	343	C
1	2	344	C
1	2	346	U
1	2	347	U
1	2	348	U
1	2	349	G
1	2	350	G

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Mol	Chain	Res	Type
1	2	352	A
1	2	353	U
1	2	354	A
1	2	355	U
1	2	356	G
1	2	357	C
1	2	358	A
1	2	359	A
1	2	360	A
1	2	361	U
1	2	362	A
1	2	363	A
1	2	364	A
1	2	365	A
1	2	366	A
1	2	367	A
1	2	368	U
1	2	370	A
1	2	371	C
1	2	372	A
1	2	373	U
1	2	374	U
1	2	375	A
1	2	376	A
1	2	377	U
1	2	382	A
1	2	383	A
1	2	386	A
1	2	388	A
1	2	389	U
1	2	390	U
1	2	391	A
1	2	395	U
1	2	396	A
1	2	397	U
1	2	399	U
1	2	400	U
1	2	401	U
1	2	402	A
1	2	403	U
1	2	404	U
1	2	405	C

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Mol	Chain	Res	Type
1	2	406	A
1	2	407	U
1	2	408	U
1	2	409	U
1	2	410	A
1	2	411	A
1	2	412	G
1	2	413	U
1	2	414	C
1	2	415	A
1	2	416	A
1	2	417	C
1	2	418	A
1	2	419	A
1	2	420	U
1	2	421	A
1	2	422	U
1	2	423	C
1	2	424	U
1	2	425	A
1	2	426	U
1	2	427	U
1	2	428	U
1	2	429	A
1	2	430	C
1	2	431	U
1	2	432	G
1	2	433	U
1	2	434	U
1	2	435	U
1	2	436	U
1	2	437	U
1	2	438	G
1	2	439	A
1	2	441	A
1	2	442	A
1	2	443	C
1	2	444	A
1	2	446	G
1	2	447	A
1	2	448	U
1	2	449	A

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Mol	Chain	Res	Type
1	2	450	A
1	2	452	G
1	2	453	A
1	2	454	U
1	2	455	U
1	2	456	A
1	2	457	U
1	2	458	A
1	2	459	A
1	2	460	A
1	2	461	U
1	2	462	G
1	2	463	G
1	2	464	U
1	2	465	A
1	2	466	U
1	2	467	U
1	2	468	G
1	2	469	C
1	2	470	A
1	2	471	A
1	2	473	U
1	2	476	U
1	2	477	A
1	2	478	U
1	2	479	A
1	2	480	A
1	2	481	U
1	2	482	C
1	2	483	A
1	2	484	A
1	2	485	A
1	2	486	A
1	2	487	C
1	2	488	U
1	2	489	A
1	2	490	A
1	2	492	U
1	2	493	U
1	2	494	A
1	2	495	U
1	2	496	U

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Mol	Chain	Res	Type
1	2	497	A
1	2	498	U
1	2	500	U
1	2	501	U
1	2	502	A
1	2	503	A
1	2	504	A
1	2	505	U
1	2	506	U
1	2	507	A
1	2	508	G
1	2	509	C
1	2	510	A
1	2	511	U
1	2	512	G
1	2	513	U
1	2	514	U
1	2	515	U
1	2	516	A
1	2	517	G
1	2	518	A
1	2	519	U
1	2	520	A
1	2	522	A
1	2	523	A
1	2	524	C
1	2	525	A
1	2	527	U
1	2	528	A
1	2	529	A
1	2	530	A
1	2	531	U
1	2	532	U
1	2	533	U
1	2	534	A
1	2	535	G
1	2	536	A
1	2	537	A
1	2	538	G
1	2	541	A
1	2	542	U
1	2	543	U

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Mol	Chain	Res	Type
1	2	544	G
1	2	545	U
1	2	546	U
1	2	547	G
1	2	548	C
1	2	549	C
1	2	550	C
1	2	551	A
1	2	552	C
1	2	553	C
1	2	554	A
1	2	556	U
1	2	557	C
1	2	558	U
1	2	559	U
1	2	560	U
1	2	561	G
1	2	563	A
1	2	564	A
1	2	565	U
1	2	566	A
1	2	567	A
1	2	568	A
1	2	570	A
1	2	571	C
1	2	573	A
1	2	574	C
1	2	575	G
1	2	578	C
1	2	582	A
1	2	583	A
1	2	585	U
1	2	586	A
1	2	587	A
1	2	588	U
1	2	589	G
1	2	590	U
1	2	592	U
1	2	593	U
1	2	595	A
1	2	596	U
1	2	597	A

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Mol	Chain	Res	Type
1	2	598	A
1	2	599	A
1	2	605	A
1	2	606	U
1	2	607	U
1	2	608	U
1	2	609	U
1	2	610	U
1	2	611	U
1	2	612	U
1	2	613	U
1	2	614	U
1	2	615	U
1	2	616	U
1	2	617	U
1	1	38	A
1	1	39	U
1	1	40	C
1	1	41	A
1	1	42	A
1	1	43	A
1	1	44	G
1	1	45	U
1	1	46	U
1	1	47	A
1	1	48	U
1	1	49	U
1	1	50	A
1	1	51	U
1	1	52	U
1	1	53	A
1	1	58	A
1	1	59	U
1	1	62	U
1	1	63	G
1	1	64	A
1	1	66	U
1	1	67	U
1	1	68	U
1	1	69	G
1	1	70	G
1	1	71	A

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Mol	Chain	Res	Type
1	1	72	U
1	1	73	G
1	1	74	A
1	1	75	A
1	1	76	U
1	1	79	A
1	1	81	U
1	1	83	U
1	1	84	U
1	1	88	U
1	1	89	U
1	1	90	A
1	1	91	U
1	1	92	A
1	1	93	U
1	1	96	U
1	1	98	G
1	1	99	A
1	1	102	U
1	1	103	U
1	1	104	U
1	1	106	A
1	1	107	U
1	1	108	U
1	1	110	U
1	1	111	A
1	1	113	U
1	1	115	U
1	1	116	U
1	1	117	U
1	1	118	U
1	1	119	G
1	1	120	A
1	1	126	U
1	1	127	A
1	1	128	U
1	1	130	U
1	1	132	U
1	1	134	A
1	1	135	A
1	1	136	A
1	1	137	U

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Mol	Chain	Res	Type
1	1	138	A
1	1	139	U
1	1	141	A
1	1	142	U
1	1	143	A
1	1	144	U
1	1	145	A
1	1	146	U
1	1	147	U
1	1	148	U
1	1	149	U
1	1	150	A
1	1	152	A
1	1	153	U
1	1	154	U
1	1	155	U
1	1	156	A
1	1	158	A
1	1	160	U
1	1	161	U
1	1	162	G
1	1	163	U
1	1	164	U
1	1	165	G
1	1	166	U
1	1	167	U
1	1	184	G
1	1	185	U
1	1	187	U
1	1	188	A
1	1	189	U
1	1	190	A
1	1	192	A
1	1	193	U
1	1	198	A
1	1	201	U
1	1	202	A
1	1	203	A
1	1	204	U
1	1	205	U
1	1	206	U
1	1	207	G

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Mol	Chain	Res	Type
1	1	208	U
1	1	209	U
1	1	210	U
1	1	211	U
1	1	212	A
1	1	214	U
1	1	215	U
1	1	221	U
1	1	225	U
1	1	226	A
1	1	230	A
1	1	233	G
1	1	238	U
1	1	239	U
1	1	240	A
1	1	241	U
1	1	245	U
1	1	246	U
1	1	247	A
1	1	249	U
1	1	250	A
1	1	251	U
1	1	252	U
1	1	253	U
1	1	254	U
1	1	256	A
1	1	257	G
1	1	259	U
1	1	268	A
1	1	270	A
1	1	271	U
1	1	272	A
1	1	280	A
1	1	282	U
1	1	283	G
1	1	284	A
1	1	285	U
1	1	286	G
1	1	287	G
1	1	288	C
1	1	289	A
1	1	290	C

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Mol	Chain	Res	Type
1	1	292	G
1	1	293	U
1	1	294	U
1	1	298	C
1	1	299	U
1	1	300	A
1	1	301	U
1	1	302	A
1	1	303	U
1	1	304	G
1	1	306	A
1	1	307	C
1	1	308	C
1	1	309	U
1	1	310	A
1	1	311	U
1	1	312	A
1	1	314	A
1	1	316	A
1	1	317	A
1	1	319	A
1	1	320	G
1	1	322	A
1	1	323	A
1	1	327	U
1	1	328	A
1	1	329	U
1	1	331	U
1	1	333	A
1	1	336	U
1	1	339	A
1	1	343	A
1	1	344	U
1	1	345	A
1	1	346	A
1	1	347	A
1	1	350	A
1	1	359	C
1	1	360	U
1	1	361	A
1	1	362	A
1	1	363	U

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Mol	Chain	Res	Type
1	1	364	U
1	1	365	U
1	1	370	U
1	1	374	U
1	1	377	U
1	1	379	U
1	1	380	G
1	1	381	A
1	1	382	A
1	1	383	A
1	1	384	A
1	1	388	U
1	1	391	A
1	1	392	A
1	1	393	A
1	1	394	U
1	1	396	A
1	1	397	A
1	1	398	U
1	1	399	U
1	1	400	U
1	1	401	U
1	1	402	U
1	1	404	U
1	1	405	U
1	1	407	C
1	1	411	U
1	1	412	U
1	1	413	U
1	1	414	U
1	1	415	U
1	1	416	A
1	1	418	A
1	1	420	A
1	1	421	U
1	1	422	U
1	1	423	G
1	1	424	A
1	1	425	A
1	1	426	G
1	1	427	U
1	1	429	A

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Mol	Chain	Res	Type
1	1	431	A
1	1	432	U
1	1	433	G
1	1	434	U
1	1	435	A
1	1	439	A
1	1	440	A
1	1	443	G
1	1	446	U
1	1	447	A
1	1	449	U
1	1	450	A
1	1	451	A
1	1	452	A
1	1	453	A
1	1	454	A
1	1	455	U
1	1	457	C
1	1	458	A
1	1	459	A
1	1	460	A
1	1	465	A
1	1	466	U
1	1	468	U
1	1	471	A
1	1	472	A
1	1	473	U
1	1	474	U
1	1	475	A
1	1	476	A
1	1	477	U
1	1	478	A
1	1	479	A
1	1	480	A
1	1	481	U
1	1	482	A
1	1	483	U
1	1	484	A
1	1	486	U
1	1	488	U
1	1	489	A
1	1	492	U

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Mol	Chain	Res	Type
1	1	495	A
1	1	496	U
1	1	497	A
1	1	498	G
1	1	500	U
1	1	501	G
1	1	504	U
1	1	506	A
1	1	507	U
1	1	508	G
1	1	509	U
1	1	510	U
1	1	511	A
1	1	512	A
1	1	514	U
1	1	515	A
1	1	516	A
1	1	517	U
1	1	518	U
1	1	519	U
1	1	520	A
1	1	521	U
1	1	522	U
1	1	523	A
1	1	524	U
1	1	525	U
1	1	526	U
1	1	527	U
1	1	528	A
1	1	529	A
1	1	532	U
1	1	536	A
1	1	537	U
1	1	538	A
1	1	543	U
1	1	544	U
1	1	545	U
1	1	546	A
1	1	547	U
1	1	548	A
1	1	549	C
1	1	550	A

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Mol	Chain	Res	Type
1	1	552	A
1	1	555	U
1	1	556	A
1	1	557	A
1	1	558	C
1	1	559	U
1	1	560	U
1	1	561	U
1	1	562	U
1	1	564	U
1	1	565	U
1	1	566	G
1	1	567	A
1	1	568	A
1	1	572	A
1	1	573	A
1	1	574	A
1	1	575	G
1	1	576	A
1	1	578	U
1	1	580	A
1	1	581	U
1	1	582	U
1	1	583	A
1	1	584	U
1	1	587	U
1	1	588	A
1	1	589	A
1	1	590	A
1	1	591	U
1	1	592	A
1	1	593	U
1	1	594	U
1	1	595	A
1	1	596	U
1	1	597	U
1	1	598	U
1	1	599	U
1	1	600	A
1	1	601	A
1	1	602	A
1	1	604	A

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Mol	Chain	Res	Type
1	1	608	A
1	1	609	A
1	1	612	A
1	1	617	G
1	1	618	U
1	1	621	A
1	1	622	U
1	1	624	A
1	1	625	A
1	1	626	A
1	1	627	U
1	1	629	A
1	1	630	U
1	1	631	C
1	1	632	A
1	1	633	A
1	1	634	G
1	1	641	A
1	1	642	A
1	1	643	G
1	1	644	C
1	1	645	G
1	1	647	U
1	1	648	U
1	1	649	A
1	1	650	U
1	1	651	U
1	1	652	A
1	1	653	A
1	1	655	U
1	1	661	G
1	1	665	U
1	1	666	A
1	1	667	A
1	1	668	G
1	1	669	U
1	1	670	A
1	1	675	A
1	1	679	A
1	1	680	A
1	1	684	U
1	1	685	A

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Mol	Chain	Res	Type
1	1	690	U
1	1	691	G
1	1	697	A
1	1	698	G
1	1	699	A
1	1	700	U
1	1	701	U
1	1	702	U
1	1	704	U
1	1	705	A
1	1	710	A
1	1	712	U
1	1	749	U
1	1	750	U
1	1	751	A
1	1	754	A
1	1	755	G
1	1	756	U
1	1	760	A
1	1	763	G
1	1	764	U
1	1	765	A
1	1	768	U
1	1	769	U
1	1	772	U
1	1	775	C
1	1	776	U
1	1	781	A
1	1	782	U
1	1	783	U
1	1	784	A
1	1	785	A
1	1	786	A
1	1	787	G
1	1	788	C
1	1	789	G
1	1	790	U
1	1	791	U
1	1	794	A
1	1	795	U
1	1	796	A
1	1	798	A

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Mol	Chain	Res	Type
1	1	799	A
1	1	802	U
1	1	807	A
1	1	808	A
1	1	809	A
1	1	810	U
1	1	811	U
1	1	812	A
1	1	813	U
1	1	815	A
1	1	816	C
1	1	817	A
1	1	821	U
1	1	822	A
1	1	830	A
1	1	835	A
1	1	836	U
1	1	837	U
1	1	839	A
1	1	845	A
1	1	847	A
1	1	848	U
1	1	850	U
1	1	851	U
1	1	856	A
1	1	857	A
1	1	862	A
1	1	863	A
1	1	864	A
1	1	868	U
1	1	869	A
1	1	870	A
1	1	873	U
1	1	876	G
1	1	887	C
1	1	888	U
1	1	889	C
1	1	890	U
1	1	892	C
1	1	893	U
1	1	894	U
1	1	895	U

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Mol	Chain	Res	Type
1	1	896	A
1	1	902	A
1	1	903	G
1	1	904	A
1	1	905	A
1	1	906	C
1	1	907	G
1	1	908	U
1	1	910	U
1	1	911	A
1	1	914	U
1	1	915	G
1	1	916	U
1	1	917	A
1	1	918	A
1	1	919	U
1	1	924	U
1	1	925	G
1	1	927	U
1	1	928	U
1	1	929	G
1	1	930	A
1	1	933	G
1	1	934	G
1	1	939	A
1	1	940	U
1	1	941	A
1	1	943	U
1	1	944	A
1	1	945	U
1	1	948	C
1	1	949	U
1	1	952	U
1	1	953	U
1	1	954	A
1	1	955	U
1	1	960	A
1	1	961	A
1	1	962	A
1	1	963	A
1	1	964	A
1	1	969	U

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Mol	Chain	Res	Type
1	1	971	U
1	1	972	A
1	1	973	U
1	1	974	U
1	1	975	U
1	1	977	U
1	1	978	U
1	1	980	A
1	1	982	A
1	1	983	U
1	1	984	A
1	1	985	A
1	1	988	A
1	1	990	A
1	1	992	G
1	1	993	U
1	1	995	C
1	1	996	G
1	1	997	A
1	1	998	G
1	1	999	C
1	1	1002	G
1	1	1003	U
1	1	1004	U
1	1	1005	A
1	1	1006	A
1	1	1007	C
1	1	1008	A
1	1	1009	A
1	1	1010	G
1	1	1011	C
1	1	1012	A
1	1	1013	U
1	1	1014	U
1	1	1015	A
1	1	1016	A
1	1	1017	U
1	1	1018	A
1	1	1019	C
1	1	1025	G
1	1	1028	U
1	1	1031	C

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Mol	Chain	Res	Type
1	1	1032	A
1	1	1033	U
1	1	1034	C
1	1	1035	G
1	1	1036	U
1	1	1037	C
1	1	1038	U
1	1	1040	C
1	1	1041	U
1	1	1044	U
1	1	1045	U
1	1	1046	G
1	1	1047	C
1	1	1050	A
1	1	1051	A
1	1	1053	U
1	1	1054	A
1	1	1055	U
1	1	1056	A
1	1	1059	U
1	1	1062	U
1	1	1063	U
1	1	1064	G
1	1	1065	U
1	1	1066	U
1	1	1068	A
1	1	1069	U
1	1	1072	A
1	1	1073	A
1	1	1074	A
1	1	1075	A
1	1	1086	U
1	1	1093	G
1	1	1095	U
1	1	1096	A
1	1	1097	A
1	1	1098	A
1	1	1099	A
1	1	1100	U
1	1	1101	C
1	1	1103	U
1	1	1105	G

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Mol	Chain	Res	Type
1	1	1107	A
1	1	1111	C
1	1	1116	U
1	1	1117	U
1	1	1118	G
1	1	1122	A
1	1	1123	U
1	1	1124	A
1	1	1125	U
1	1	1126	A
1	1	1127	U
1	1	1128	U
1	1	1129	U
1	1	1135	U
1	1	1136	U
1	1	1137	G
1	1	1138	U
1	1	1139	A
1	1	1140	U
1	1	1141	A
1	1	1146	U
1	1	1157	A
1	1	1158	U

All (329) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1	G
1	2	2	U
1	2	3	C
1	2	5	A
1	2	27	U
1	2	28	U
1	2	32	A
1	2	46	U
1	2	53	U
1	2	54	A
1	2	60	U
1	2	65	U
1	2	83	A
1	2	87	A
1	2	92	U

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Mol	Chain	Res	Type
1	2	100	A
1	2	102	U
1	2	108	A
1	2	109	U
1	2	111	A
1	2	123	G
1	2	133	G
1	2	134	U
1	2	147	U
1	2	149	A
1	2	150	A
1	2	156	U
1	2	165	A
1	2	166	G
1	2	167	U
1	2	171	A
1	2	172	A
1	2	174	U
1	2	175	U
1	2	176	U
1	2	179	G
1	2	183	U
1	2	188	A
1	2	190	A
1	2	194	U
1	2	195	A
1	2	198	U
1	2	200	A
1	2	210	U
1	2	213	U
1	2	218	A
1	2	227	U
1	2	234	C
1	2	241	G
1	2	242	U
1	2	243	A
1	2	247	U
1	2	255	U
1	2	257	U
1	2	258	A
1	2	259	A
1	2	267	A

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Mol	Chain	Res	Type
1	2	271	U
1	2	272	U
1	2	274	U
1	2	286	G
1	2	291	U
1	2	304	U
1	2	306	A
1	2	311	A
1	2	312	A
1	2	315	A
1	2	325	U
1	2	326	U
1	2	327	U
1	2	333	U
1	2	335	U
1	2	338	A
1	2	353	U
1	2	358	A
1	2	361	U
1	2	371	C
1	2	372	A
1	2	373	U
1	2	381	U
1	2	387	U
1	2	390	U
1	2	397	U
1	2	399	U
1	2	400	U
1	2	401	U
1	2	403	U
1	2	404	U
1	2	405	C
1	2	406	A
1	2	407	U
1	2	408	U
1	2	409	U
1	2	410	A
1	2	411	A
1	2	412	G
1	2	413	U
1	2	414	C
1	2	415	A

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Mol	Chain	Res	Type
1	2	416	A
1	2	417	C
1	2	418	A
1	2	419	A
1	2	420	U
1	2	421	A
1	2	422	U
1	2	423	C
1	2	424	U
1	2	425	A
1	2	426	U
1	2	427	U
1	2	428	U
1	2	429	A
1	2	430	C
1	2	431	U
1	2	432	G
1	2	433	U
1	2	434	U
1	2	435	U
1	2	436	U
1	2	442	A
1	2	446	G
1	2	448	U
1	2	452	G
1	2	453	A
1	2	454	U
1	2	455	U
1	2	456	A
1	2	457	U
1	2	459	A
1	2	461	U
1	2	462	G
1	2	463	G
1	2	464	U
1	2	465	A
1	2	466	U
1	2	468	G
1	2	469	C
1	2	470	A
1	2	472	A
1	2	476	U

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Mol	Chain	Res	Type
1	2	478	U
1	2	483	A
1	2	484	A
1	2	485	A
1	2	486	A
1	2	487	C
1	2	488	U
1	2	489	A
1	2	492	U
1	2	493	U
1	2	494	A
1	2	495	U
1	2	496	U
1	2	497	A
1	2	500	U
1	2	503	A
1	2	504	A
1	2	505	U
1	2	506	U
1	2	507	A
1	2	508	G
1	2	509	C
1	2	510	A
1	2	511	U
1	2	512	G
1	2	513	U
1	2	514	U
1	2	515	U
1	2	516	A
1	2	517	G
1	2	518	A
1	2	519	U
1	2	523	A
1	2	524	C
1	2	528	A
1	2	529	A
1	2	530	A
1	2	531	U
1	2	532	U
1	2	533	U
1	2	534	A
1	2	535	G

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Mol	Chain	Res	Type
1	2	536	A
1	2	537	A
1	2	540	U
1	2	543	U
1	2	545	U
1	2	555	U
1	2	556	U
1	2	559	U
1	2	560	U
1	2	565	U
1	2	570	A
1	2	572	A
1	2	578	C
1	2	585	U
1	2	607	U
1	2	611	U
1	2	616	U
1	1	39	U
1	1	40	C
1	1	41	A
1	1	45	U
1	1	47	A
1	1	50	A
1	1	65	U
1	1	70	G
1	1	74	A
1	1	97	U
1	1	98	G
1	1	106	A
1	1	131	U
1	1	135	A
1	1	136	A
1	1	137	U
1	1	146	U
1	1	155	U
1	1	161	U
1	1	164	U
1	1	191	A
1	1	201	U
1	1	202	A
1	1	203	A
1	1	204	U

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Mol	Chain	Res	Type
1	1	206	U
1	1	207	G
1	1	208	U
1	1	209	U
1	1	210	U
1	1	239	U
1	1	249	U
1	1	269	A
1	1	282	U
1	1	284	A
1	1	293	U
1	1	299	U
1	1	303	U
1	1	309	U
1	1	343	A
1	1	346	A
1	1	369	A
1	1	381	A
1	1	398	U
1	1	401	U
1	1	403	U
1	1	406	U
1	1	414	U
1	1	424	A
1	1	430	U
1	1	433	G
1	1	450	A
1	1	477	U
1	1	487	U
1	1	491	U
1	1	506	A
1	1	508	G
1	1	509	U
1	1	511	A
1	1	513	U
1	1	519	U
1	1	523	A
1	1	547	U
1	1	565	U
1	1	572	A
1	1	589	A
1	1	590	A

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Mol	Chain	Res	Type
1	1	591	U
1	1	592	A
1	1	593	U
1	1	595	A
1	1	596	U
1	1	617	G
1	1	626	A
1	1	628	U
1	1	632	A
1	1	642	A
1	1	643	G
1	1	649	A
1	1	650	U
1	1	652	A
1	1	660	C
1	1	668	G
1	1	689	U
1	1	697	A
1	1	698	G
1	1	703	U
1	1	704	U
1	1	754	A
1	1	759	C
1	1	763	G
1	1	781	A
1	1	782	U
1	1	790	U
1	1	798	A
1	1	811	U
1	1	821	U
1	1	835	A
1	1	844	A
1	1	847	A
1	1	849	U
1	1	856	A
1	1	861	A
1	1	862	A
1	1	905	A
1	1	906	C
1	1	910	U
1	1	915	G
1	1	916	U

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Mol	Chain	Res	Type
1	1	928	U
1	1	929	G
1	1	932	U
1	1	944	A
1	1	951	U
1	1	960	A
1	1	974	U
1	1	1015	A
1	1	1044	U
1	1	1054	A
1	1	1067	C
1	1	1074	A
1	1	1097	A
1	1	1121	U
1	1	1122	A
1	1	1125	U
1	1	1126	A
1	1	1127	U
1	1	1128	U
1	1	1157	A

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 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	$\#\|Z\|>2$
125	NAD	Ag	301	-	42,48,48	0.61	0	50,73,73	1.12	5 (10%)

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
125	NAD	Ag	301	-	-	11/26/62/62	0/5/5/5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
125	Ag	301	NAD	O4D-C1D-C2D	-4.10	100.93	106.93
125	Ag	301	NAD	C3D-C2D-C1D	3.28	105.91	100.98
125	Ag	301	NAD	C6N-N1N-C2N	-2.20	119.97	121.97
125	Ag	301	NAD	C5A-C6A-N6A	2.15	123.62	120.35
125	Ag	301	NAD	O4B-C4B-C3B	-2.09	100.98	105.11

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
125	Ag	301	NAD	C5B-O5B-PA-O3
125	Ag	301	NAD	C2D-C1D-N1N-C2N
125	Ag	301	NAD	C4B-C5B-O5B-PA
125	Ag	301	NAD	PN-O3-PA-O5B
125	Ag	301	NAD	PA-O3-PN-O5D
125	Ag	301	NAD	C4D-C5D-O5D-PN
125	Ag	301	NAD	C5B-O5B-PA-O1A
125	Ag	301	NAD	PA-O3-PN-O1N
125	Ag	301	NAD	PN-O3-PA-O2A
125	Ag	301	NAD	C2D-C1D-N1N-C6N
125	Ag	301	NAD	C5D-O5D-PN-O1N

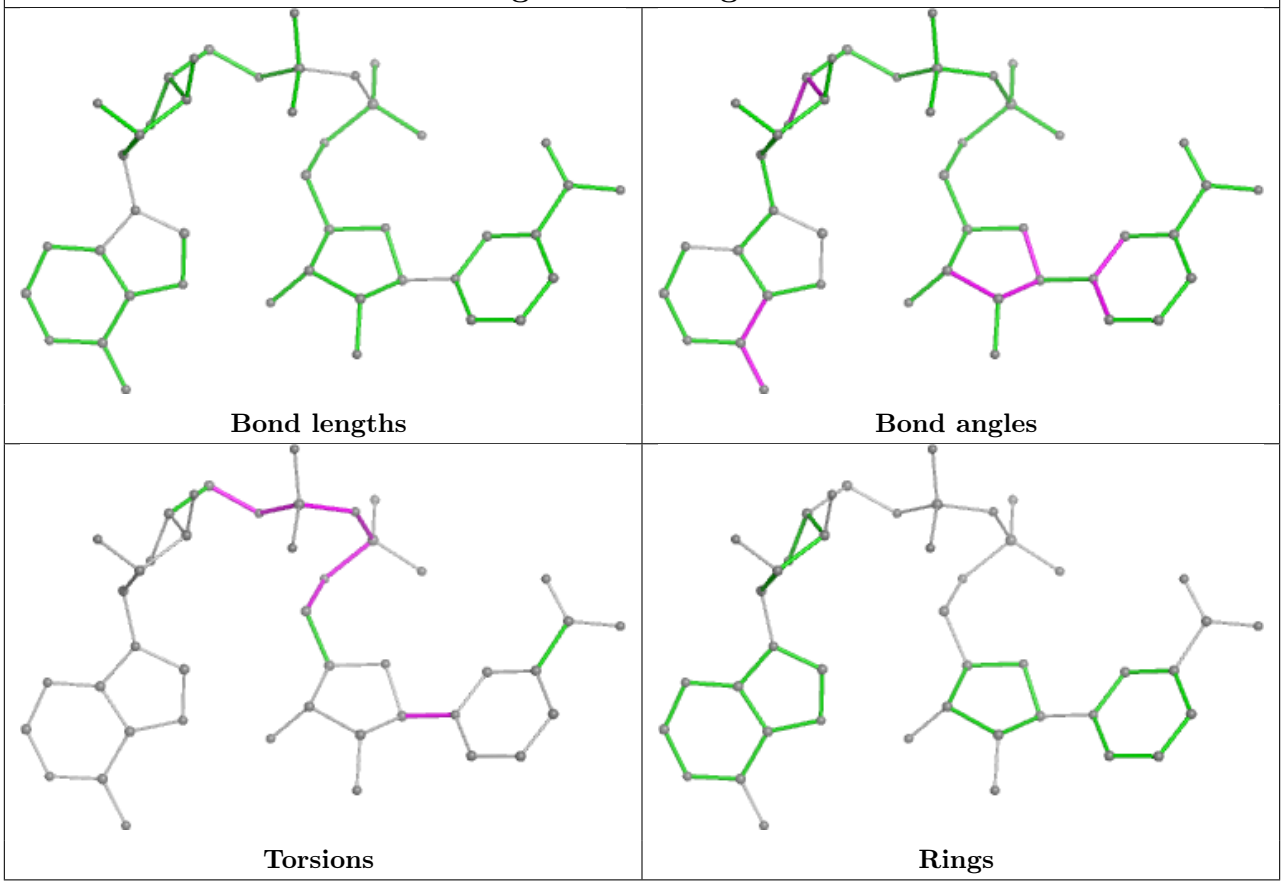
There are no ring outliers.

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 NAD Ag 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	am	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	am	121:GLU	C	122:ASN	N	3.38

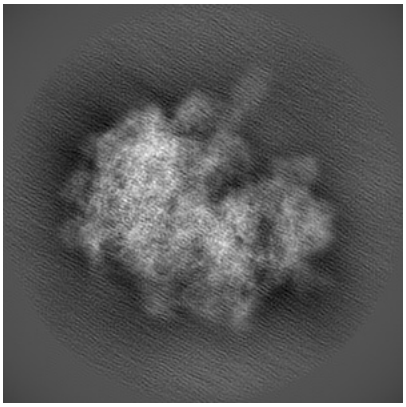
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11829. These allow visual inspection of the internal detail of the map and identification of artifacts.

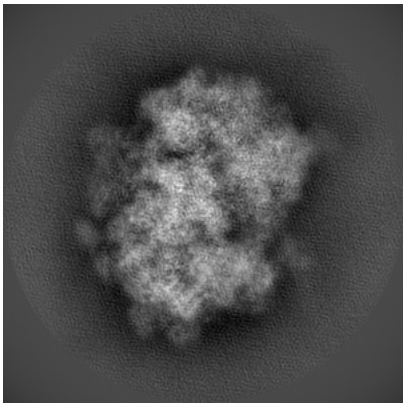
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

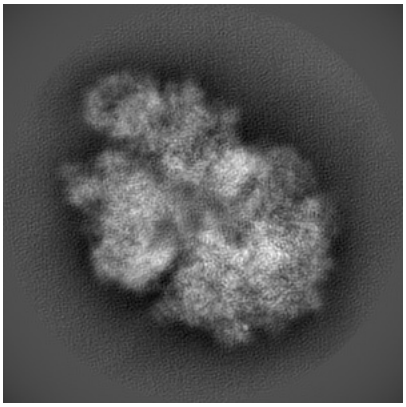
6.1.1 Primary map



X



Y

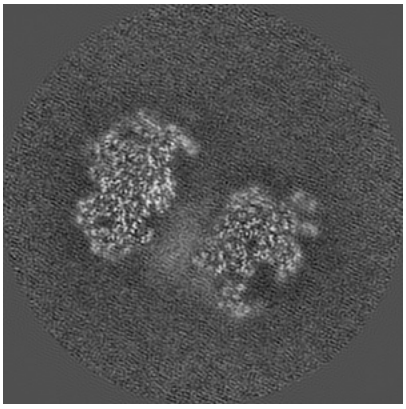


Z

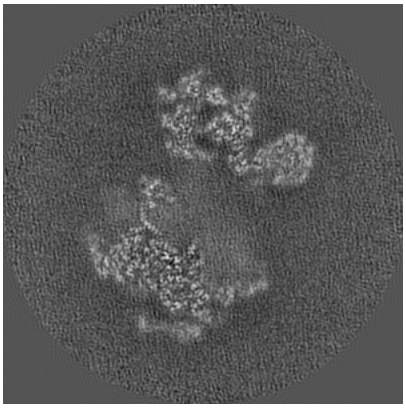
The images above show the map projected in three orthogonal directions.

6.2 Central slices

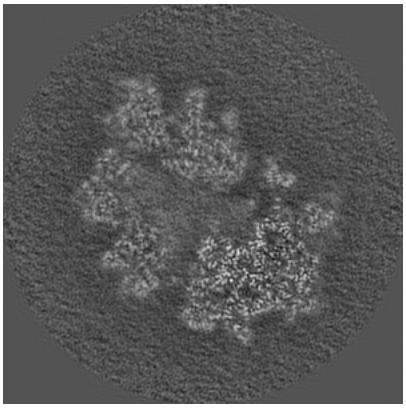
6.2.1 Primary map



X Index: 200



Y Index: 200

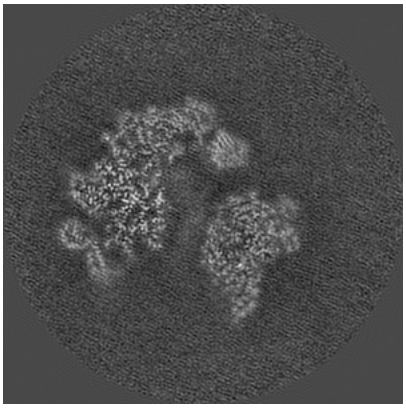


Z Index: 200

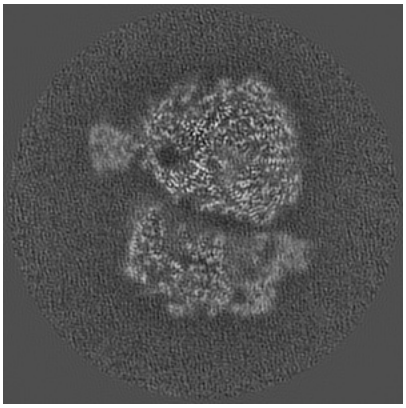
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

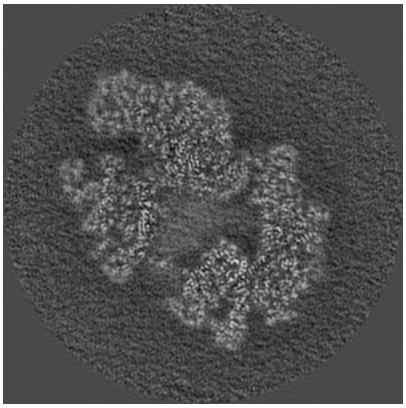
6.3.1 Primary map



X Index: 224



Y Index: 150

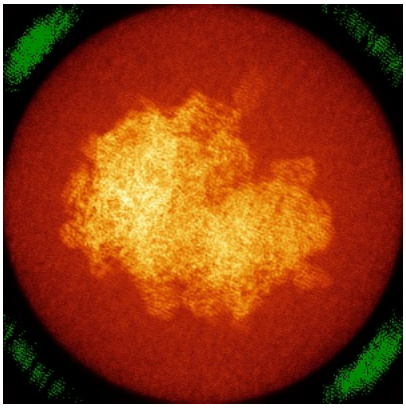


Z Index: 173

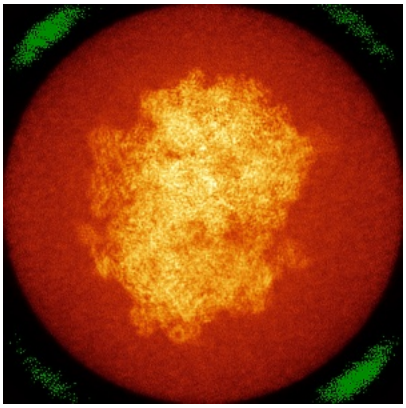
The images above show the largest variance slices of the map in three orthogonal directions.

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

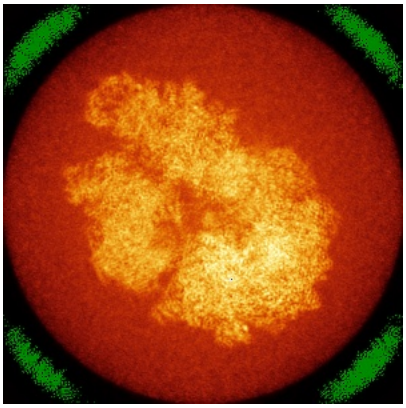
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

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.

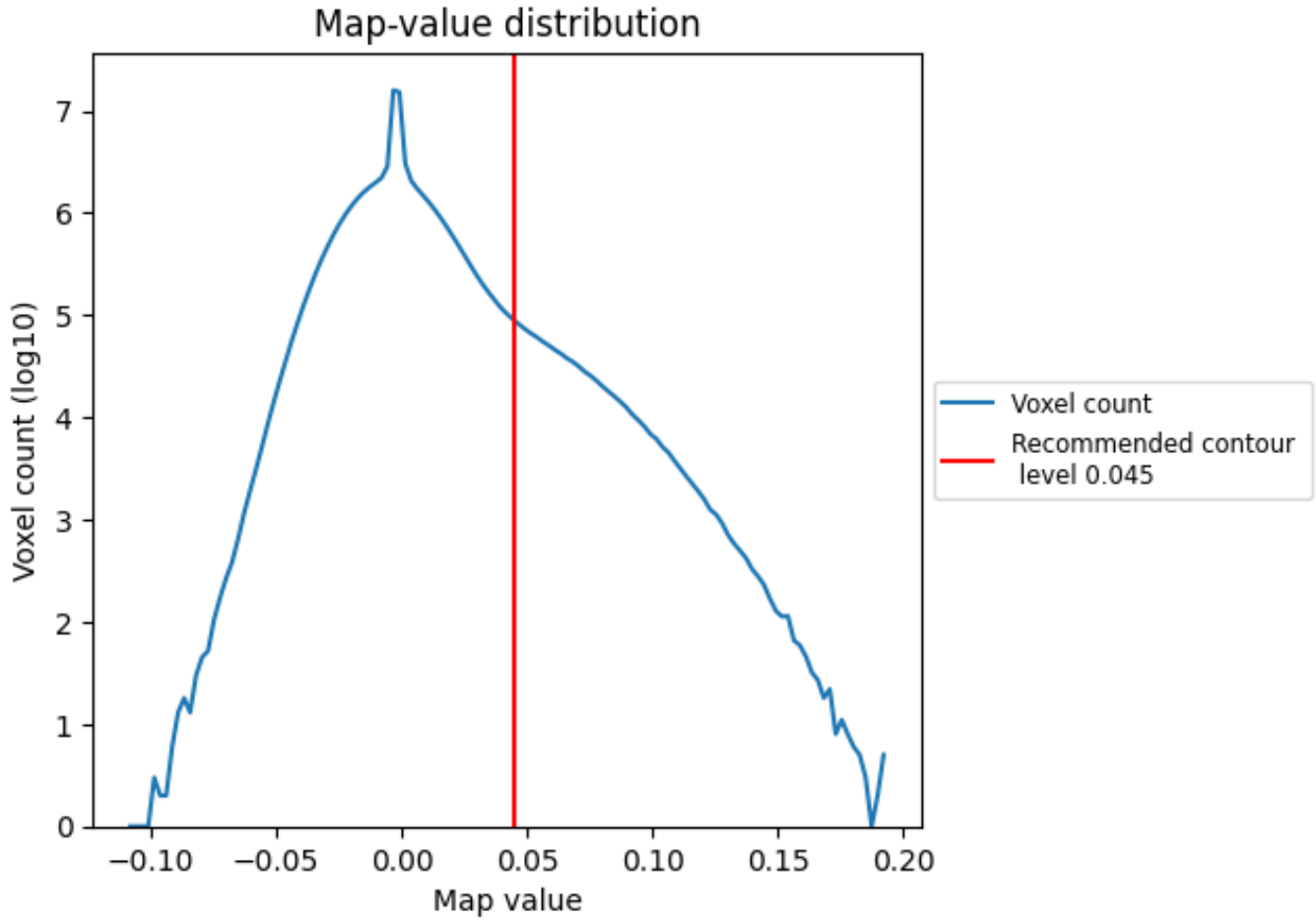
6.6 Mask visualisation (i)

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

7 Map analysis

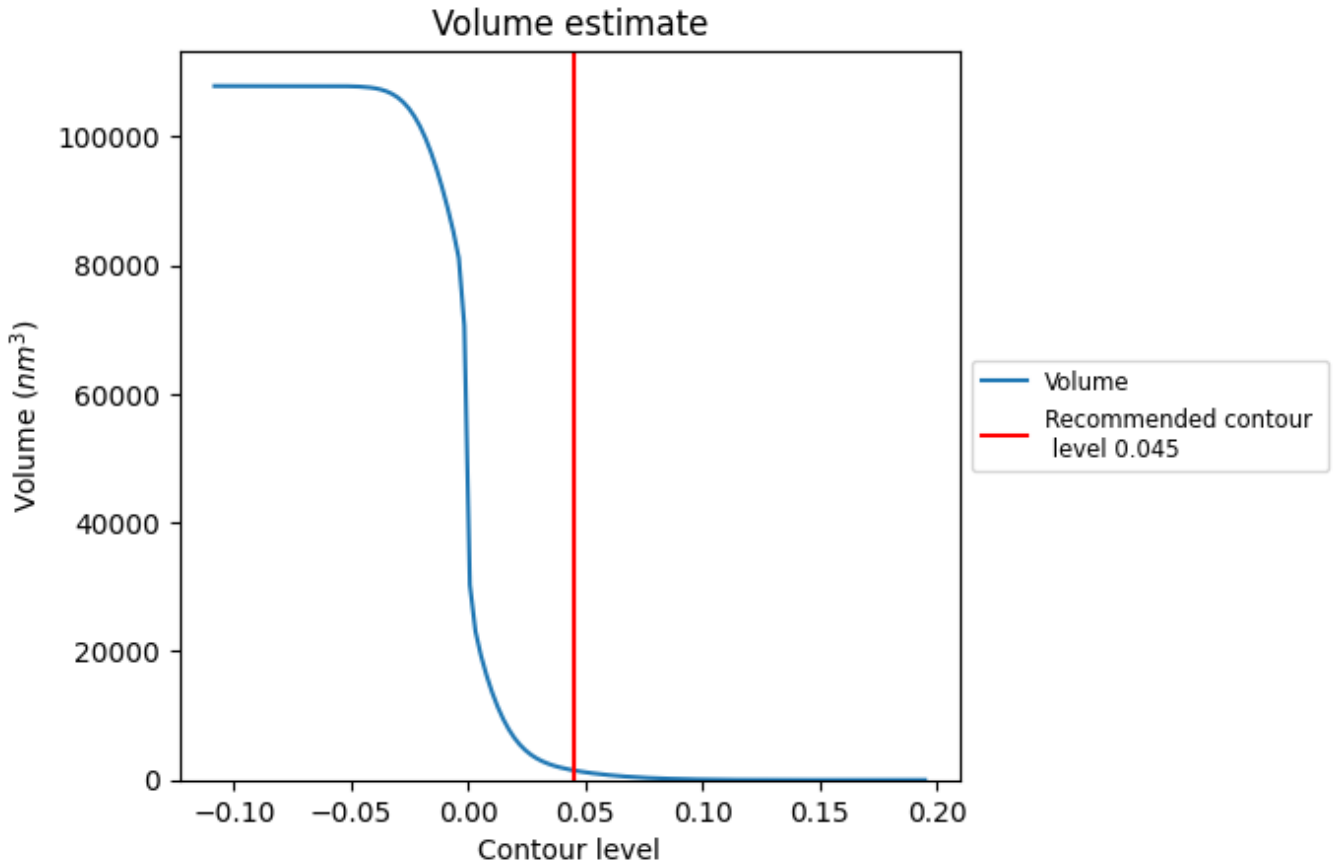
This section contains the results of statistical analysis of the map.

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.

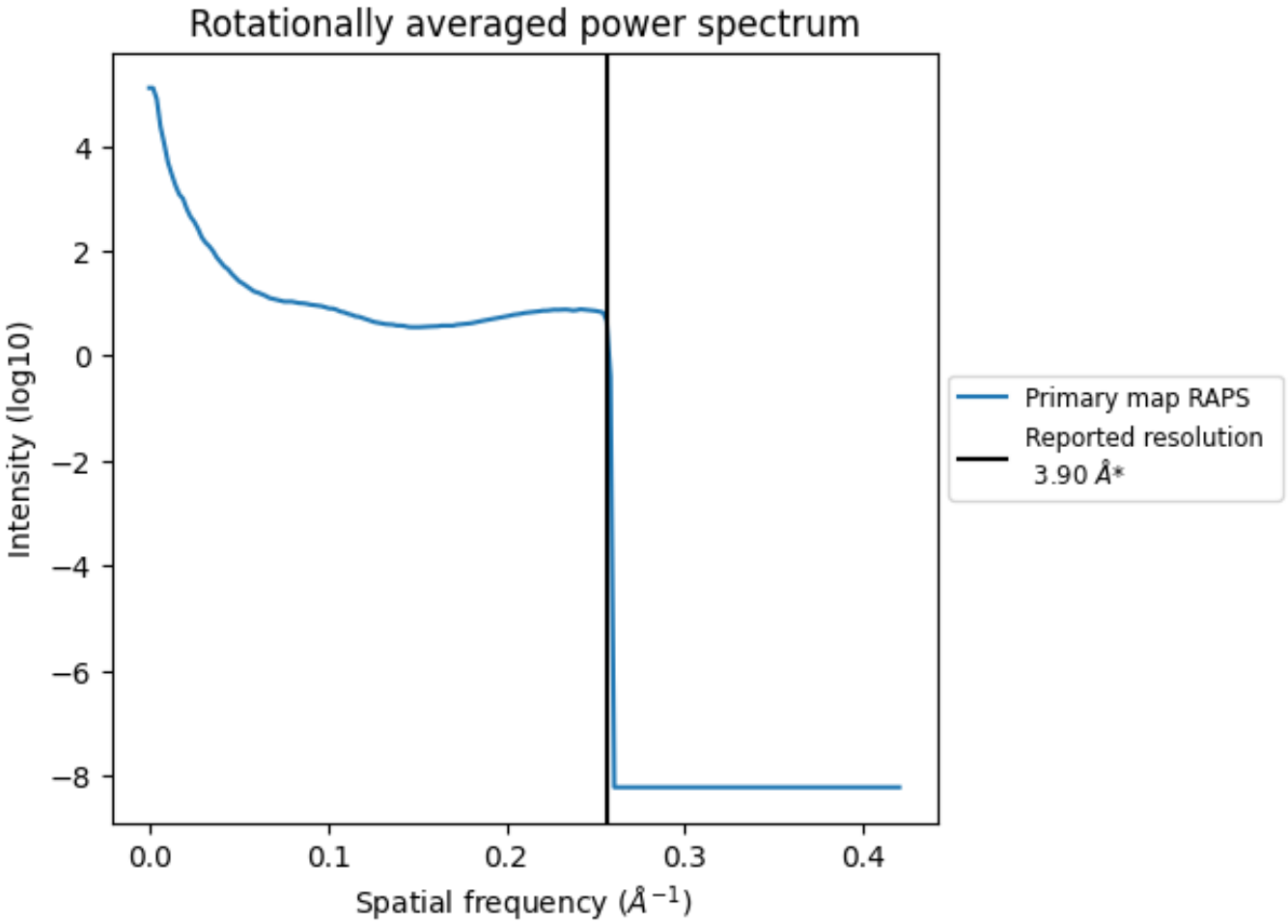
7.2 Volume estimate



The volume at the recommended contour level is 1487 nm^3; this corresponds to an approximate mass of 1343 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

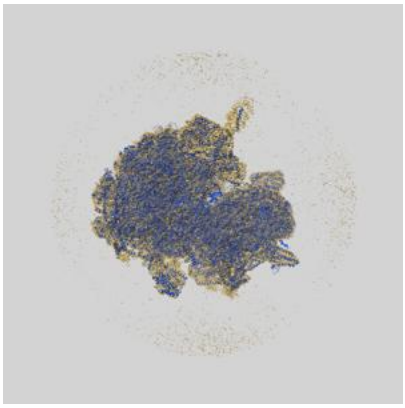
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

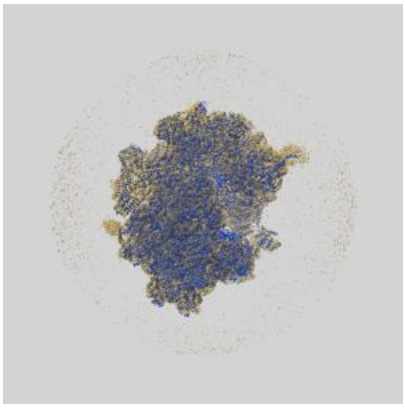
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11829 and PDB model 7ANE. Per-residue inclusion information can be found in section 3 on page 27.

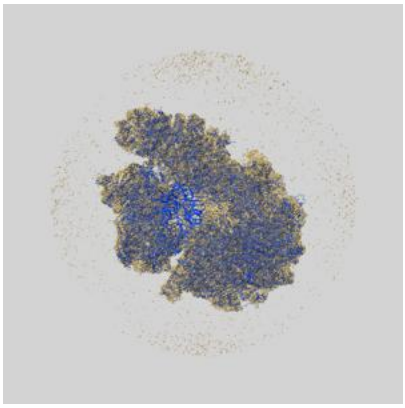
9.1 Map-model overlay



X



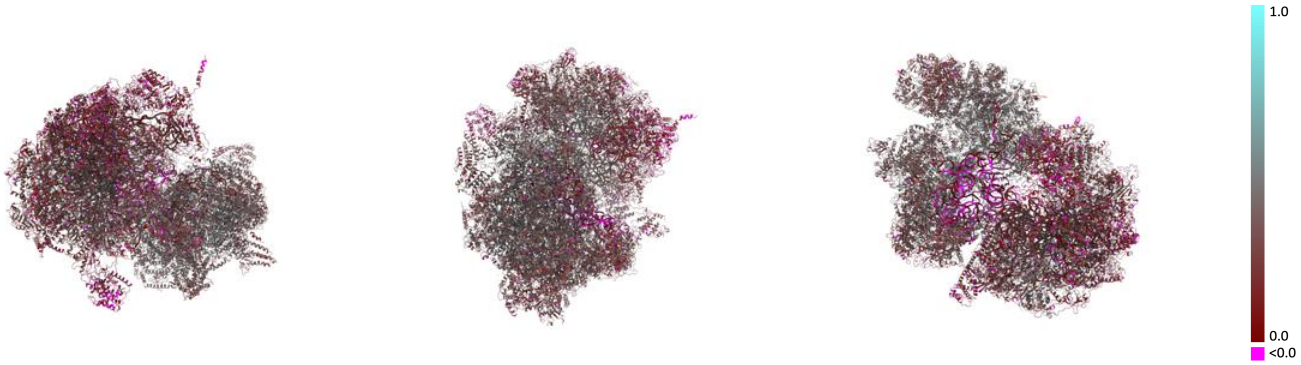
Y



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.

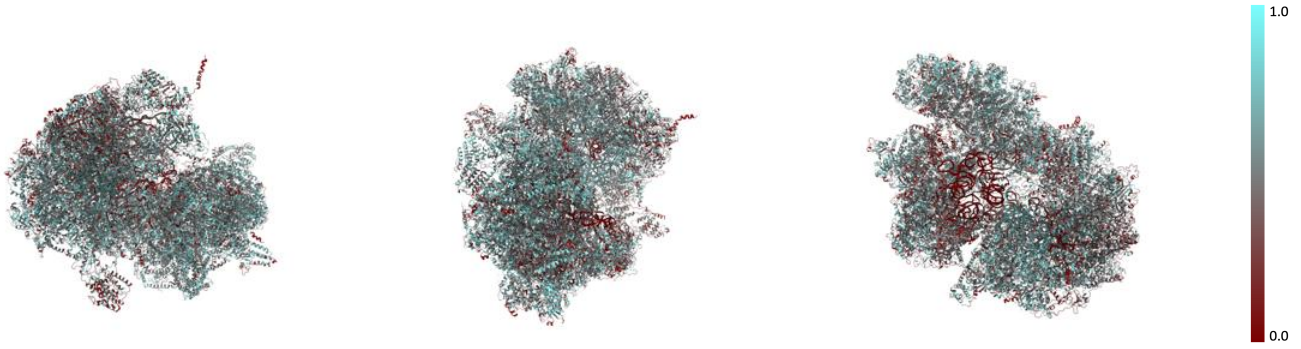
9.2 Q-score mapped to coordinate model (i)



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.

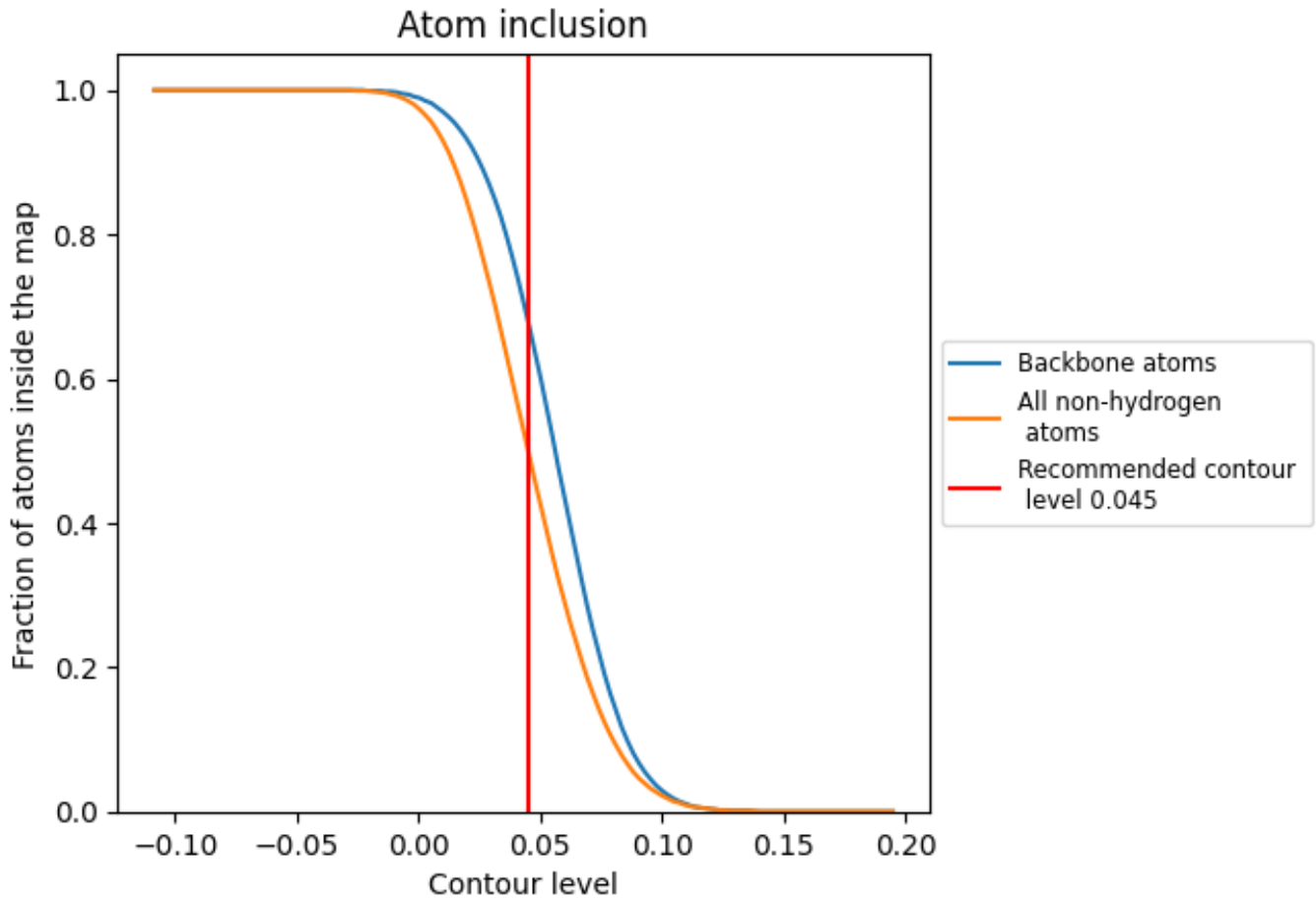
9.3 Atom inclusion mapped to coordinate model (i)



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 (i)



At the recommended contour level, 68% of all backbone atoms, 50% 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	0.5010	0.3210
1	0.6440	0.3250
2	0.1120	0.0360
A	0.4610	0.2040
Aa	0.3690	0.2020
Ab	0.4850	0.2250
Ac	0.5310	0.3030
Ad	0.4300	0.2790
Ae	0.4230	0.1760
Af	0.4190	0.2100
Ag	0.5820	0.3550
Ah	0.5310	0.2640
Ai	0.5150	0.2900
Aj	0.4460	0.2260
Ak	0.5080	0.2390
Al	0.5480	0.2700
Am	0.4360	0.1610
An	0.5300	0.2960
Ao	0.5800	0.3180
Ap	0.4250	0.1900
Aq	0.5120	0.3570
Ar	0.5580	0.3460
As	0.4710	0.1780
At	0.5100	0.2510
Au	0.5970	0.3460
Av	0.4840	0.2070
Aw	0.5140	0.2570
Ax	0.5600	0.3310
Ay	0.5790	0.2930
Az	0.6210	0.3700
B	0.5050	0.2890
BA	0.4840	0.2390
BB	0.4210	0.1810
BC	0.5510	0.3630
BD	0.5930	0.3220

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Chain	Atom inclusion	Q-score
BE	0.4470	0.1690
BF	0.5210	0.3430
BG	0.5290	0.3080
BH	0.4620	0.2390
BI	0.5840	0.2960
BL	0.5730	0.3350
BM	0.3460	0.1220
BO	0.4170	0.2090
BP	0.4470	0.2500
Bj	0.4920	0.3330
C	0.5840	0.3250
D	0.3250	0.1210
E	0.4720	0.1750
F	0.4170	0.2200
G	0.5290	0.3200
H	0.4850	0.3200
I	0.4870	0.2790
J	0.4400	0.1980
K	0.4380	0.2300
L	0.4190	0.2030
M	0.5270	0.3060
N	0.6120	0.4010
O	0.4020	0.2560
P	0.5730	0.3810
Q	0.5820	0.3370
R	0.5320	0.2830
S	0.4750	0.2740
T	0.5820	0.3010
U	0.5240	0.3610
UA	0.6670	0.2890
UB	0.5370	0.3040
UC	0.3280	0.1890
UD	0.5030	0.1910
V	0.5590	0.3960
W	0.4600	0.2770
X	0.4890	0.2890
Y	0.5370	0.3210
Z	0.6180	0.3990
a	0.4880	0.4310
aa	0.5240	0.3740
ab	0.5000	0.4030
ac	0.4990	0.3150

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Chain	Atom inclusion	Q-score
ad	0.4910	0.3690
ae	0.5580	0.3940
af	0.5580	0.3690
ag	0.4930	0.4050
ai	0.5610	0.3960
aj	0.6130	0.4020
ak	0.4450	0.3460
am	0.4960	0.4470
an	0.5890	0.4180
ao	0.5520	0.4140
ap	0.6240	0.3810
aq	0.3490	0.2790
ar	0.4900	0.3620
as	0.4150	0.3030
at	0.2090	0.2680
au	0.5050	0.3990
av	0.3970	0.3520
aw	0.5600	0.4370
ax	0.5370	0.4190
ay	0.5480	0.4160
az	0.6230	0.4420
b	0.5500	0.3990
ba	0.0730	0.3450
bd	0.4940	0.4070
c	0.4700	0.4340
d	0.5590	0.4430
e	0.5400	0.4250
f	0.4810	0.3670
g	0.3030	0.3410
h	0.5830	0.4480
i	0.5020	0.4050
j	0.4610	0.3630
k	0.5070	0.4440
l	0.4720	0.3280
m	0.5350	0.4250
n	0.4920	0.4150
o	0.4140	0.3920
p	0.5950	0.4110
q	0.5720	0.3820
r	0.6050	0.4200
s	0.5520	0.4360
t	0.4240	0.3090

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Chain	Atom inclusion	Q-score
u	0.5160	0.3860
v	0.5070	0.3990
w	0.2920	0.2890
x	0.5900	0.4250
y	0.5590	0.3560
z	0.5650	0.4190