wwPDB EM Validation Summary Report

Mar 20, 2024 – 04:51 AM JST

PDB ID	:	6KE6
EMDB ID	:	EMD-9964
Title	:	3.4 angstrom cryo-EM structure of yeast 90S small subunit preribosome
Authors	:	Du, Y.; Ye, K.; An, W.
Deposited on	:	2019-07-03
Resolution	:	3.40 Å(reported)
Based on initial models	:	5WYJ, 5WLC

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

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

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

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

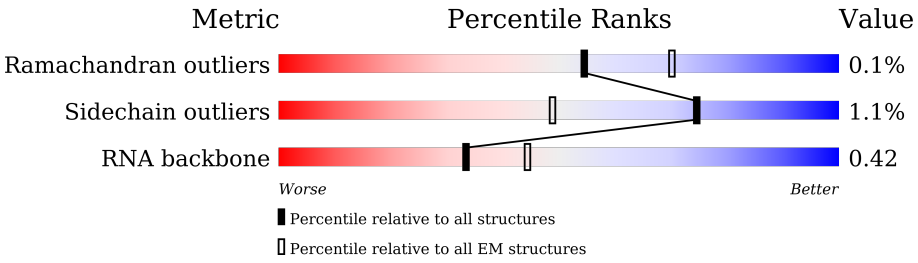
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 Å.

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



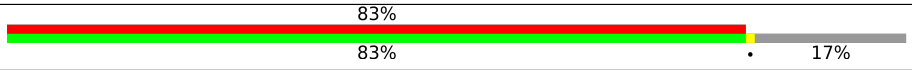
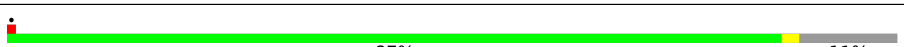
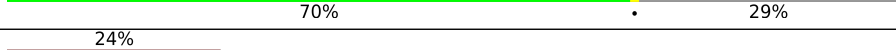
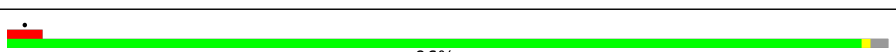
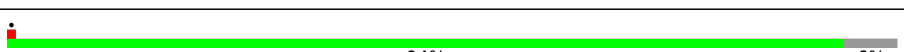
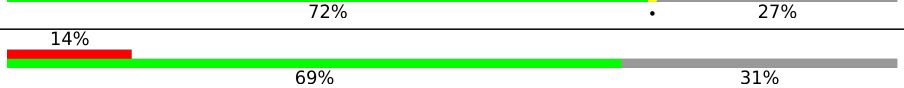
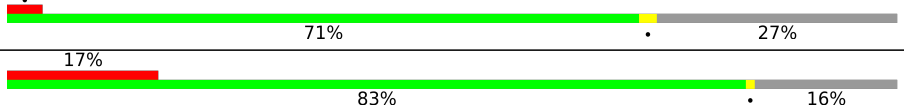
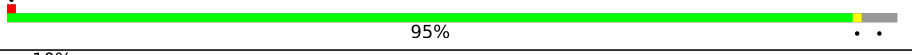
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	3A	333	36% 14% 47%
2	5A	700	10% 51% 20% 25%
3	SA	1807	33% 43% 26% 28%
4	SC	255	82% 14%
5	SF	261	62% 85% 12%
6	SG	225	94% 5%
7	SH	236	47% 46% 53%
8	SI	190	31% 85% 13%

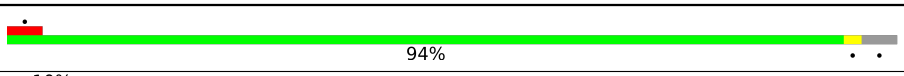
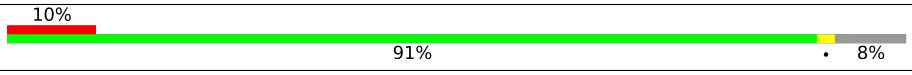
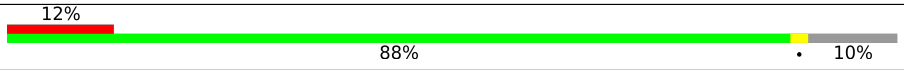
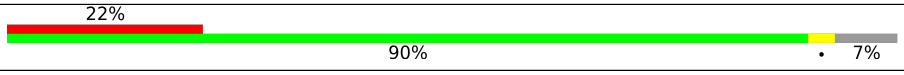
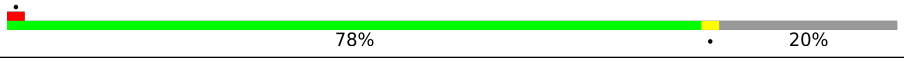
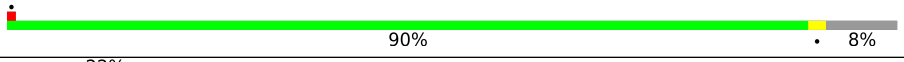
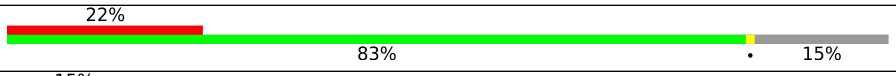
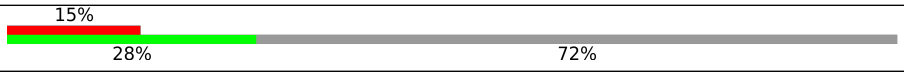
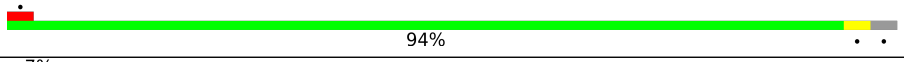
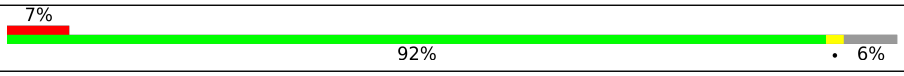
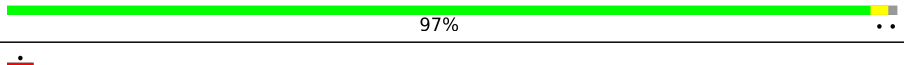
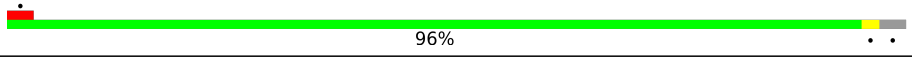
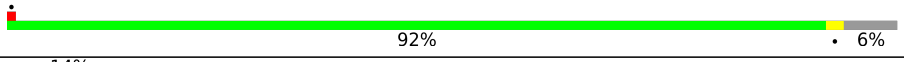
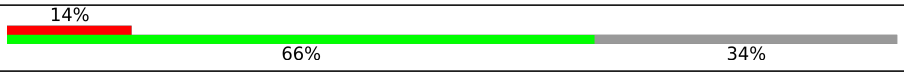
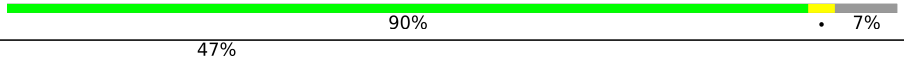
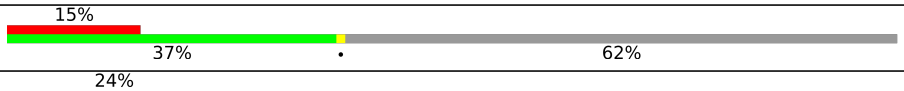
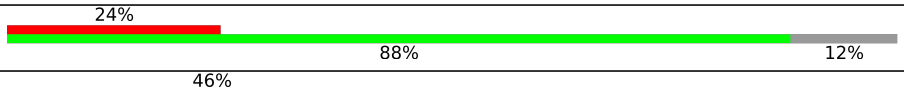
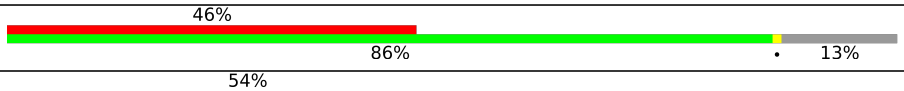
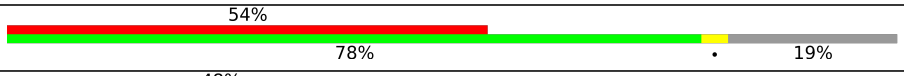
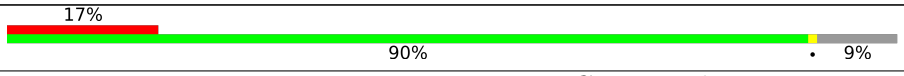
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	SJ	200	
10	SK	197	
11	SM	156	
12	SN	143	
13	SO	151	
14	SP	137	
15	SR	143	
16	ST	146	
17	SX	130	
18	SY	145	
19	SZ	135	
20	Sc	82	
21	Sd	67	
22	3B	327	
22	3C	327	
23	3D	504	
24	3E	511	
25	3F	573	
26	3G	126	
26	3H	126	
27	A4	776	
28	A5	643	
29	A8	713	
30	A9	575	
31	AE	1769	

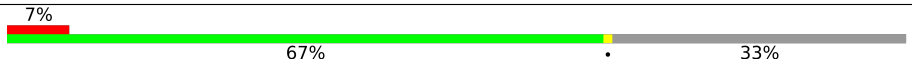
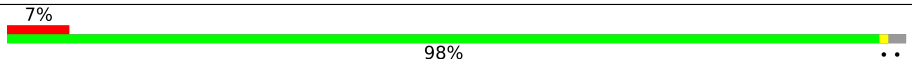
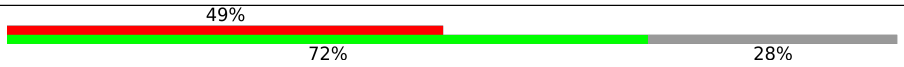
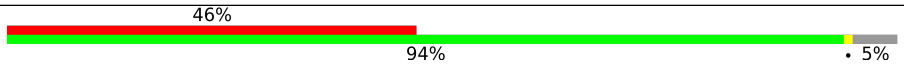
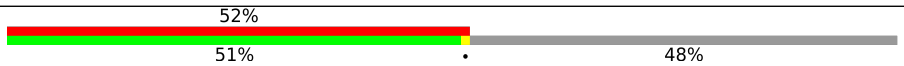
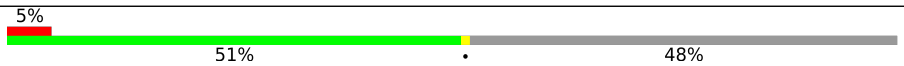
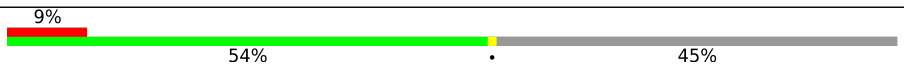
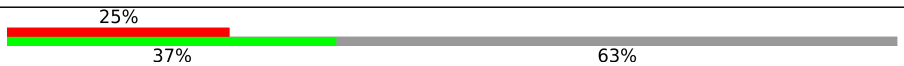
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
32	AF	513	
33	AG	896	
34	B1	923	
35	B2	943	
36	B3	817	
37	B8	594	
38	BE	939	
39	B6	440	
40	5B	214	
41	5C	554	
42	5D	250	
43	5E	593	
44	5F	183	
45	5G	290	
46	5H	610	
47	5I	489	
48	5J	217	
49	5K	189	
50	RA	707	
51	RB	357	
52	RC	316	
53	RE	1237	
54	RF	297	
55	RG	252	
55	RH	252	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
56	RI	274	
57	RJ	1183	
58	RK	367	
59	RL	1056	
59	RM	1056	
60	RN	810	
61	RO	552	
62	RP	2493	
63	RQ	899	
64	RS	483	
65	RT	326	
66	RV	346	
67	X1	347	

2 Entry composition (i)

There are 70 unique types of molecules in this entry. The entry contains 224791 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 U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	3A	175	3711	1661	648	1227	175	0	0

- Molecule 2 is a RNA chain called 5' ETS.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5A	522	11143	4979	1982	3660	522	0	0

- Molecule 3 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	SA	1310	27940	12487	4981	9162	1310	0	0

- Molecule 4 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SC	219	1751	1109	321	317	4	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SF	229	1815	1161	331	320	3	0	0

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SG	213	1669	1045	307	314	3	0	0

- Molecule 7 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SH	112	Total	C	N	O	S	0	0
			879	562	155	160	2		

- Molecule 8 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	SI	165	Total	C	N	O	0	0
			1321	853	226	242		

- Molecule 9 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SJ	166	Total	C	N	O	S	0	0
			1324	824	262	236	2		

- Molecule 10 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SK	171	Total	C	N	O	S	0	0
			1388	879	268	240	1		

- Molecule 11 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SM	123	Total	C	N	O	S	0	0
			997	641	189	164	3		

- Molecule 12 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SN	119	Total	C	N	O	S	0	0
			865	545	151	167	2		

- Molecule 13 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SO	134	Total	C	N	O	S	0	0
			1087	698	202	186	1		

- Molecule 14 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SP	118	Total 868	C 536	N 164	O 165	S 3	0	0

- Molecule 15 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	SR	125	Total 973	C 625	N 174	O 174	0	0

- Molecule 16 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	ST	113	Total 918	C 578	N 174	O 164	S 2	0	0

- Molecule 17 is a protein called 40S ribosomal protein S22-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SX	127	Total 1003	C 640	N 183	O 177	S 3	0	0

- Molecule 18 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SY	103	Total 786	C 503	N 144	O 137	S 2	0	0

- Molecule 19 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	SZ	102	Total 809	C 517	N 148	O 144	0	0

- Molecule 20 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Sc	80	Total 603	C 377	N 109	O 112	S 5	0	0

- Molecule 21 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Sd	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 22 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3B	240	Total	C	N	O	S	0	0
			1865	1184	333	338	10		
22	3C	225	Total	C	N	O	S	0	0
			1763	1120	316	317	10		

- Molecule 23 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3D	369	Total	C	N	O	S	0	0
			2848	1811	489	540	8		

- Molecule 24 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3E	431	Total	C	N	O	S	0	0
			3028	1888	543	588	9		

- Molecule 25 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3F	434	Total	C	N	O	S	0	0
			3473	2211	603	649	10		

- Molecule 26 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3G	121	Total	C	N	O	S	0	0
			916	583	158	171	4		
26	3H	121	Total	C	N	O	S	0	0
			916	583	158	171	4		

- Molecule 27 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A4	662	Total	C	N	O	S	0	0
			5226	3309	910	986	21		

- Molecule 28 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A5	514	Total	C	N	O	S	0	0
			3976	2520	688	755	13		

- Molecule 29 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A8	548	Total	C	N	O	S	0	0
			3307	2054	608	642	3		

- Molecule 30 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A9	128	Total	C	N	O	S	0	0
			939	594	173	170	2		

- Molecule 31 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AE	777	Total	C	N	O	S	0	0
			6197	3998	1014	1166	19		

- Molecule 32 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AF	493	Total	C	N	O	S	0	0
			3911	2462	702	735	12		

- Molecule 33 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AG	826	Total	C	N	O	S	0	0
			6570	4181	1111	1259	19		

- Molecule 34 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B1	834	Total	C	N	O	S	0	0
			6635	4223	1140	1253	19		

- Molecule 35 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B2	851	Total	C	N	O	S	0	0
			6723	4294	1133	1269	27		

- Molecule 36 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B3	757	Total	C	N	O	S	0	0
			5919	3769	993	1130	27		

- Molecule 37 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B8	477	Total	C	N	O	S	0	0
			3764	2387	662	705	10		

- Molecule 38 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BE	865	Total	C	N	O	S	0	0
			6810	4322	1175	1292	21		

- Molecule 39 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B6	374	Total	C	N	O	S	0	0
			2800	1782	501	505	12		

- Molecule 40 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	5B	60	Total	C	N	O	0	0
			495	310	101	84		

- Molecule 41 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	5C	535	Total	C	N	O	S	0	0
			4237	2656	762	807	12		

- Molecule 42 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	5D	235	Total	C	N	O	S	0	0
			1972	1226	380	359	7		

- Molecule 43 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	5E	204	Total	C	N	O	S	0	0
			1647	1021	294	328	4		

- Molecule 44 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	5F	182	Total	C	N	O	S	0	0
			1530	967	287	269	7		

- Molecule 45 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	5G	282	Total	C	N	O	S	0	0
			2296	1441	430	418	7		

- Molecule 46 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	5H	136	Total	C	N	O	0	0
			1065	658	211	196		

- Molecule 47 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5I	461	Total	C	N	O	S	0	0
			3765	2354	686	709	16		

- Molecule 48 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5J	144	Total	C	N	O	S	0	0
			1219	769	230	215	5		

- Molecule 49 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	5K	175	Total	C	N	O	S	0	0
			1403	896	256	241	10		

- Molecule 50 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	RA	338	Total	C	N	O	S	0	0
			2709	1713	463	524	9		

- Molecule 51 is a protein called U3 small nucleolar ribonucleoprotein protein LCP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	RB	134	Total	C	N	O	S	0	0
			1108	664	227	214	3		

- Molecule 52 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	RC	278	Total	C	N	O	S	0	0
			2207	1408	391	395	13		

- Molecule 53 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	RE	1079	Total	C	N	O	S	0	0
			8716	5666	1437	1589	24		

- Molecule 54 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	RF	241	Total	C	N	O	S	0	0
			1963	1253	335	367	8		

- Molecule 55 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	RG	216	Total	C	N	O	S	0	0
			1701	1079	296	315	11		
55	RH	230	Total	C	N	O	S	0	0
			1799	1142	313	333	11		

- Molecule 56 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	RI	252	Total	C	N	O	S	0	0
			2045	1309	362	366	8		

- Molecule 57 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	RJ	796	Total	C	N	O	S	0	0
			6379	4086	1136	1128	29		

- Molecule 58 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	RK	360	Total	C	N	O	S	0	0
			2781	1781	473	516	11		

- Molecule 59 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	RL	805	Total	C	N	O	S	0	0
			4539	2760	885	887	7		
59	RM	765	Total	C	N	O		0	0
			3774	2244	765	765			

- Molecule 60 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	RN	587	Total	C	N	O	S	0	0
			4363	2758	791	803	11		

- Molecule 61 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	RO	525	Total	C	N	O	S	0	0
			3766	2412	646	696	12		

- Molecule 62 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	RP	2052	Total	C	N	O	0	0
			10202	6098	2052	2052		

- Molecule 63 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	RQ	226	Total	C	N	O	S	0	0
			1651	1023	313	313	2		

- Molecule 64 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	RS	251	Total	C	N	O	S	0	0
			2051	1340	349	359	3		

- Molecule 65 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	RT	171	Total	C	N	O	S	0	0
			1357	864	249	240	4		

- Molecule 66 is a protein called Protein FAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	RV	190	Total	C	N	O	S	0	0
			1448	891	290	264	3		

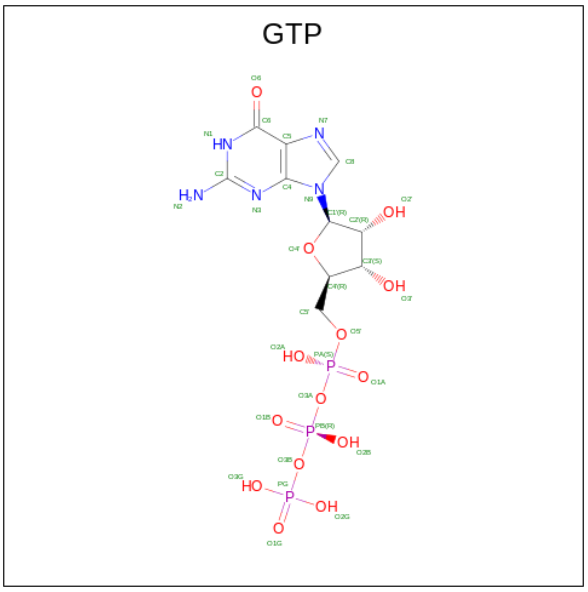
- Molecule 67 is a protein called Unassigned helices.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	X1	127	Total	C	N	O	0	0
			635	381	127	127		

- Molecule 68 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
68	Sc	1	Total	Zn	0
			1	1	
68	5K	1	Total	Zn	0
			1	1	

- Molecule 69 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

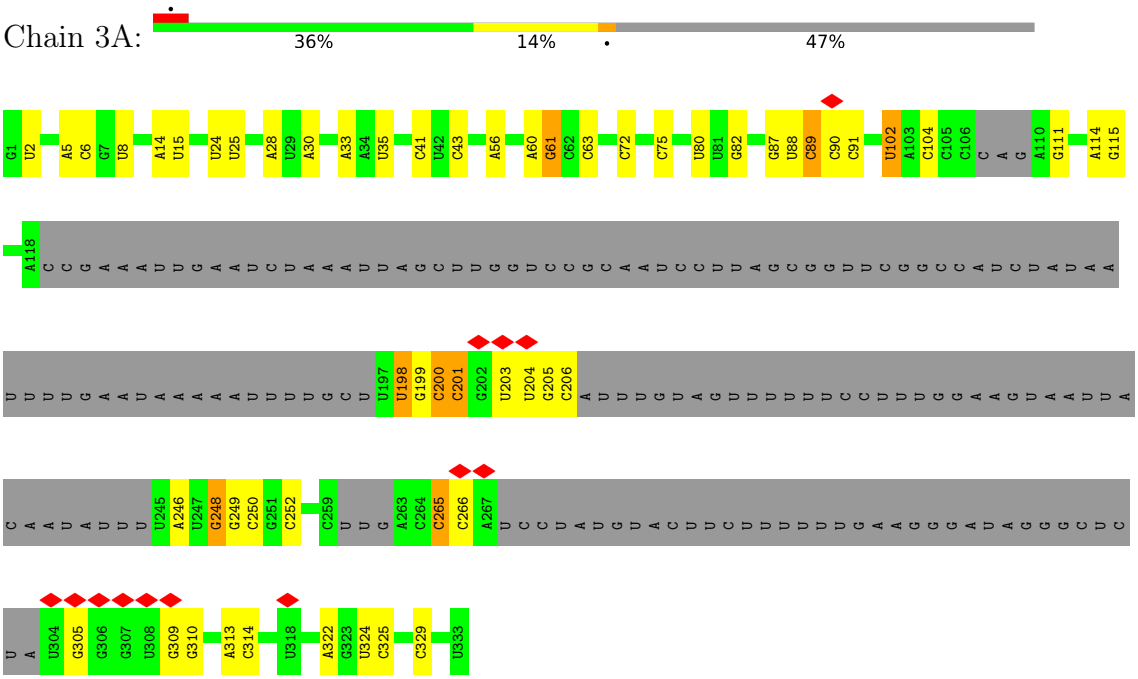
- Molecule 70 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
70	RJ	1	Total	Mg	0
			1	1	

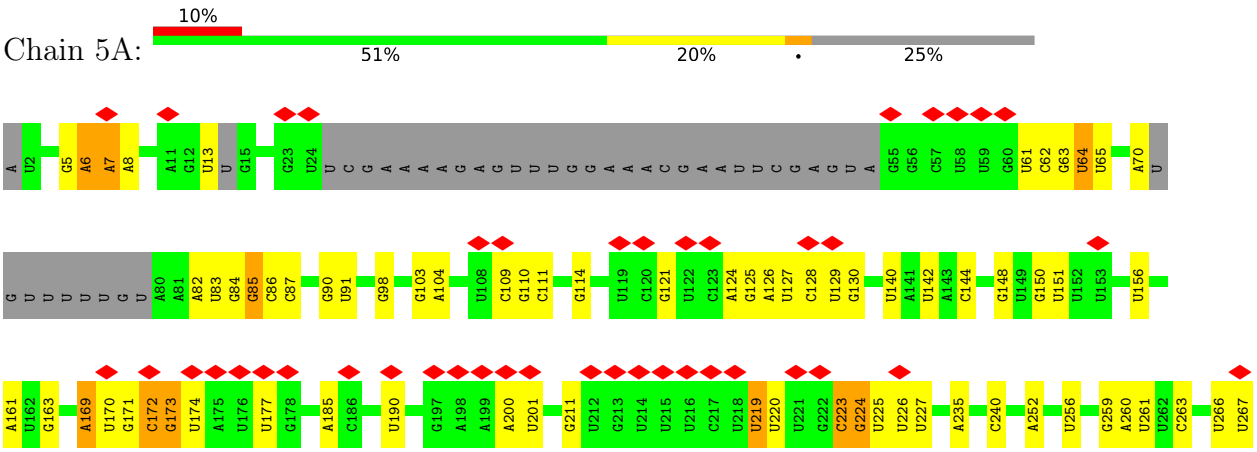
3 Residue-property plots

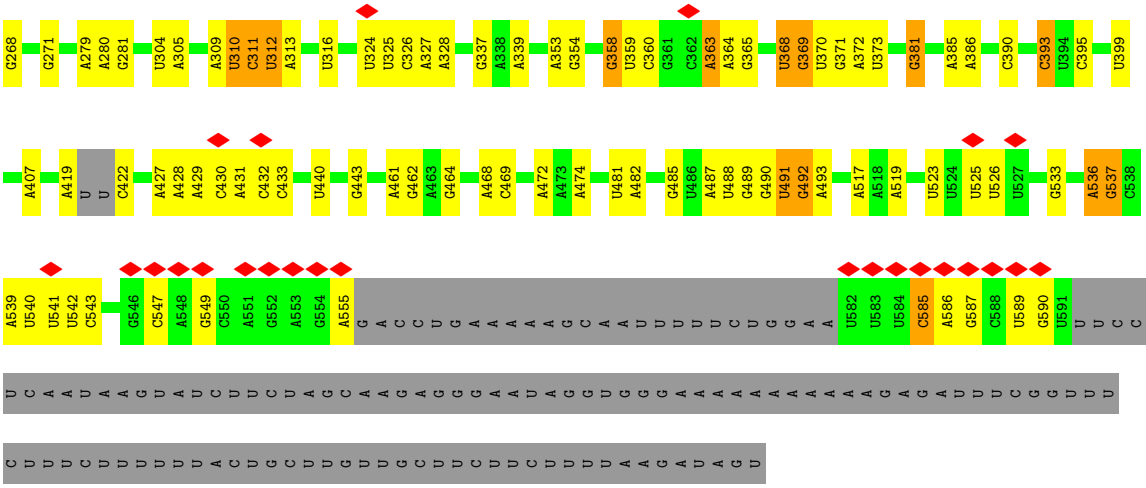
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: U3 snoRNA



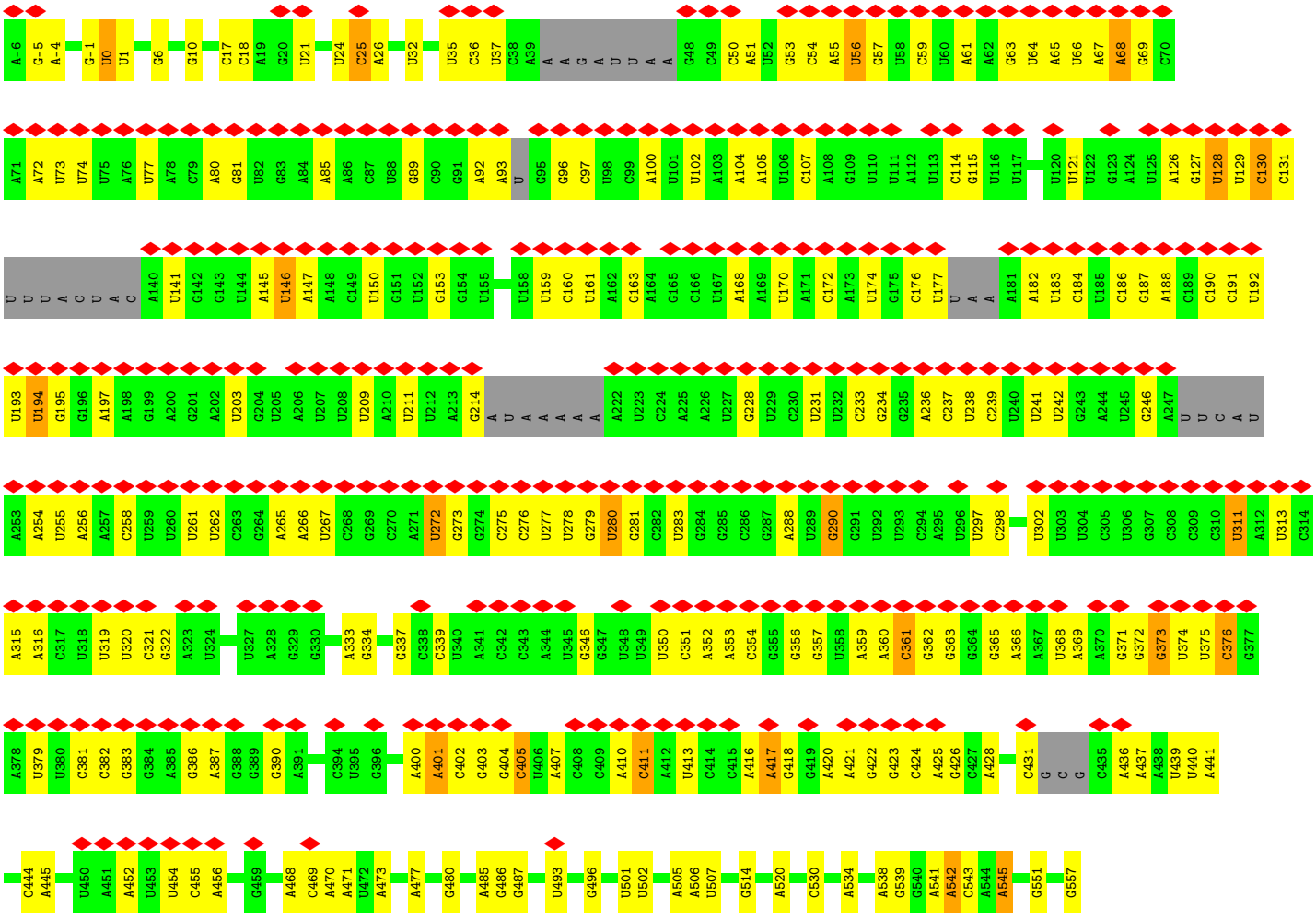
- Molecule 2: 5' ETS

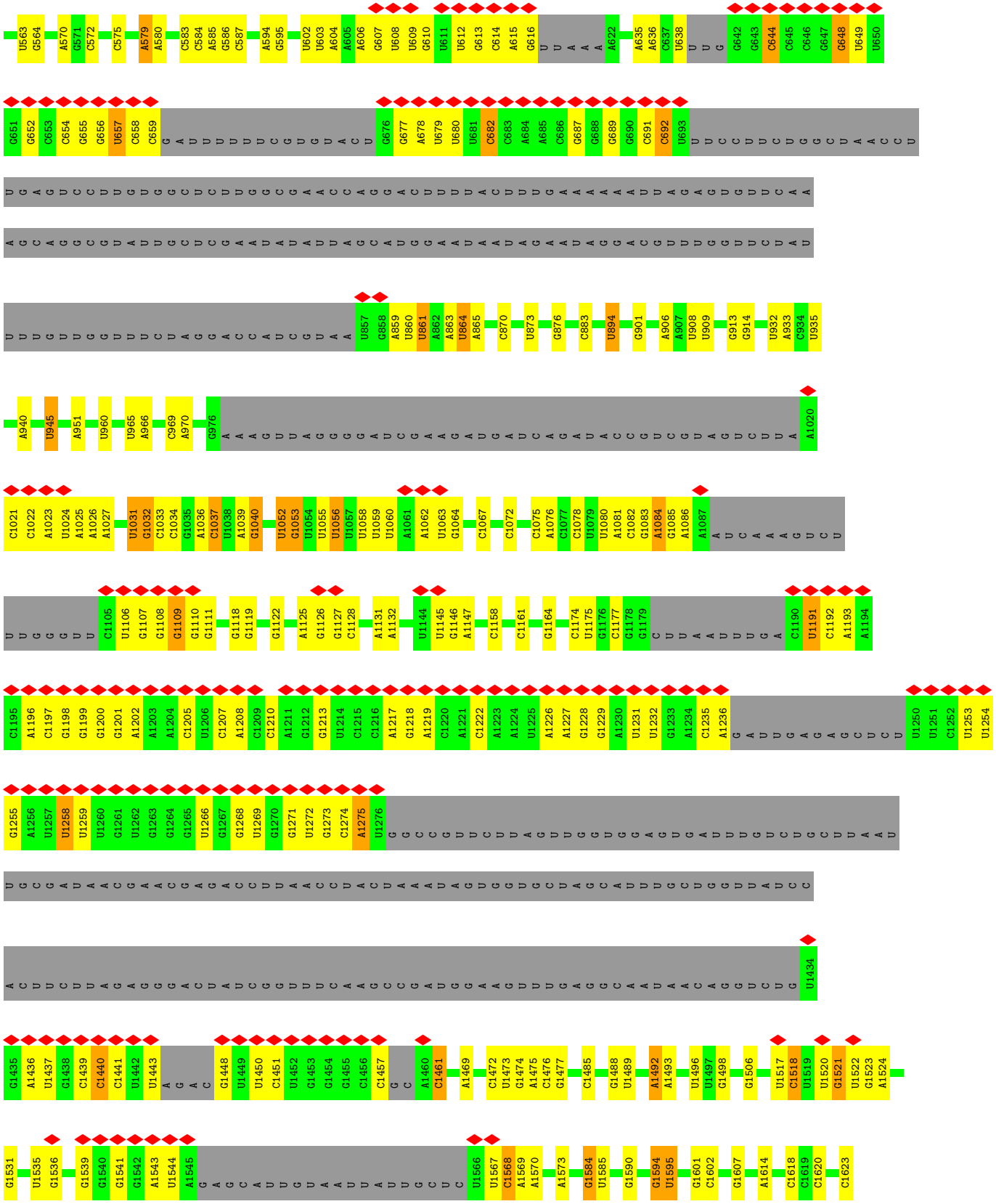




• Molecule 3: 18S rRNA

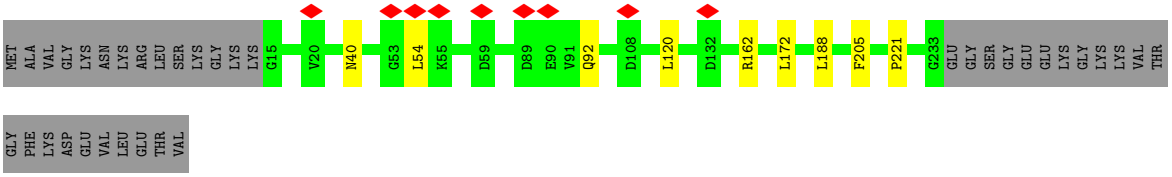
Chain SA:





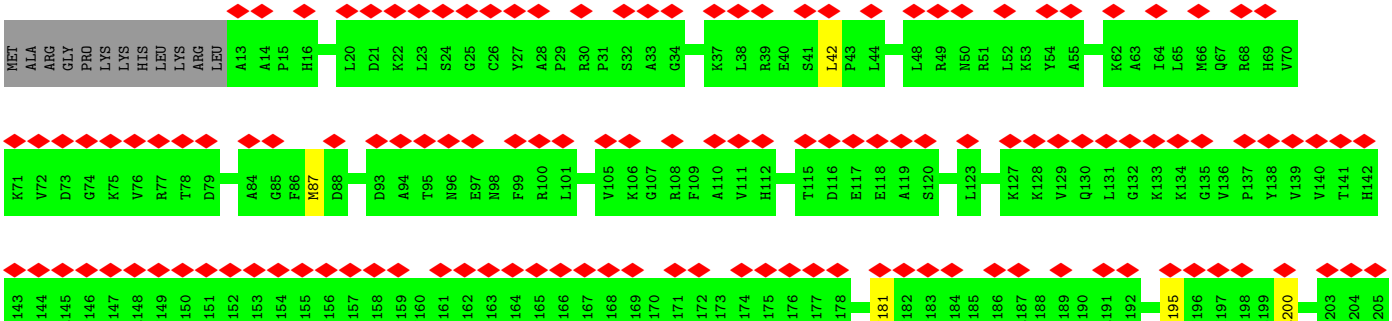
• Molecule 4: 40S ribosomal protein S1-A

Chain SC:



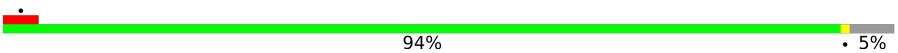
• Molecule 5: 40S ribosomal protein S4-A

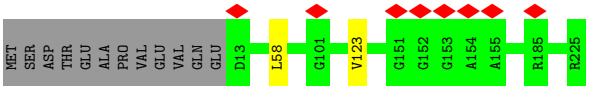
Chain SF:



• Molecule 6: 40S ribosomal protein S5

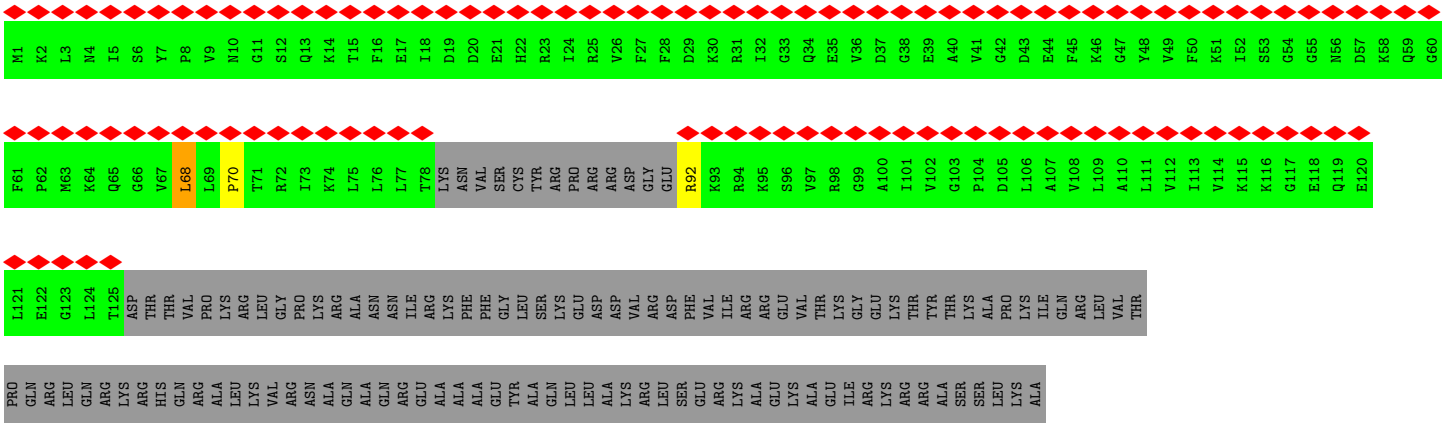
Chain SG:





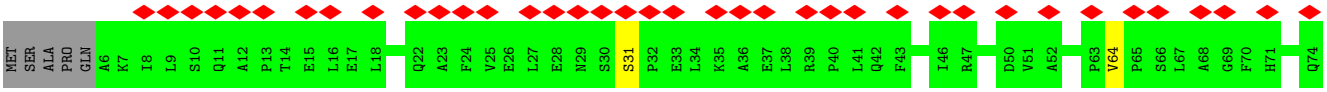
• Molecule 7: 40S ribosomal protein S6-A

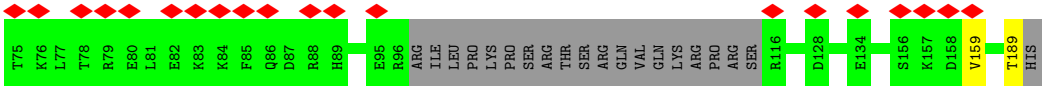
Chain SH:



• Molecule 8: 40S ribosomal protein S7-A

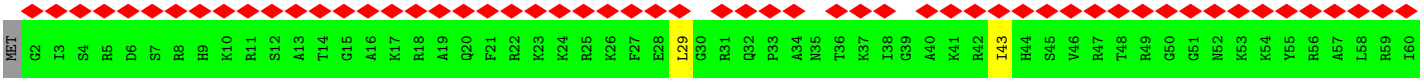
Chain SI:

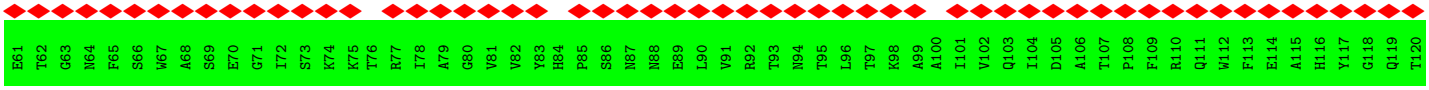


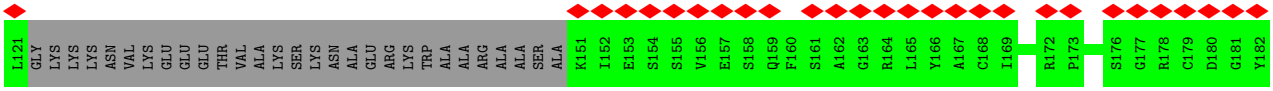


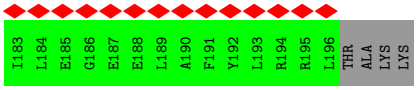
• Molecule 9: 40S ribosomal protein S8-A

Chain SJ:





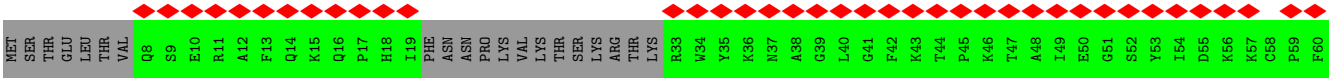


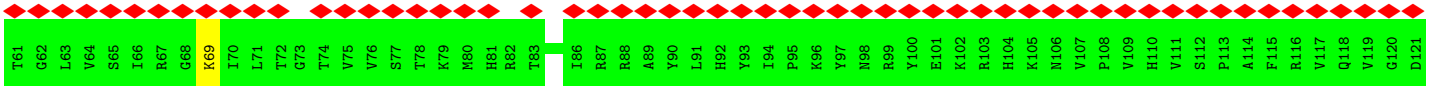


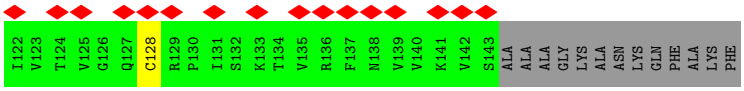
• Molecule 10: 40S ribosomal protein S9-A

Chain SK:

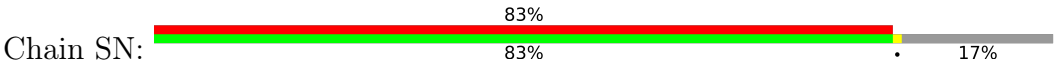
• Molecule 11: 40S ribosomal protein S11-A

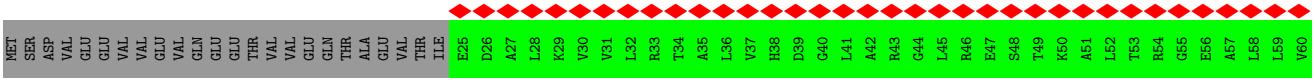


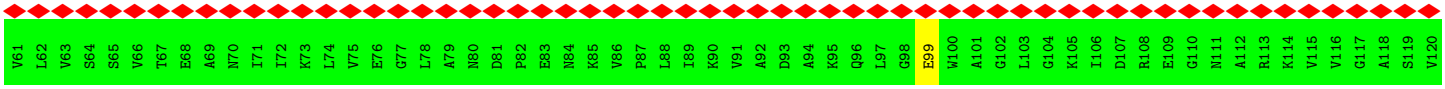


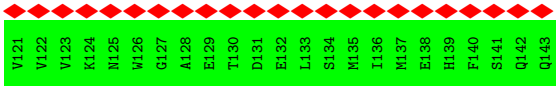


• Molecule 12: 40S ribosomal protein S12

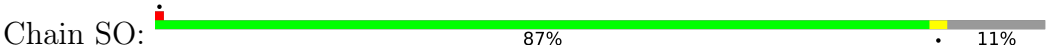


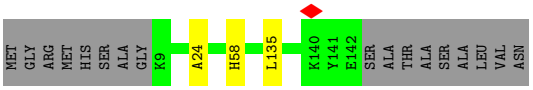




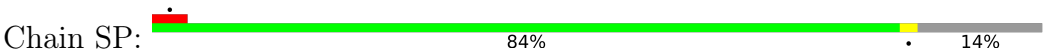


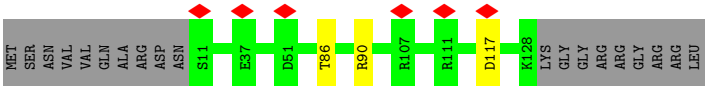
• Molecule 13: 40S ribosomal protein S13





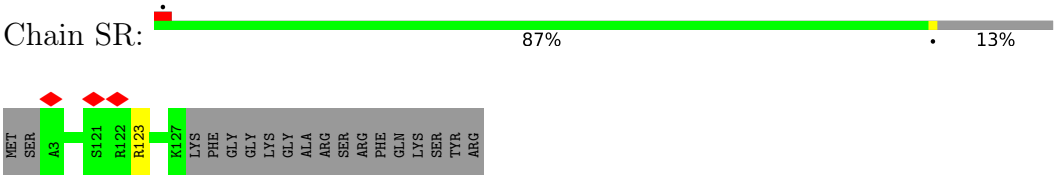
• Molecule 14: 40S ribosomal protein S14-A





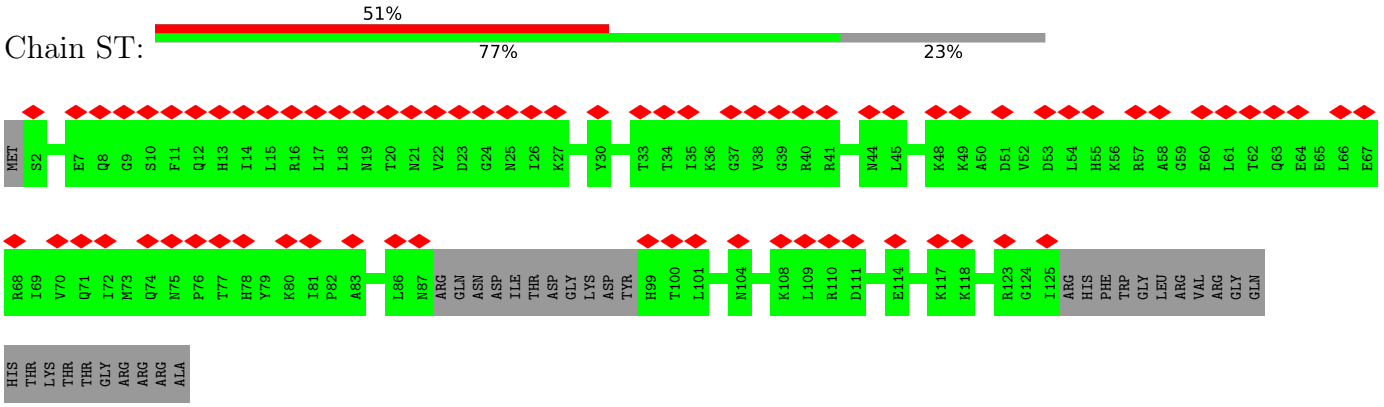
• Molecule 15: 40S ribosomal protein S16-A

Chain SR:



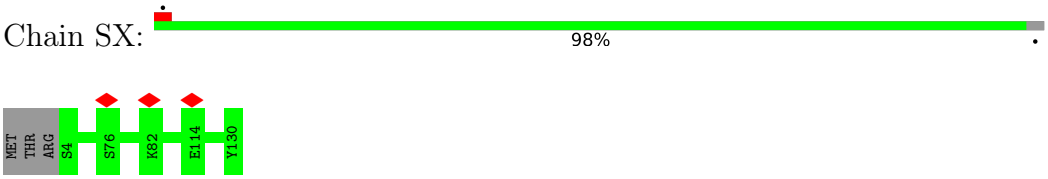
• Molecule 16: 40S ribosomal protein S18-A

Chain ST:



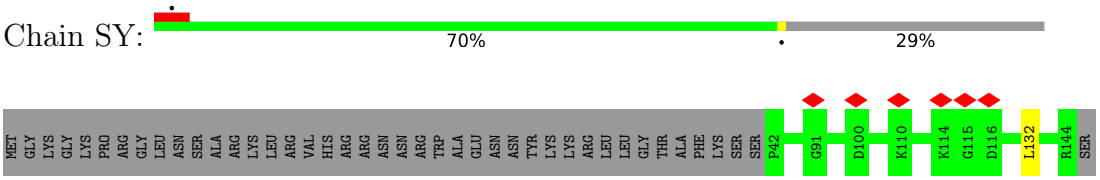
• Molecule 17: 40S ribosomal protein S22-B

Chain SX:



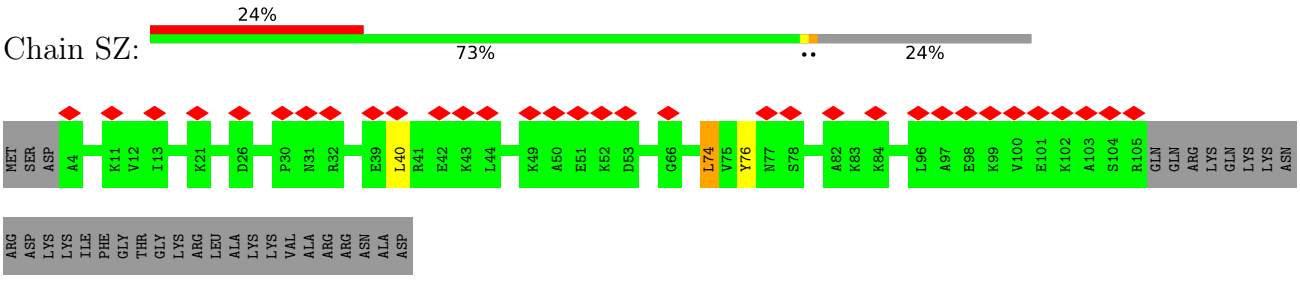
• Molecule 18: 40S ribosomal protein S23-A

Chain SY:



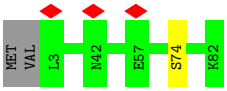
• Molecule 19: 40S ribosomal protein S24-A

Chain SZ:



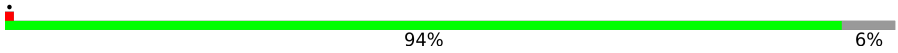
• Molecule 20: 40S ribosomal protein S27-A

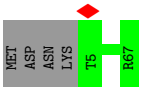
Chain Sc:



• Molecule 21: 40S ribosomal protein S28-A

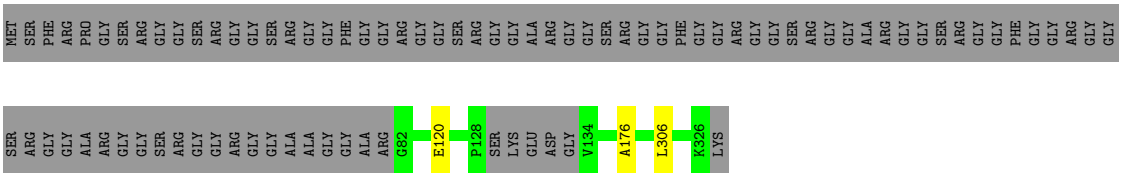
Chain Sd:





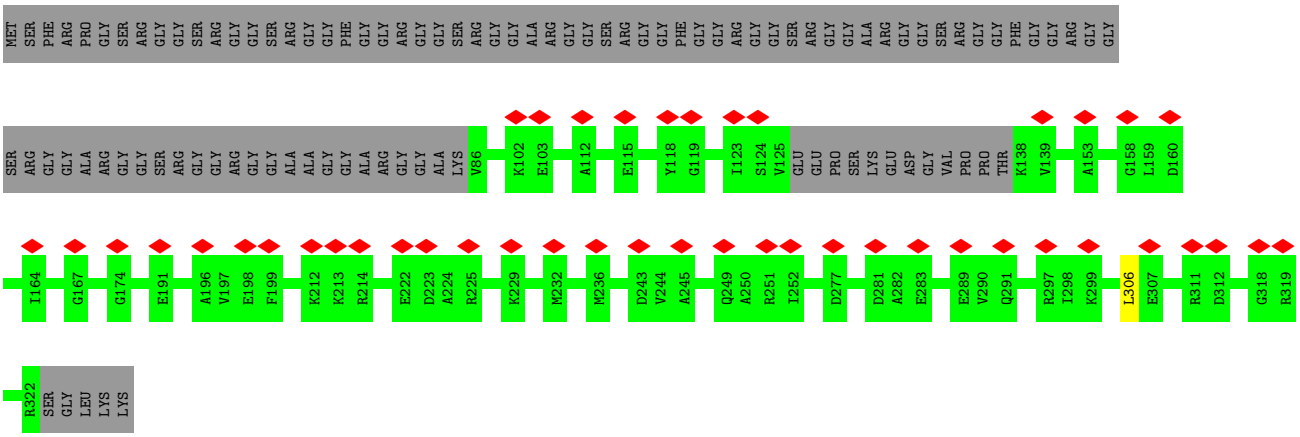
• Molecule 22: rRNA 2'-O-methyltransferase fibrillarin

Chain 3B:



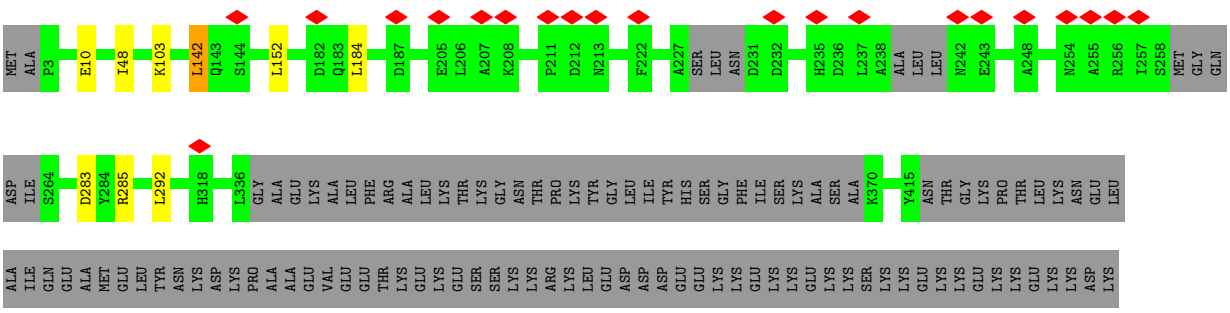
• Molecule 22: rRNA 2'-O-methyltransferase fibrillarin

Chain 3C:



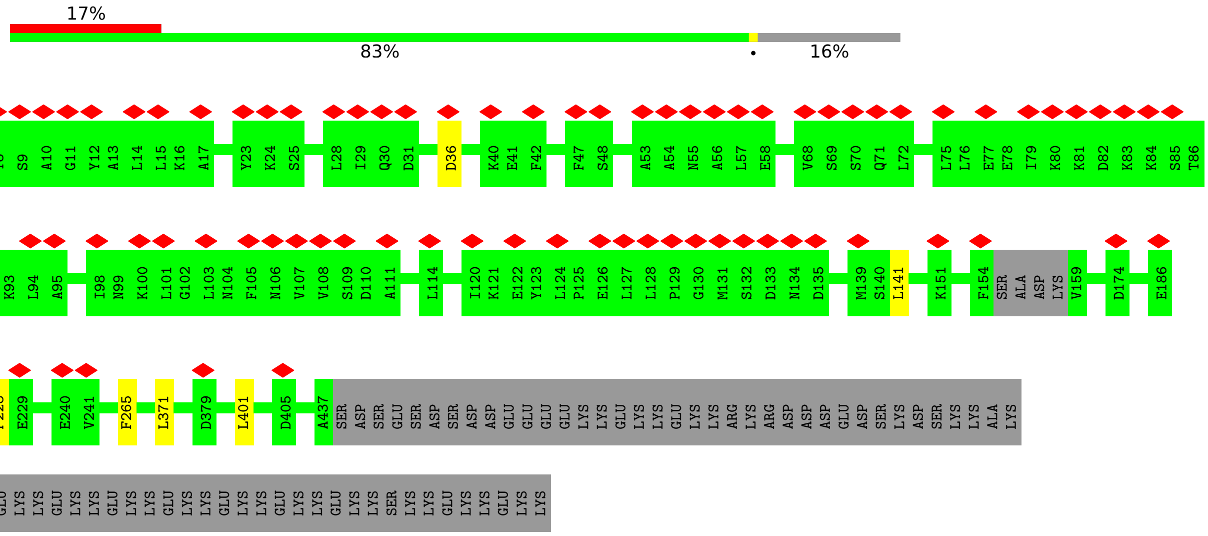
• Molecule 23: Nucleolar protein 56

Chain 3D:



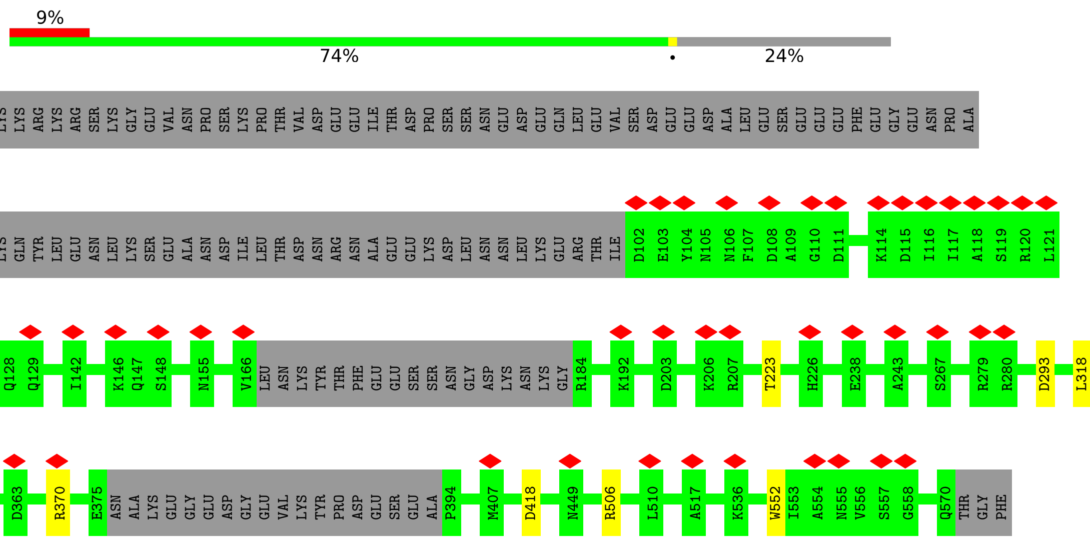
• Molecule 24: Nucleolar protein 58

Chain 3E:



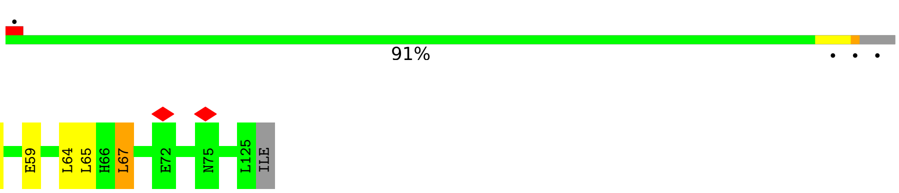
• Molecule 25: Ribosomal RNA-processing protein 9

Chain 3F:



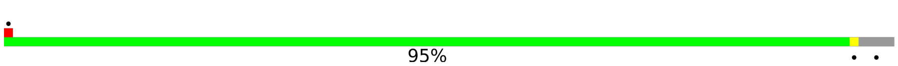
• Molecule 26: 13 kDa ribonucleoprotein-associated protein

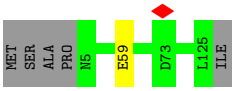
Chain 3G:



• Molecule 26: 13 kDa ribonucleoprotein-associated protein

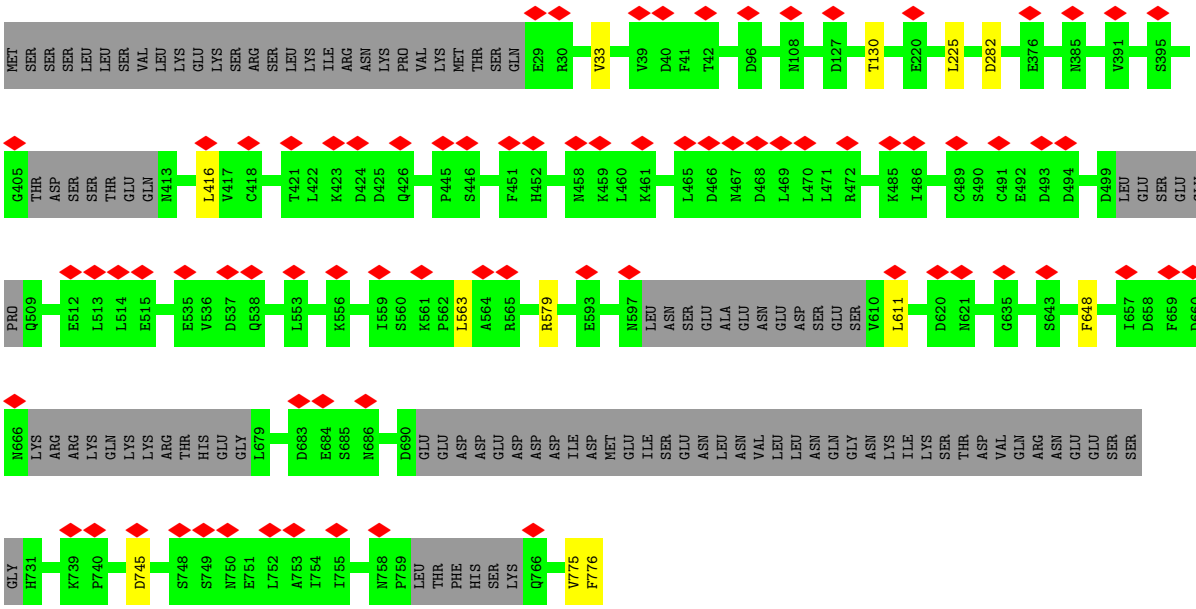
Chain 3H:





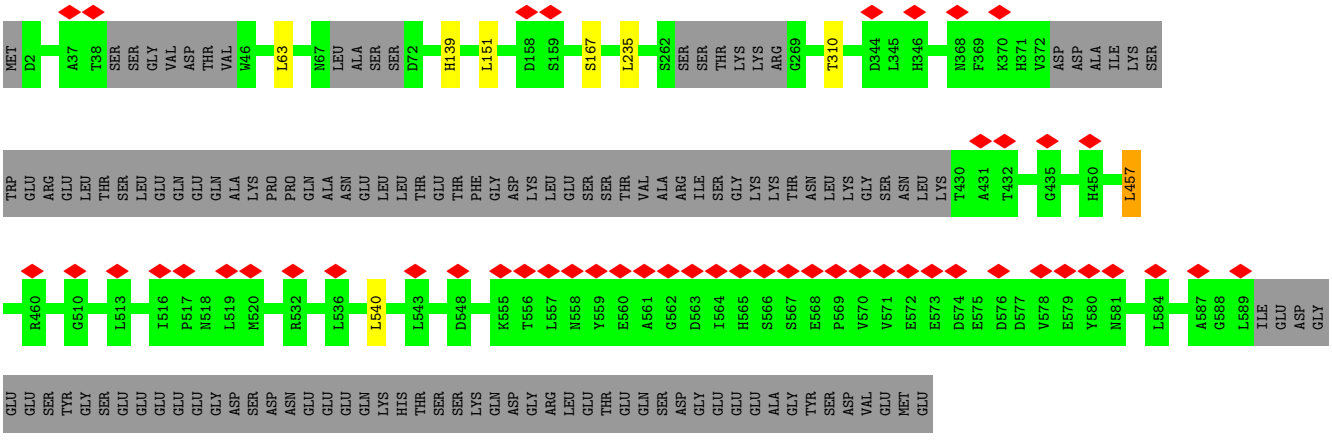
• Molecule 27: U3 small nucleolar RNA-associated protein 4

Chain A4:



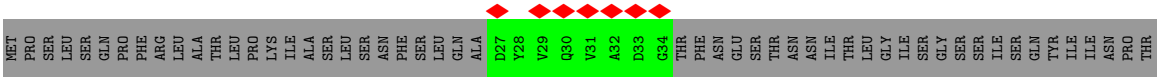
• Molecule 28: U3 small nucleolar RNA-associated protein 5

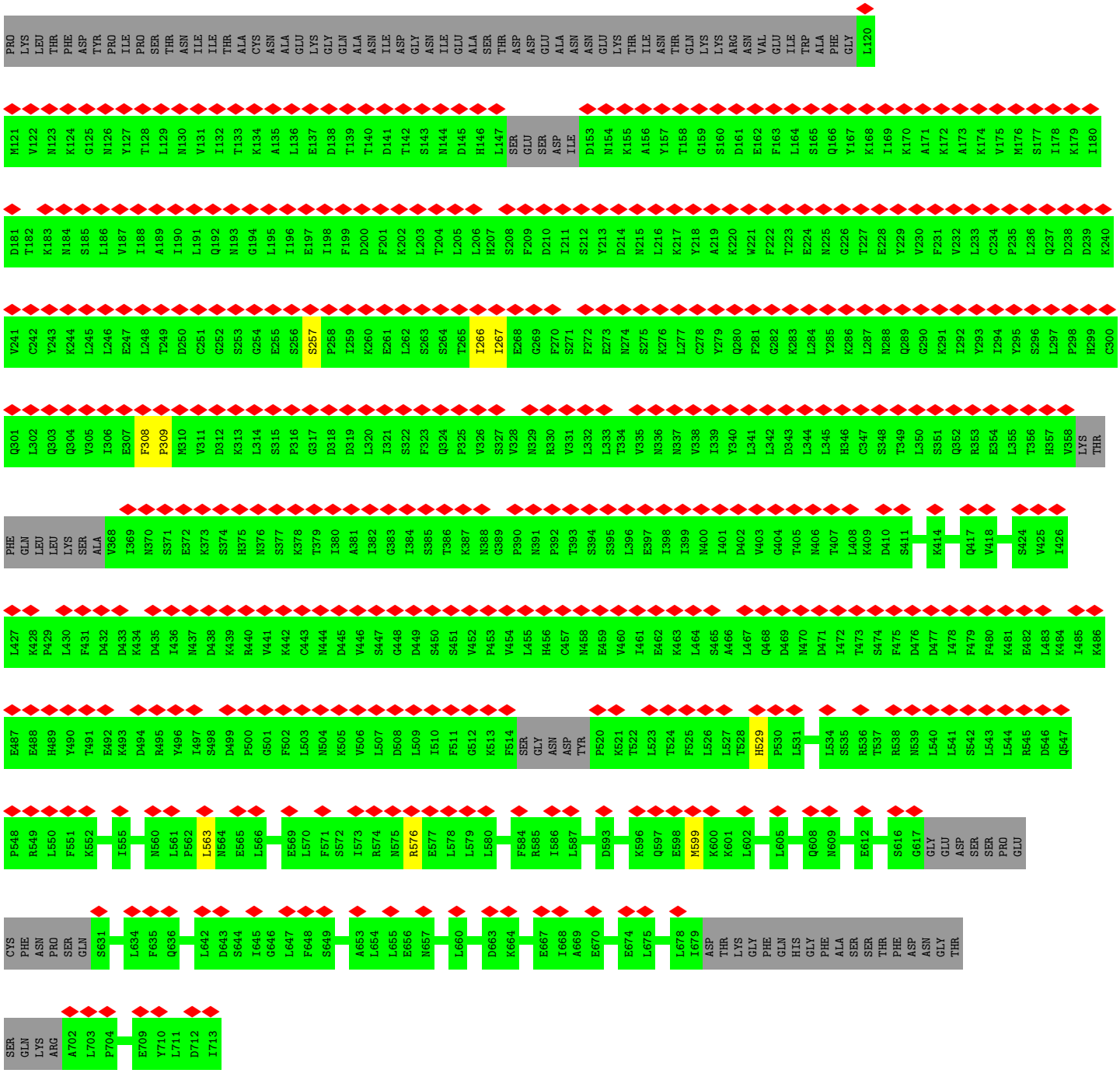
Chain A5:



• Molecule 29: U3 small nucleolar RNA-associated protein 8

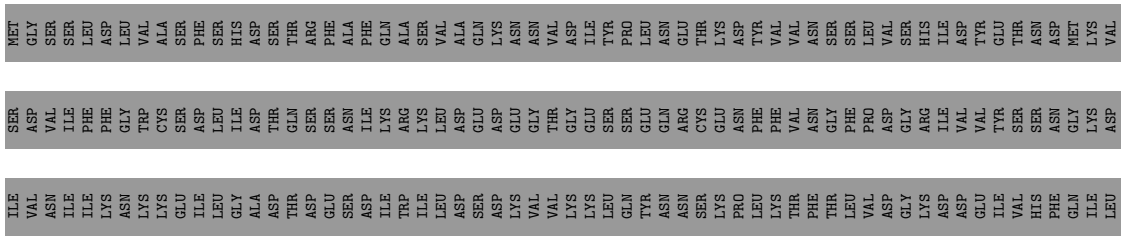
Chain A8:

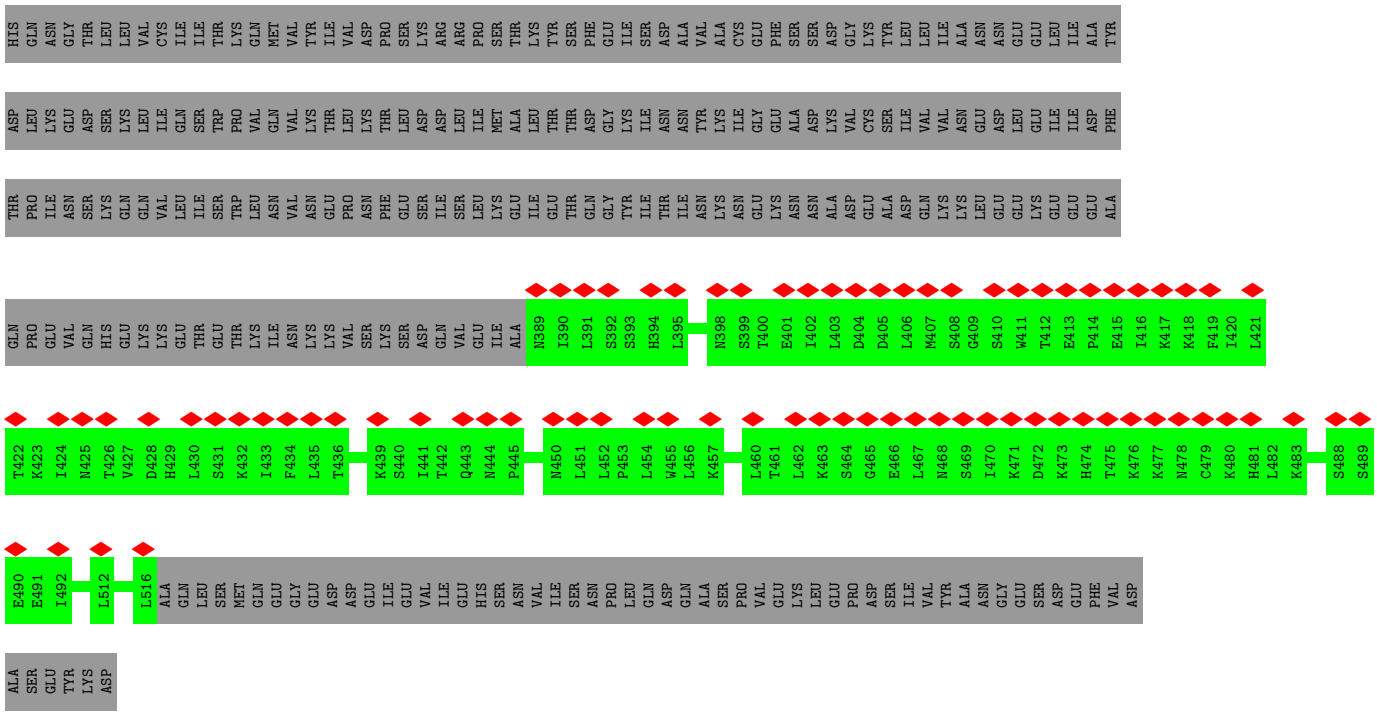




• Molecule 30: U3 small nucleolar RNA-associated protein 9

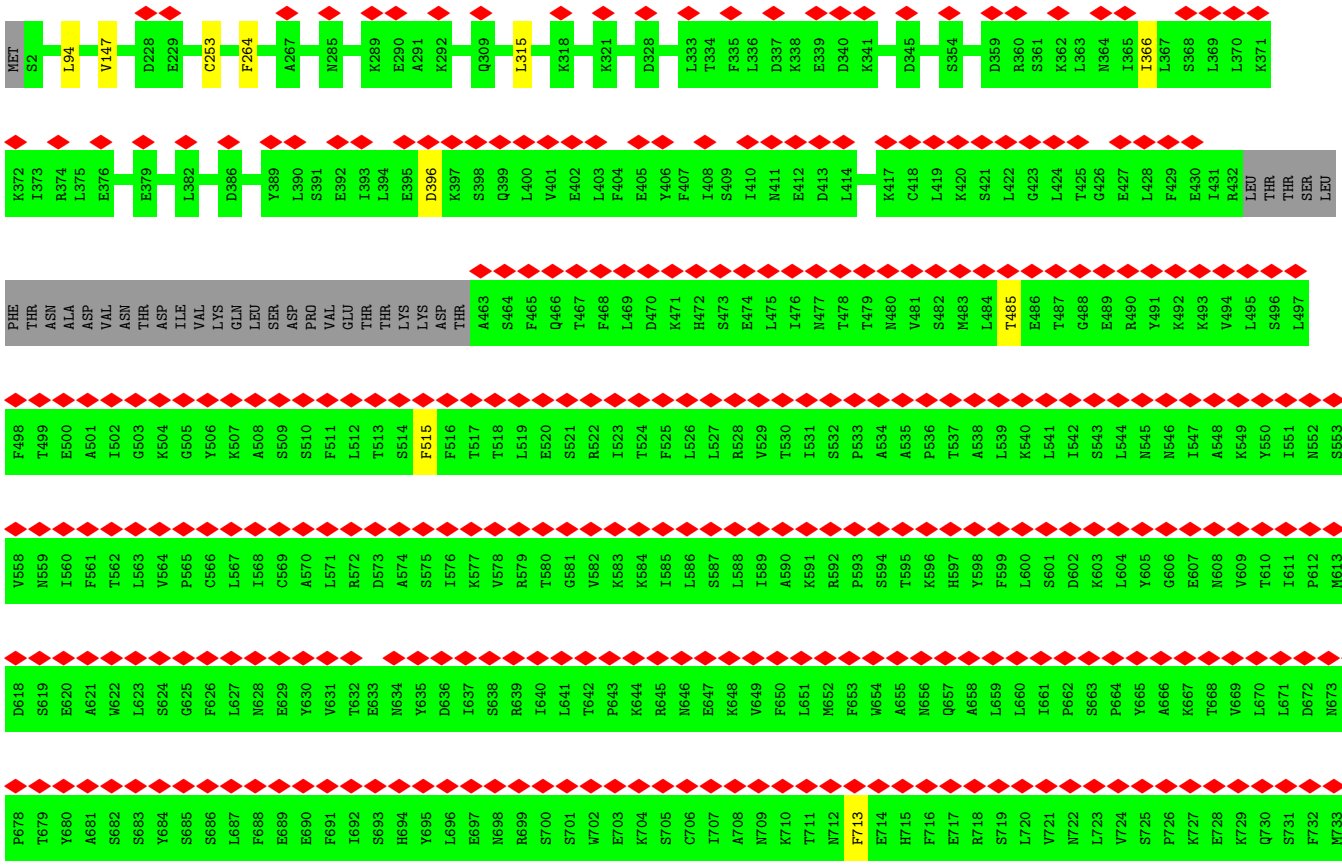
Chain A9:

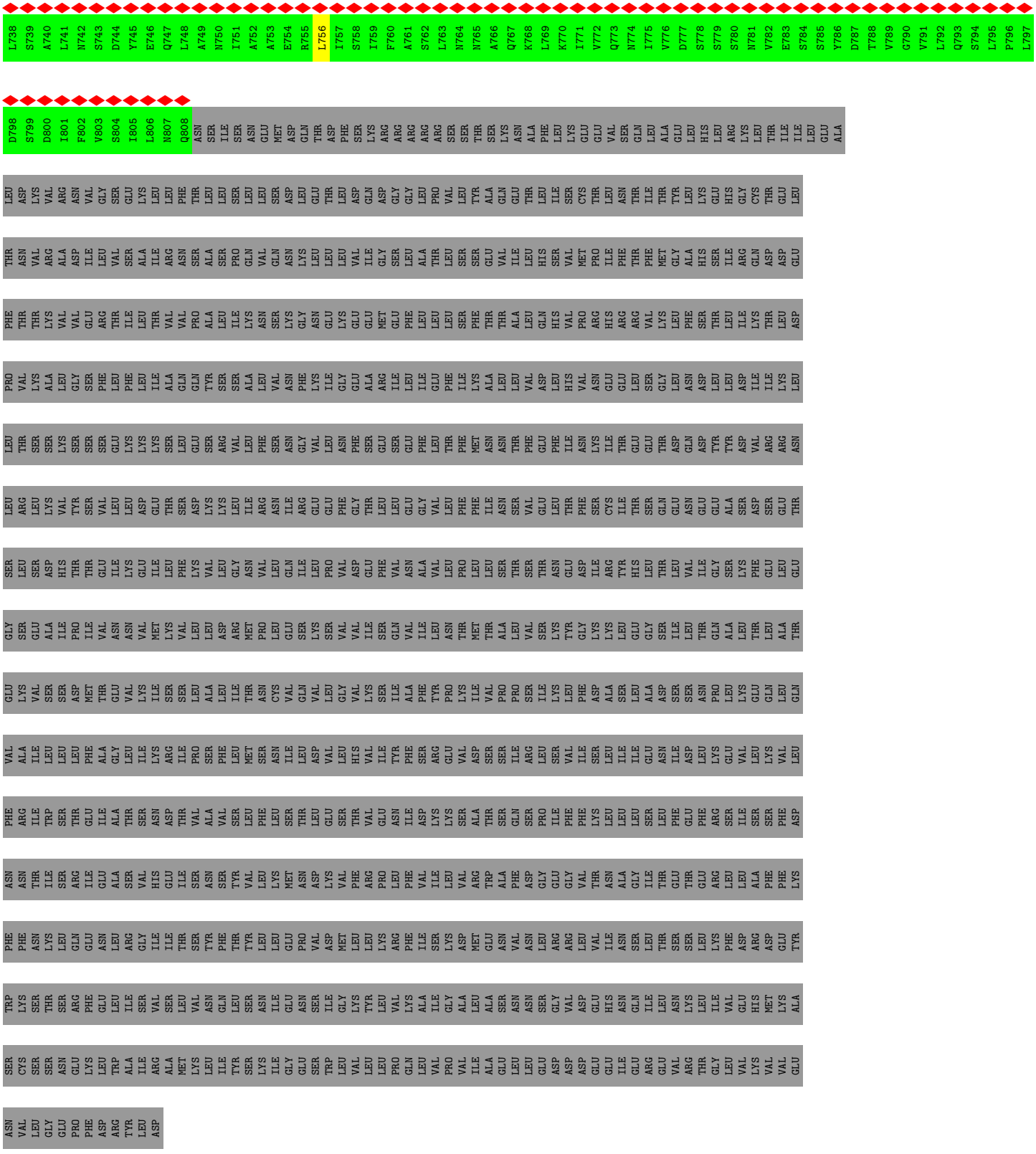




• Molecule 31: U3 small nucleolar RNA-associated protein 10

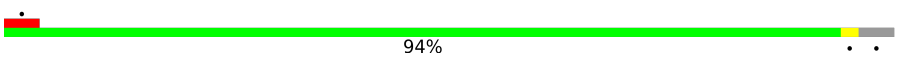
Chain AE:

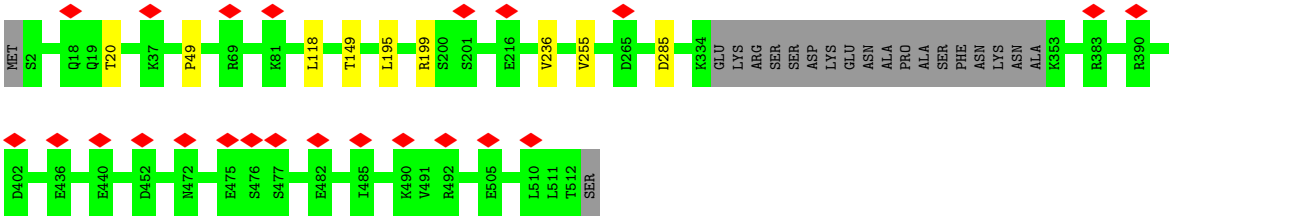




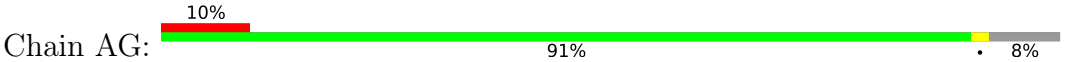
• Molecule 32: U3 small nucleolar RNA-associated protein 15

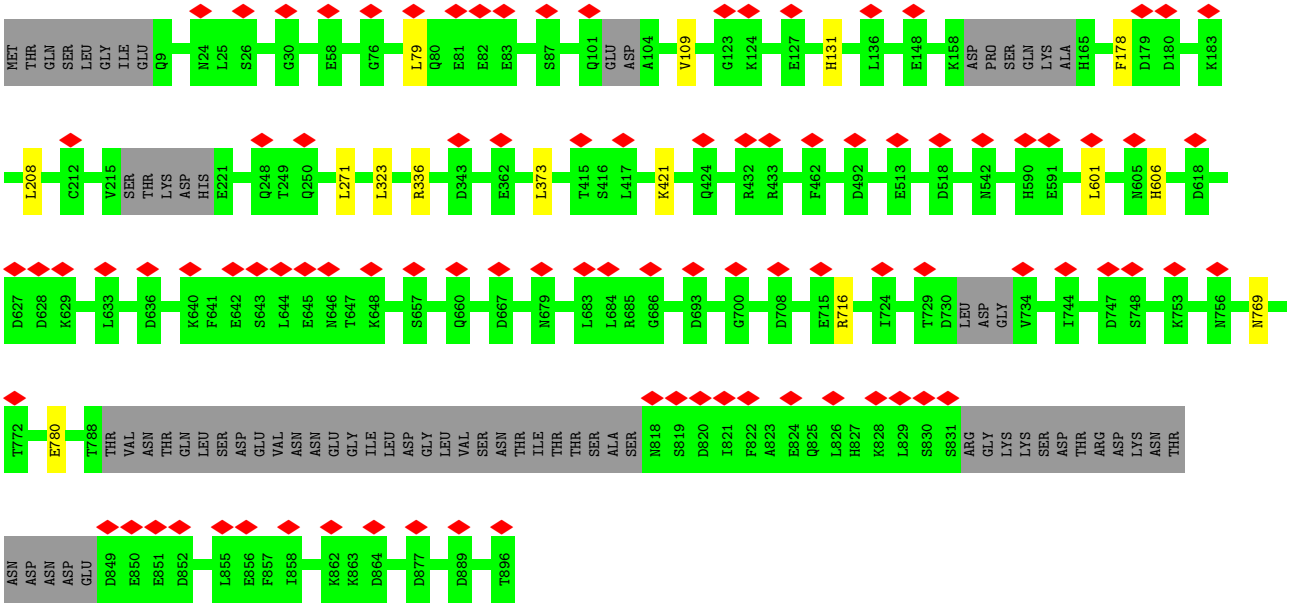
Chain AF:



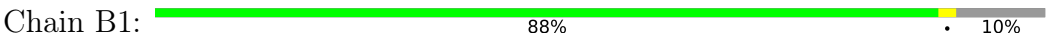


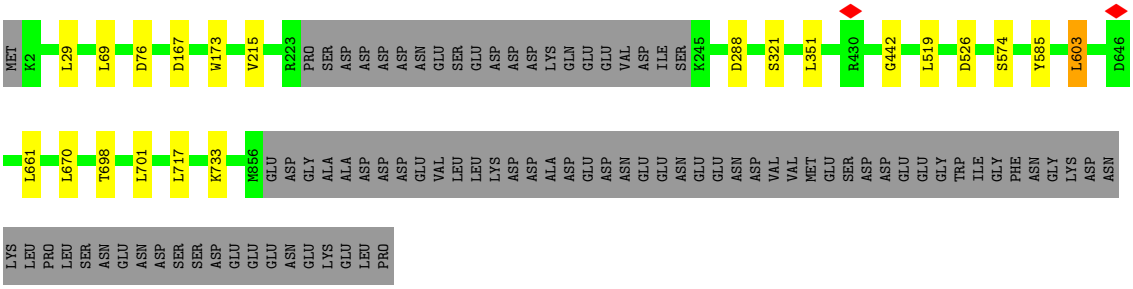
• Molecule 33: NET1-associated nuclear protein 1



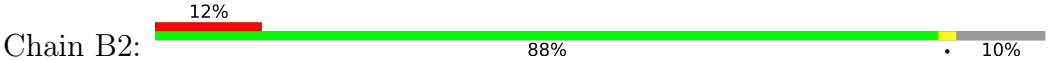


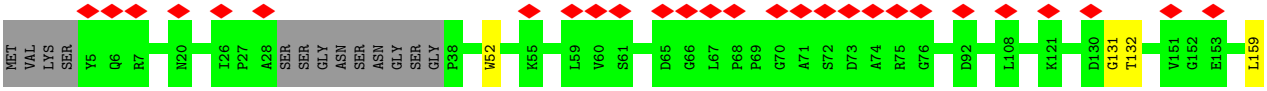
• Molecule 34: Periodic tryptophan protein 2





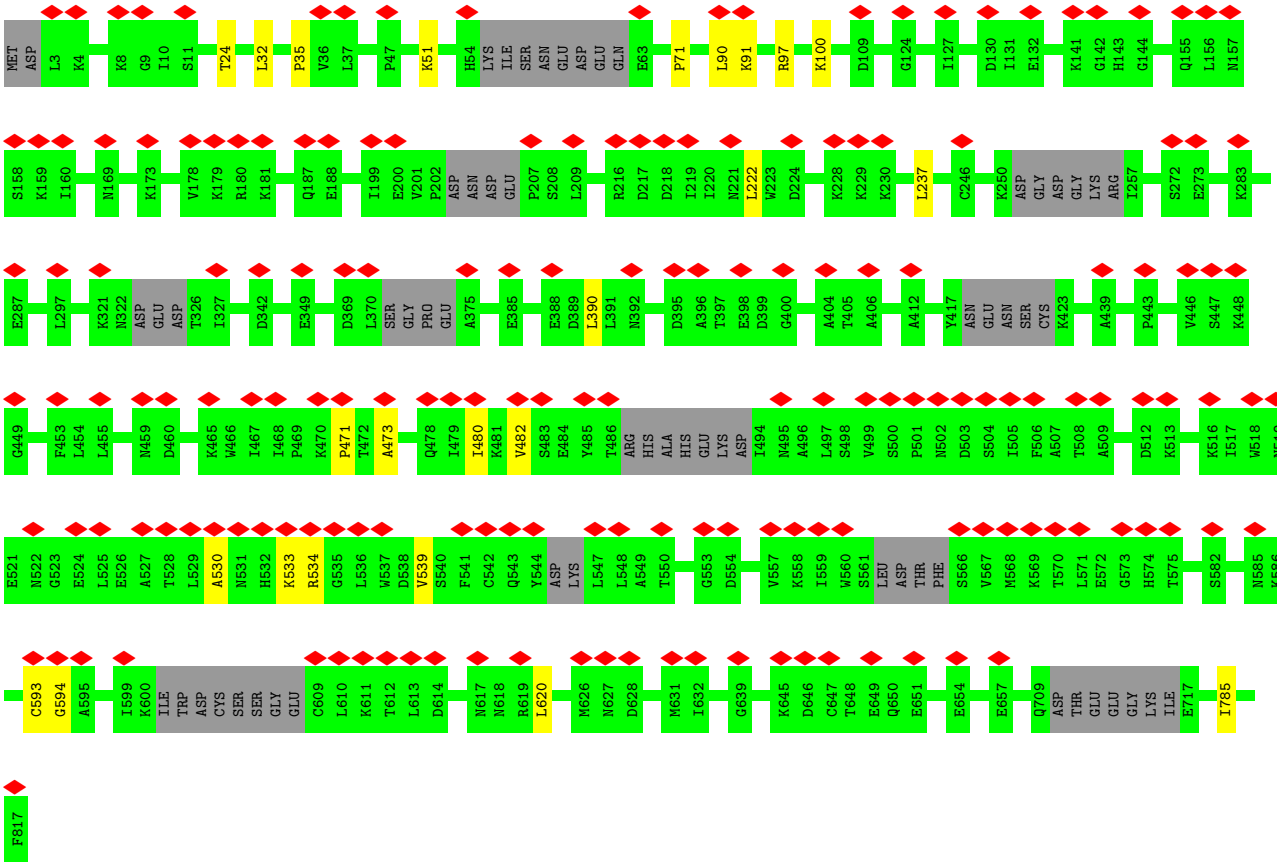
• Molecule 35: U3 small nucleolar RNA-associated protein 12





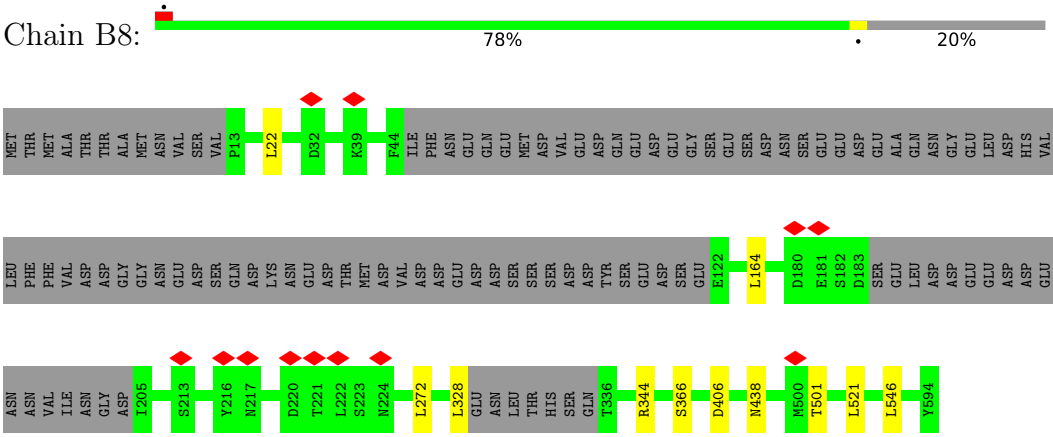
• Molecule 36: U3 small nucleolar RNA-associated protein 13

Chain B3:



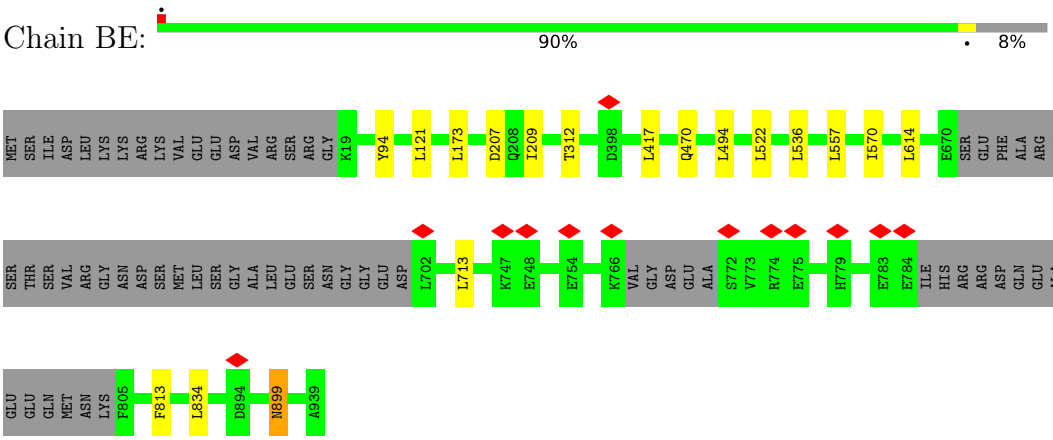
• Molecule 37: U3 small nucleolar RNA-associated protein 18

Chain B8:



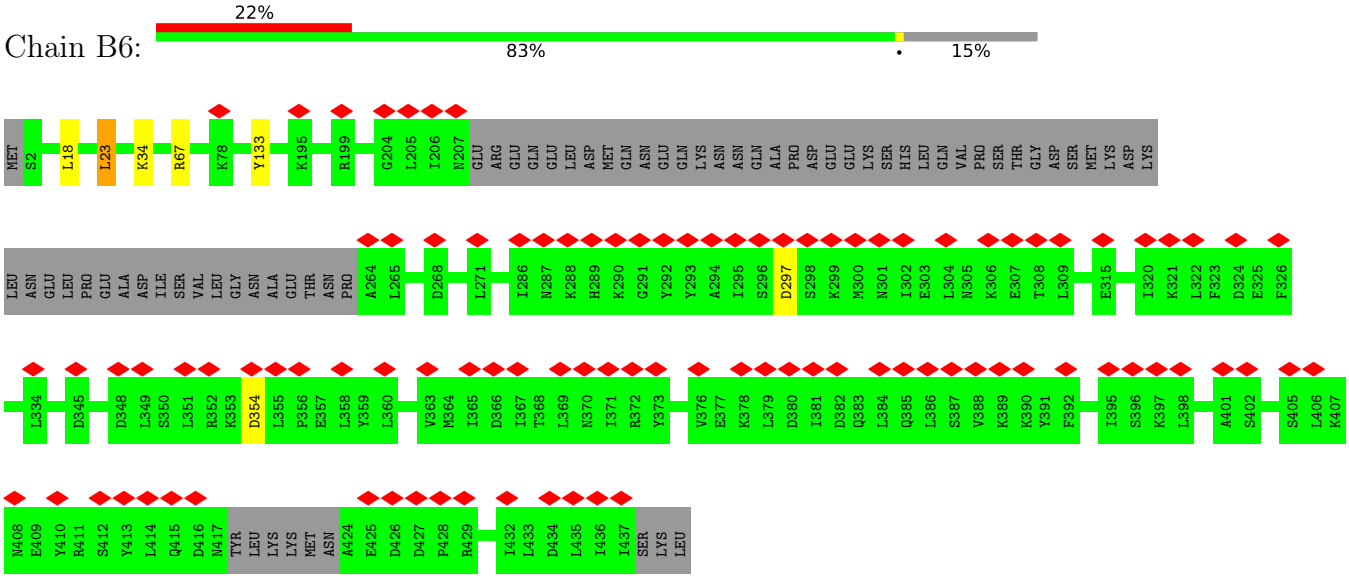
• Molecule 38: U3 small nucleolar RNA-associated protein 21

Chain BE:



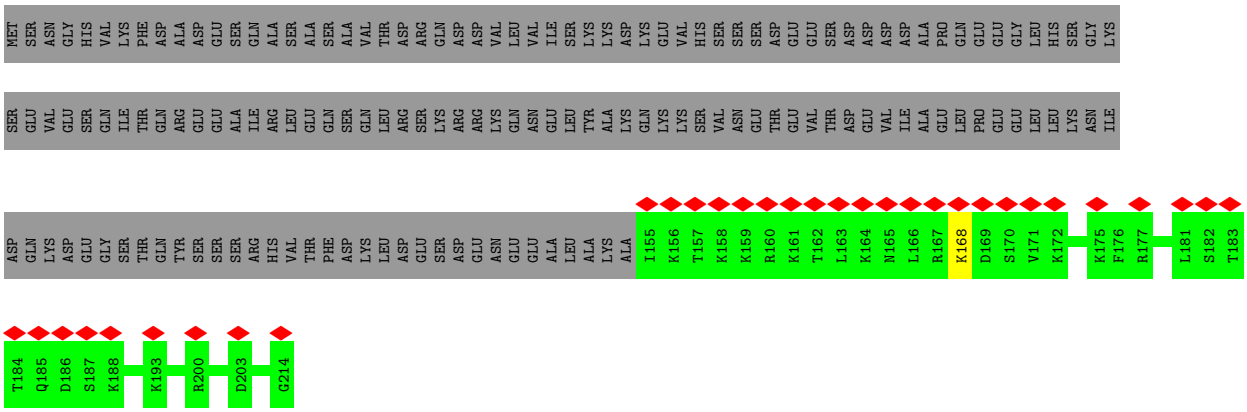
• Molecule 39: U3 small nucleolar RNA-associated protein 6

Chain B6:



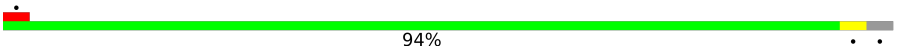
• Molecule 40: Bud site selection protein 21

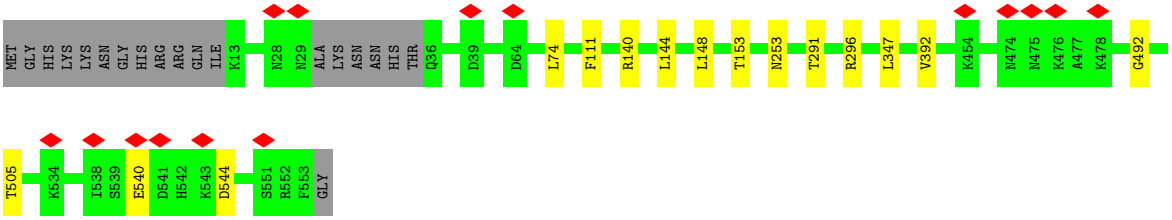
Chain 5B:



• Molecule 41: U3 small nucleolar RNA-associated protein 7

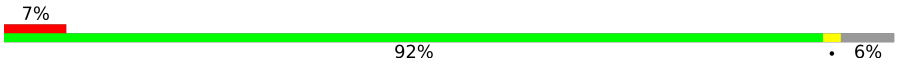
Chain 5C:

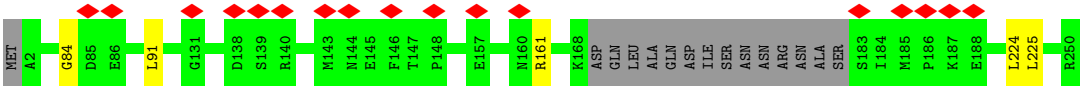




• Molecule 42: U3 small nucleolar RNA-associated protein 11

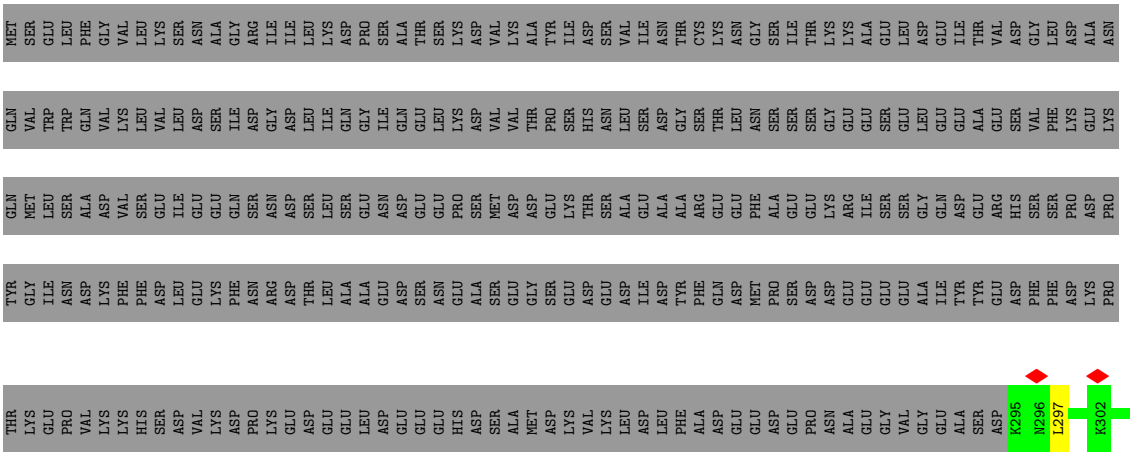
Chain 5D:

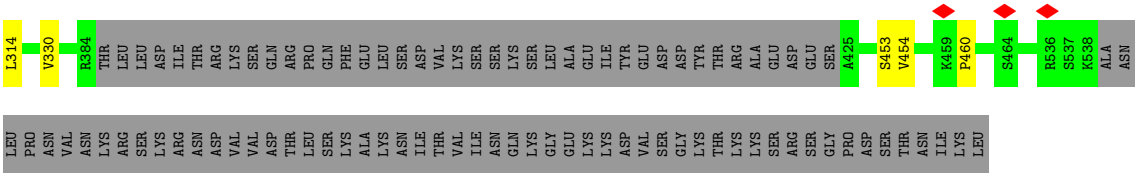




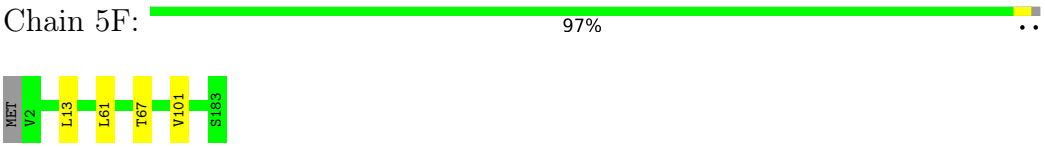
• Molecule 43: U3 small nucleolar RNA-associated protein MPP10

Chain 5E:

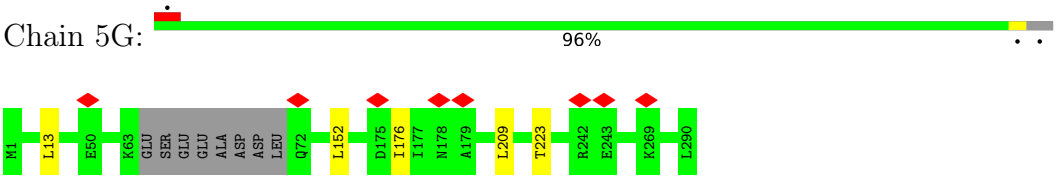




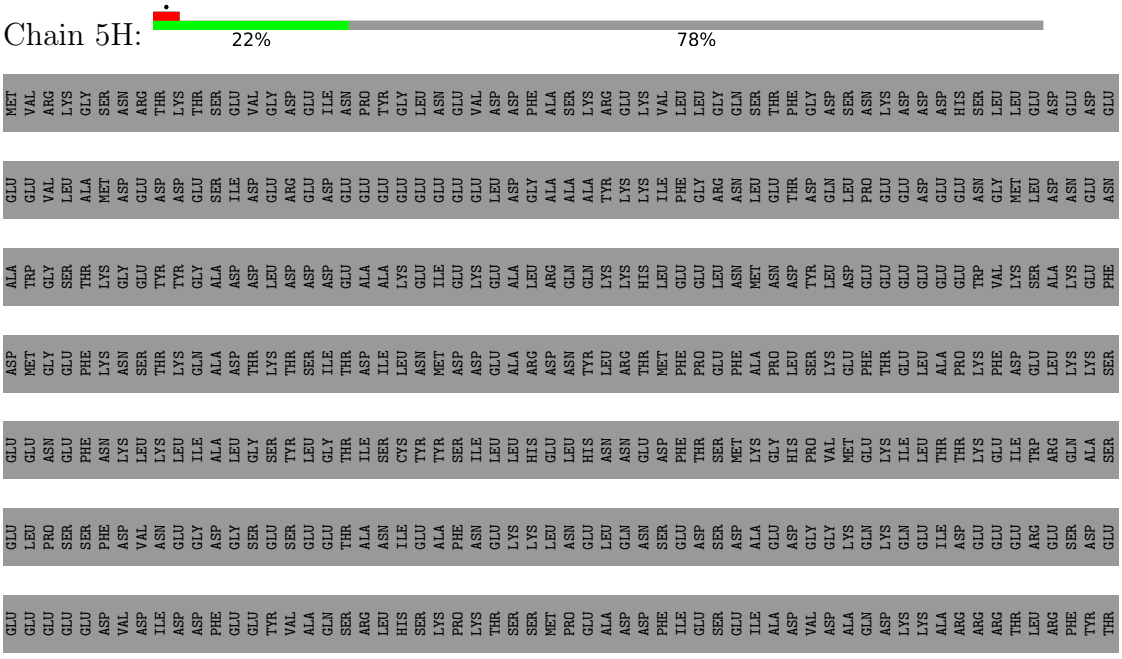
• Molecule 44: U3 small nucleolar ribonucleoprotein protein IMP3



• Molecule 45: U3 small nucleolar ribonucleoprotein protein IMP4

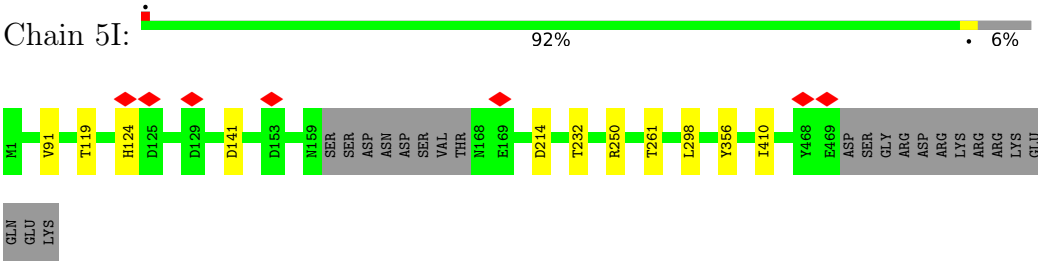


• Molecule 46: Something about silencing protein 10



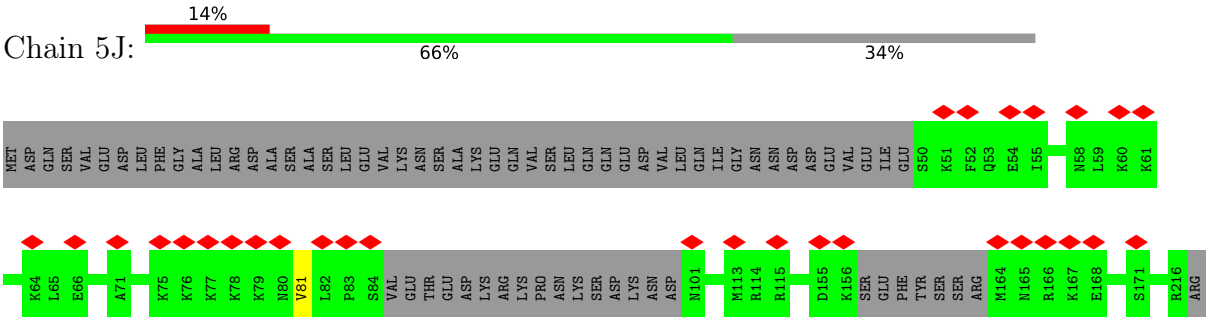
• Molecule 47: Protein SOF1

Chain 5I:



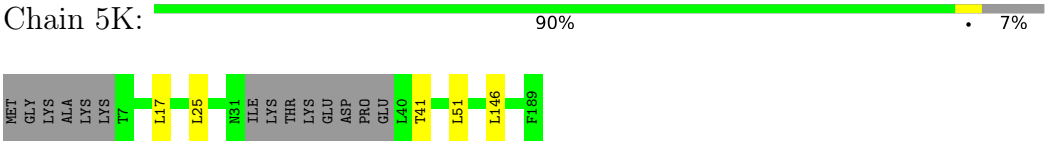
• Molecule 48: rRNA-processing protein FCF2

Chain 5J:



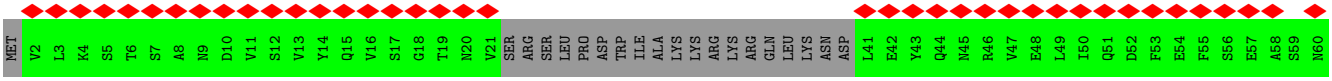
• Molecule 49: rRNA-processing protein FCF1

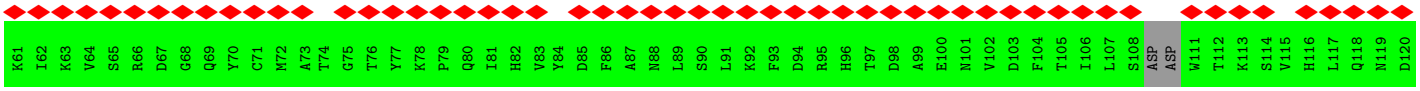
Chain 5K:

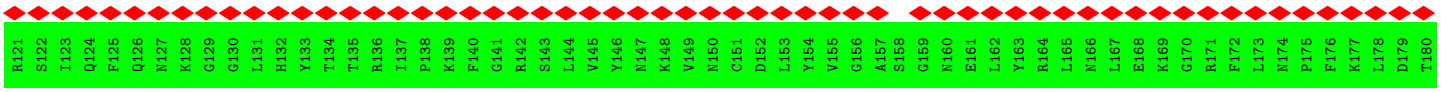


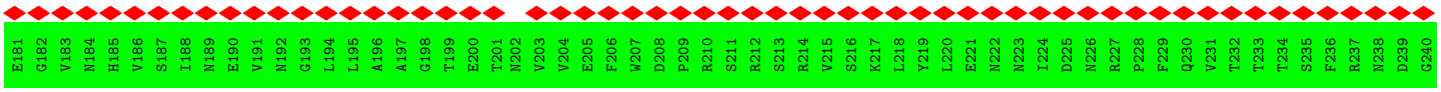
• Molecule 50: Ribosome biogenesis protein ENP2

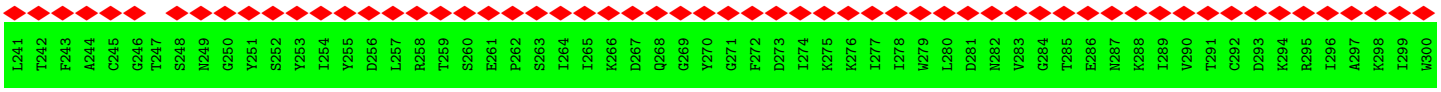
Chain RA:

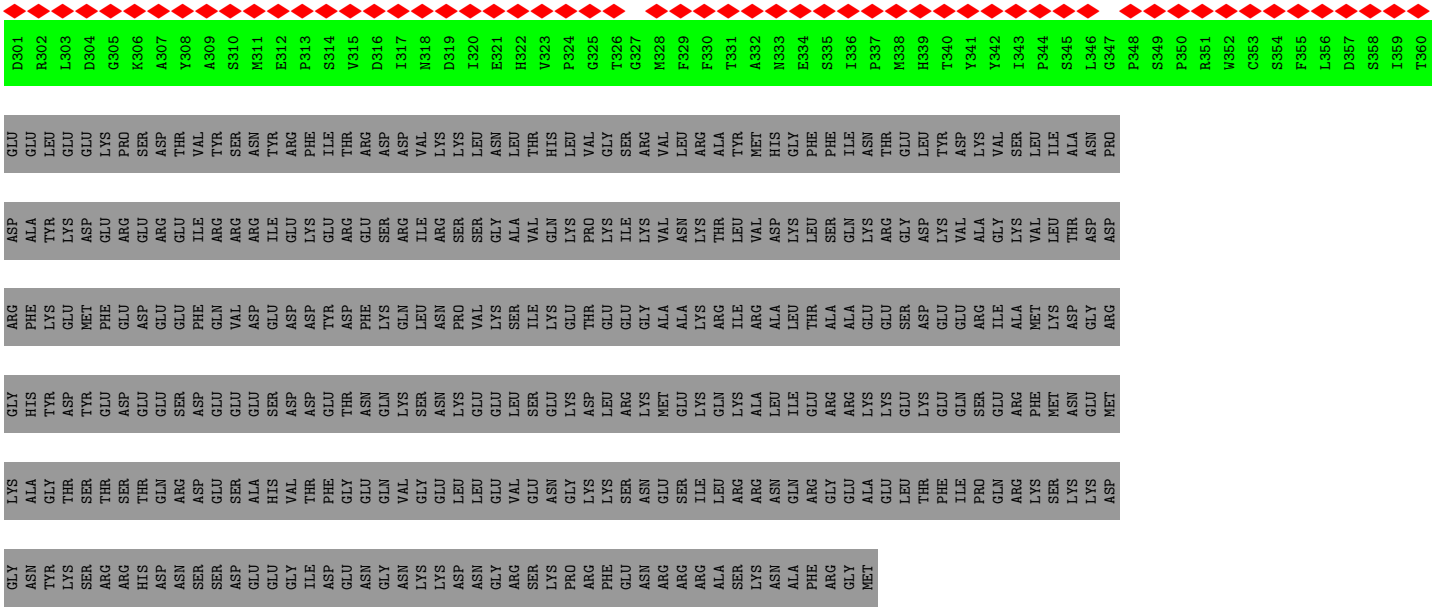




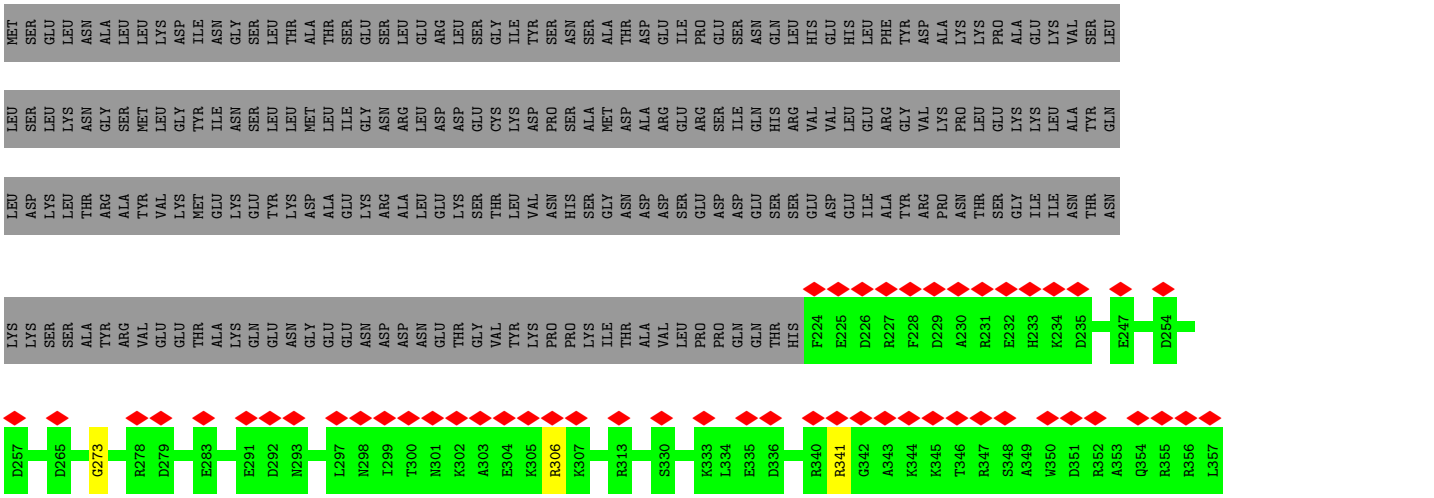




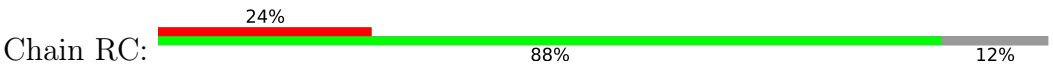


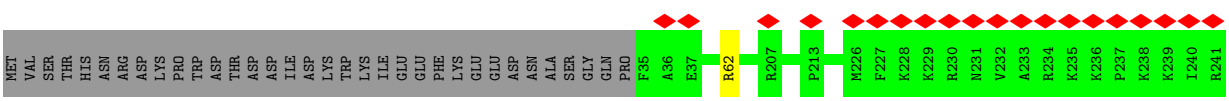


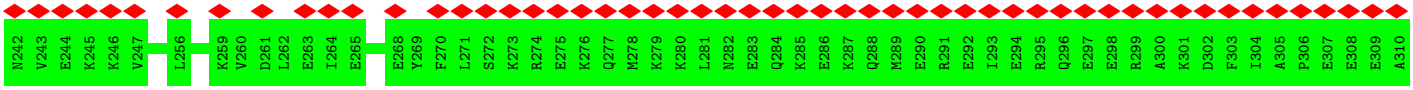
• Molecule 51: U3 small nucleolar ribonucleoprotein protein LCP5

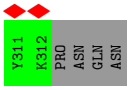


• Molecule 52: KRR1 small subunit processome component



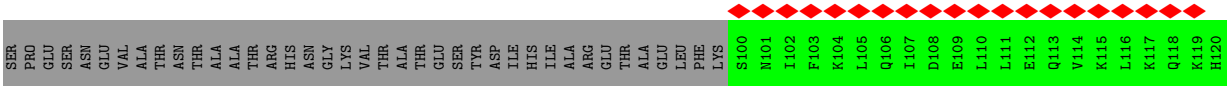


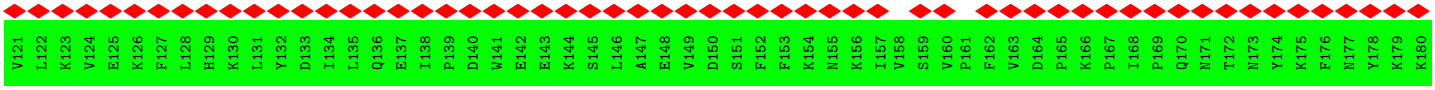


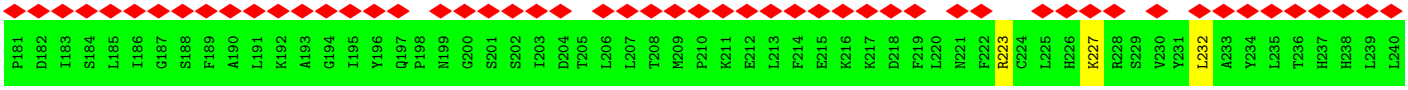


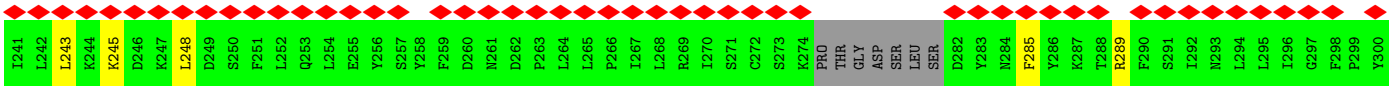
• Molecule 53: U3 small nucleolar RNA-associated protein 22

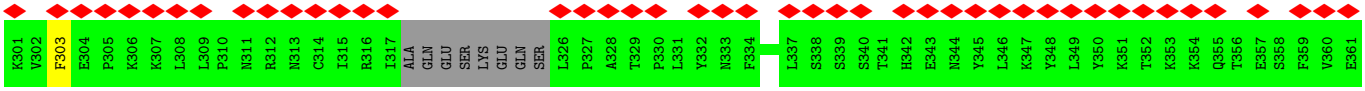
Chain RE:

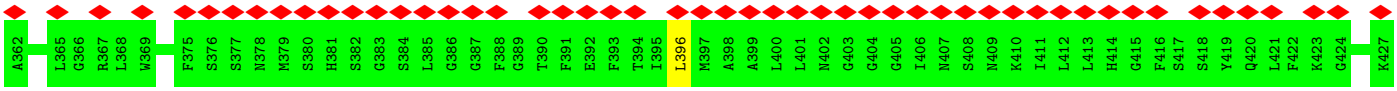


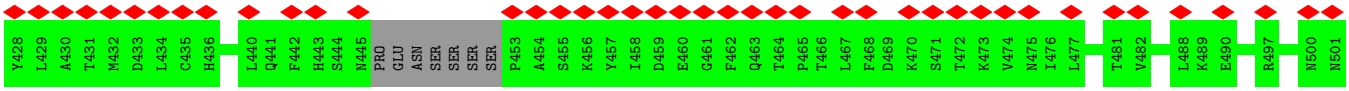


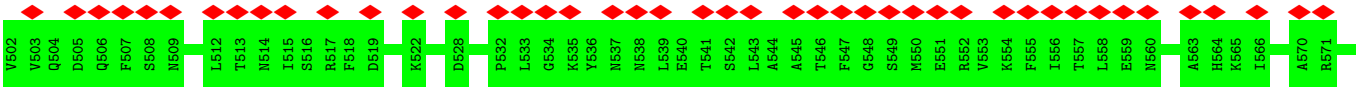


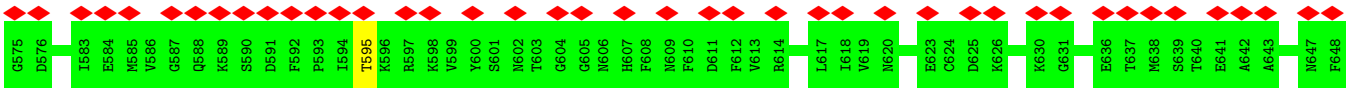


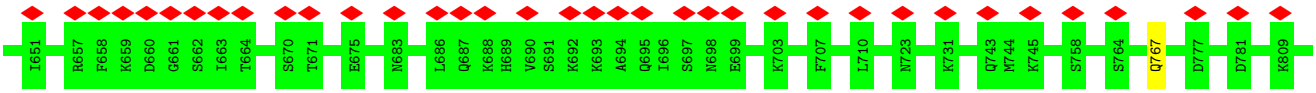


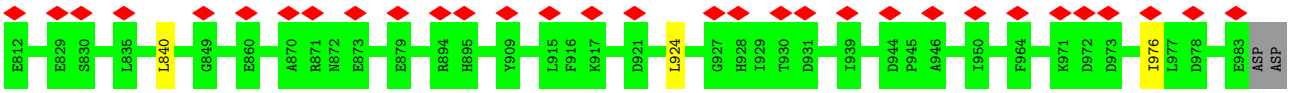


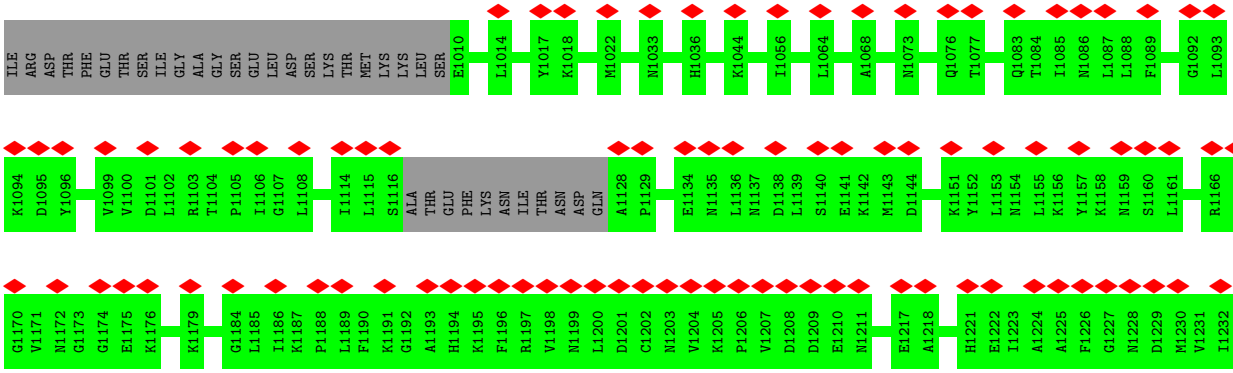






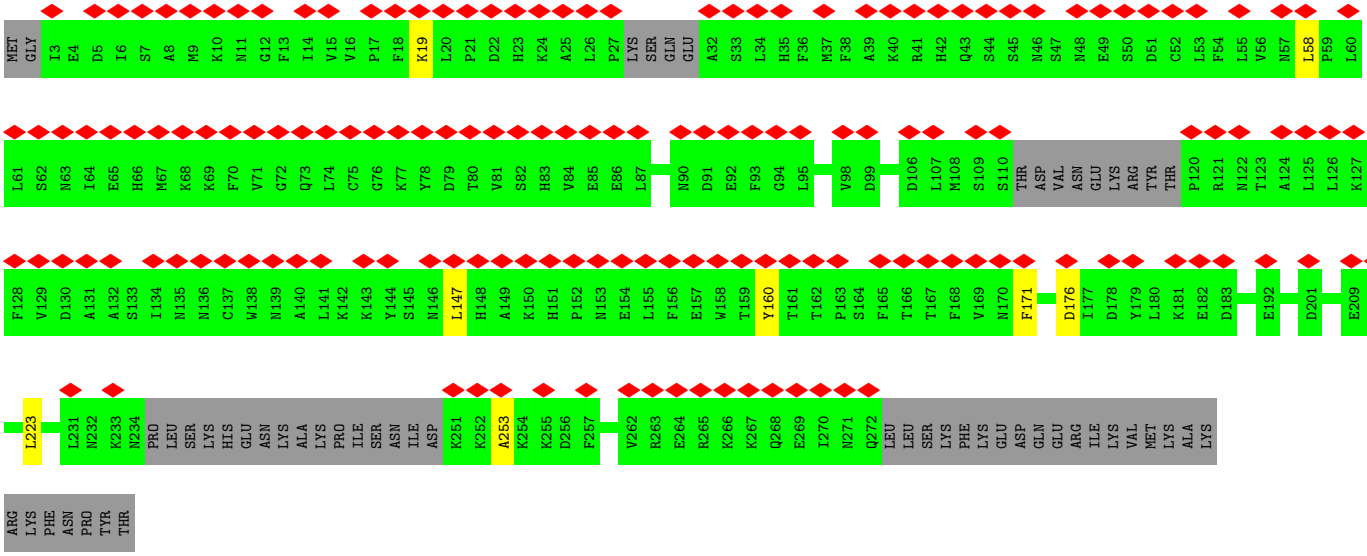






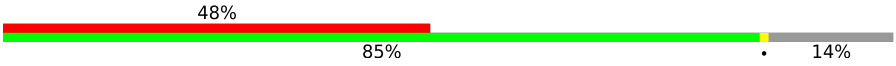
• Molecule 54: Ribosomal RNA-processing protein 7

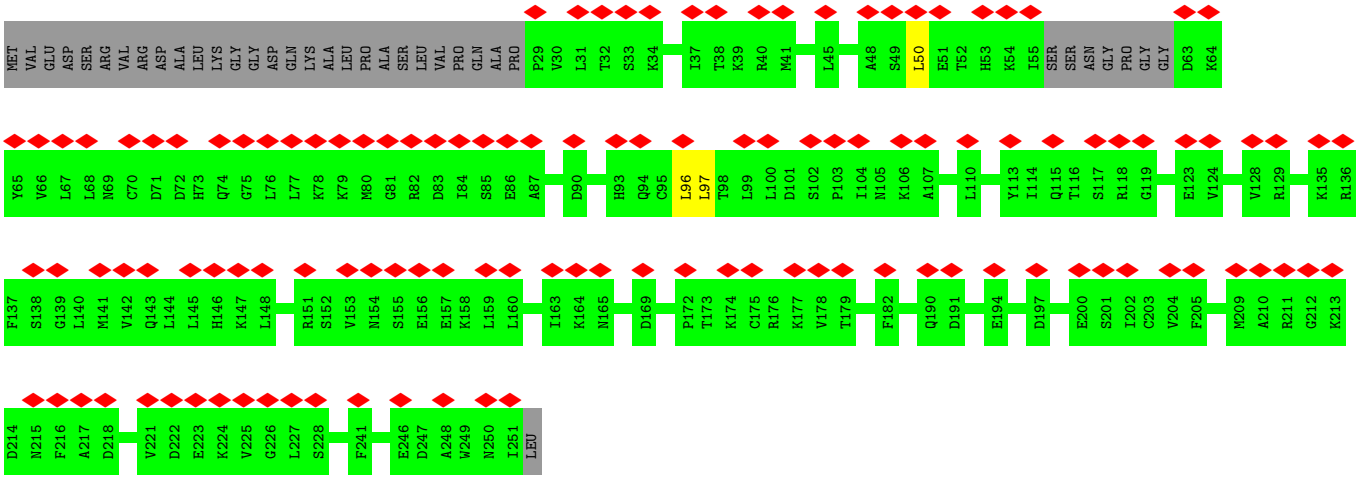
Chain RF:



• Molecule 55: Ribosomal RNA small subunit methyltransferase NEP1

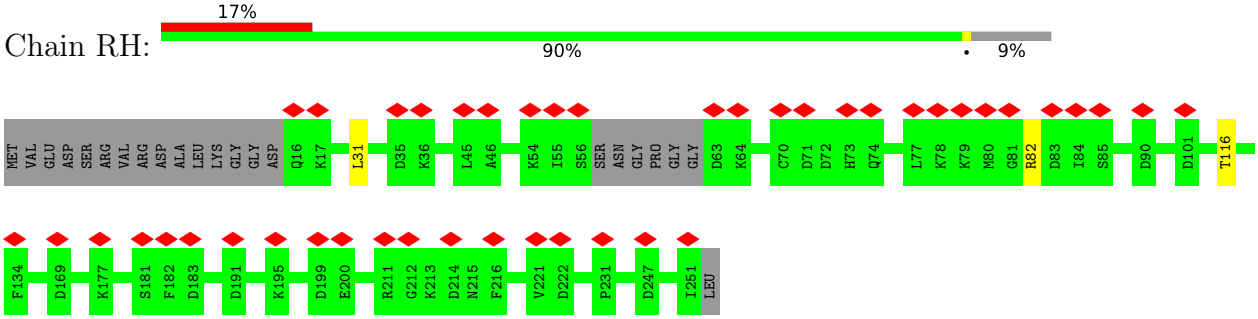
Chain RG:





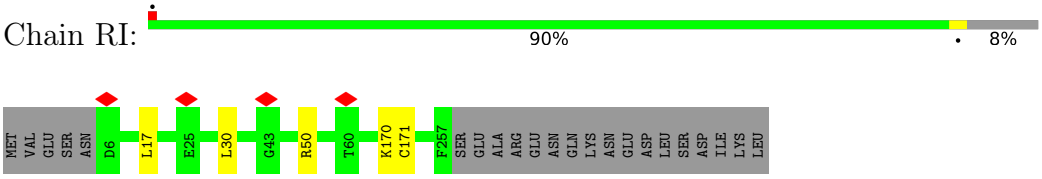
• Molecule 55: Ribosomal RNA small subunit methyltransferase NEP1

Chain RH:



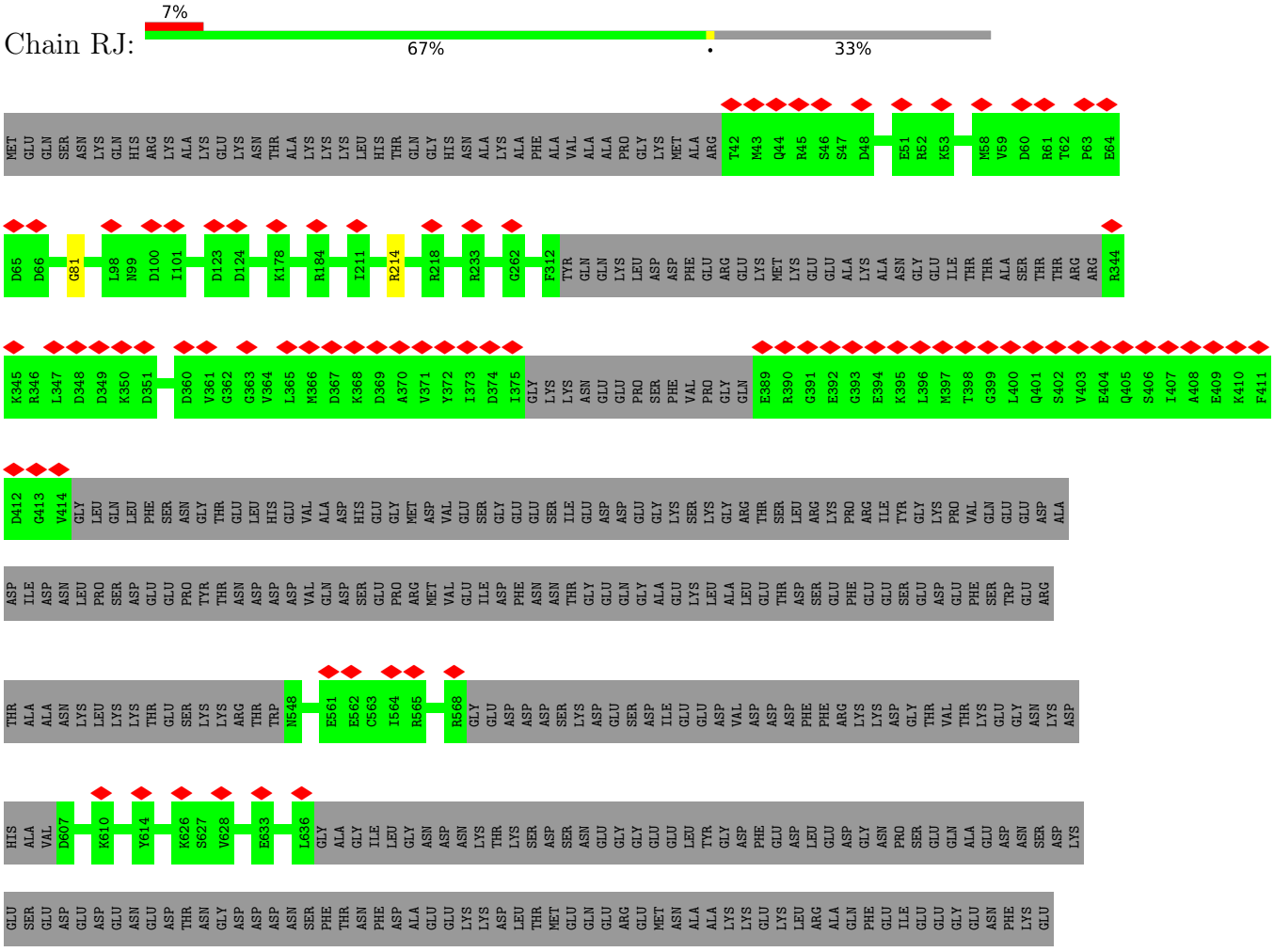
• Molecule 56: Ribosome biogenesis protein UTP30

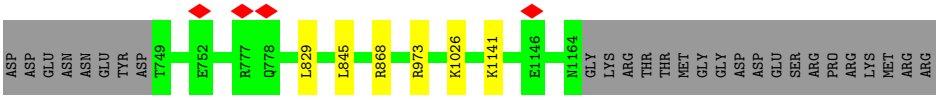
Chain RI:



• Molecule 57: Ribosome biogenesis protein BMS1

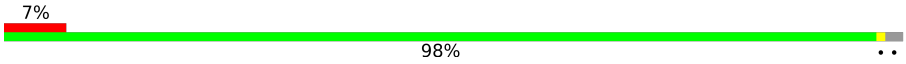
Chain RJ:

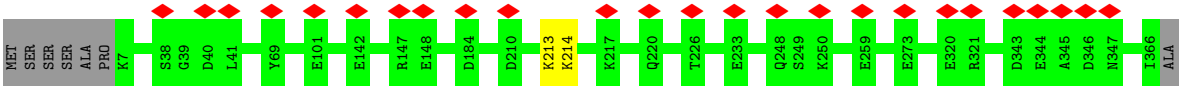




• Molecule 58: RNA 3'-terminal phosphate cyclase-like protein

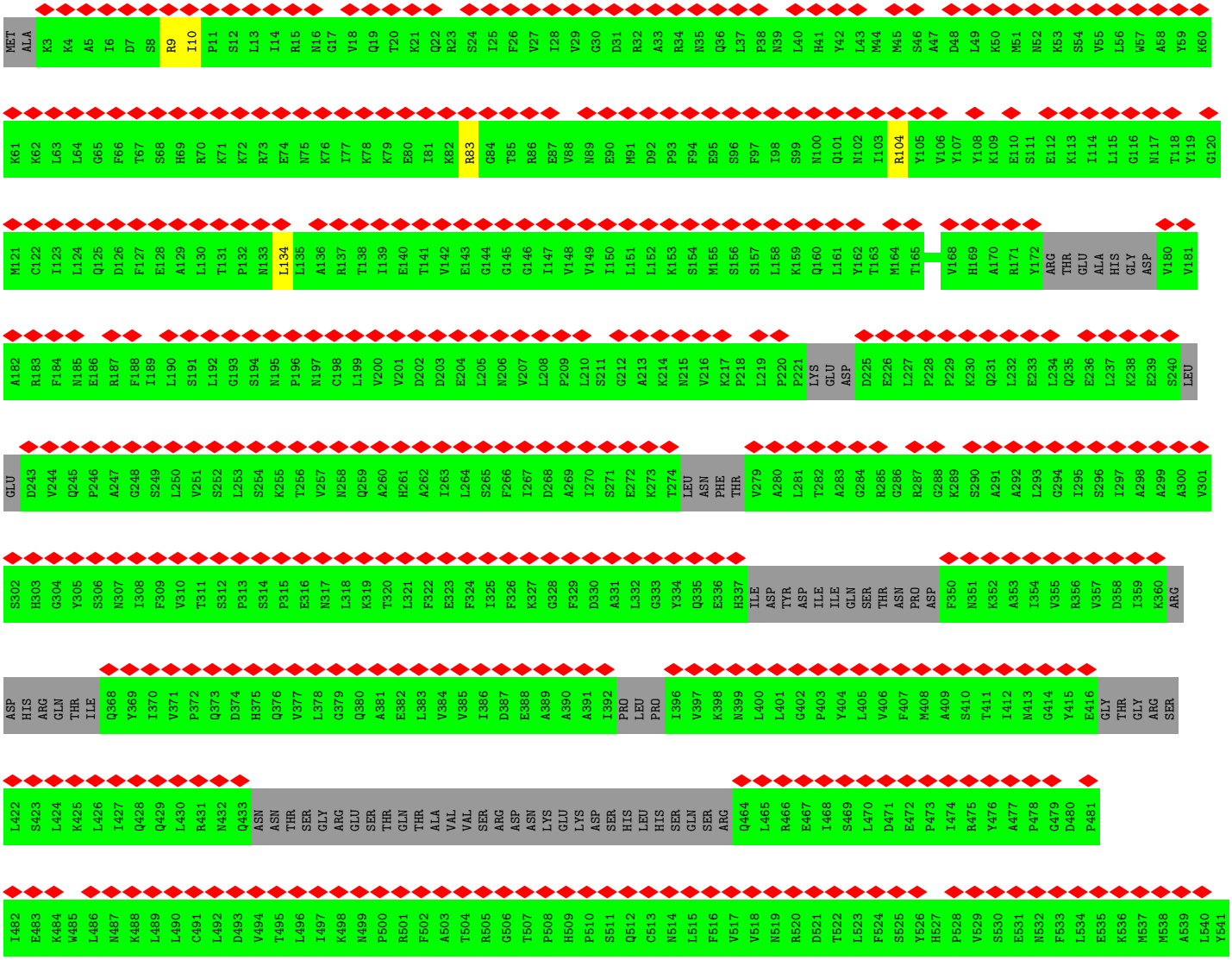
Chain RK:

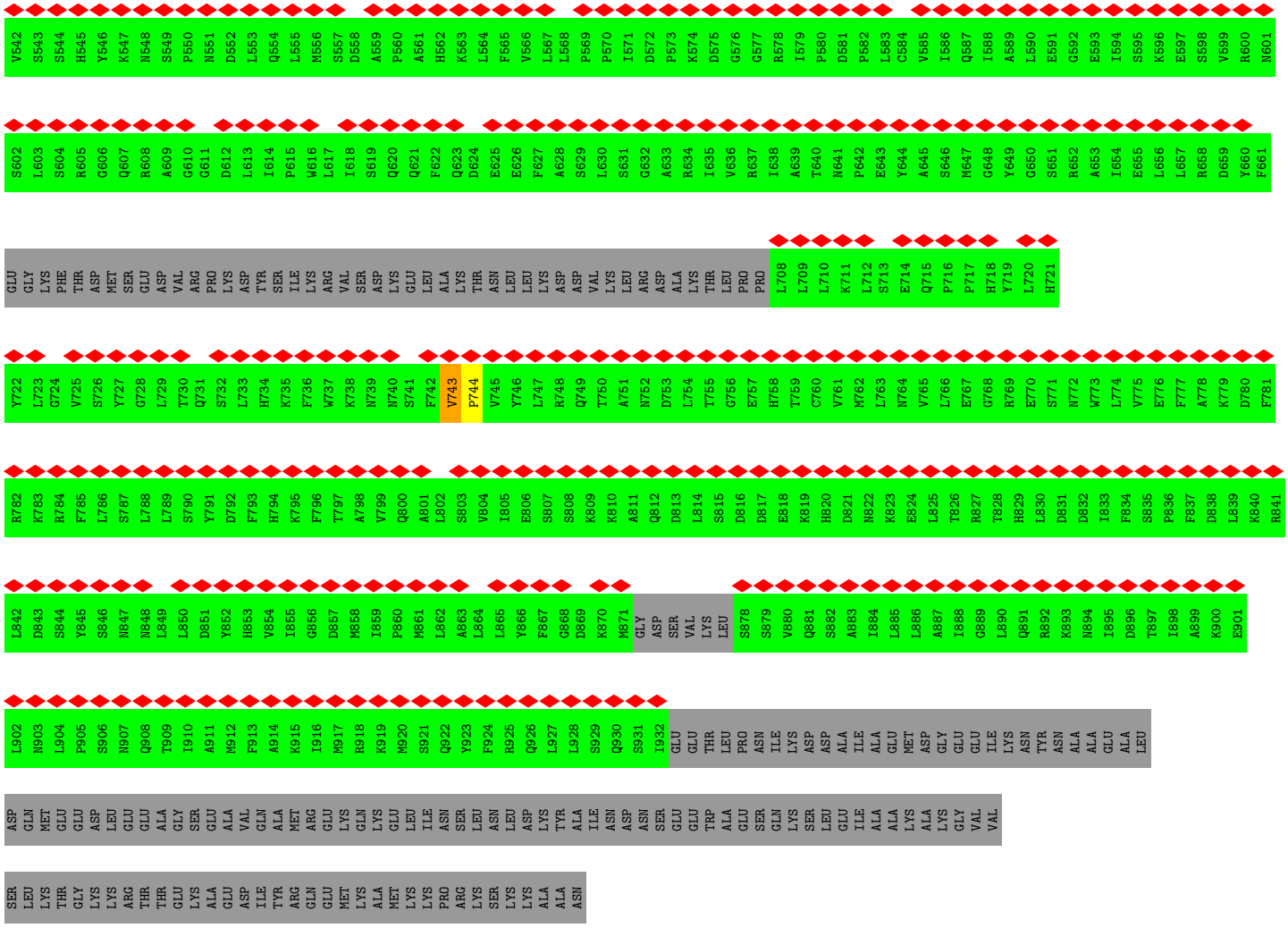




• Molecule 59: RNA cytidine acetyltransferase

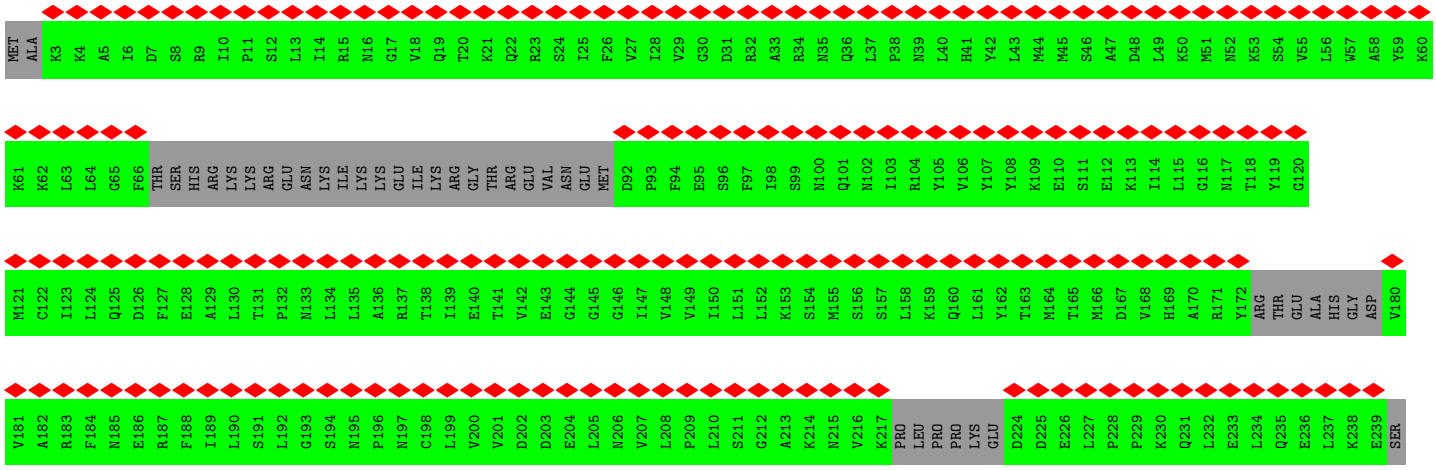
Chain RL:

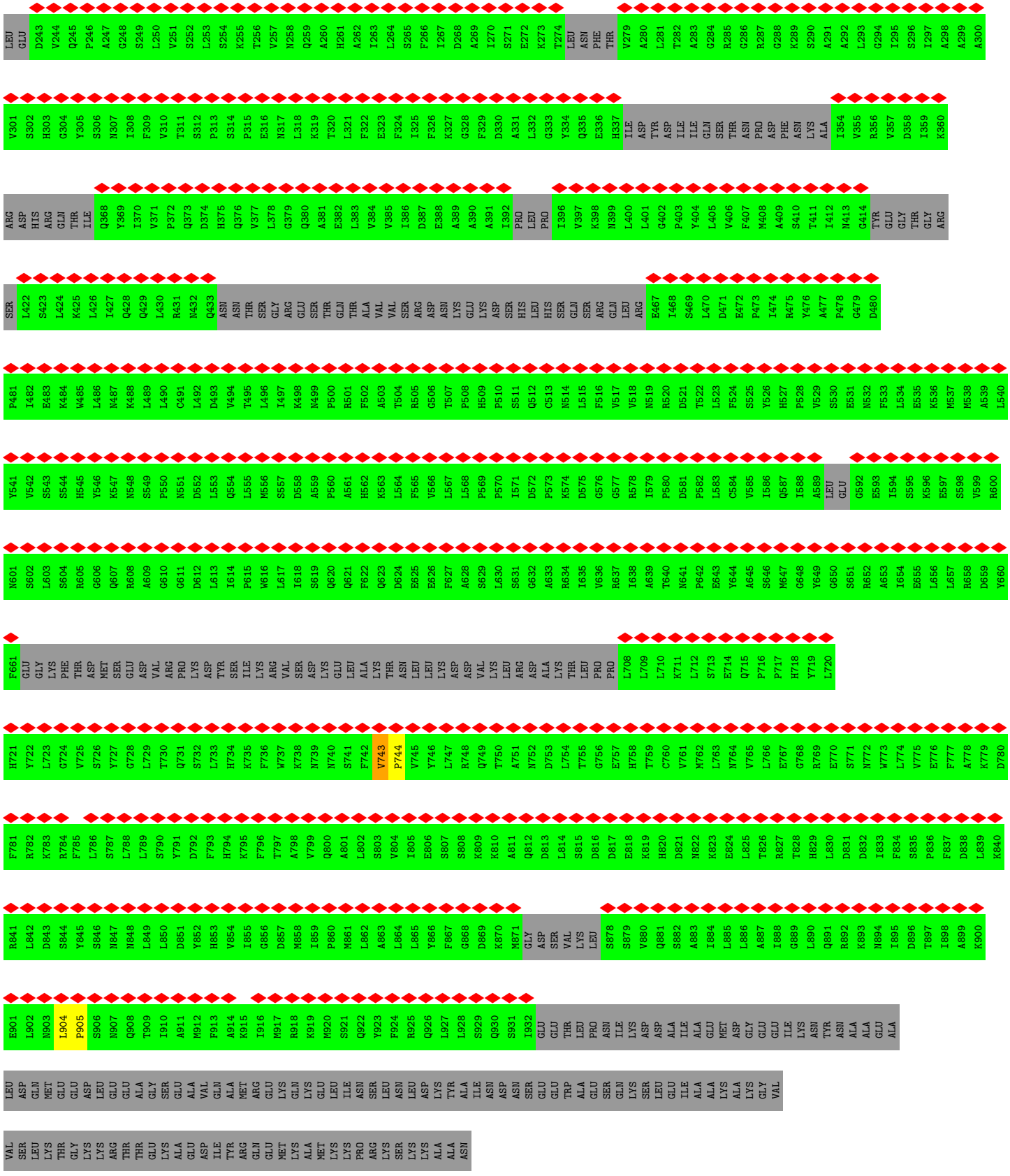




- Molecule 59: RNA cytidine acetyltransferase

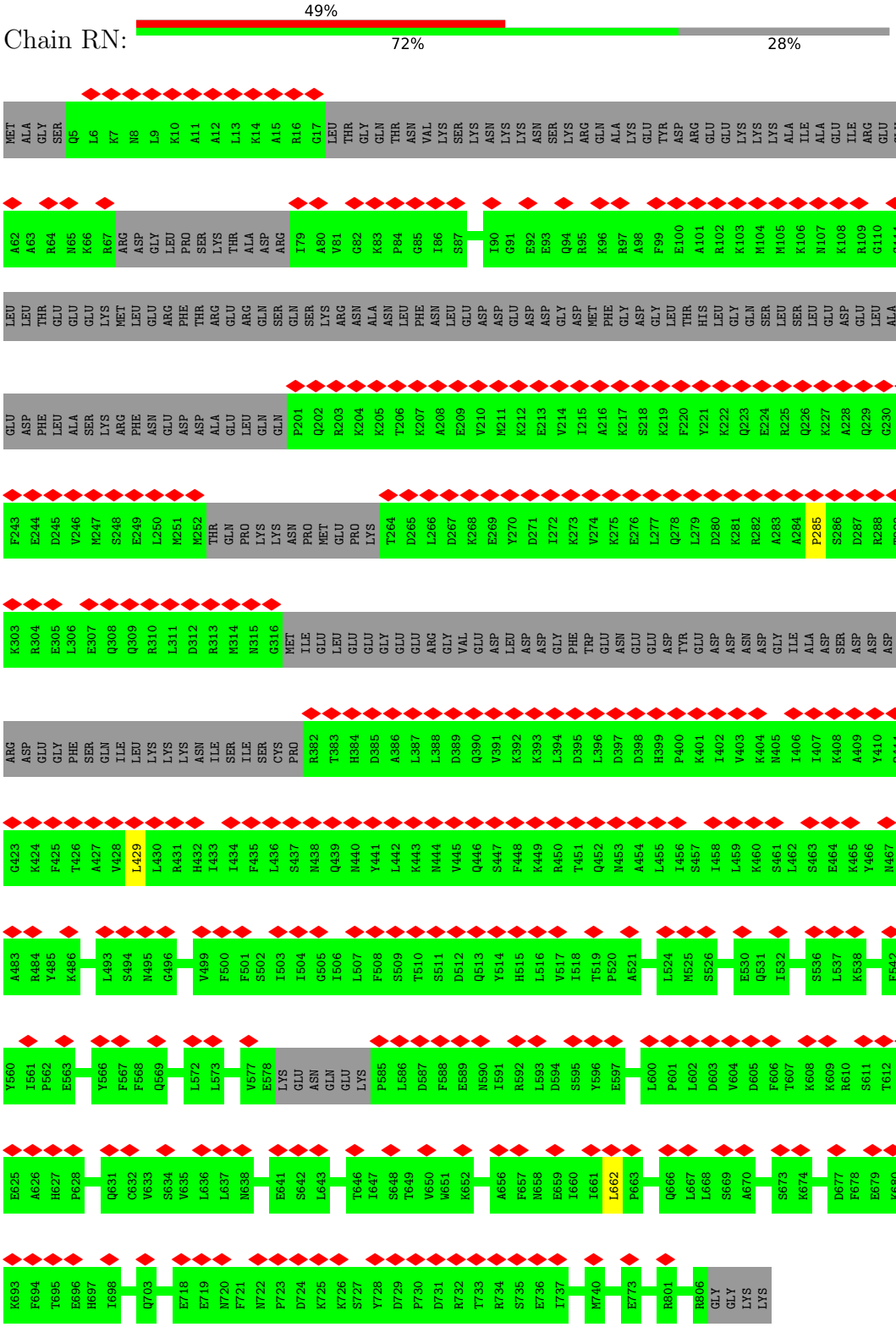
Chain RM:





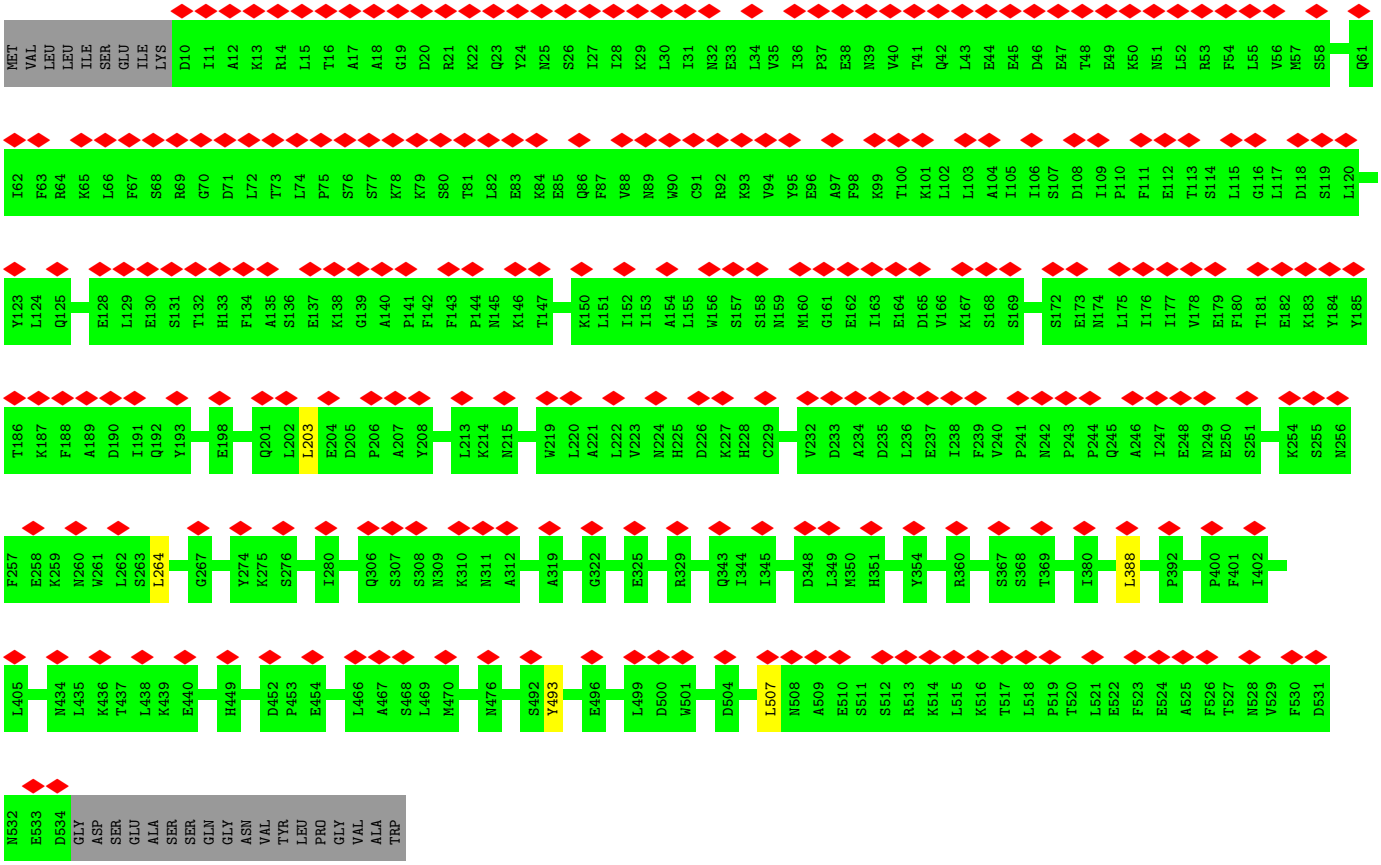
• Molecule 60: Nucleolar complex protein 14

Chain RN:



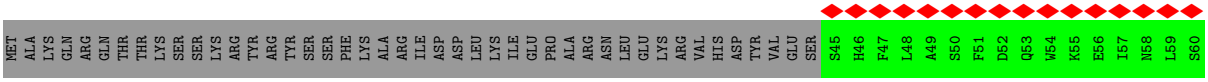
• Molecule 61: Nucleolar complex protein 4

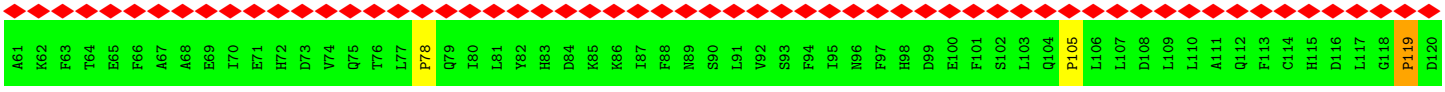
Chain RO:

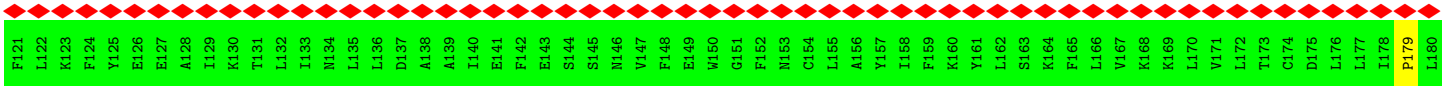


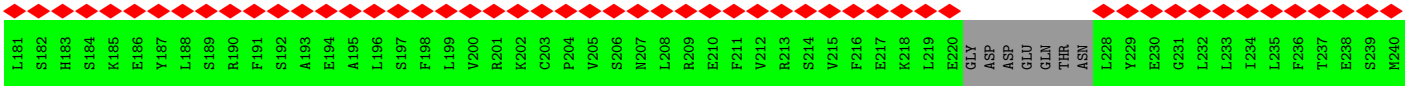
• Molecule 62: U3 small nucleolar RNA-associated protein 20

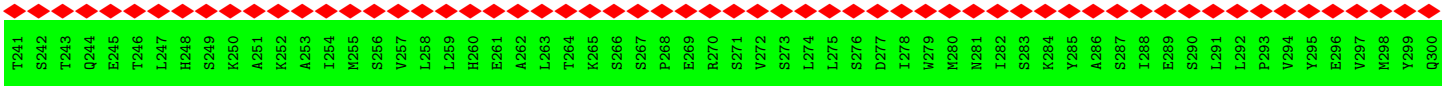
Chain RP:

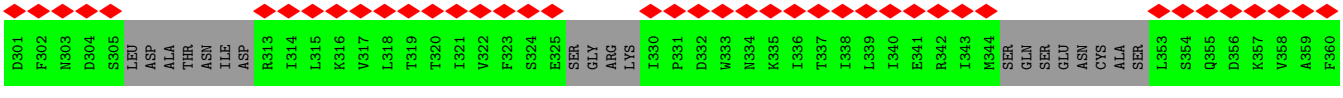


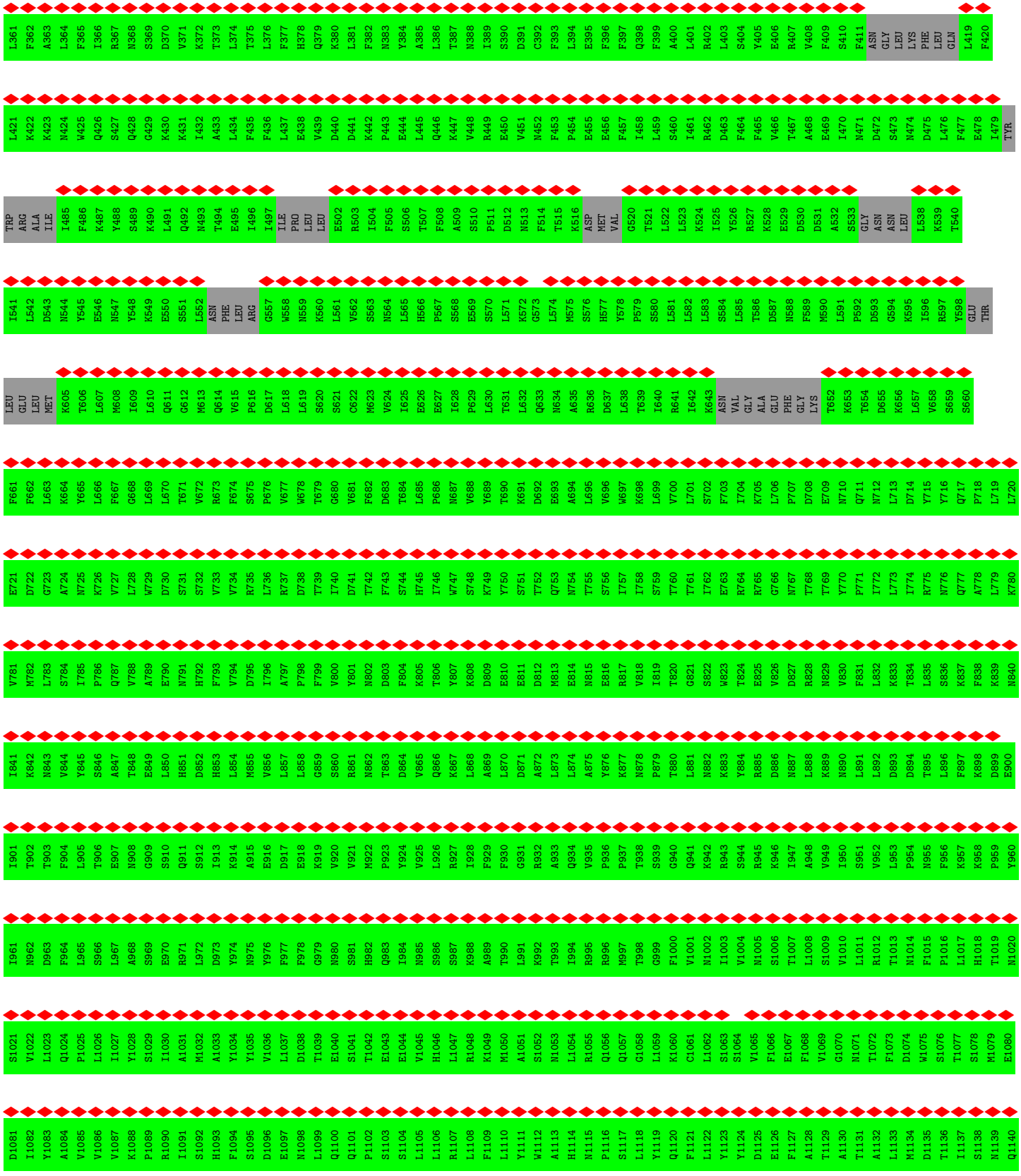


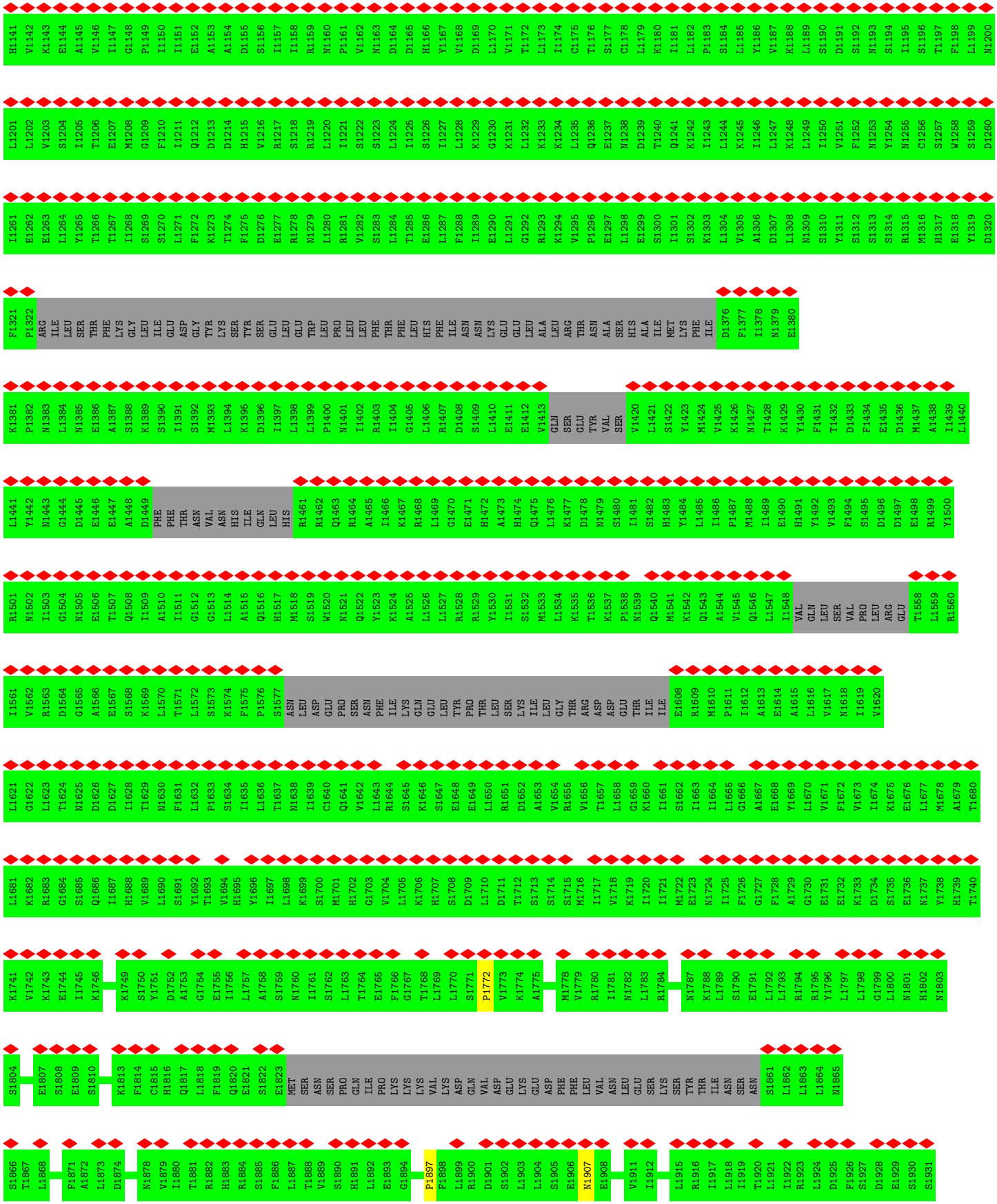


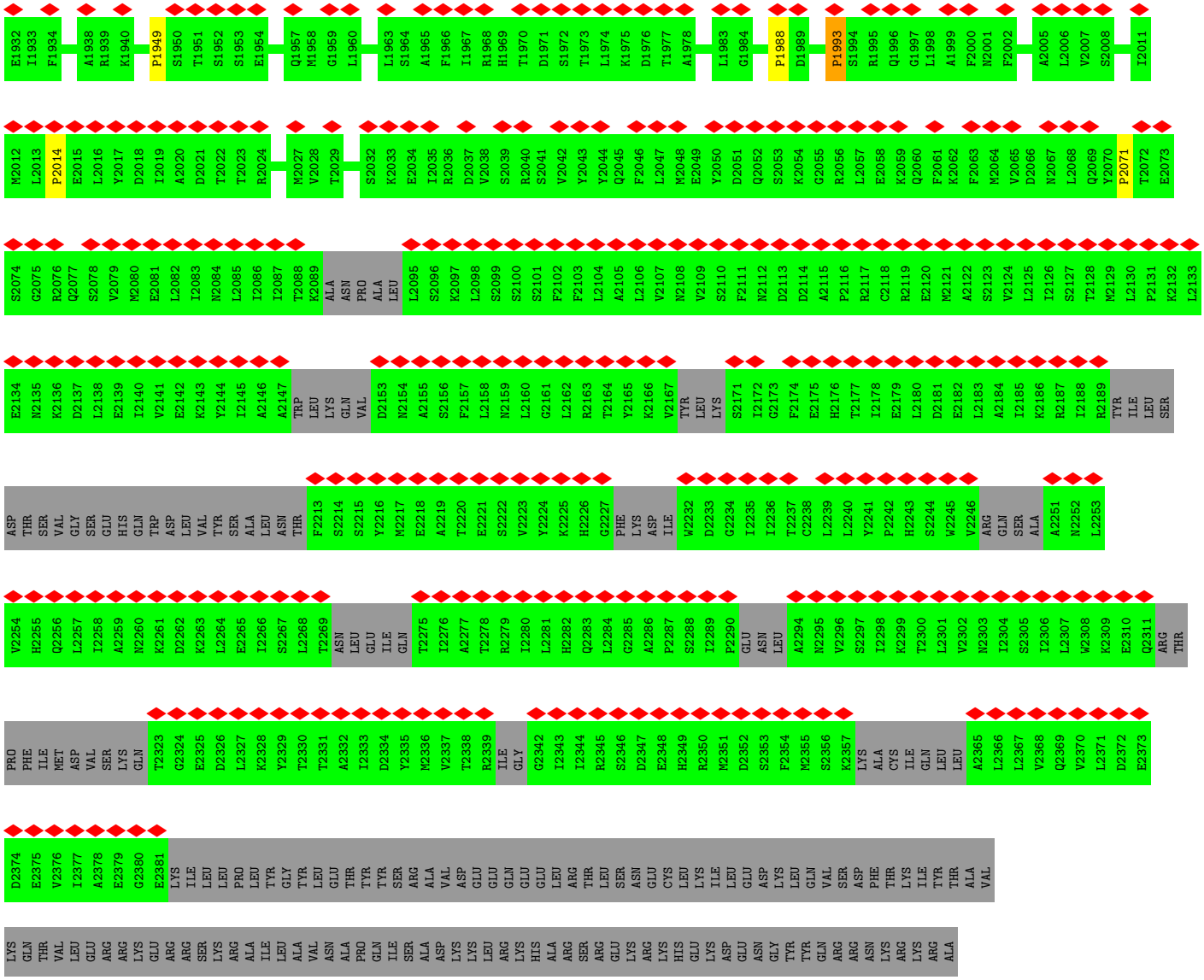






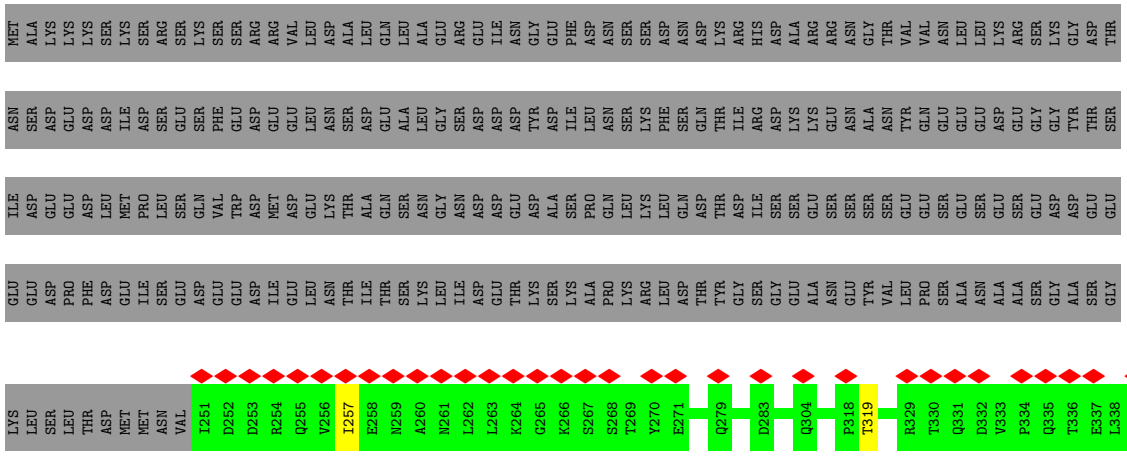

L361 F362 A363 L364 F365 I366 R367 N368 S369 D370 V371 K372 T373 L374 T375 L376 F377 H378 Q379 K380 L381 F382 N383 Y384 A385 L386 T387 N388 I389 S390 D391 C392 F393 L394 E395 F396 F397 Q398 F399 A400 L401 R402 L403 S404 Y405 E406 R407 V408 F409 S410 F411 ASN GLY LEU LYS PHE LEU GLN L419 F420
L421 K422 K423 N424 W425 Q426 S427 Q428 G429 K430 K431 I432 A433 L434 F435 F436 L437 E438 V439 D440 D441 K442 P443 E444 L445 Q446 K447 V448 R449 E450 V451 N452 F453 P454 E455 E456 F457 I458 L459 S460 I461 R462 D463 F464 F465 V466 T467 A468 E469 I470 N471 D472 S473 N474 D475 L476 F477 E478 I479 TYR
TRP ARG ALA ILE I485 F486 K487 Y488 S489 K490 L491 Q492 N493 T494 E495 I496 I497 ILE PRO LEU LEU E502 R503 I504 F505 S506 T507 F508 A509 S510 P511 D512 N513 F514 T515 K516 ASP MET VAL G520 T521 L522 L523 K524 I525 Y526 R527 K528 E529 D530 D531 A532 S533 GLY ASN ASN LEU L538 K539 T540
I541 L542 D543 N544 Y545 E546 N547 Y548 K549 E550 S551 L552 ASN PHE LEU ARG G557 W558 N559 K560 L561 V562 S563 N564 L565 H566 P567 S568 E569 S570 L571 K572 G573 L574 M575 S576 H577 Y578 P579 S580 L581 L582 L583 S584 L585 T586 D587 N588 F589 M590 L591 P592 D593 G594 K595 I596 R597 Y598 GLU THR
LEU GLU LEU MET K605 T606 L607 M608 I609 L610 Q611 G612 M613 Q614 V615 P616 D617 L618 L619 S620 S621 C622 M623 V624 I625 E626 E627 I628 P629 L630 T631 L632 Q633 N634 A635 R636 D637 L638 T639 I640 R641 I642 K643 ASN VAL GLY ALA GLU PHE GLY LYS T652 K653 T654 D655 K656 L657 V658 S659 S660
F661 F662 L663 K664 Y665 L666 F667 G668 L669 L670 T671 V672 R673 F674 S675 P676 V677 W678 T679 G680 V681 F682 D683 T684 L685 P686 N687 V688 Y689 T690 K691 D692 E693 A694 L695 V696 W697 K698 L699 V700 L701 S702 F703 I704 K705 L706 P707 D708 E709 N710 Q711 N712 L713 D714 Y715 Y716 Q717 P718 L719 L720
E721 D722 G723 A724 N725 K726 V727 L728 W729 D730 S731 S732 V733 V734 R735 L736 R737 D738 T739 I740 D741 T742 F743 S744 H745 I746 W747 S748 K749 Y750 S751 T752 Q753 N754 T755 S756 I757 T758 S759 T760 T761 I762 E763 R764 R765 G766 N767 T768 T769 Y770 P771 I772 L773 I774 R775 N776 Q777 A778 L779 K780
V781 M782 L783 S784 I785 P786 Q787 V788 A789 E790 N791 H792 F793 V794 D795 I796 A797 P798 F799 V800 Y801 N802 D803 F804 K805 T806 Y807 K808 D809 E810 E811 D812 M813 E814 N815 E816 R817 V818 I819 T820 G821 S822 W823 T824 E825 V826 D827 R828 N829 V830 F831 L832 K833 T834 L835 S836 K837 F838 K839 N840
I841 K842 N843 V844 Y845 S846 A847 T848 E849 L850 H851 D852 H853 L854 M855 V856 L857 L858 G859 S860 R861 N862 T863 D864 V865 Q866 K867 L868 A869 L870 D871 A872 L873 L874 A875 Y876 K877 N878 P879 T880 L881 N882 K883 Y884 R885 D886 N887 L888 K889 N890 L891 L892 D893 D894 T895 L896 F897 K898 D899 E900
I901 T902 T903 F904 L905 T906 E907 N908 G909 S910 Q911 S912 I913 K914 A915 E916 D917 E918 K919 V920 V921 M922 P923 Y924 V925 L926 R927 I928 F929 F930 G931 R932 A933 Q934 V935 P936 P937 T938 S939 G940 Q941 K942 R943 S944 R945 K946 I947 A948 V949 I950 S951 V952 L953 P954 N955 F956 K957 K958 P959 Y960
I961 N962 D963 F964 L965 S966 L967 A968 S969 E970 R971 L972 D973 Y974 N975 Y976 F977 F978 G979 N980 S981 H982 Q983 I984 N985 S986 S987 K988 A989 T990 L991 K992 T993 I994 R995 R996 M997 T998 G999 F1000 V1001 N1002 I1003 V1004 N1005 S1006 T1007 L1008 S1009 V1010 L1011 R1012 T1013 N1014 F1015 P1016 L1017 H1018 T1019 N1020
S1021 V1022 L1023 Q1024 P1025 L1026 I1027 Y1028 S1029 I1030 A1031 M1032 A1033 Y1034 Y1035 V1036 L1037 D1038 T1039 E1040 S1041 T1042 E1043 E1044 V1045 H1046 L1047 R1048 K1049 M1050 A1051 S1052 N1053 L1054 R1055 Q1056 Q1057 G1058 L1059 K1060 C1061 L1062 S1063 S1064 V1065 F1066 E1067 F1068 V1069 G1070 N1071 T1072 F1073 D1074 W1075 S1076 T1077 S1078 M1079 E1080
D1081 I1082 Y1083 A1084 V1085 V1086 V1087 K1088 P1089 R1090 I1091 S1092 H1093 F1094 S1095 D1096 E1097 N1098 L1099 Q1100 Q1101 P1102 S1103 S1104 L1105 L1106 R1107 L1108 F1109 L1110 Y1111 W1112 A1113 H1114 N1115 P1116 S1117 L1118 Y1119 Q1120 F1121 L1122 Y1123 Y1124 D1125 E1126 F1127 A1128 T1129 A1130 T1131 A1132 L1133 M1134 D1135 T1136 I1137 S1138 N1139 Q1140

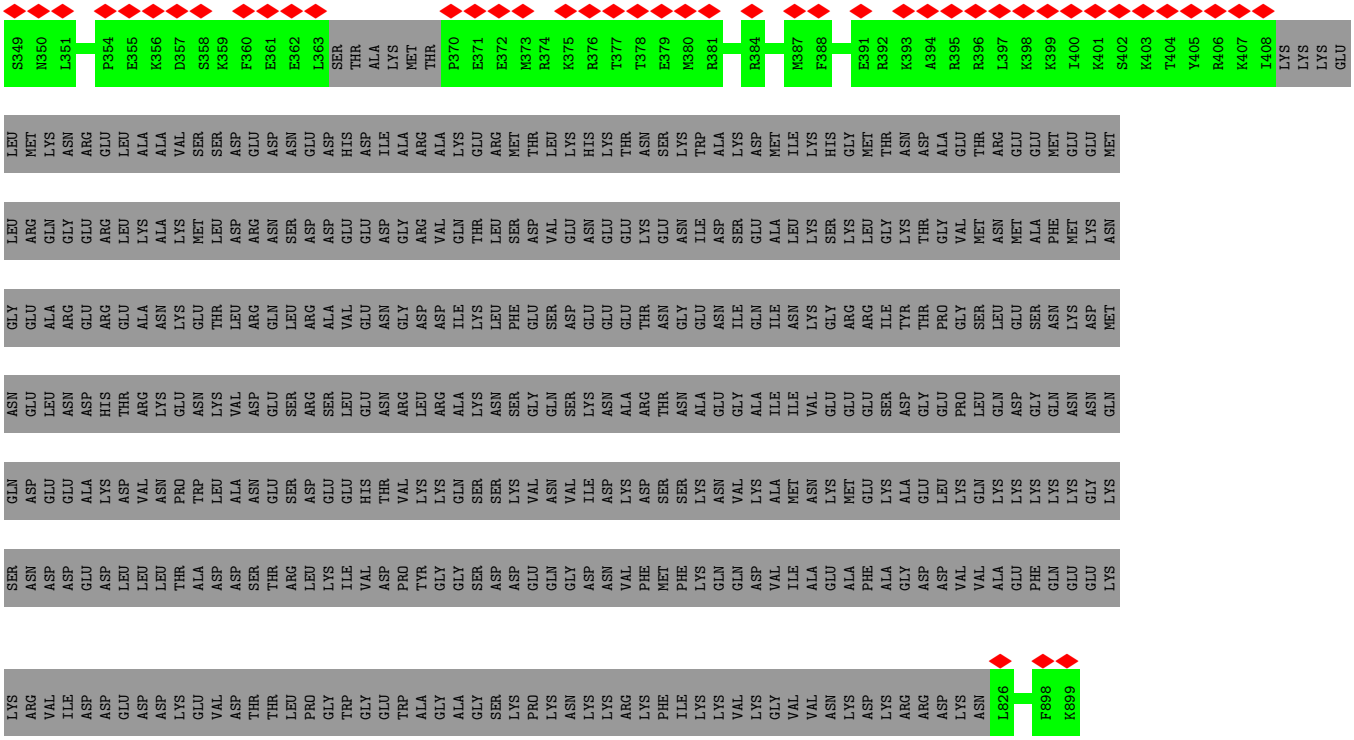

H1141 V1142 K1143 E1144 A1145 V1146 I1147 G1148 P1149 I1150 I1151 E1152 A1153 A1154 D1155 S1156 I1157 I1158 R1159 N1160 P1161 V1162 N1163 D1164 D1165 H1166 Y1167 V1168 D1169 L1170 V1171 T1172 L1173 I1174 C1175 T1176 S1177 C1178 L1179 K1180 I1181 L1182 P1183 S1184 L1185 Y1186 V1187 K1188 L1189 S1190 D1191 S1192 N1193 S1194 I1195 S1196 T1197 F1198 L1199 N1200
L1201 L1202 V1203 S1204 I1205 T1206 E1207 M1208 G1209 F1210 I1211 Q1212 D1213 D1214 H1215 V1216 R1217 S1218 R1219 L1220 I1221 S1222 S1223 L1224 I1225 S1226 I1227 L1228 K1229 G1230 K1231 L1232 K1233 K1234 L1235 Q1236 E1237 N1238 D1239 T1240 Q1241 K1242 I1243 L1244 K1245 I1246 L1247 K1248 L1249 I1250 V1251 F1252 N1253 Y1254 N1255 C1256 S1257 V1258 S1259 D1260
I1261 E1262 E1263 L1264 Y1265 T1266 T1267 I1268 S1269 S1270 L1271 F1272 K1273 T1274 F1275 D1276 E1277 R1278 N1279 L1280 R1281 V1282 S1283 L1284 T1285 E1286 L1287 F1288 I1289 E1290 L1291 G1292 R1293 K1294 V1295 P1296 E1297 L1298 E1299 S1300 I1301 S1302 K1303 L1304 V1305 A1306 D1307 L1308 N1309 S1310 Y1311 S1312 S1313 S1314 R1315 M1316 H1317 E1318 Y1319 D1320
F1321 P1322 ARG ILE LEU SER THR PHE LYS GLY LEU ILE GLU ASP GLY TYR LYS SER TYR SER GLU LEU GLU TRP LEU PRO LEU LEU PHE THR LEU HIS PHE ILE ASN ASN LYS GLU GLU LEU ALA LEU ARG THR ASN ALA SER HIS ALA ILE MET LYS PHE ILE D1376 F1377 I1378 N1379 E1380
K1381 P1382 N1383 L1384 N1385 E1386 A1387 S1388 K1389 S1390 I1391 S1392 M1393 L1394 K1395 D1396 I1397 L1398 L1399 P1400 N1401 I1402 R1403 I1404 G1405 L1406 R1407 D1408 S1409 L1410 E1411 E1412 V1413 GLN SER GLU TYR VAL SER V1420 L1421 S1422 Y1423 M1424 V1425 K1426 N1427 T1428 K1429 Y1430 F1431 T1432 D1433 F1434 E1435 D1436 M1437 A1438 I1439 L1440
L1441 Y1442 N1443 G1444 D1445 E1446 E1447 A1448 D1449 PHE PHE THR ASN VAL ASN HIS ILE GLN LEU HIS R1461 R1462 Q1463 R1464 A1465 I1466 K1467 R1468 L1469 G1470 E1471 H1472 A1473 H1474 Q1475 L1476 K1477 D1478 N1479 S1480 I1481 S1482 H1483 Y1484 L1485 I1486 P1487 M1488 I1489 E1490 H1491 Y1492 V1493 F1494 S1495 D1496 D1497 E1498 R1499 Y1500
R1501 N1502 I1503 G1504 N1505 E1506 T1507 Q1508 I1509 A1510 I1511 G1512 G1513 L1514 A1515 Q1516 H1517 M1518 S1519 W1520 N1521 Q1522 Y1523 K1524 A1525 L1526 L1527 R1528 R1529 Y1530 R1531 S1532 M1533 L1534 K1535 T1536 K1537 P1538 N1539 Q1540 M1541 K1542 Q1543 A1544 V1545 Q1546 L1547 I1548 VAL GLN LEU SER VAL PRO LEU ARG GLU T1558 L1559 R1560
I1561 V1562 R1563 D1564 G1565 A1566 E1567 S1568 K1569 L1570 T1571 L1572 S1573 K1574 F1575 P1576 S1577 ASN LEU ASP GLU PRO SER ASN PHE ILE LYS GLN GLU LEU TYR PRO THR LEU SER LYS ILE LEU GLY THR ARG ASP ASP GLU THR ILE ILE E1608 R1609 M1610 P1611 I1612 A1613 E1614 A1615 L1616 V1617 N1618 I1619 V1620
L1621 G1622 L1623 T1624 N1625 D1626 D1627 I1628 T1629 N1630 F1631 L1632 P1633 S1634 I1635 L1636 T1637 N1638 I1639 C1640 Q1641 V1642 L1643 R1644 S1645 K1646 S1647 E1648 E1649 L1650 R1651 D1652 A1653 V1654 R1655 V1656 T1657 L1658 G1659 K1660 I1661 S1662 I1663 I1664 L1665 G1666 A1667 E1668 Y1669 L1670 V1671 F1672 V1673 I1674 K1675 E1676 L1677 M1678 A1679 T1680
L1681 K1682 R1683 G1684 S1685 Q1686 I1687 H1688 V1689 L1690 S1691 Y1692 T1693 V1694 H1695 Y1696 I1697 L1698 K1699 S1700 M1701 H1702 G1703 V1704 L1705 K1706 H1707 S1708 D1709 L1710 D1711 T1712 S1713 S1714 S1715 M1716 I1717 V1718 K1719 I1720 I1721 M1722 E1723 I1724 I1725 F1726 G1727 F1728 A1729 G1730 E1731 E1732 K1733 D1734 S1735 E1736 N1737 Y1738 H1739 T1740
K1741 V1742 K1743 E1744 I1745 K1746 K1749 S1750 Y1751 D1752 A1753 G1754 E1755 I1756 L1757 A1758 S1759 N1760 I1761 S1762 L1763 T1764 E1765 F1766 G1767 T1768 L1769 L1770 S1771 P1772 V1773 K1774 A1775 M1778 V1779 R1780 I1781 N1782 L1783 R1784 N1787 K1788 L1789 S1790 E1791 L1792 L1793 R1794 R1795 Y1796 L1797 L1798 G1799 L1800 N1801 H1802 N1803
S1804 E1807 S1808 E1809 S1810 K1813 F1814 C1815 H1816 Q1817 L1818 F1819 Q1820 E1821 S1822 E1823 MET SER ASN SER PRO GLN ILE PRO LYS LYS LYS VAL LYS ASP GLN VAL ASP GLU LYS GLU ASP PHE PHE LEU VAL ASN LEU GLU SER LYS SER TYR THR ILE ASN SER ASN S1861 L1862 L1863 L1864 N1865
S1866 T1867 L1868 F1871 A1872 L1873 D1874 N1878 V1879 I1880 T1881 R1882 H1883 R1884 S1885 F1886 L1887 T1888 V1889 S1890 H1891 L1892 E1893 G1894 P1897 F1898 L1899 R1900 D1901 S1902 L1903 L1904 S1905 E1906 N1907 E1908 V1911 I1912 L1915 R1916 I1917 L1918 I1919 T1920 L1921 I1922 R1923 L1924 D1925 F1926 S1927 D1928 E1929 S1930 S1931



• Molecule 63: U3 small nucleolar RNA-associated protein 14

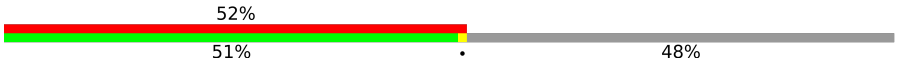
Chain RQ:

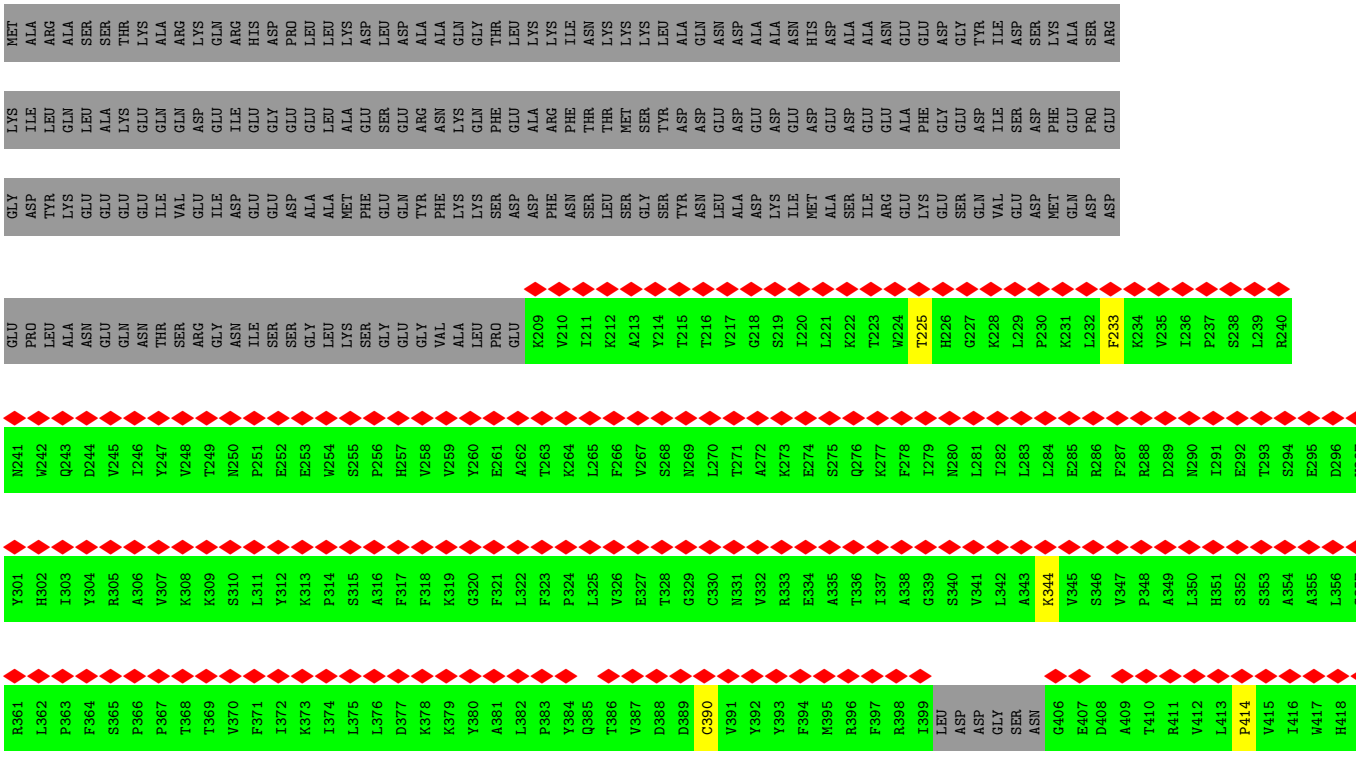


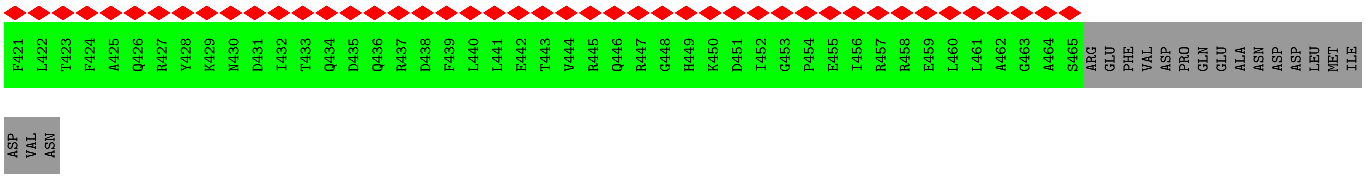


• Molecule 64: Essential nuclear protein 1

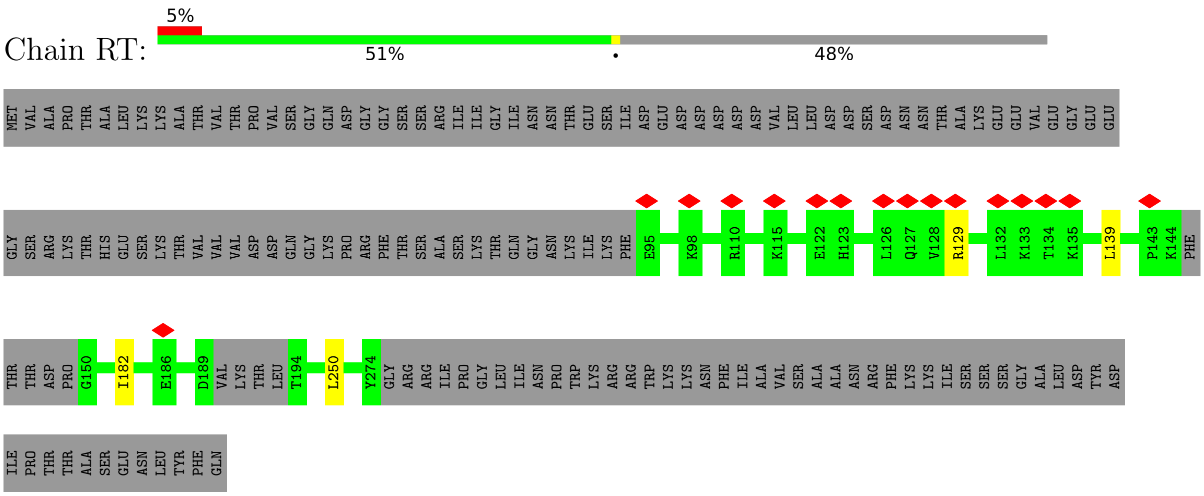
Chain RS:



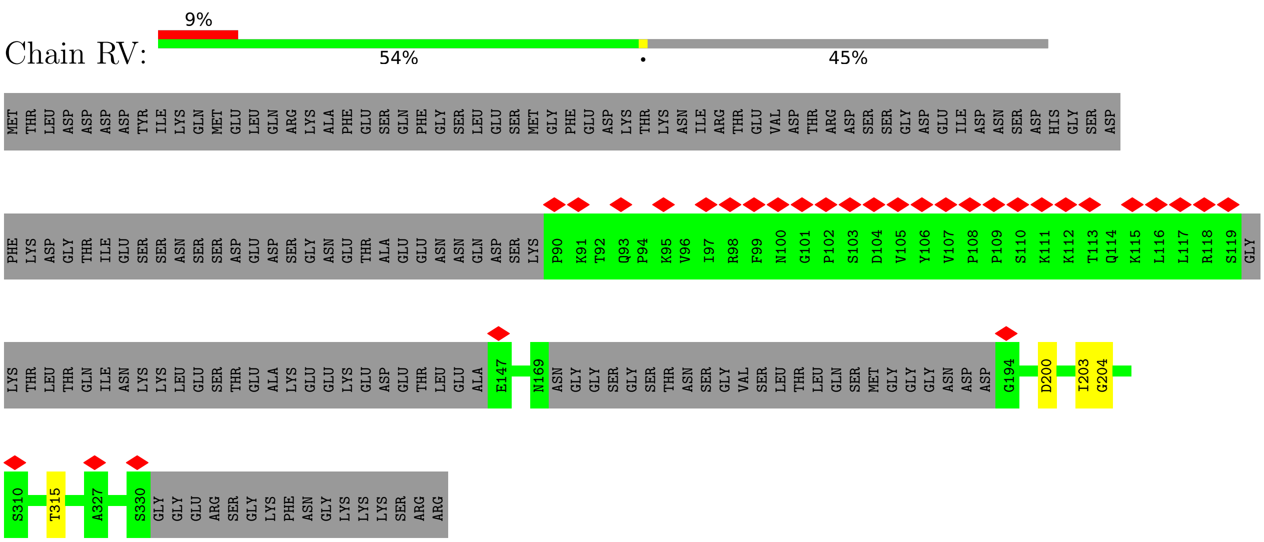




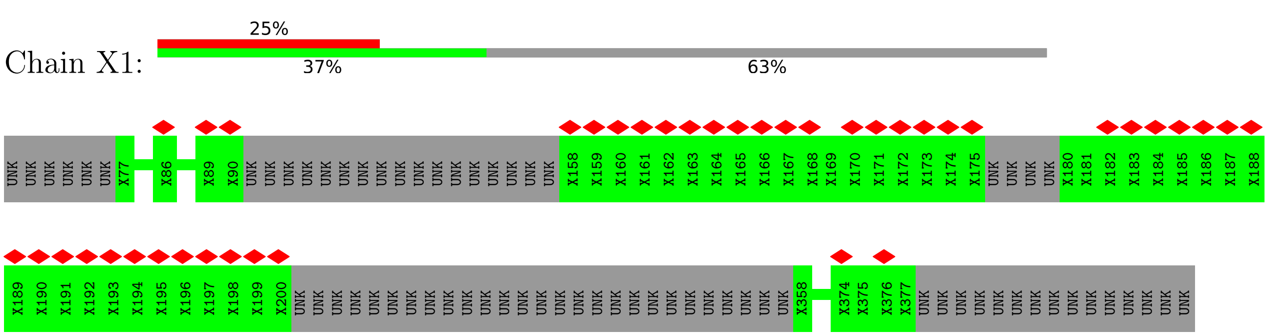
• Molecule 65: Pre-rRNA-processing protein PNO1

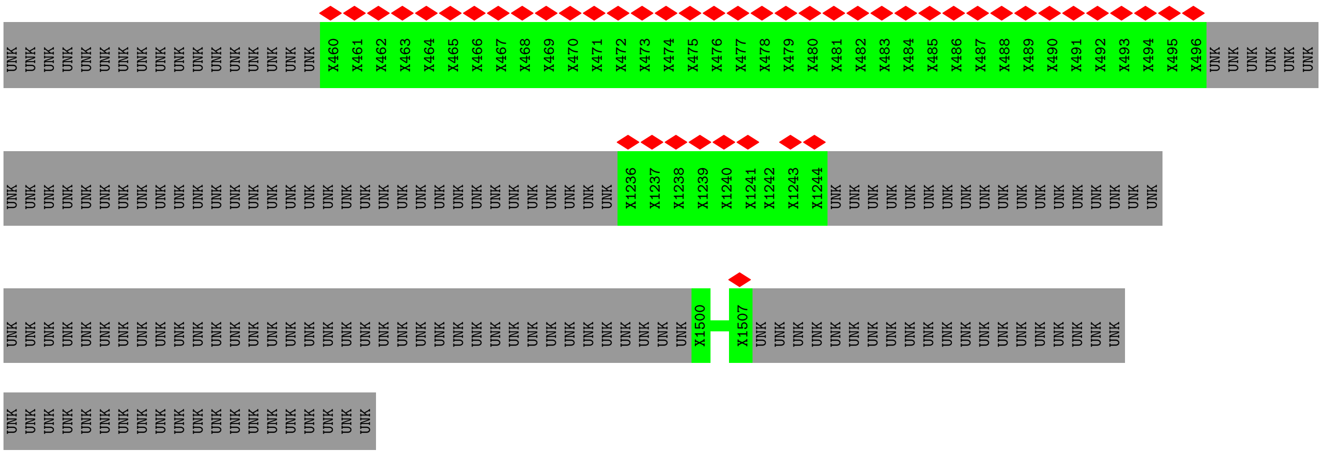


• Molecule 66: Protein FAF1



• Molecule 67: Unassigned helices




UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
X460 X461 X462 X463 X464 X465 X466 X467 X468 X469 X470 X471 X472 X473 X474 X475 X476 X477 X478 X479 X480 X481 X482 X483 X484 X485 X486 X487 X488 X489 X490 X491 X492 X493 X494 X495 X496
UNK UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
X1236 X1237 X1238 X1239 X1240 X1241 X1242 X1243 X1244
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
X1500 X1507
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	121139	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	25000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	3A	1.23	0/4141	1.27	34/6433 (0.5%)
2	5A	1.10	0/12462	1.20	78/19411 (0.4%)
3	SA	0.85	0/31237	1.22	263/48637 (0.5%)
4	SC	0.56	0/1777	0.77	4/2388 (0.2%)
5	SF	0.35	0/1854	0.69	2/2504 (0.1%)
6	SG	0.67	0/1690	0.65	0/2285
7	SH	0.36	0/890	0.67	1/1189 (0.1%)
8	SI	0.43	0/1341	0.70	0/1806
9	SJ	0.33	0/1347	0.59	1/1801 (0.1%)
10	SK	0.62	0/1410	0.66	1/1888 (0.1%)
11	SM	0.36	0/1020	0.63	0/1374
12	SN	0.29	0/873	0.66	0/1185
13	SO	0.50	0/1109	0.65	0/1495
14	SP	0.55	0/879	0.66	0/1186
15	SR	0.84	0/990	0.79	2/1335 (0.1%)
16	ST	0.37	0/930	0.64	0/1251
17	SX	0.63	0/1020	0.69	0/1371
18	SY	0.65	0/798	0.74	1/1065 (0.1%)
19	SZ	0.42	0/822	0.69	2/1103 (0.2%)
20	Sc	0.51	0/613	0.68	0/828
21	Sd	0.71	0/499	0.71	0/670
22	3B	0.81	0/1901	0.74	1/2567 (0.0%)
22	3C	0.46	0/1796	0.64	1/2424 (0.0%)
23	3D	0.55	0/2891	0.67	5/3895 (0.1%)
24	3E	0.50	0/3059	0.65	2/4153 (0.0%)
25	3F	0.47	0/3544	0.68	2/4775 (0.0%)
26	3G	0.67	0/928	0.77	2/1262 (0.2%)
26	3H	0.56	0/928	0.71	0/1262
27	A4	0.49	0/5321	0.68	4/7207 (0.1%)
28	A5	0.57	0/4044	0.70	4/5493 (0.1%)
29	A8	0.30	0/3328	0.64	1/4565 (0.0%)
30	A9	0.32	0/951	0.61	0/1287

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
31	AE	0.48	0/6308	0.67	3/8543 (0.0%)
32	AF	0.54	0/3993	0.68	3/5413 (0.1%)
33	AG	0.46	0/6699	0.66	5/9077 (0.1%)
34	B1	0.87	0/6780	0.75	6/9175 (0.1%)
35	B2	0.45	0/6853	0.69	2/9256 (0.0%)
36	B3	0.45	0/6014	0.72	5/8137 (0.1%)
37	B8	0.72	0/3848	0.71	4/5218 (0.1%)
38	BE	0.75	0/6948	0.70	7/9391 (0.1%)
39	B6	0.53	0/2849	0.60	2/3853 (0.1%)
40	5B	0.36	0/499	0.66	0/659
41	5C	0.79	0/4321	0.72	3/5832 (0.1%)
42	5D	0.67	0/1998	0.71	2/2644 (0.1%)
43	5E	0.58	0/1665	0.66	1/2233 (0.0%)
44	5F	0.96	0/1559	0.85	3/2097 (0.1%)
45	5G	0.72	0/2337	0.71	3/3148 (0.1%)
46	5H	0.57	0/1074	0.58	0/1422
47	5I	0.80	0/3844	0.72	1/5174 (0.0%)
48	5J	0.58	0/1238	0.62	1/1641 (0.1%)
49	5K	0.76	0/1426	0.74	1/1917 (0.1%)
50	RA	0.35	0/2769	0.66	0/3753
51	RB	0.40	0/1121	0.65	0/1487
52	RC	0.55	0/2245	0.63	0/3021
53	RE	0.39	0/8924	0.64	5/12070 (0.0%)
54	RF	0.37	0/2004	0.66	3/2697 (0.1%)
55	RG	0.36	0/1727	0.71	2/2329 (0.1%)
55	RH	0.43	0/1828	0.64	0/2470
56	RI	0.54	0/2080	0.67	0/2797
57	RJ	0.60	0/6514	0.63	2/8768 (0.0%)
58	RK	0.45	0/2832	0.65	0/3825
59	RL	0.29	0/4549	0.52	0/6241
59	RM	0.25	0/3760	0.47	0/5211
60	RN	0.37	0/4423	0.61	2/5965 (0.0%)
61	RO	0.38	0/3849	0.62	2/5261 (0.0%)
62	RP	0.25	0/10172	0.46	11/14158 (0.1%)
63	RQ	0.52	0/1678	0.61	0/2282
64	RS	0.34	0/2104	0.69	1/2854 (0.0%)
65	RT	0.42	0/1379	0.62	1/1853 (0.1%)
66	RV	0.60	0/1456	0.69	2/1937 (0.1%)
All	All	0.65	0/232060	0.82	494/323904 (0.2%)

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
4	SC	0	1
5	SF	0	1
6	SG	0	1
7	SH	0	1
8	SI	0	2
11	SM	0	1
12	SN	0	1
13	SO	0	1
14	SP	0	1
19	SZ	0	1
20	Sc	0	1
22	3B	0	1
23	3D	0	1
24	3E	0	2
26	3G	0	3
26	3H	0	1
28	A5	0	2
29	A8	0	4
33	AG	0	3
34	B1	0	3
35	B2	0	9
36	B3	0	8
37	B8	0	3
38	BE	0	3
39	B6	0	1
41	5C	0	3
42	5D	0	1
43	5E	0	1
44	5F	0	1
47	5I	0	1
49	5K	0	2
51	RB	0	1
53	RE	0	1
54	RF	0	1
56	RI	0	1
57	RJ	0	2
59	RL	0	1
59	RM	0	1
62	RP	0	1
63	RQ	0	1
66	RV	0	1
All	All	0	76

There are no bond length outliers.

The worst 5 of 494 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	5F	13	LEU	CA-CB-CG	10.94	140.47	115.30
3	SA	1034	C	C5-C6-N1	10.38	126.19	121.00
3	SA	1254	U	C2-N1-C1'	10.13	129.85	117.70
2	5A	312	U	O4'-C1'-N1	9.96	116.17	108.20
2	5A	310	U	N3-C2-O2	-9.45	115.59	122.20

There are no chirality outliers.

5 of 76 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	SC	40	ASN	Peptide
5	SF	195	ILE	Peptide
6	SG	58	LEU	Peptide
7	SH	68	LEU	Peptide
8	SI	31	SER	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
4	SC	217/255 (85%)	186 (86%)	30 (14%)	1 (0%)	29 61
5	SF	227/261 (87%)	192 (85%)	35 (15%)	0	100 100
6	SG	211/225 (94%)	197 (93%)	14 (7%)	0	100 100
7	SH	108/236 (46%)	98 (91%)	9 (8%)	1 (1%)	17 49
8	SI	161/190 (85%)	139 (86%)	22 (14%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	SJ	162/200 (81%)	141 (87%)	21 (13%)	0	100	100
10	SK	169/197 (86%)	163 (96%)	6 (4%)	0	100	100
11	SM	119/156 (76%)	99 (83%)	20 (17%)	0	100	100
12	SN	117/143 (82%)	96 (82%)	21 (18%)	0	100	100
13	SO	132/151 (87%)	125 (95%)	7 (5%)	0	100	100
14	SP	116/137 (85%)	102 (88%)	14 (12%)	0	100	100
15	SR	123/143 (86%)	113 (92%)	10 (8%)	0	100	100
16	ST	109/146 (75%)	100 (92%)	9 (8%)	0	100	100
17	SX	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
18	SY	101/145 (70%)	91 (90%)	10 (10%)	0	100	100
19	SZ	100/135 (74%)	86 (86%)	14 (14%)	0	100	100
20	Sc	78/82 (95%)	68 (87%)	10 (13%)	0	100	100
21	Sd	61/67 (91%)	55 (90%)	6 (10%)	0	100	100
22	3B	236/327 (72%)	222 (94%)	14 (6%)	0	100	100
22	3C	221/327 (68%)	203 (92%)	18 (8%)	0	100	100
23	3D	359/504 (71%)	344 (96%)	15 (4%)	0	100	100
24	3E	427/511 (84%)	394 (92%)	33 (8%)	0	100	100
25	3F	428/573 (75%)	384 (90%)	43 (10%)	1 (0%)	47	78
26	3G	119/126 (94%)	109 (92%)	9 (8%)	1 (1%)	19	51
26	3H	119/126 (94%)	110 (92%)	9 (8%)	0	100	100
27	A4	648/776 (84%)	576 (89%)	72 (11%)	0	100	100
28	A5	504/643 (78%)	460 (91%)	44 (9%)	0	100	100
29	A8	534/713 (75%)	407 (76%)	124 (23%)	3 (1%)	25	57
30	A9	126/575 (22%)	119 (94%)	7 (6%)	0	100	100
31	AE	773/1769 (44%)	710 (92%)	63 (8%)	0	100	100
32	AF	489/513 (95%)	437 (89%)	51 (10%)	1 (0%)	47	78
33	AG	812/896 (91%)	730 (90%)	82 (10%)	0	100	100
34	B1	830/923 (90%)	752 (91%)	76 (9%)	2 (0%)	47	78
35	B2	839/943 (89%)	750 (89%)	88 (10%)	1 (0%)	51	82
36	B3	733/817 (90%)	599 (82%)	132 (18%)	2 (0%)	41	72
37	B8	469/594 (79%)	423 (90%)	46 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BE	857/939 (91%)	792 (92%)	65 (8%)	0	100	100
39	B6	368/440 (84%)	337 (92%)	31 (8%)	0	100	100
40	5B	58/214 (27%)	55 (95%)	3 (5%)	0	100	100
41	5C	531/554 (96%)	472 (89%)	58 (11%)	1 (0%)	47	78
42	5D	231/250 (92%)	204 (88%)	27 (12%)	0	100	100
43	5E	200/593 (34%)	187 (94%)	11 (6%)	2 (1%)	15	46
44	5F	180/183 (98%)	169 (94%)	11 (6%)	0	100	100
45	5G	278/290 (96%)	249 (90%)	29 (10%)	0	100	100
46	5H	132/610 (22%)	121 (92%)	11 (8%)	0	100	100
47	5I	457/489 (94%)	420 (92%)	37 (8%)	0	100	100
48	5J	138/217 (64%)	129 (94%)	9 (6%)	0	100	100
49	5K	171/189 (90%)	160 (94%)	11 (6%)	0	100	100
50	RA	332/707 (47%)	287 (86%)	45 (14%)	0	100	100
51	RB	132/357 (37%)	116 (88%)	16 (12%)	0	100	100
52	RC	276/316 (87%)	260 (94%)	16 (6%)	0	100	100
53	RE	1067/1237 (86%)	984 (92%)	83 (8%)	0	100	100
54	RF	233/297 (78%)	214 (92%)	19 (8%)	0	100	100
55	RG	212/252 (84%)	186 (88%)	26 (12%)	0	100	100
55	RH	226/252 (90%)	212 (94%)	14 (6%)	0	100	100
56	RI	250/274 (91%)	228 (91%)	22 (9%)	0	100	100
57	RJ	784/1183 (66%)	723 (92%)	61 (8%)	0	100	100
58	RK	358/367 (98%)	335 (94%)	23 (6%)	0	100	100
59	RL	781/1056 (74%)	670 (86%)	109 (14%)	2 (0%)	41	72
59	RM	737/1056 (70%)	640 (87%)	93 (13%)	4 (0%)	29	61
60	RN	573/810 (71%)	524 (91%)	48 (8%)	1 (0%)	47	78
61	RO	523/552 (95%)	457 (87%)	66 (13%)	0	100	100
62	RP	1992/2493 (80%)	1801 (90%)	189 (10%)	2 (0%)	51	82
63	RQ	220/899 (24%)	197 (90%)	23 (10%)	0	100	100
64	RS	247/483 (51%)	223 (90%)	23 (9%)	1 (0%)	34	67
65	RT	165/326 (51%)	151 (92%)	14 (8%)	0	100	100
66	RV	184/346 (53%)	168 (91%)	16 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	23995/32886 (73%)	21566 (90%)	2403 (10%)	26 (0%)	54 82

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	5E	454	VAL
59	RL	744	PRO
59	RM	744	PRO
62	RP	119	PRO
29	A8	309	PRO

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
4	SC	195/224 (87%)	192 (98%)	3 (2%)	65 82
5	SF	196/222 (88%)	191 (97%)	5 (3%)	46 72
6	SG	180/191 (94%)	179 (99%)	1 (1%)	86 94
7	SH	95/201 (47%)	94 (99%)	1 (1%)	73 86
8	SI	146/170 (86%)	144 (99%)	2 (1%)	67 83
9	SJ	136/161 (84%)	135 (99%)	1 (1%)	84 92
10	SK	147/166 (89%)	144 (98%)	3 (2%)	55 77
11	SM	110/137 (80%)	109 (99%)	1 (1%)	78 90
12	SN	88/119 (74%)	88 (100%)	0	100 100
13	SO	117/128 (91%)	115 (98%)	2 (2%)	60 80
14	SP	90/105 (86%)	88 (98%)	2 (2%)	52 75
15	SR	105/119 (88%)	105 (100%)	0	100 100
16	ST	101/129 (78%)	101 (100%)	0	100 100
17	SX	108/111 (97%)	108 (100%)	0	100 100
18	SY	85/120 (71%)	85 (100%)	0	100 100
19	SZ	85/113 (75%)	84 (99%)	1 (1%)	71 85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	Sc	69/71 (97%)	69 (100%)	0	100	100
21	Sd	56/60 (93%)	56 (100%)	0	100	100
22	3B	201/240 (84%)	200 (100%)	1 (0%)	88	94
22	3C	190/240 (79%)	190 (100%)	0	100	100
23	3D	296/435 (68%)	292 (99%)	4 (1%)	67	83
24	3E	262/433 (60%)	260 (99%)	2 (1%)	81	91
25	3F	378/503 (75%)	373 (99%)	5 (1%)	69	84
26	3G	100/104 (96%)	99 (99%)	1 (1%)	76	88
26	3H	100/104 (96%)	100 (100%)	0	100	100
27	A4	591/713 (83%)	583 (99%)	8 (1%)	67	83
28	A5	433/574 (75%)	430 (99%)	3 (1%)	84	92
29	A8	174/657 (26%)	173 (99%)	1 (1%)	86	94
30	A9	89/533 (17%)	89 (100%)	0	100	100
31	AE	708/1633 (43%)	700 (99%)	8 (1%)	73	86
32	AF	437/454 (96%)	432 (99%)	5 (1%)	73	86
33	AG	750/826 (91%)	743 (99%)	7 (1%)	78	90
34	B1	730/812 (90%)	719 (98%)	11 (2%)	65	82
35	B2	736/832 (88%)	729 (99%)	7 (1%)	76	88
36	B3	665/719 (92%)	654 (98%)	11 (2%)	60	80
37	B8	421/529 (80%)	417 (99%)	4 (1%)	76	88
38	BE	757/819 (92%)	748 (99%)	9 (1%)	71	85
39	B6	251/414 (61%)	246 (98%)	5 (2%)	55	77
40	5B	57/196 (29%)	56 (98%)	1 (2%)	59	79
41	5C	465/480 (97%)	457 (98%)	8 (2%)	60	80
42	5D	221/234 (94%)	219 (99%)	2 (1%)	78	90
43	5E	185/535 (35%)	183 (99%)	2 (1%)	73	86
44	5F	171/172 (99%)	171 (100%)	0	100	100
45	5G	251/258 (97%)	249 (99%)	2 (1%)	81	91
46	5H	107/538 (20%)	106 (99%)	1 (1%)	78	90
47	5I	416/443 (94%)	407 (98%)	9 (2%)	52	75
48	5J	133/200 (66%)	133 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
49	5K	157/169 (93%)	155 (99%)	2 (1%)	69 84
50	RA	303/636 (48%)	303 (100%)	0	100 100
51	RB	117/315 (37%)	115 (98%)	2 (2%)	60 80
52	RC	231/289 (80%)	230 (100%)	1 (0%)	91 95
53	RE	984/1125 (88%)	975 (99%)	9 (1%)	78 90
54	RF	221/274 (81%)	217 (98%)	4 (2%)	59 79
55	RG	195/222 (88%)	194 (100%)	1 (0%)	88 94
55	RH	206/222 (93%)	203 (98%)	3 (2%)	65 82
56	RI	235/256 (92%)	231 (98%)	4 (2%)	60 80
57	RJ	683/1039 (66%)	679 (99%)	4 (1%)	86 94
58	RK	307/312 (98%)	305 (99%)	2 (1%)	84 92
59	RL	164/934 (18%)	159 (97%)	5 (3%)	41 68
60	RN	406/732 (56%)	406 (100%)	0	100 100
61	RO	329/506 (65%)	326 (99%)	3 (1%)	78 90
63	RQ	148/808 (18%)	147 (99%)	1 (1%)	84 92
64	RS	225/424 (53%)	221 (98%)	4 (2%)	59 79
65	RT	148/282 (52%)	145 (98%)	3 (2%)	55 77
66	RV	141/304 (46%)	140 (99%)	1 (1%)	84 92
All	All	17584/26026 (68%)	17396 (99%)	188 (1%)	74 86

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	5C	153	THR
52	RC	62	ARG
41	5C	347	LEU
47	5I	91	VAL
53	RE	595	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 285 such sidechains are listed below:

Mol	Chain	Res	Type
55	RG	105	ASN
56	RI	186	ASN
60	RN	771	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	AF	250	ASN
32	AF	72	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3A	169/333 (50%)	46 (27%)	2 (1%)
2	5A	516/700 (73%)	146 (28%)	10 (1%)
3	SA	1290/1807 (71%)	461 (35%)	16 (1%)
All	All	1975/2840 (69%)	653 (33%)	28 (1%)

5 of 653 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3A	2	U
1	3A	5	A
1	3A	14	A
1	3A	15	U
1	3A	24	U

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	SA	68	A
3	SA	1594	G
3	SA	401	A
3	SA	1052	U
3	SA	372	G

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
69	GTP	RJ	1201	70	26,34,34	1.23	1 (3%)	32,54,54	1.65	6 (18%)

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
69	GTP	RJ	1201	70	-	2/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	RJ	1201	GTP	C5-C6	-4.38	1.38	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
69	RJ	1201	GTP	PA-O3A-PB	-4.27	118.18	132.83
69	RJ	1201	GTP	PB-O3B-PG	-3.72	120.06	132.83
69	RJ	1201	GTP	C5-C6-N1	3.41	119.98	113.95
69	RJ	1201	GTP	C8-N7-C5	3.09	108.88	102.99
69	RJ	1201	GTP	C2-N1-C6	-3.06	119.46	125.10

There are no chirality outliers.

All (2) torsion outliers are listed below:

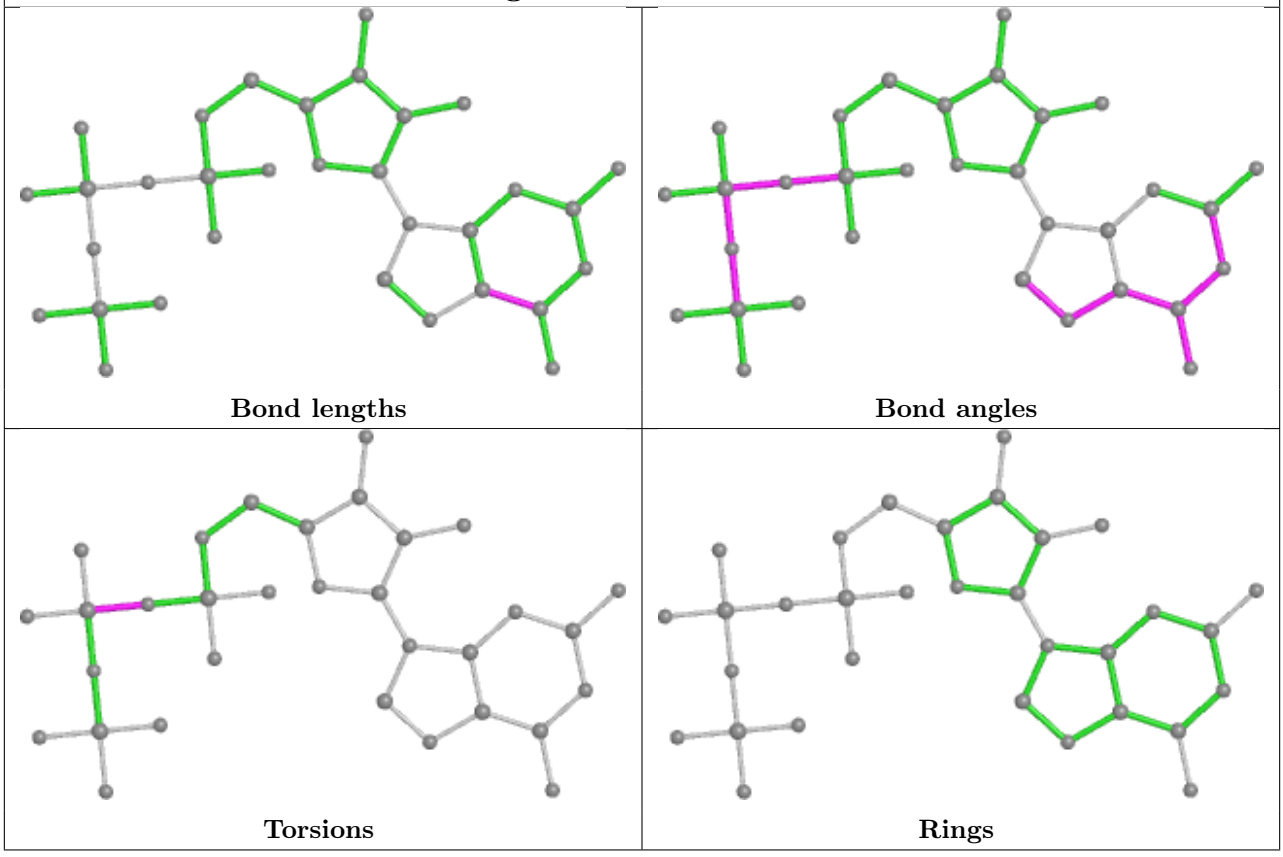
Mol	Chain	Res	Type	Atoms
69	RJ	1201	GTP	PA-O3A-PB-O2B
69	RJ	1201	GTP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand GTP RJ 1201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

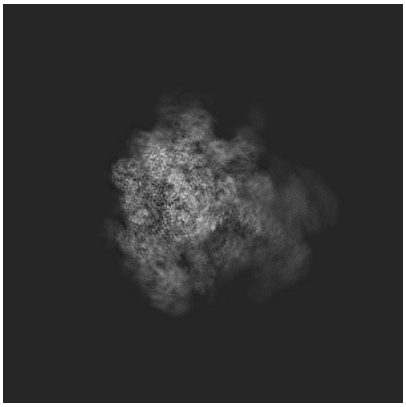
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9964. These allow visual inspection of the internal detail of the map and identification of artifacts.

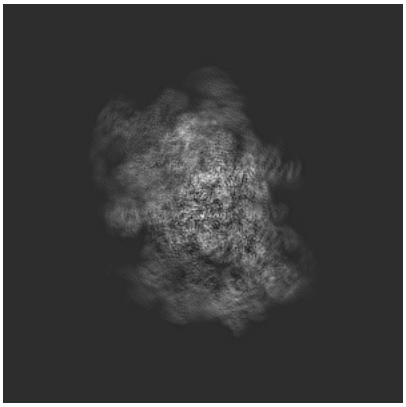
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

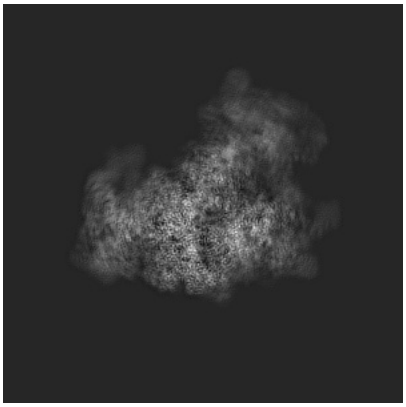
6.1.1 Primary map



X



Y

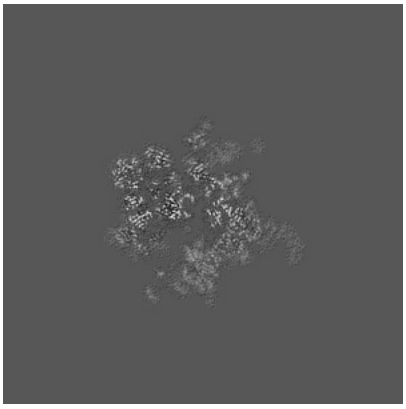


Z

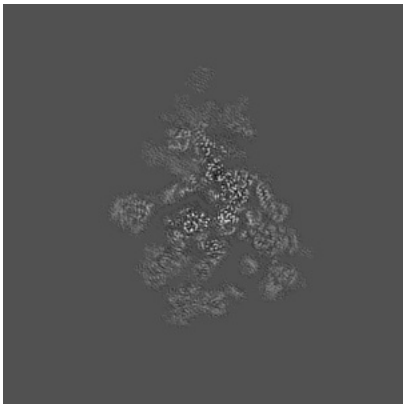
The images above show the map projected in three orthogonal directions.

6.2 Central slices

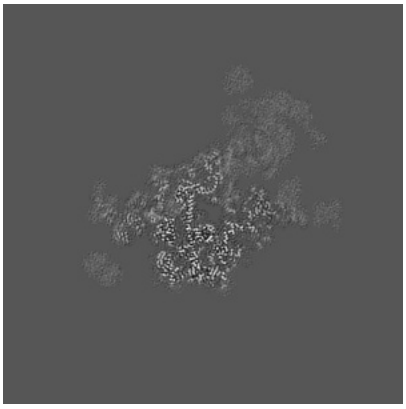
6.2.1 Primary map



X Index: 256



Y Index: 256

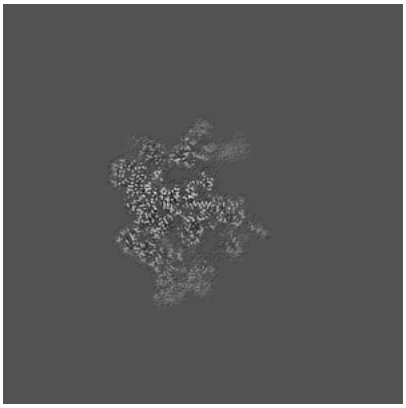


Z Index: 256

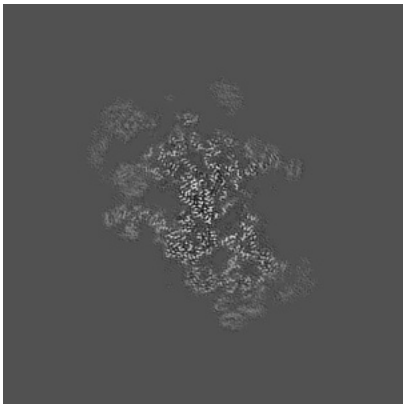
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

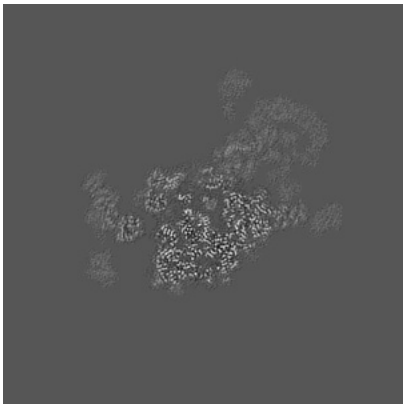
6.3.1 Primary map



X Index: 240



Y Index: 216

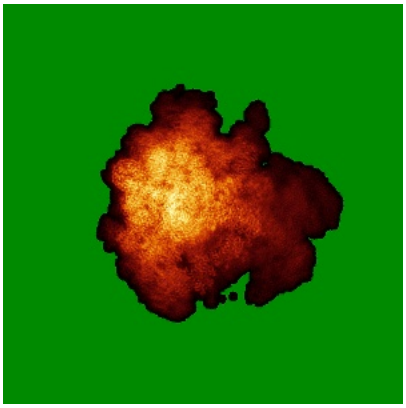


Z Index: 267

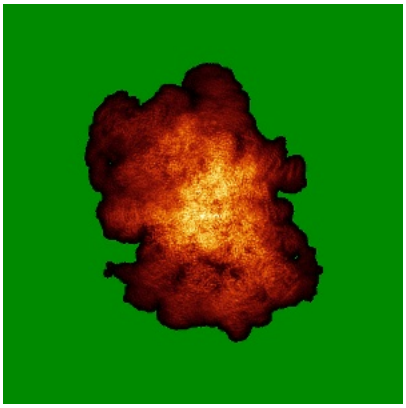
The images above show the largest variance slices of the map in three orthogonal directions.

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

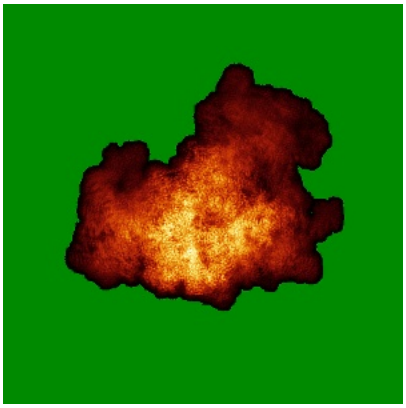
6.4.1 Primary map



X



Y

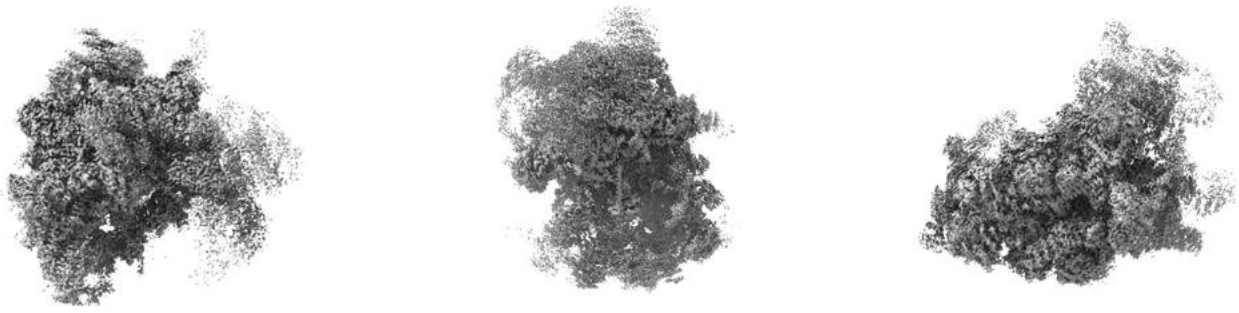


Z

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

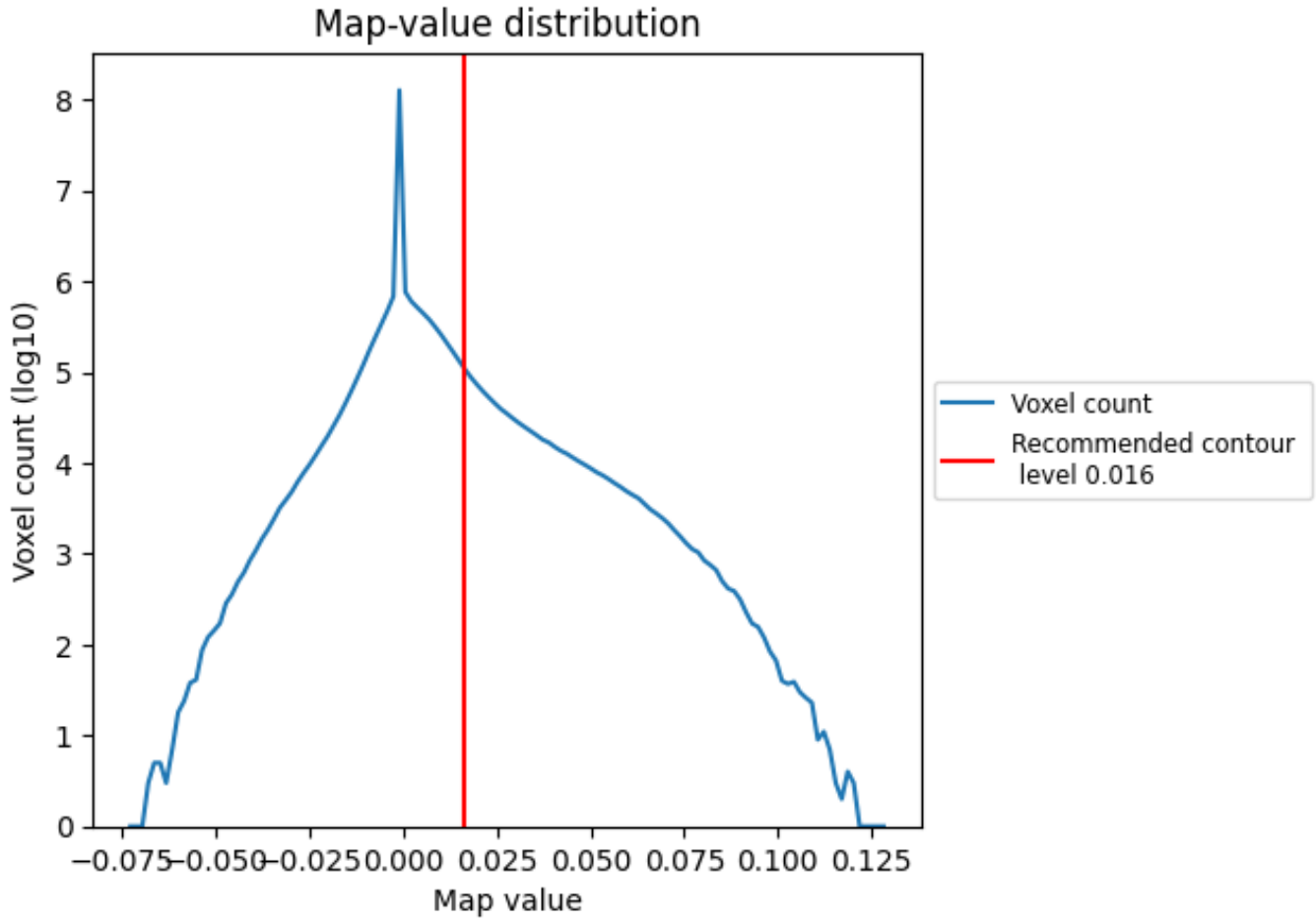
6.6 Mask visualisation (i)

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

7 Map analysis

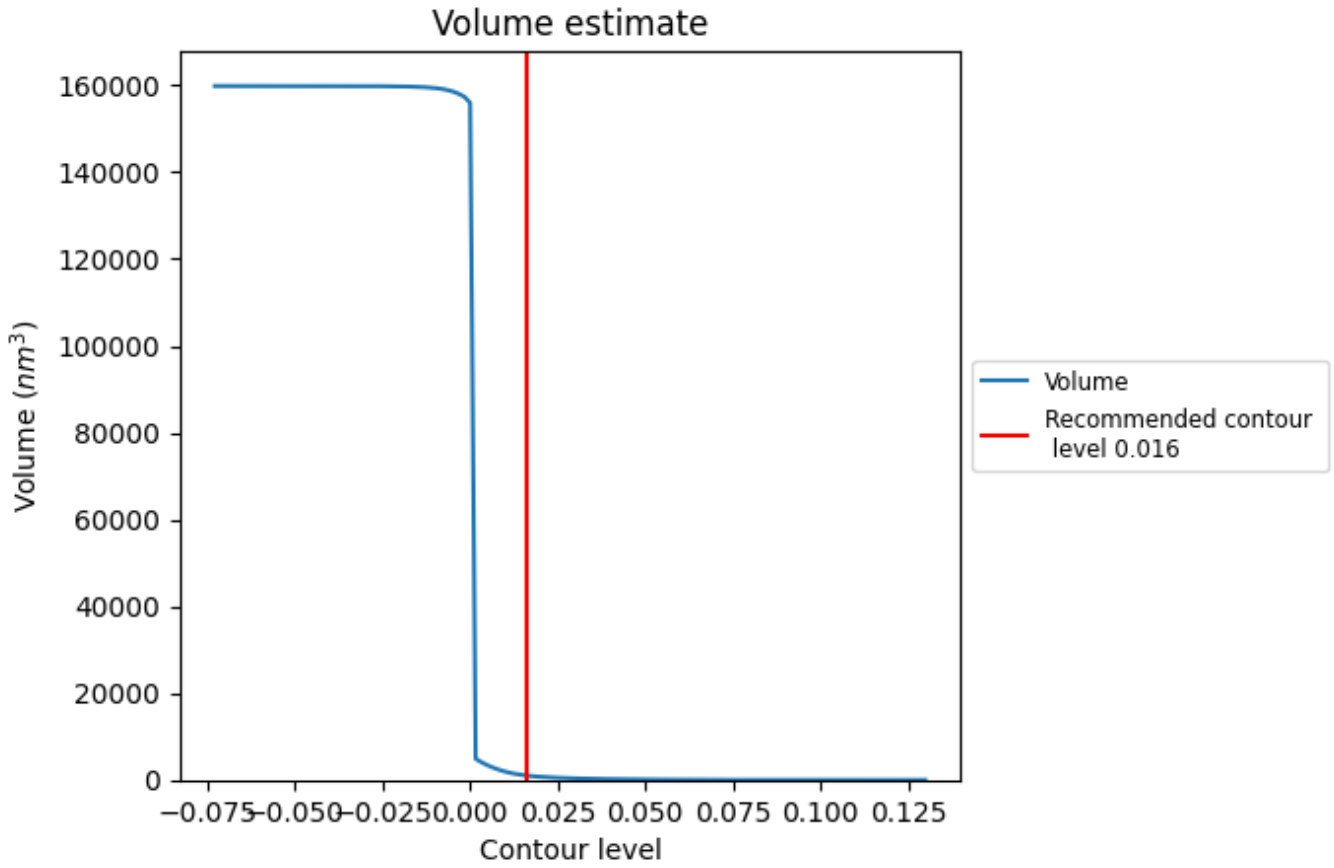
This section contains the results of statistical analysis of the map.

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.

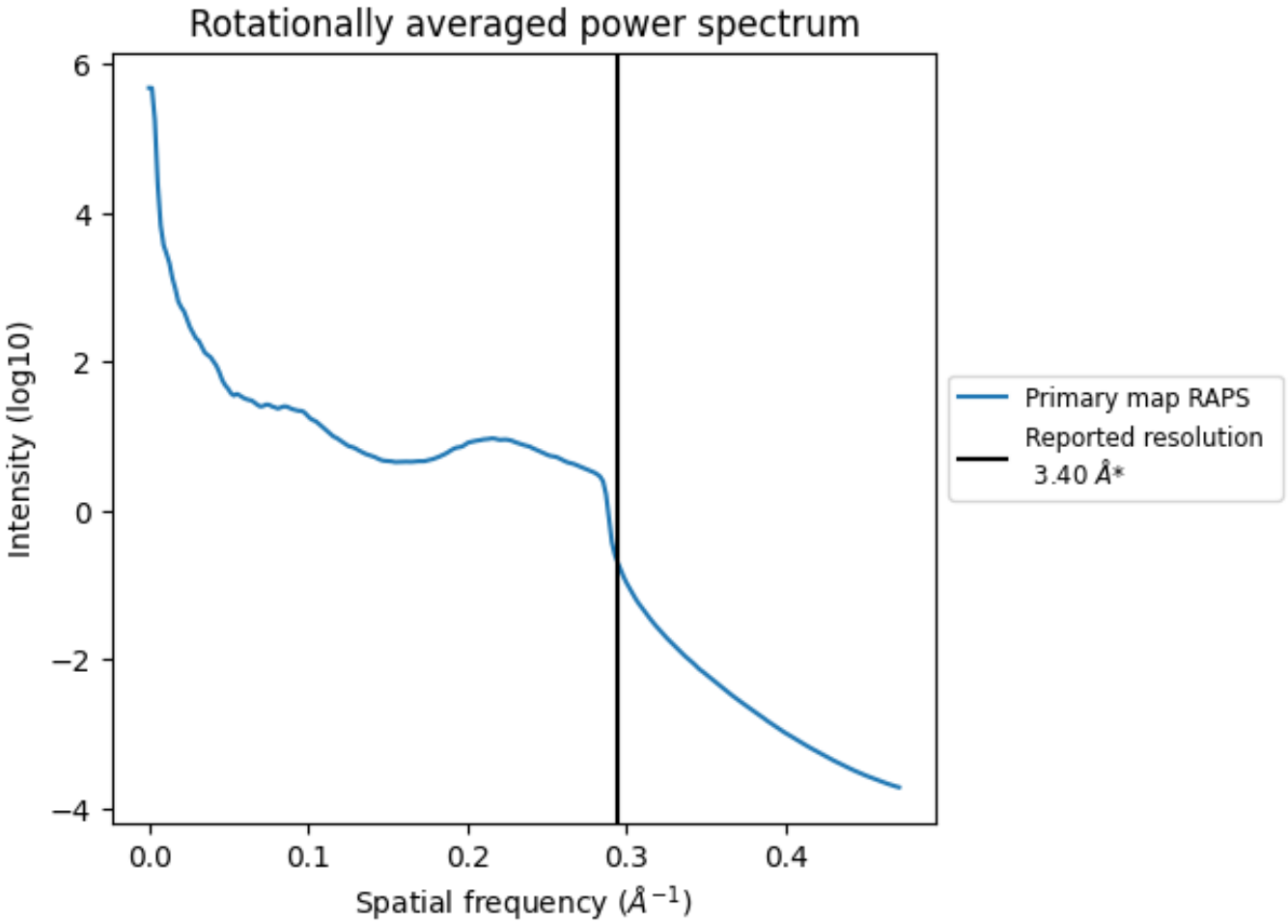
7.2 Volume estimate (i)



The volume at the recommended contour level is 1022 nm^3; this corresponds to an approximate mass of 923 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)

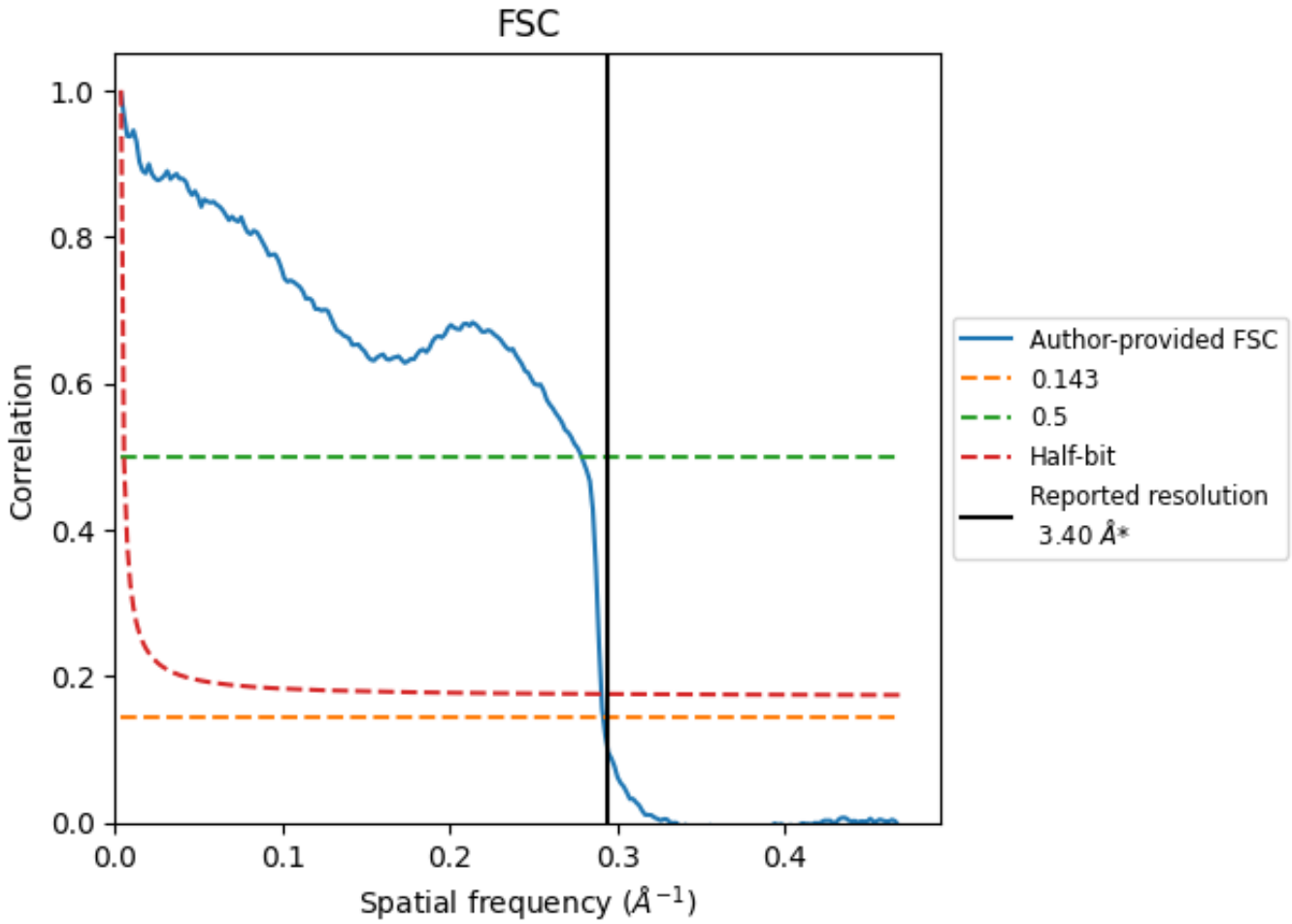


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

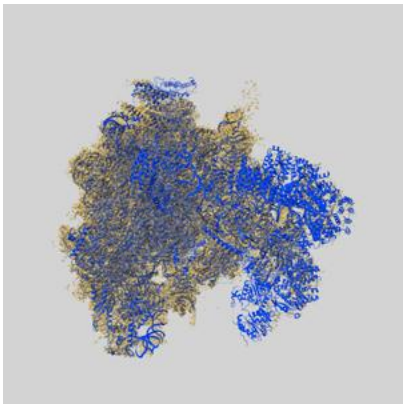
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	3.59	3.44
Unmasked-calculated*	-	-	-

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

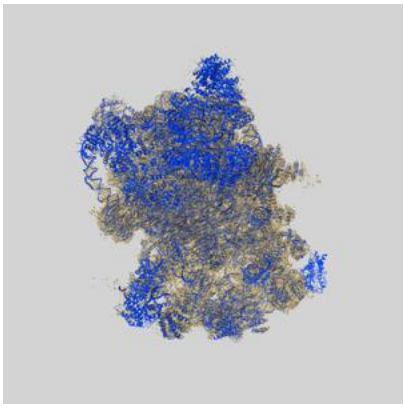
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9964 and PDB model 6KE6. Per-residue inclusion information can be found in section 3 on page 17.

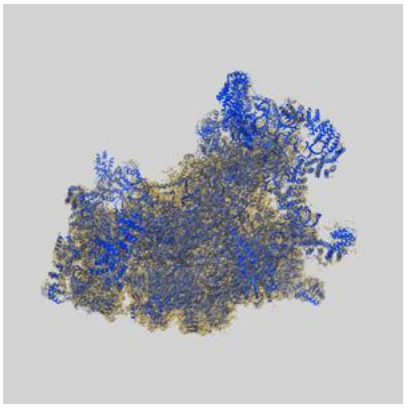
9.1 Map-model overlay



X



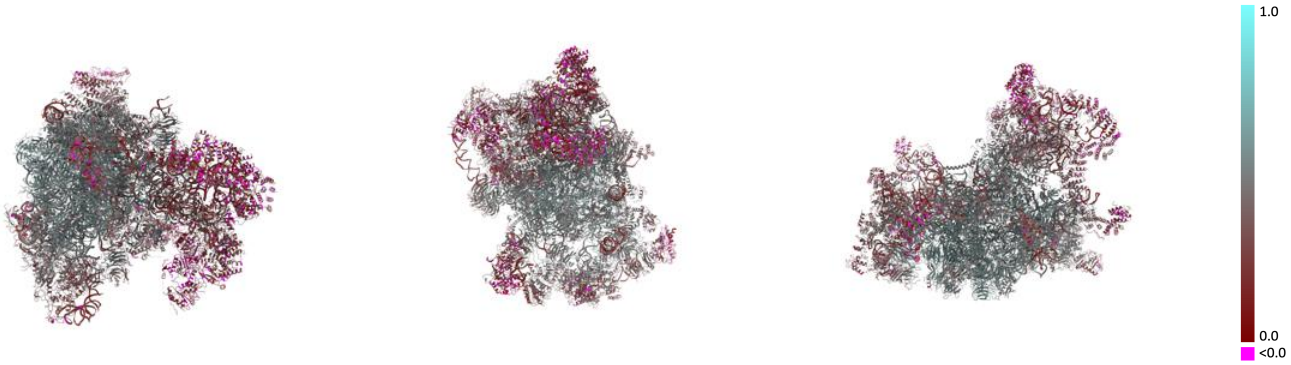
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

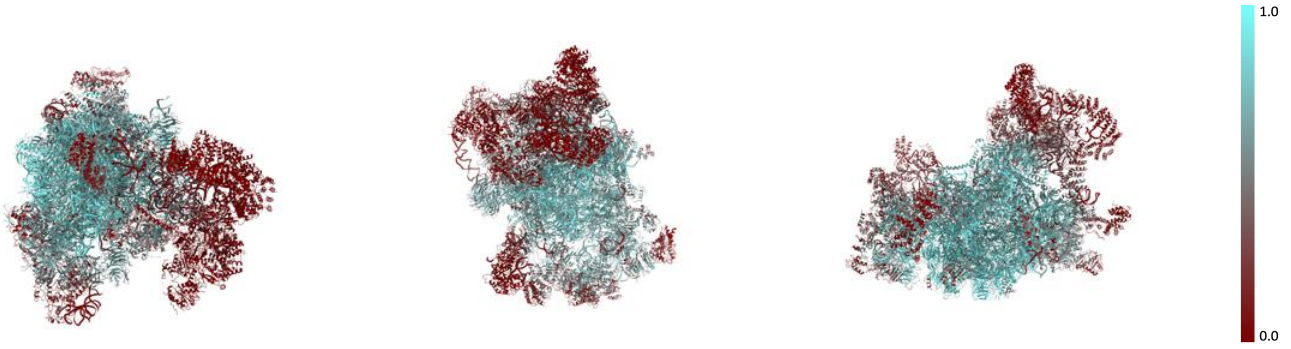
9.2 Q-score mapped to coordinate model



X Y Z

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

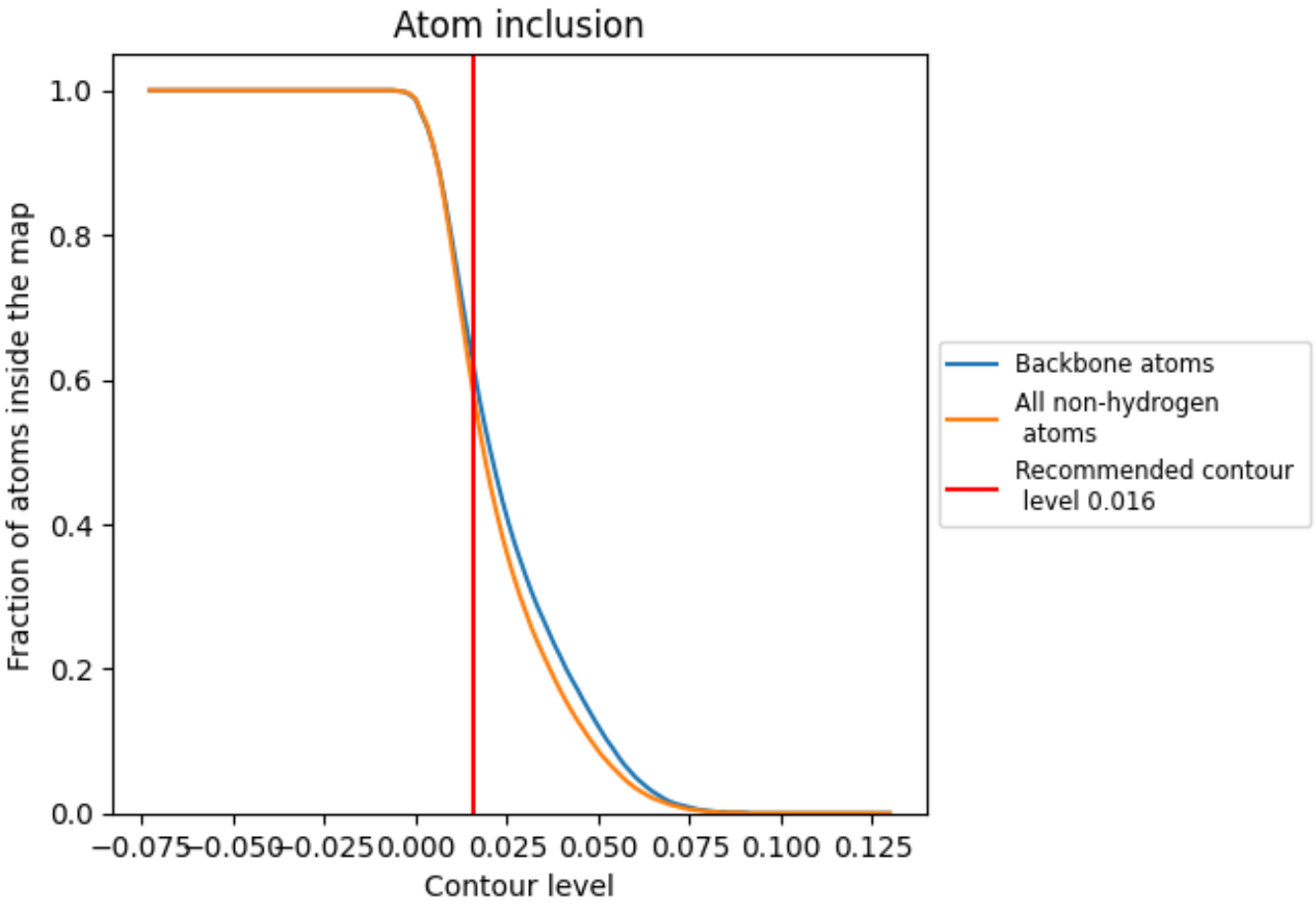
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 57% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5740	0.4270
3A	0.8270	0.4550
3B	0.8620	0.5570
3C	0.5800	0.4410
3D	0.7370	0.4890
3E	0.6830	0.4590
3F	0.6610	0.4530
3G	0.8340	0.5450
3H	0.7580	0.5110
5A	0.7640	0.4290
5B	0.4040	0.3970
5C	0.8460	0.5510
5D	0.7550	0.5110
5E	0.7530	0.5240
5F	0.8870	0.5690
5G	0.8110	0.5500
5H	0.7230	0.5000
5I	0.8630	0.5500
5J	0.6630	0.4970
5K	0.8570	0.5580
A4	0.6830	0.4510
A5	0.7530	0.4910
A8	0.2280	0.3060
A9	0.3970	0.3630
AE	0.3780	0.3480
AF	0.7590	0.5060
AG	0.6910	0.4690
B1	0.8810	0.5590
B2	0.6660	0.4520
B3	0.5920	0.4230
B6	0.6690	0.4400
B8	0.8480	0.5430
BE	0.8700	0.5550
RA	0.0960	0.2760
RB	0.4640	0.4280

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
RC	0.6170	0.4820
RE	0.3870	0.4000
RF	0.2960	0.3630
RG	0.3630	0.3870
RH	0.5720	0.4780
RI	0.7660	0.4930
RJ	0.7420	0.5030
RK	0.6830	0.4860
RL	0.1200	0.3130
RM	0.0190	0.1970
RN	0.3310	0.3780
RO	0.4480	0.3860
RP	0.0910	0.2260
RQ	0.5790	0.4680
RS	0.0370	0.2090
RT	0.6790	0.4800
RV	0.7190	0.5180
SA	0.5130	0.3620
SC	0.7480	0.5170
SF	0.2900	0.3660
SG	0.8170	0.5350
SH	0.0940	0.3450
SI	0.5210	0.4250
SJ	0.1430	0.2790
SK	0.8060	0.5300
SM	0.1530	0.2840
SN	0.0050	0.1060
SO	0.7580	0.5080
SP	0.7590	0.5120
SR	0.8490	0.5530
ST	0.3320	0.4150
SX	0.7840	0.5300
SY	0.7750	0.5270
SZ	0.4900	0.4280
Sc	0.7680	0.5200
Sd	0.8410	0.5500
X1	0.3290	0.3770