Full wwPDB EM Validation 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

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

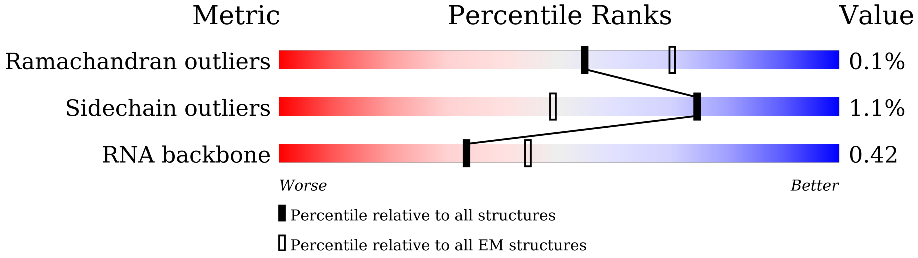
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

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

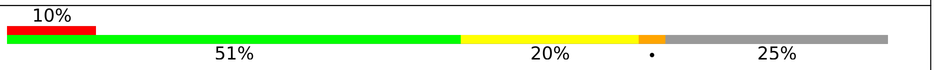
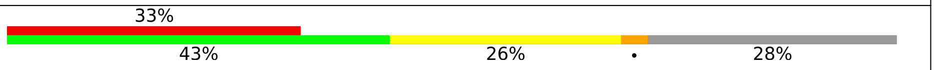
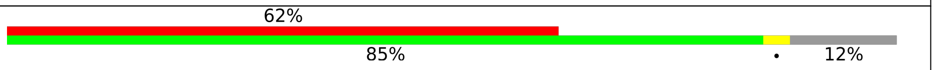
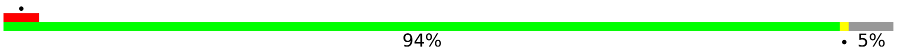
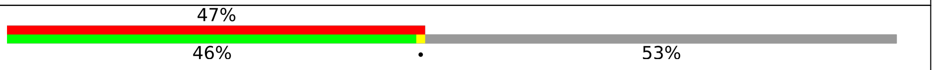
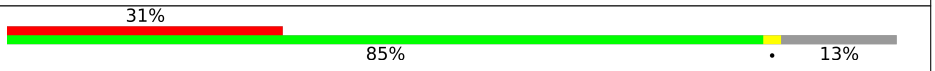
The reported resolution of this entry is 3.40 Å.

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	
2	5A	700	
3	SA	1807	
4	SC	255	
5	SF	261	
6	SG	225	
7	SH	236	
8	SI	190	

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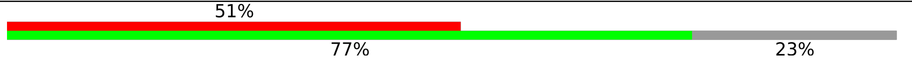
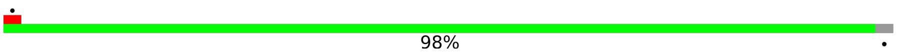
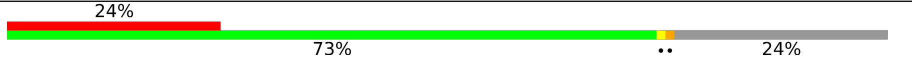
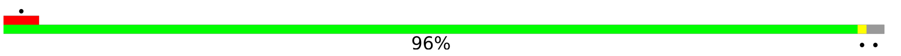
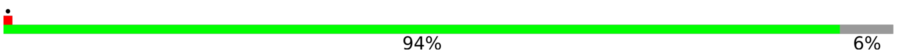
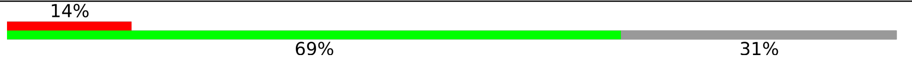
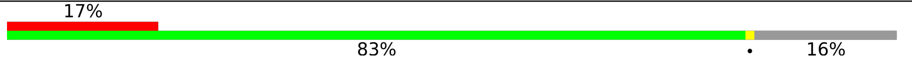
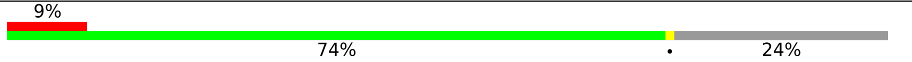
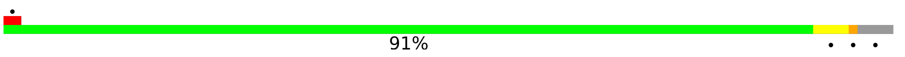
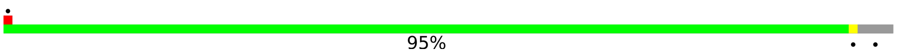
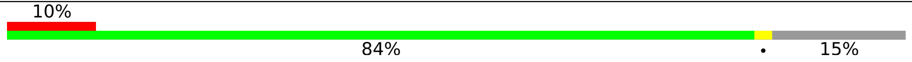
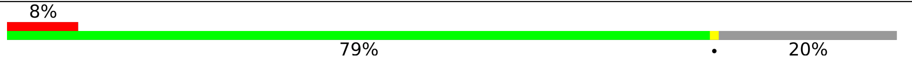
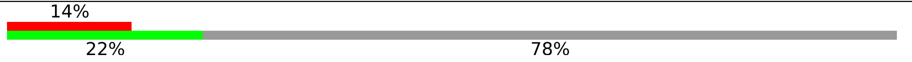
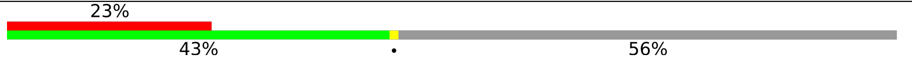
Mol	Chain	Length	Quality of chain
9	SJ	200	
10	SK	197	
11	SM	156	
12	SN	143	
13	SO	151	
14	SP	137	
15	SR	143	
16	ST	146	
17	SX	130	
18	SY	145	
19	SZ	135	
20	Sc	82	
21	Sd	67	
22	3B	327	
22	3C	327	
23	3D	504	
24	3E	511	
25	3F	573	
26	3G	126	
26	3H	126	
27	A4	776	
28	A5	643	
29	A8	713	
30	A9	575	
31	AE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

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Mol	Chain	Length	Quality of chain
32	AF	513	• 94% • •
33	AG	896	10% 91% • 8%
34	B1	923	88% • 10%
35	B2	943	12% 88% • 10%
36	B3	817	22% 90% • 7%
37	B8	594	• 78% • 20%
38	BE	939	• 90% • 8%
39	B6	440	22% 83% • 15%
40	5B	214	15% 28% 72%
41	5C	554	• 94% • •
42	5D	250	7% 92% • 6%
43	5E	593	• 33% • 66%
44	5F	183	97% • •
45	5G	290	• 96% • •
46	5H	610	• 22% 78%
47	5I	489	• 92% • 6%
48	5J	217	14% 66% 34%
49	5K	189	90% • 7%
50	RA	707	47% 48% 52%
51	RB	357	15% 37% • 62%
52	RC	316	24% 88% 12%
53	RE	1237	46% 86% • 13%
54	RF	297	54% 78% • 19%
55	RG	252	48% 85% • 14%
55	RH	252	17% 90% • 9%

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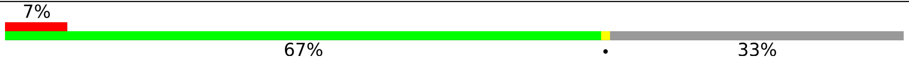
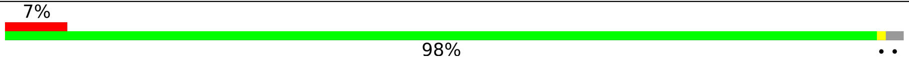
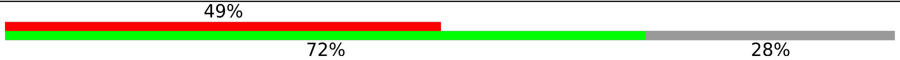
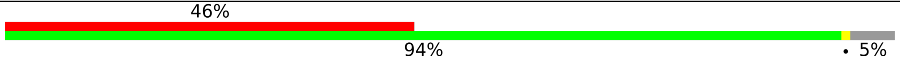
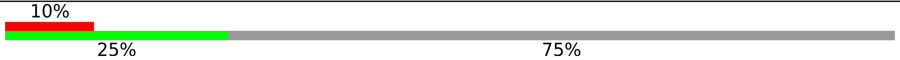
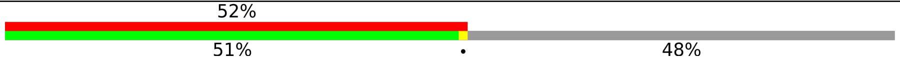
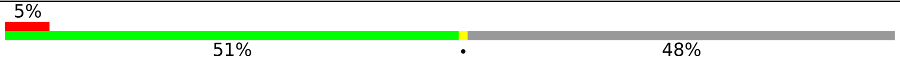
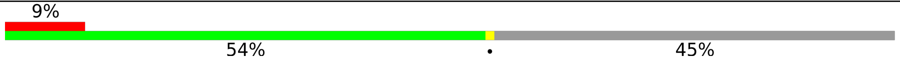
Mol	Chain	Length	Quality of chain
56	RI	274	
57	RJ	1183	
58	RK	367	
59	RL	1056	
59	RM	1056	
60	RN	810	
61	RO	552	
62	RP	2493	
63	RQ	899	
64	RS	483	
65	RT	326	
66	RV	346	
67	X1	347	

2 Entry composition

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
			Total	C	N	O	S		
7	SH	112	879	562	155	160	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
21	Sd	63	497	306	99	91	1	0	0

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

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

- Molecule 23 is a protein called Nucleolar protein 56.

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

- Molecule 24 is a protein called Nucleolar protein 58.

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
35	B2	851	6723	4294	1133	1269	27	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 47 is a protein called Protein SOF1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 59 is a protein called RNA cytidine acetyltransferase.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 66 is a protein called Protein FAF1.

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

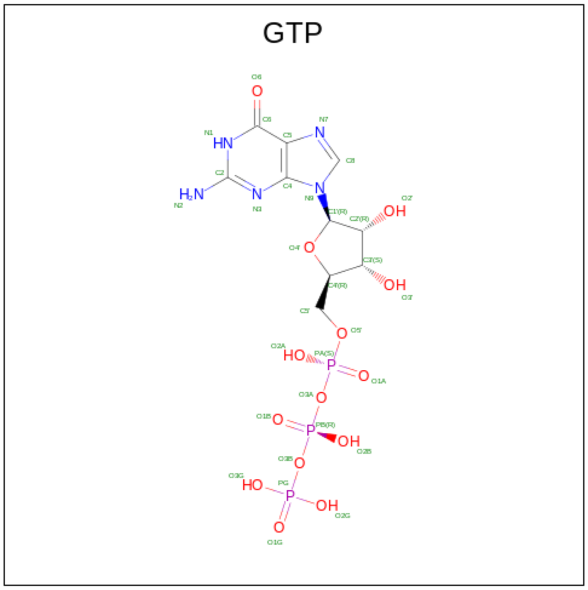
- Molecule 67 is a protein called Unassigned helices.

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

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

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

- 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
			Total	C	N	O	P	
69	RJ	1	32	10	5	14	3	0

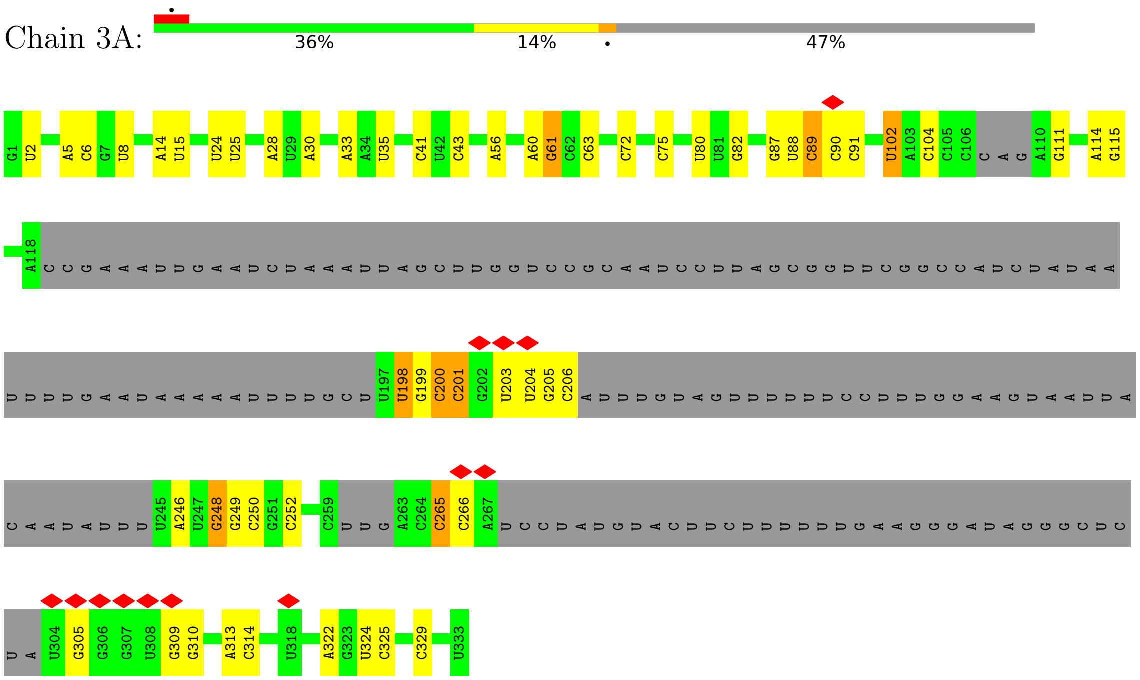
- Molecule 70 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

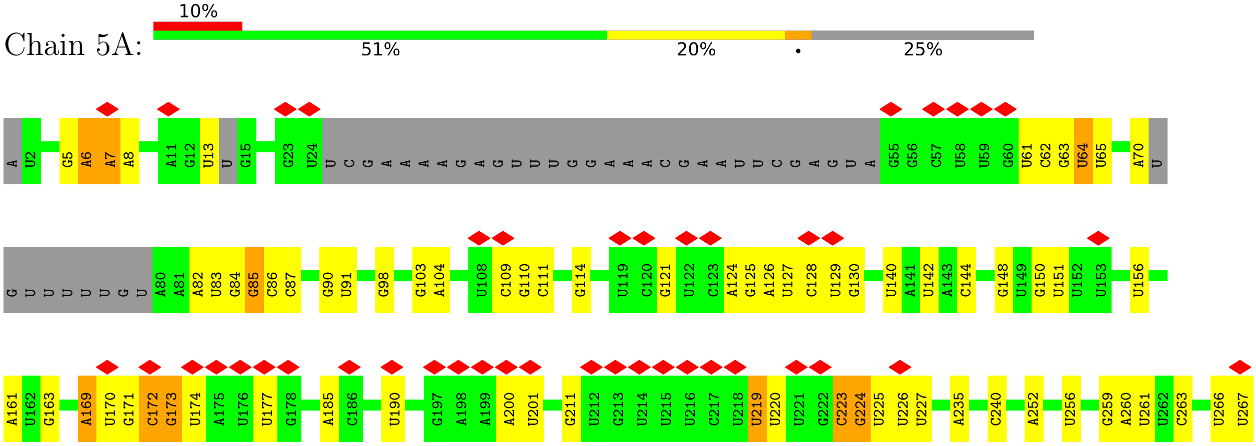
3 Residue-property plots ⓘ

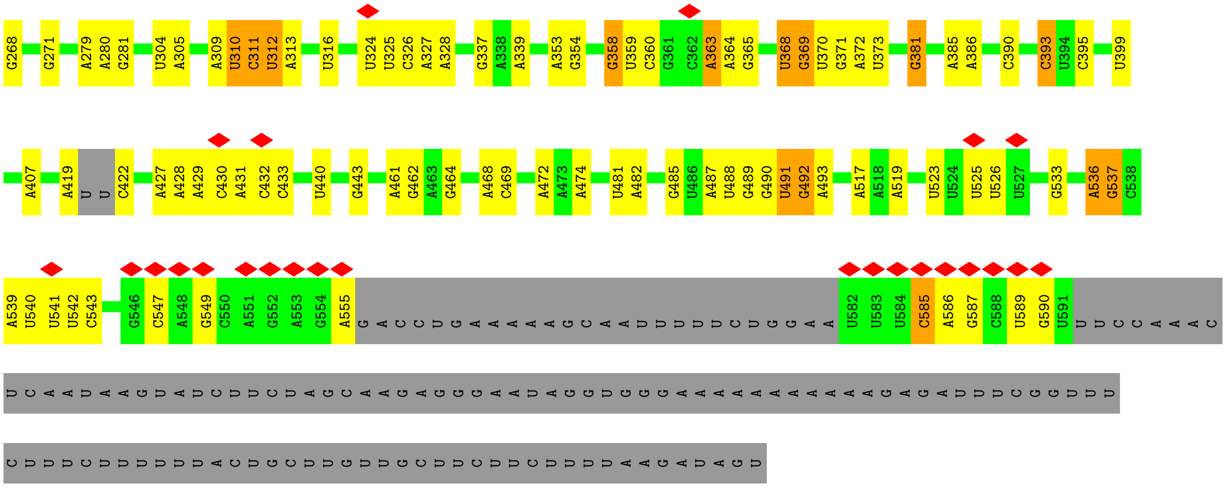
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: U3 snoRNA



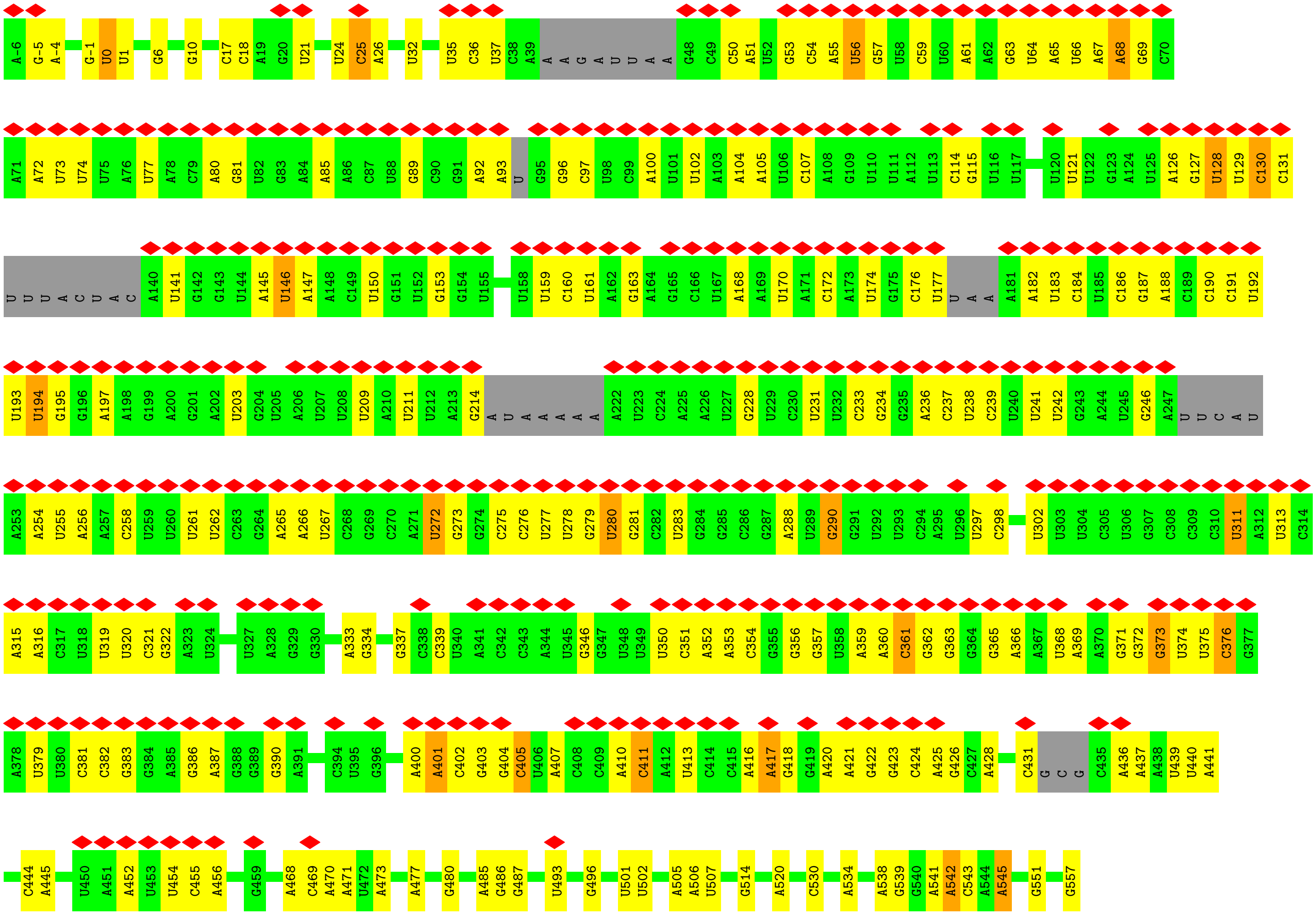
- Molecule 2: 5’ ETS

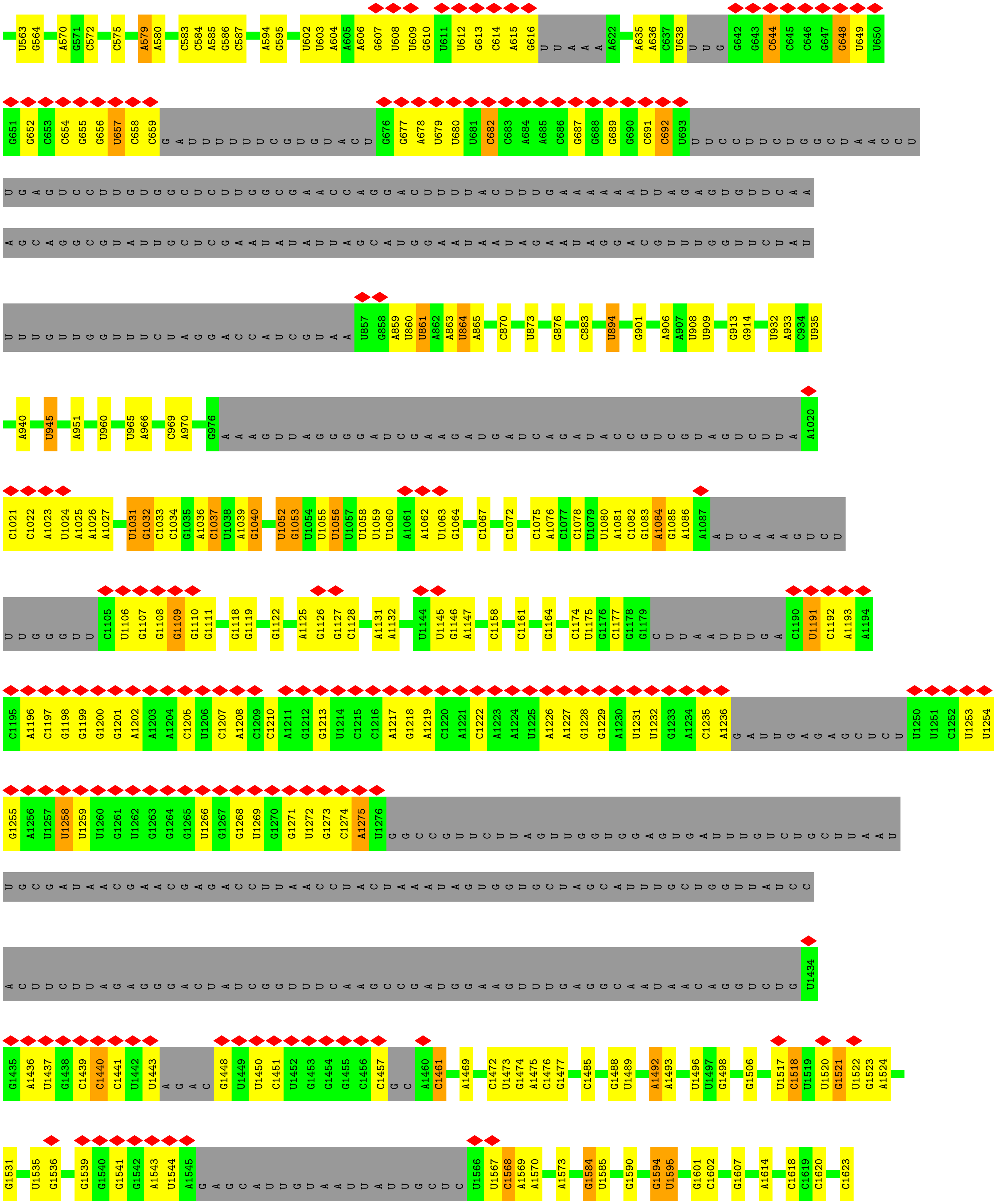




- Molecule 3: 18S rRNA

Chain SA:

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G651 G652 C653 C654 G655 G656 U657 C658 C659 G A U U U U U U C G U G U A C U G676 G677 A678 U679 U680 U681 C682 C683 A684 A685 C686 G687 G688 G689 G690 C691 C692 U693 U U C C U U C U G G C U A A C C U
U G A G U C C U U G U G G C U C U U G G C G A A C C A G G A C U U U U A C U U U G A A A A A U U A G A G U G U U C A A
A G C A G G C G U A U U G C U C G A A U A U A U U A G C A U G G A A U A A U A G A A U A G G A C G U U U G G U U C U A U
U U U G U U G G U U U U C U A G G A C C A U C G U A A U857 G858 A859 U860 U861 A862 A863 U864 A865 C870 U873 G876 C883 U894 G901 A906 A907 U908 U909 G913 G914 U932 A933 C934 U935
A940 U945 A951 U960 U965 A966 C969 A970 G976 A A A G U U A G G G G A U C G A A G A U G A U C A G A U A C C G U C G U A G U C U U A A1020
C1021 C1022 A1023 U1024 A1025 A1026 A1027 U1031 G1032 C1033 C1034 G1035 A1036 C1037 U1038 A1039 G1040 U1052 G1053 U1054 U1055 U1056 U1057 U1058 U1059 U1060 A1061 A1062 U1063 G1064 C1067 C1072 C1075 A1076 C1077 C1078 U1079 U1080 A1081 C1082 G1083 A1084 G1085 A1086 A1087 A U C A A G U C U
U U G G G U U C1105 U1106 G1107 G1108 G1109 G1110 G1111 G1118 G1119 G1122 A1125 G1126 G1127 C1128 A1131 A1132 U1144 U1145 G1146 A1147 C1158 C1161 G1164 C1174 U1175 G1176 C1177 G1178 G1179 C U U A A U U G A C1190 U1191 C1192 A1193 A1194
C1195 A1196 C1197 G1198 G1199 G1200 G1201 A1202 A1203 A1204 C1205 U1206 C1207 A1208 C1209 C1210 A1211 G1212 G1213 U1214 C1215 C1216 A1217 G1218 A1219 C1220 A1221 C1222 A1223 A1224 U1225 A1226 A1227 G1228 G1229 A1230 U1231 U1232 G1233 A1234 C1235 A1236 G A U U G A G A G C U C U U1250 U1251 C1252 U1253 U1254
G1255 A1256 U1257 U1258 U1259 U1260 G1261 U1262 G1263 G1264 G1265 U1266 G1267 G1268 U1269 G1270 G1271 U1272 G1273 C1274 A1275 U1276 G G C C G U U C U U A G U U G G U G G A G U G A U U G U C U G C U U A A U
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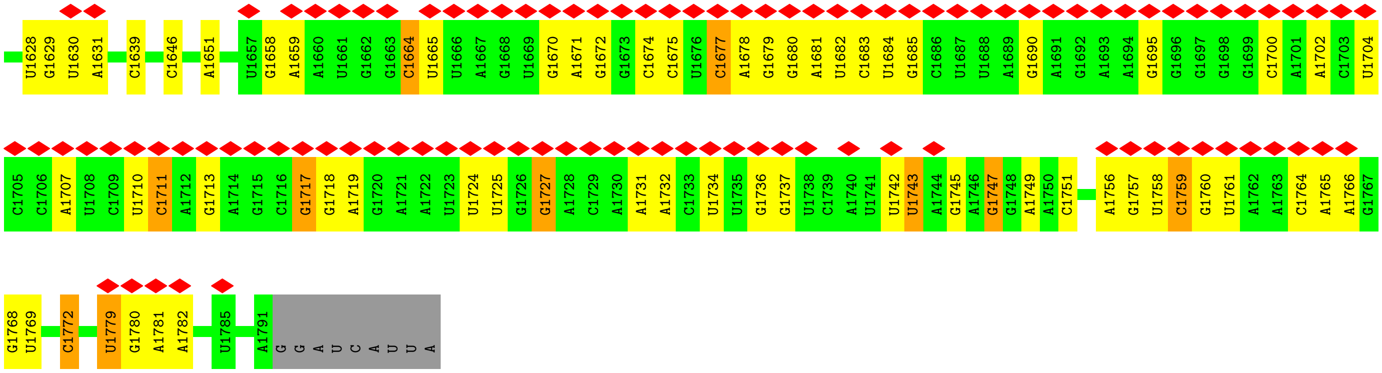
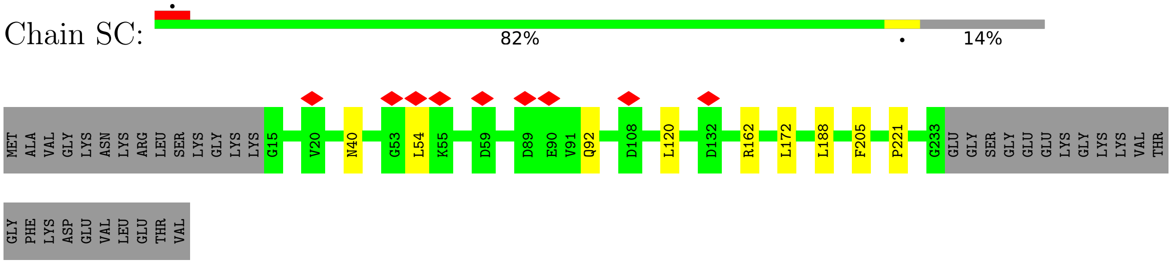
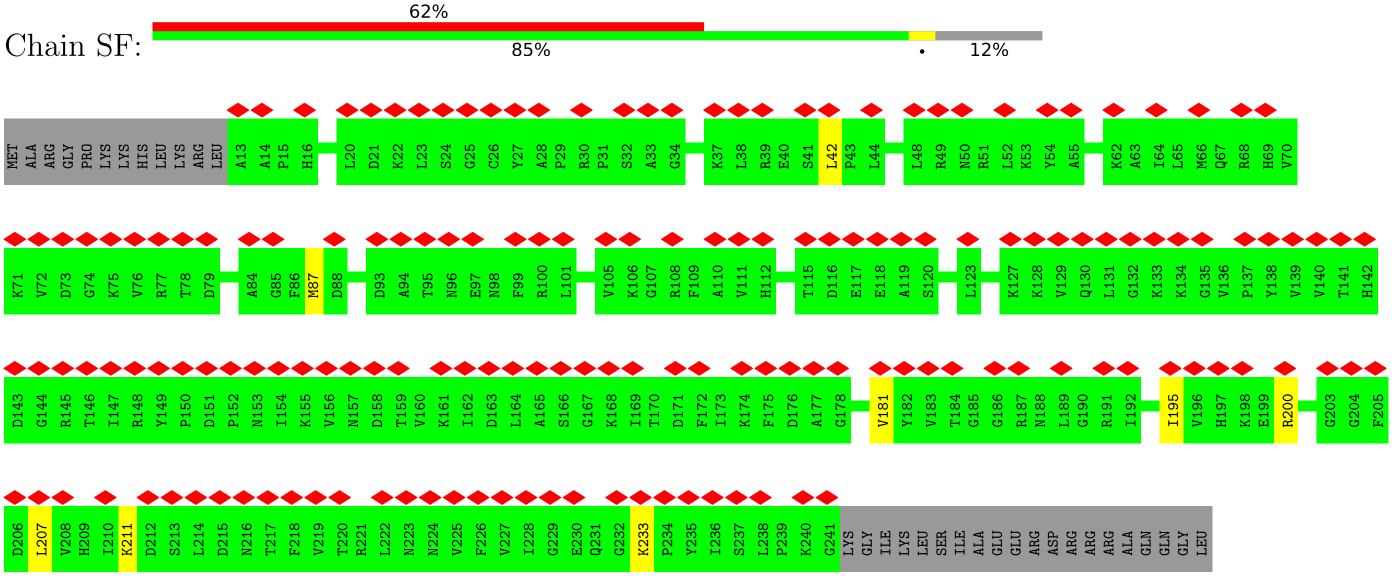
A C U U C U U A G A G G G A C U A U C G G U U U C A A G C C G A U G G A A G U U U G A G G C A A U A A C A G G U C U G U1434
G1435 A1436 U1437 G1438 C1439 C1440 C1441 U1442 U1443 A G A C G1448 U1449 U1450 C1451 U1452 G1453 G1454 G1455 C1456 C1457 G C A1460 C1461 A1469 C1472 U1473 G1474 A1475 C1476 G1477 C1485 G1488 U1489 A1492 A1493 U1496 U1497 G1498 G1506 U1517 C1518 U1519 U1520 G1521 U1522 G1523 A1524
G1531 U1535 G1536 G1539 G1540 G1541 G1542 A1543 U1544 A1545 G A G C A U U G U A A U U A U U G C U C U1566 U1567 C1568 A1569 A1570 A1573 G1584 U1585 G1590 G1594 U1595 G1601 C1602 G1607 A1614 C1618 C1619 C1620 C1623



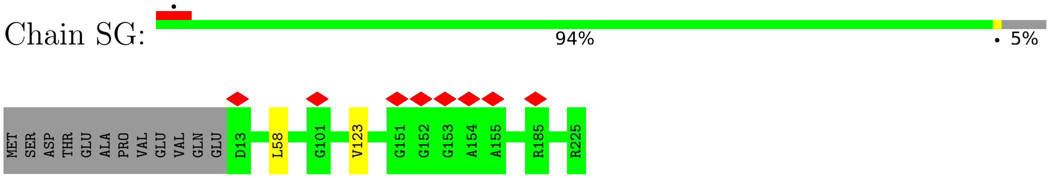
- Molecule 4: 40S ribosomal protein S1-A



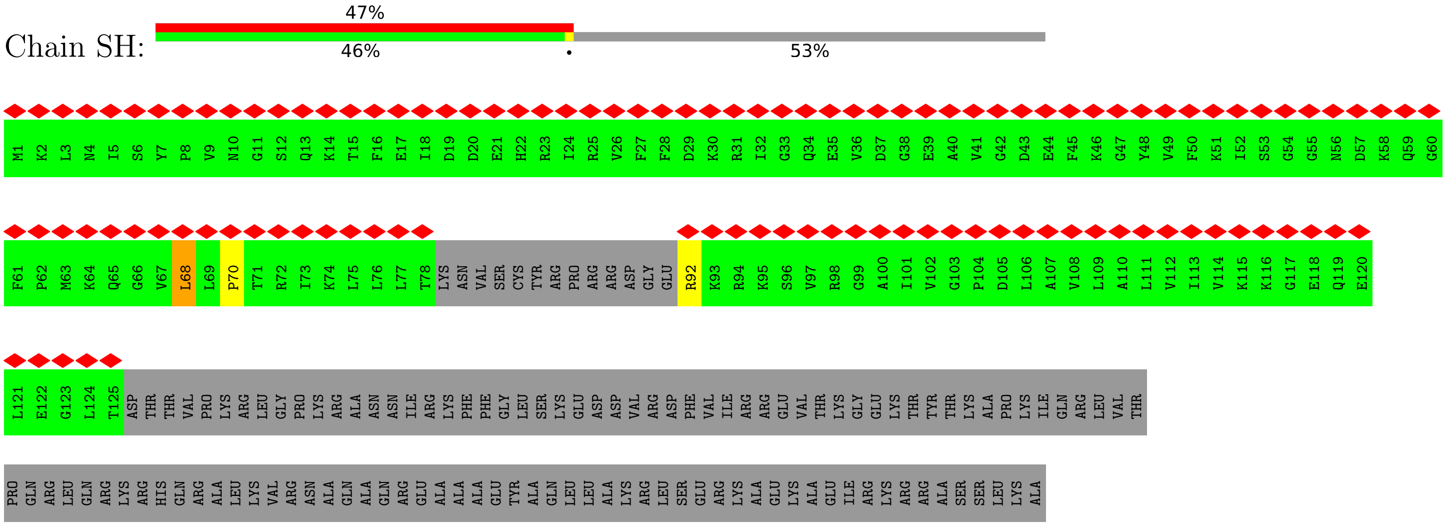
- Molecule 5: 40S ribosomal protein S4-A



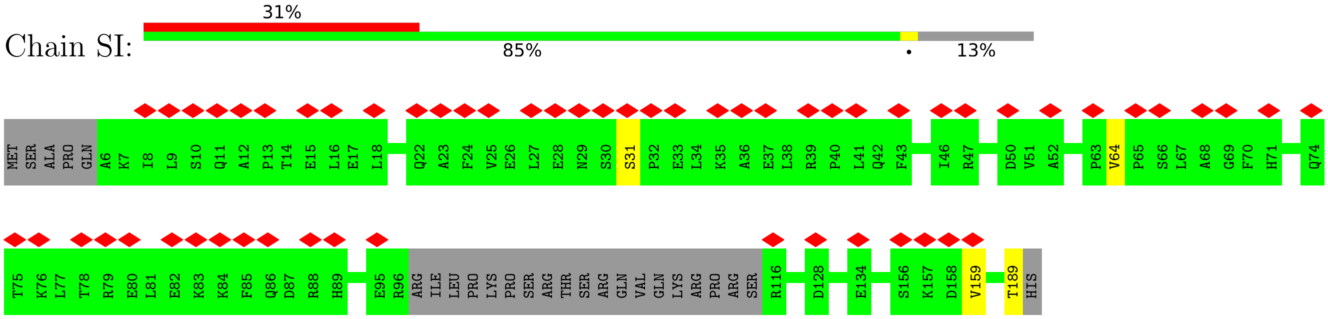
- Molecule 6: 40S ribosomal protein S5



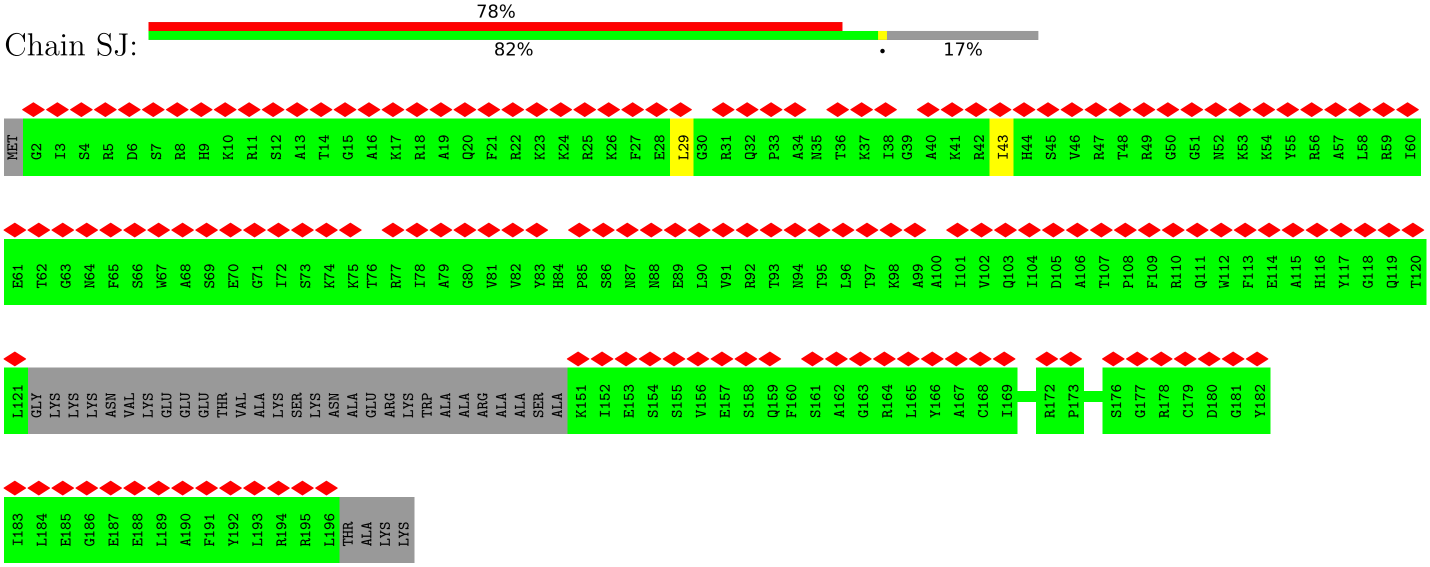
- Molecule 7: 40S ribosomal protein S6-A



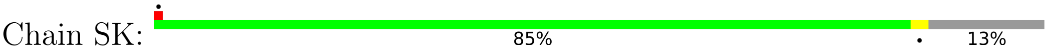
- Molecule 8: 40S ribosomal protein S7-A

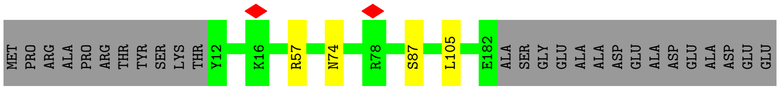


- Molecule 9: 40S ribosomal protein S8-A



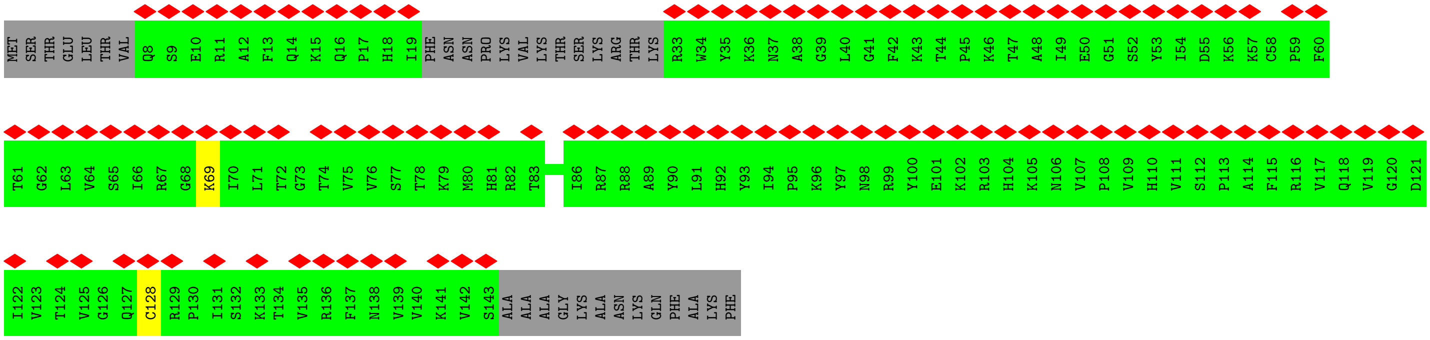
- Molecule 10: 40S ribosomal protein S9-A





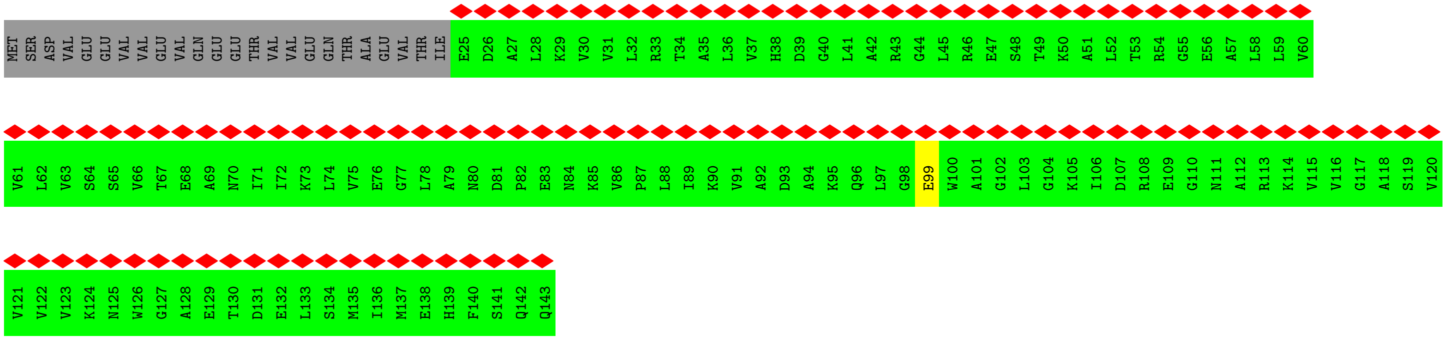
- Molecule 11: 40S ribosomal protein S11-A

Chain SM:



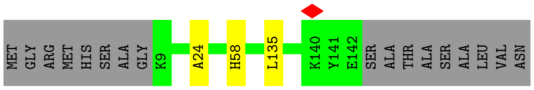
- Molecule 12: 40S ribosomal protein S12

Chain SN:



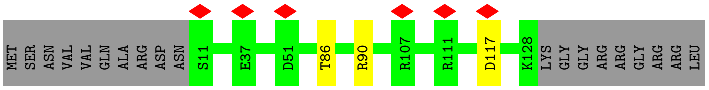
- Molecule 13: 40S ribosomal protein S13

Chain SO:

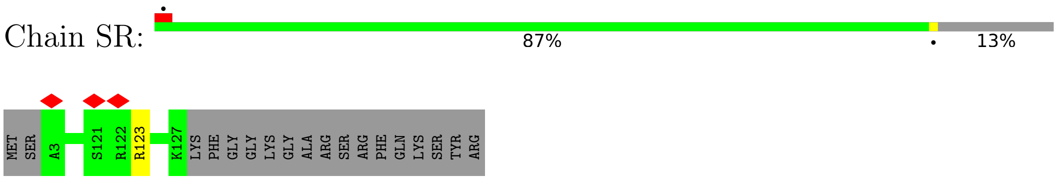


- Molecule 14: 40S ribosomal protein S14-A

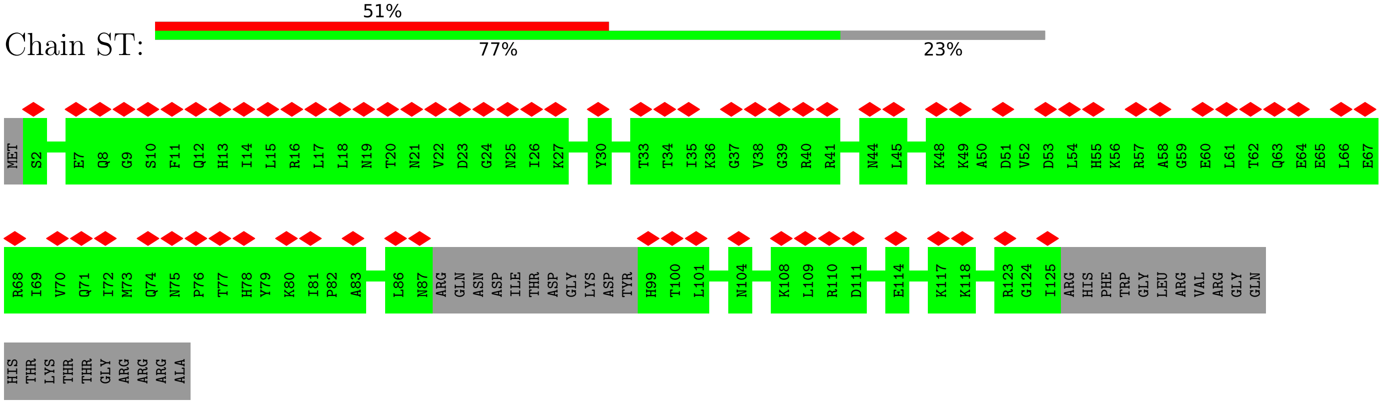
Chain SP:



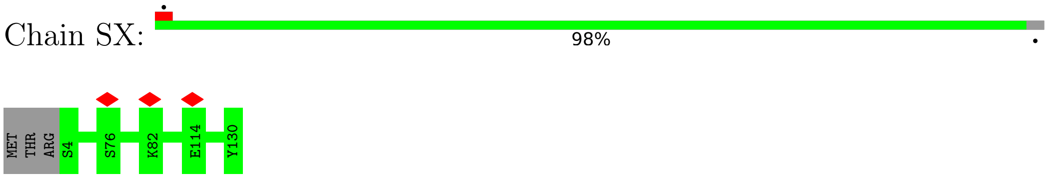
- Molecule 15: 40S ribosomal protein S16-A



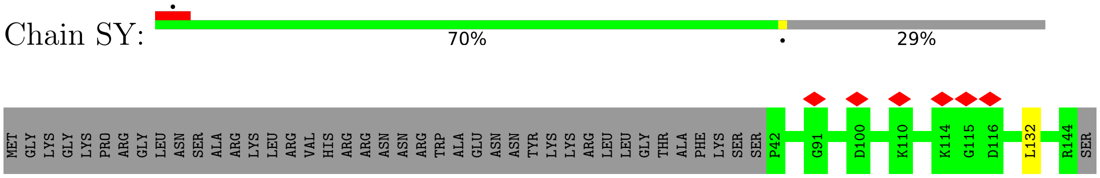
- Molecule 16: 40S ribosomal protein S18-A



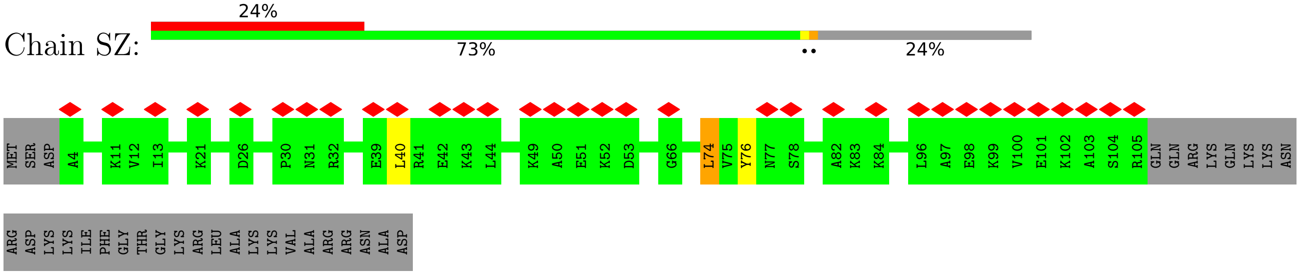
- Molecule 17: 40S ribosomal protein S22-B



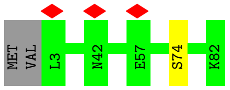
- Molecule 18: 40S ribosomal protein S23-A



- Molecule 19: 40S ribosomal protein S24-A

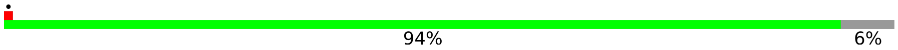


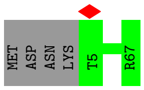
- Molecule 20: 40S ribosomal protein S27-A



- Molecule 21: 40S ribosomal protein S28-A

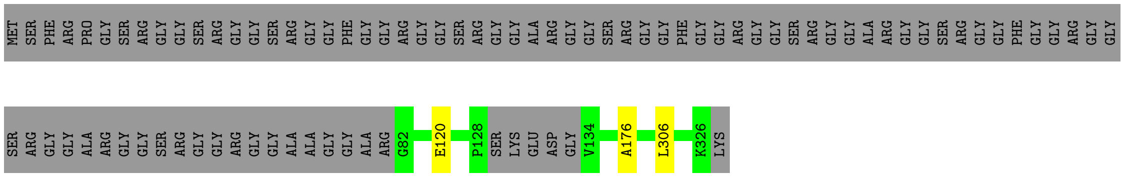
Chain Sd:





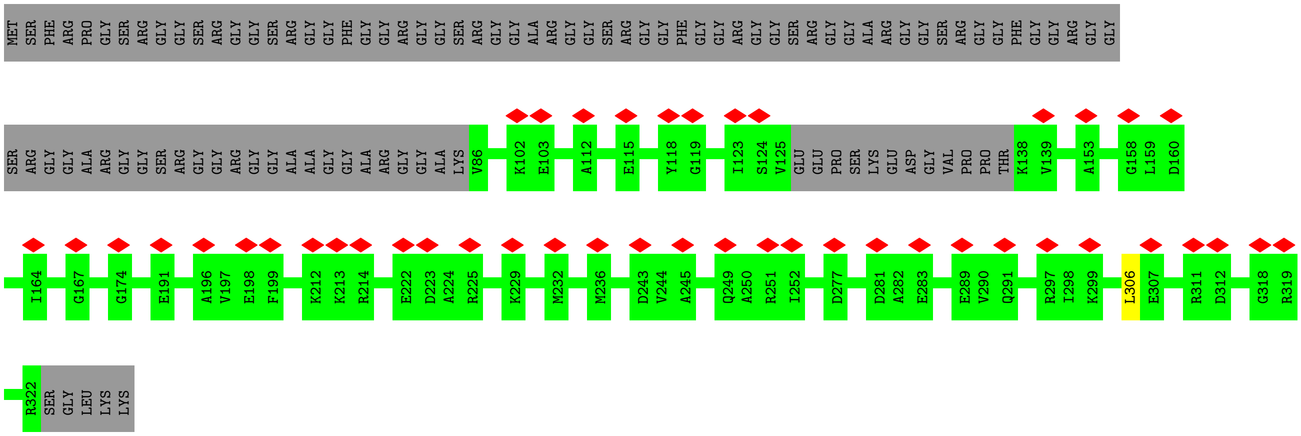
- Molecule 22: rRNA 2'-O-methyltransferase fibrillarin

Chain 3B:



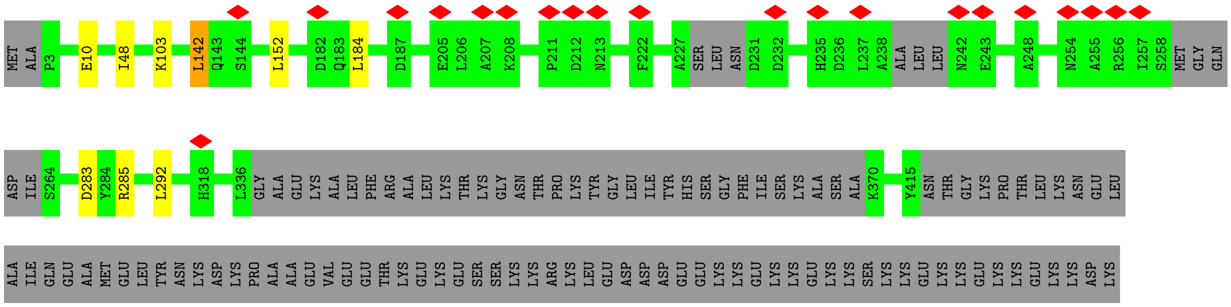
- Molecule 22: rRNA 2'-O-methyltransferase fibrillarin

Chain 3C:



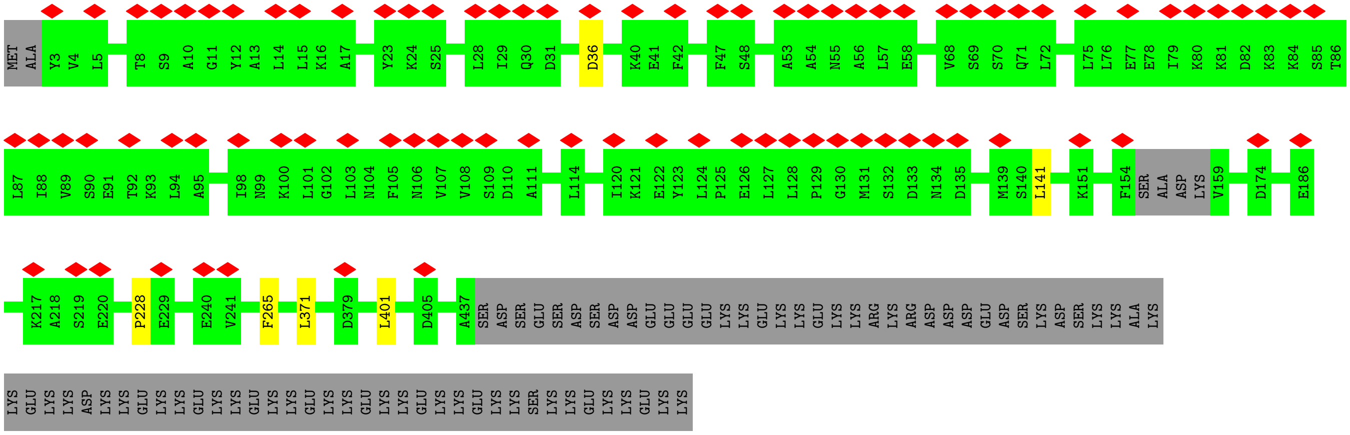
- Molecule 23: Nucleolar protein 56

Chain 3D:



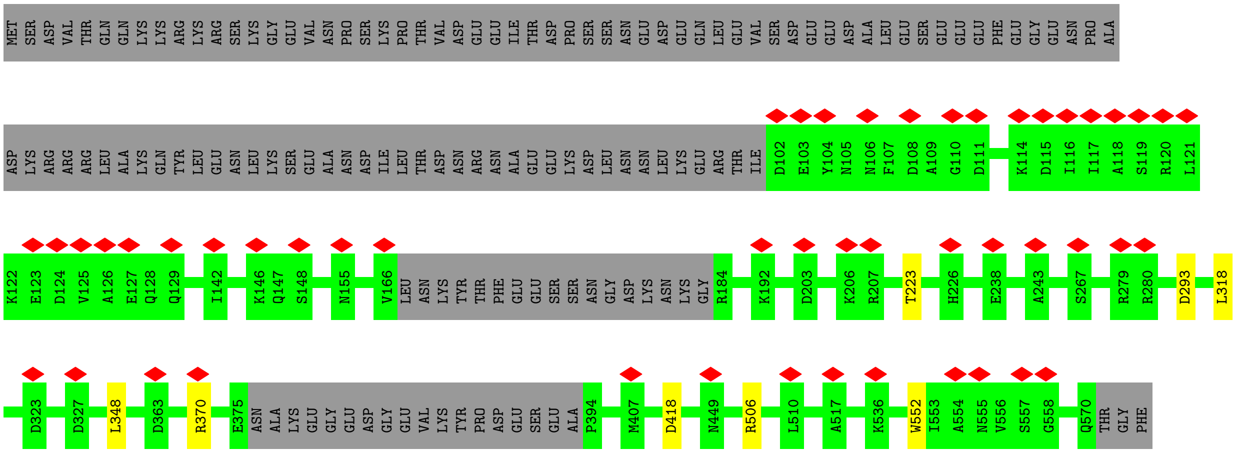
- Molecule 24: Nucleolar protein 58

Chain 3E:



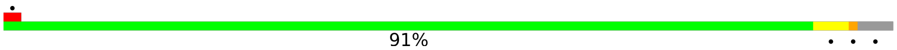
- Molecule 25: Ribosomal RNA-processing protein 9

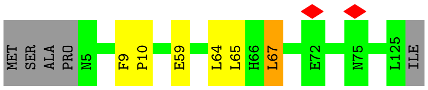
Chain 3F:



- Molecule 26: 13 kDa ribonucleoprotein-associated protein

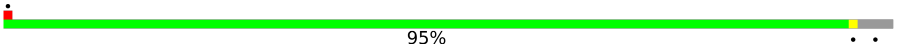
Chain 3G:

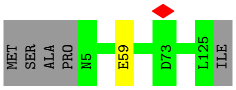




- Molecule 26: 13 kDa ribonucleoprotein-associated protein

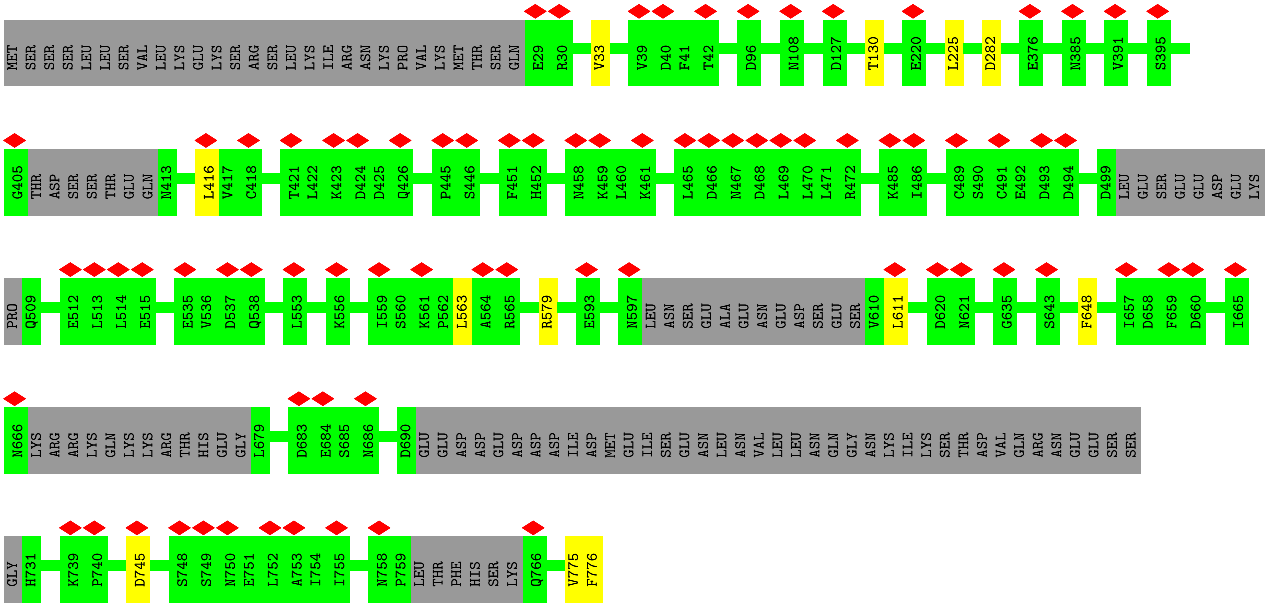
Chain 3H:





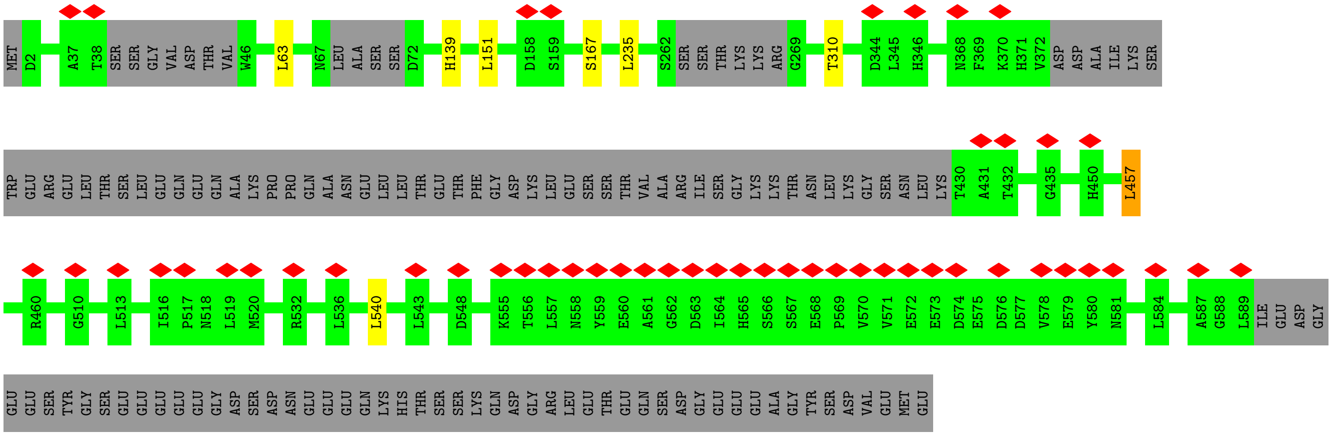
- Molecule 27: U3 small nucleolar RNA-associated protein 4

Chain A4:



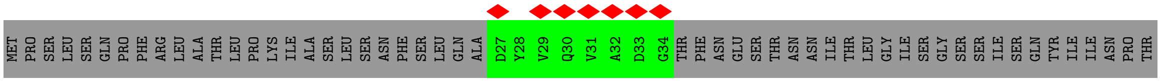
- Molecule 28: U3 small nucleolar RNA-associated protein 5

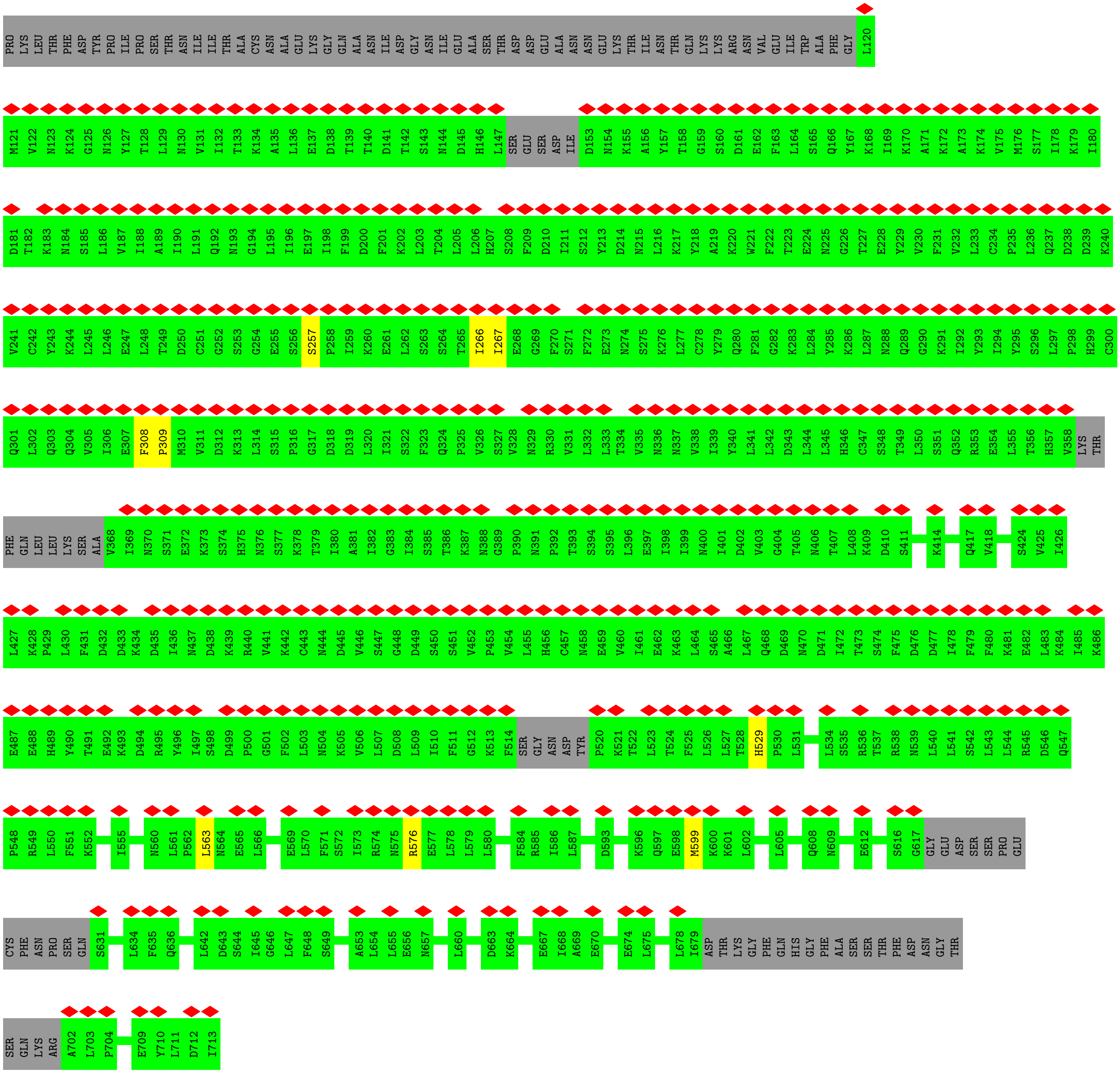
Chain A5:



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

Chain A8:





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

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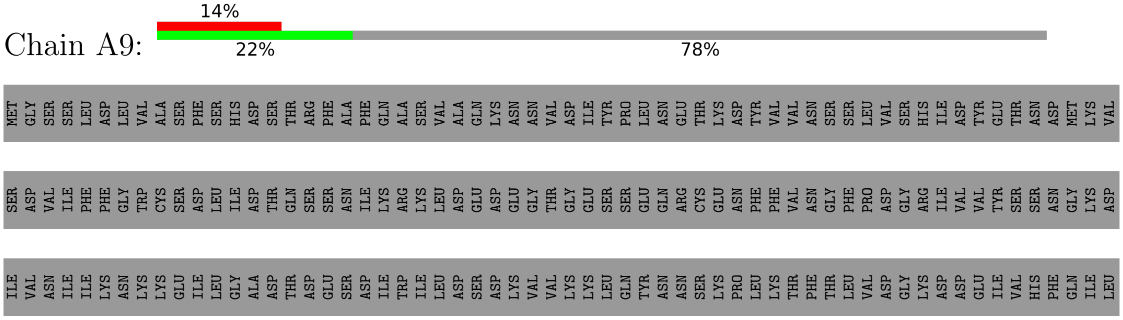
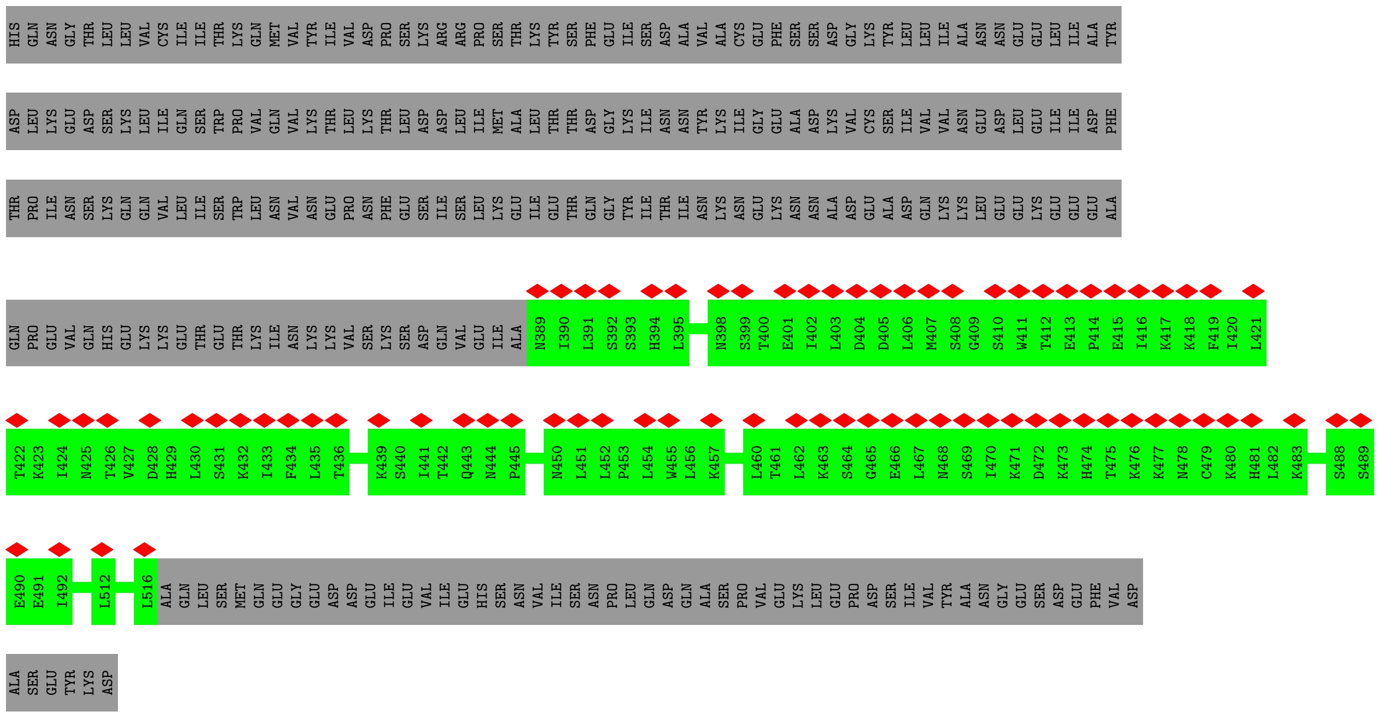
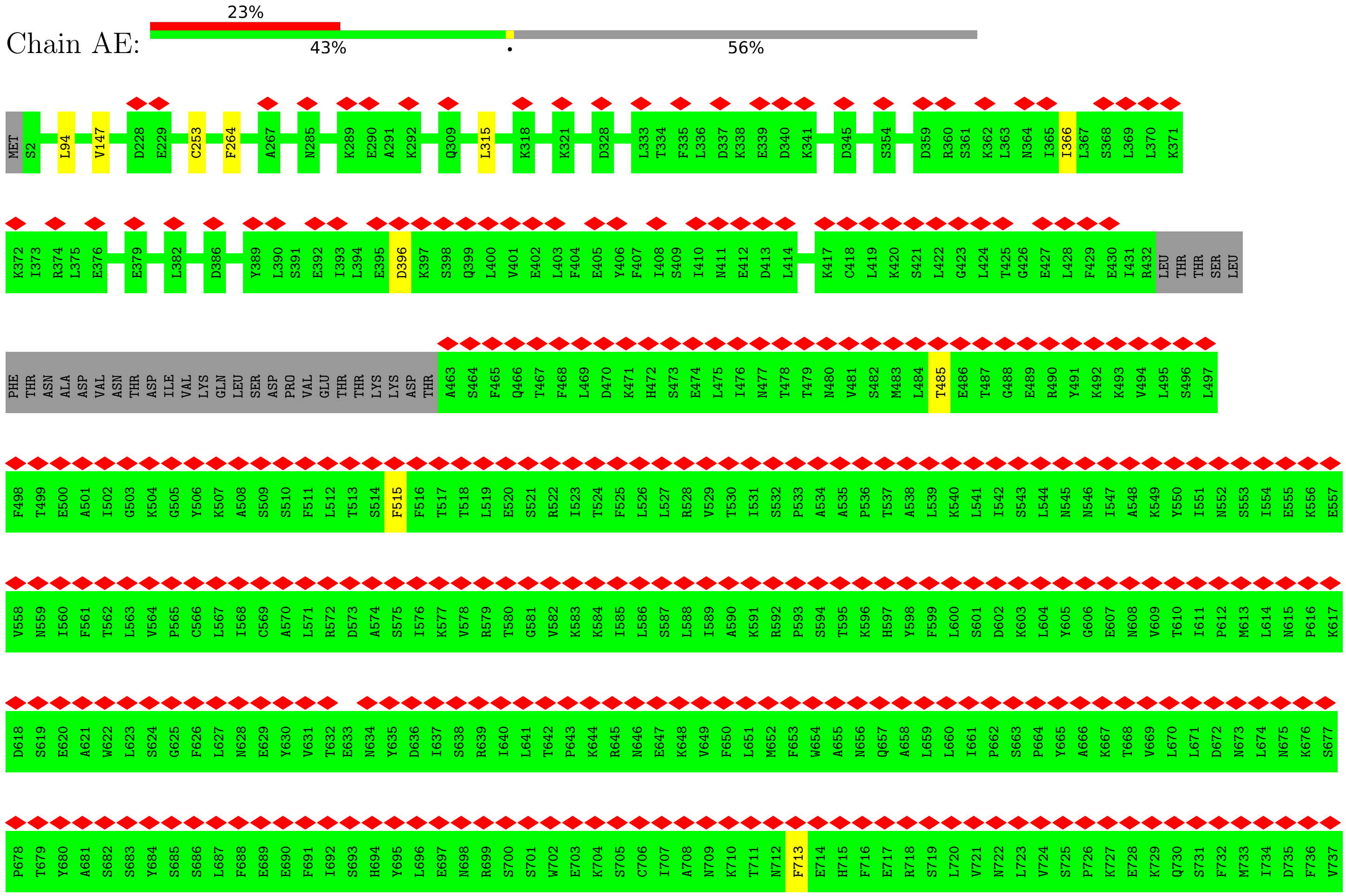




- Molecule 31: U3 small nucleolar RNA-associated protein 10

Chain AE:



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D798 S799 D800 I801 F802 V803 S804 I805 L806 N807 Q808 ASN SER ILE SER ASN GLU MET ASP GLN THR ASP PHE SER LYS ARG ARG ARG ARG ARG SER SER THR SER LYS ASN ALA PHE LEU LYS GLU GLU VAL SER GLN LEU ALA GLU LEU HIS LEU ARG LYS LEU THR ILE ILE LEU GLU ALA

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

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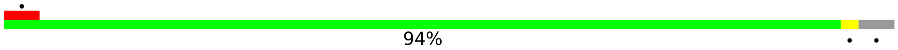
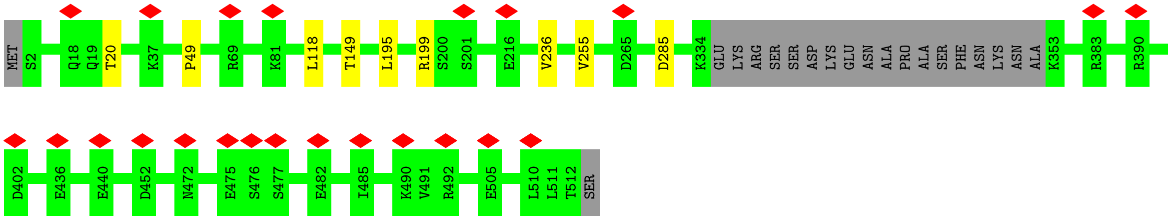
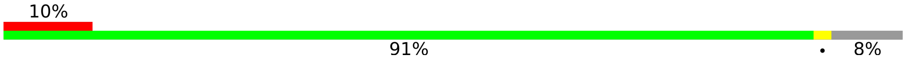
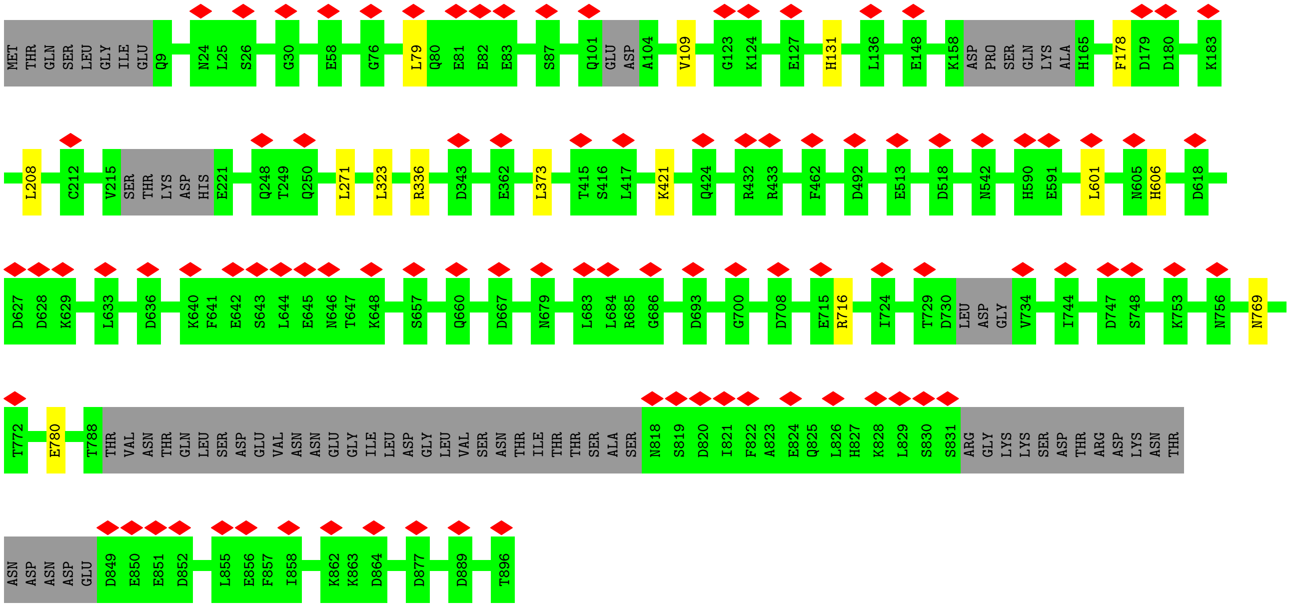




- Molecule 33: NET1-associated nuclear protein 1

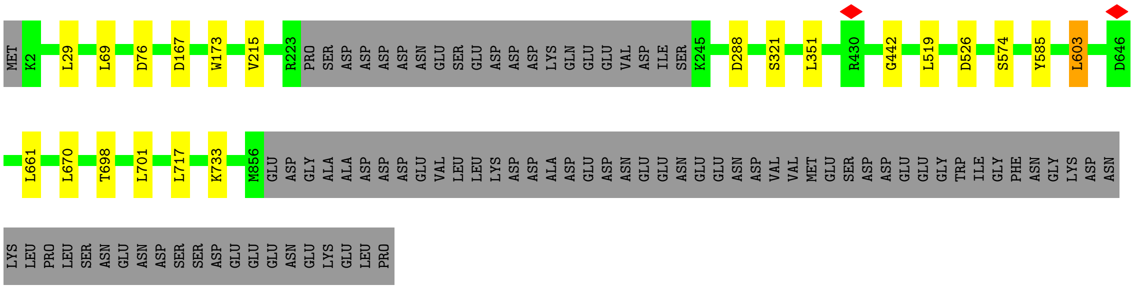
Chain AG:





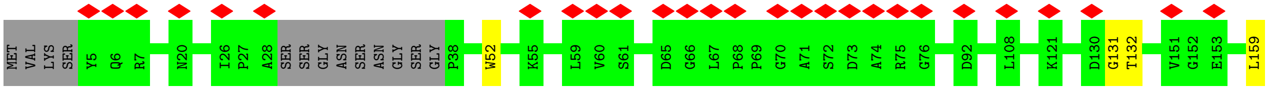
- Molecule 34: Periodic tryptophan protein 2

Chain B1:



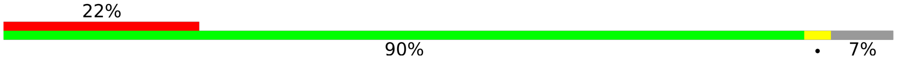
- Molecule 35: U3 small nucleolar RNA-associated protein 12

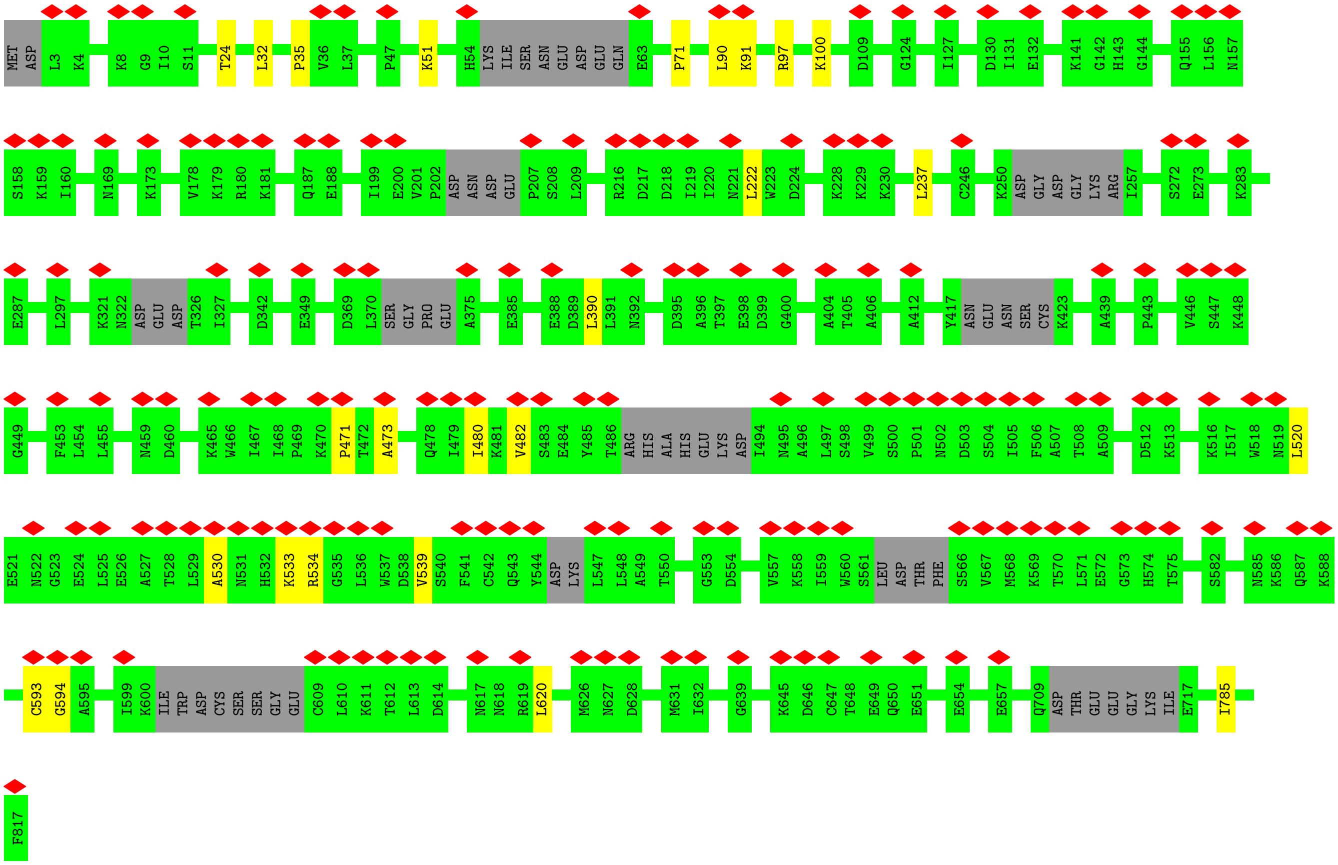
Chain B2:



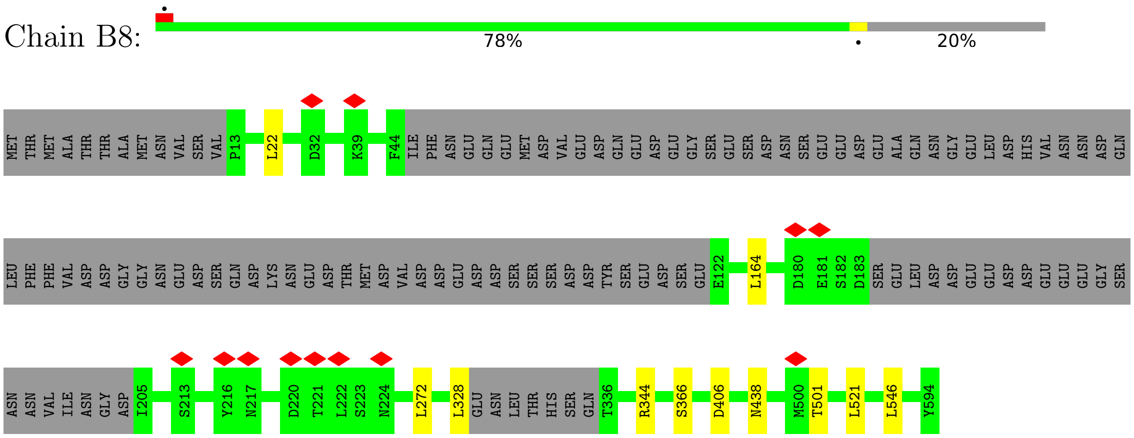
- Molecule 36: U3 small nucleolar RNA-associated protein 13

Chain B3:

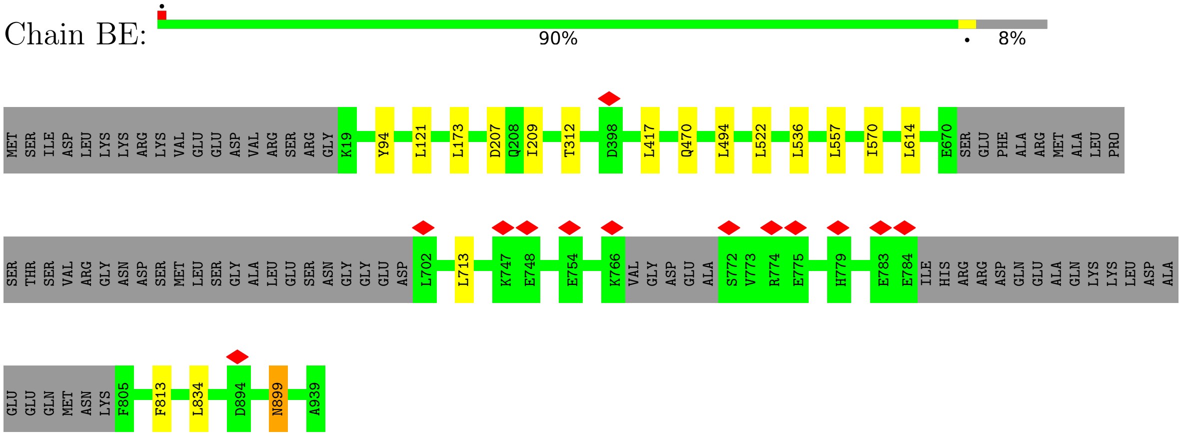




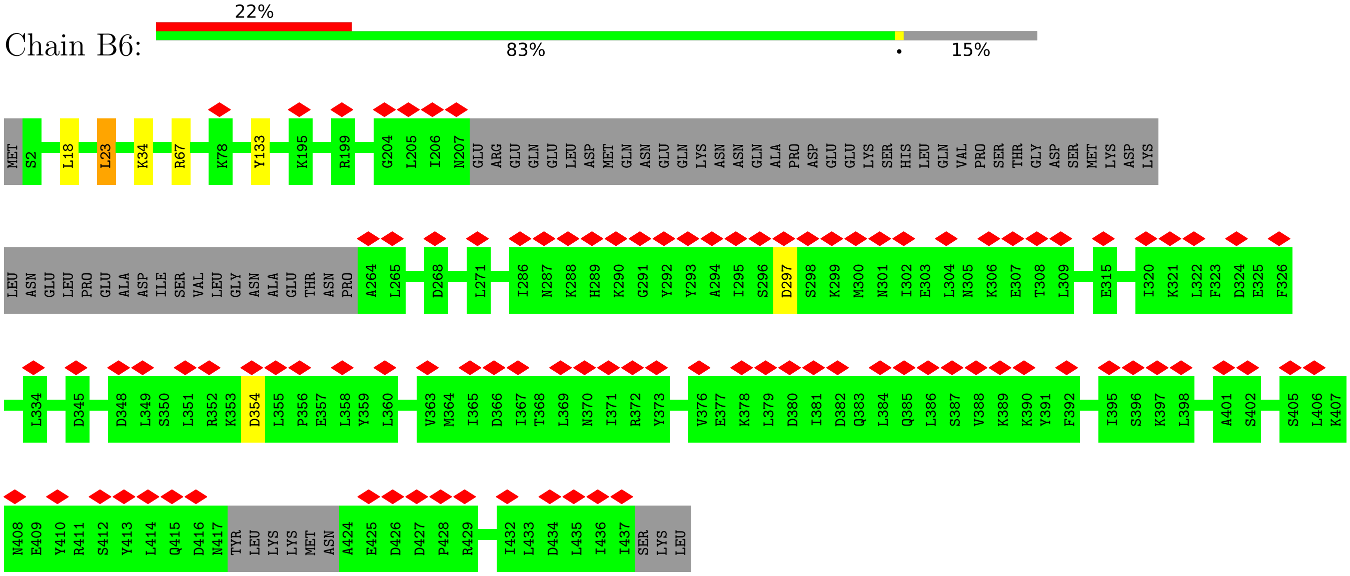
- Molecule 37: U3 small nucleolar RNA-associated protein 18



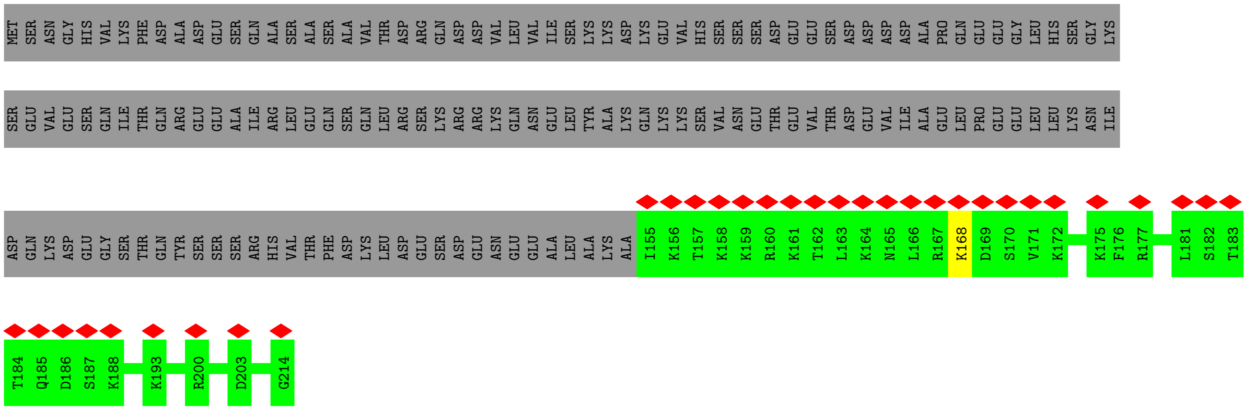
- Molecule 38: U3 small nucleolar RNA-associated protein 21



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

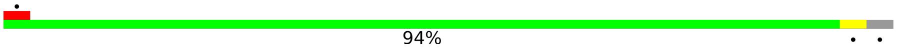


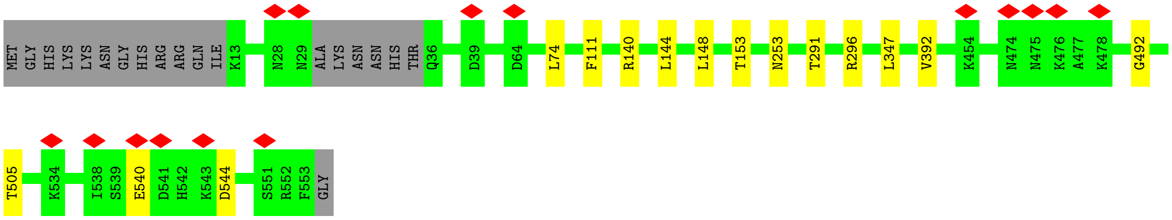
- Molecule 40: Bud site selection protein 21



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

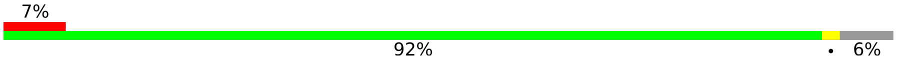
Chain 5C:

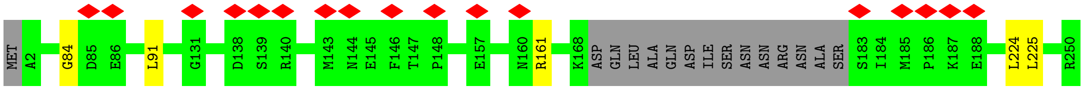




• Molecule 42: U3 small nucleolar RNA-associated protein 11

Chain 5D:





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

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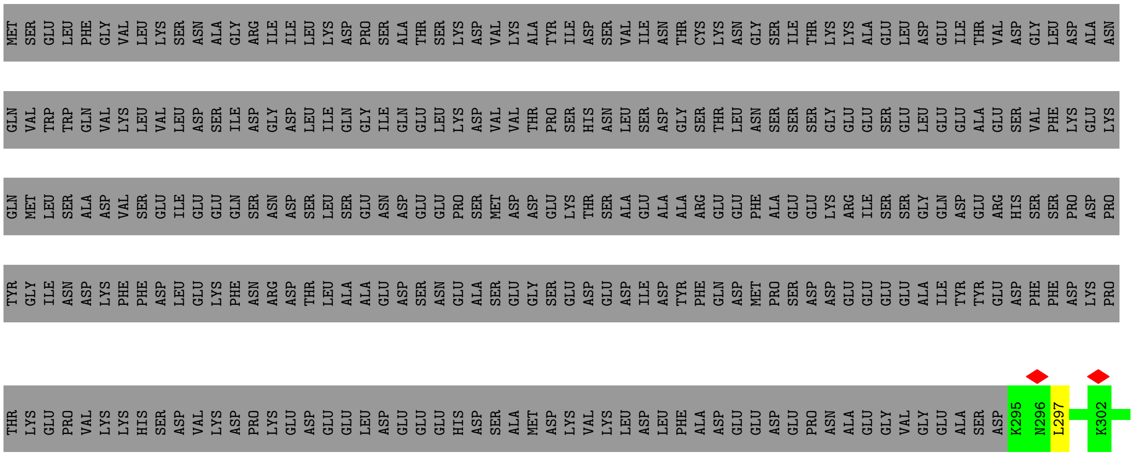
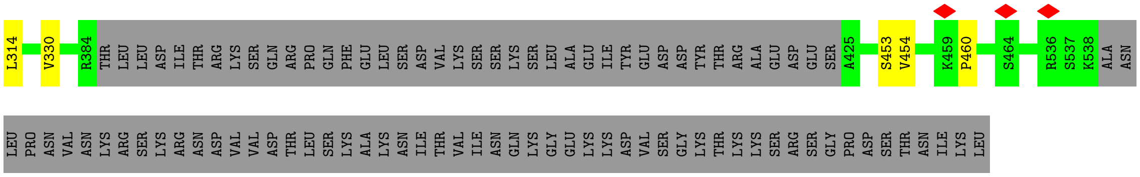
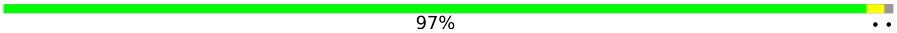
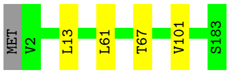




- Molecule 44: U3 small nucleolar ribonucleoprotein protein IMP3

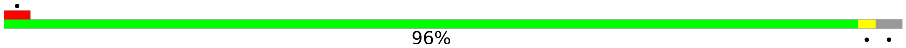
Chain 5F:

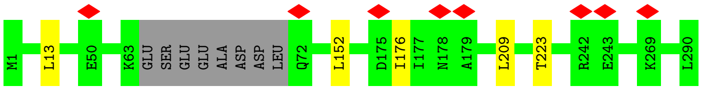




- Molecule 45: U3 small nucleolar ribonucleoprotein protein IMP4

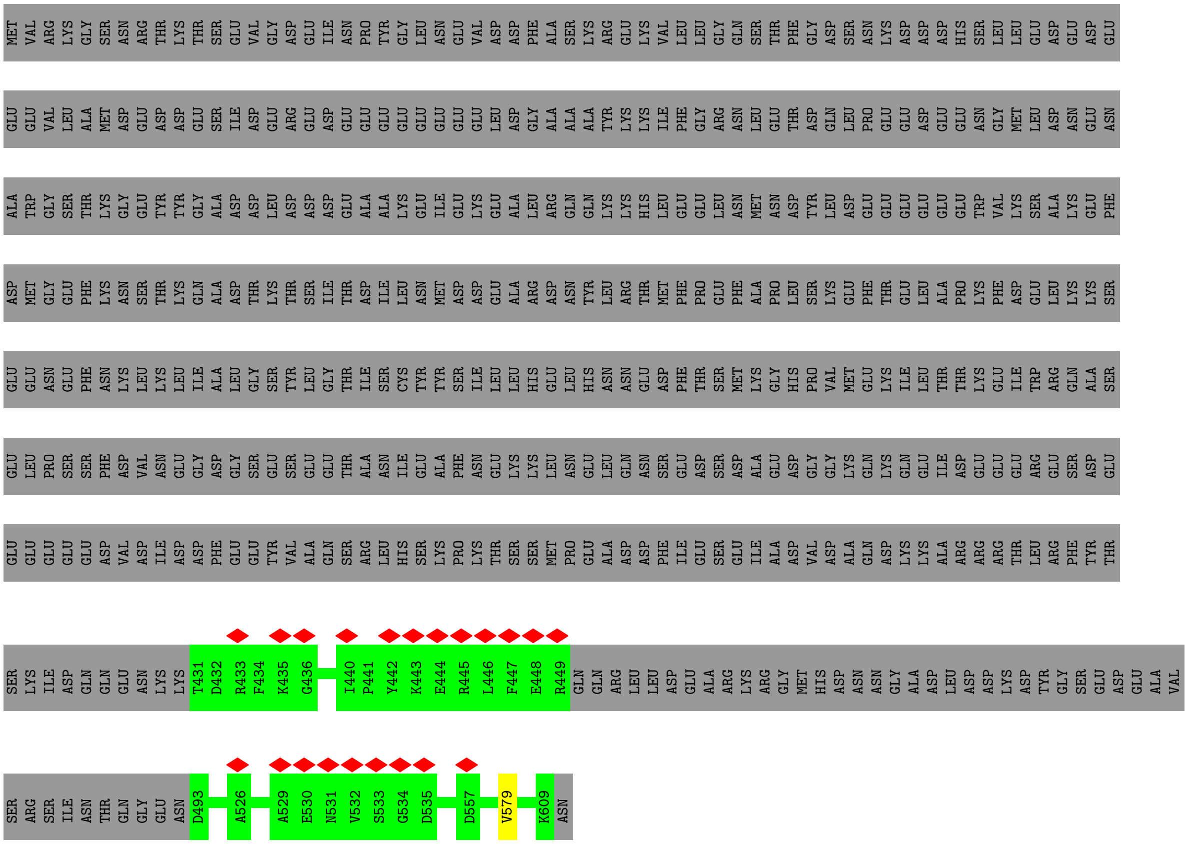
Chain 5G:





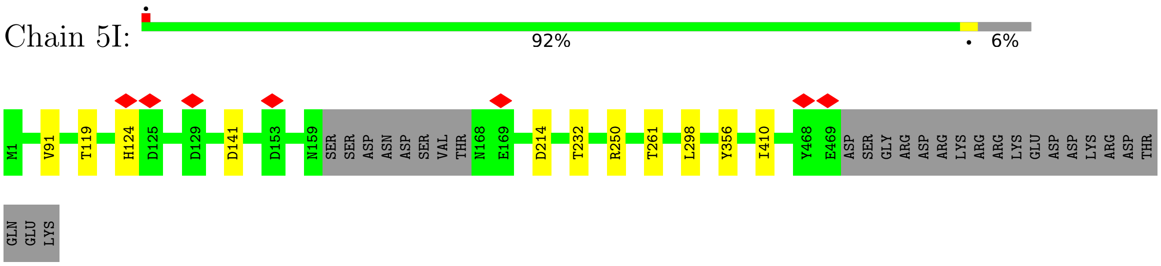
- Molecule 46: Something about silencing protein 10

Chain 5H:



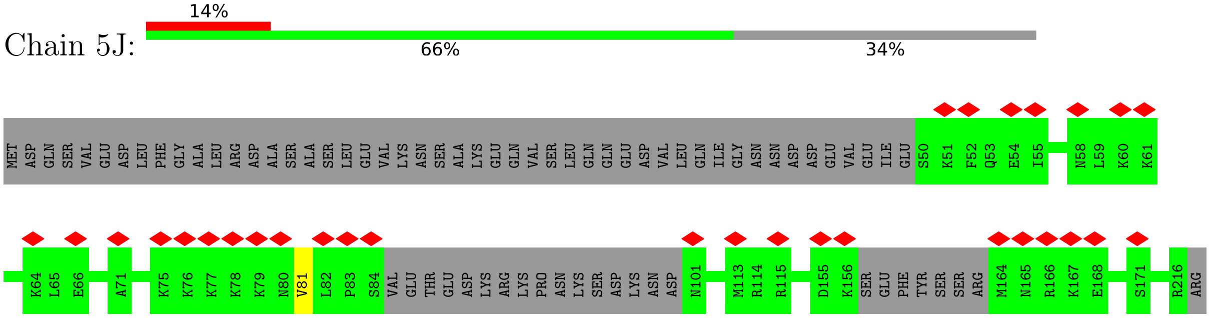
- Molecule 47: Protein SOF1

Chain 5I:



- Molecule 48: rRNA-processing protein FCF2

Chain 5J:



- Molecule 49: rRNA-processing protein FCF1

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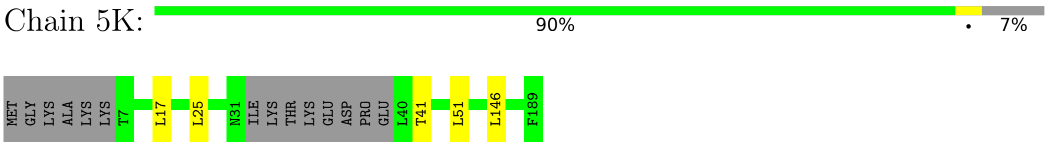
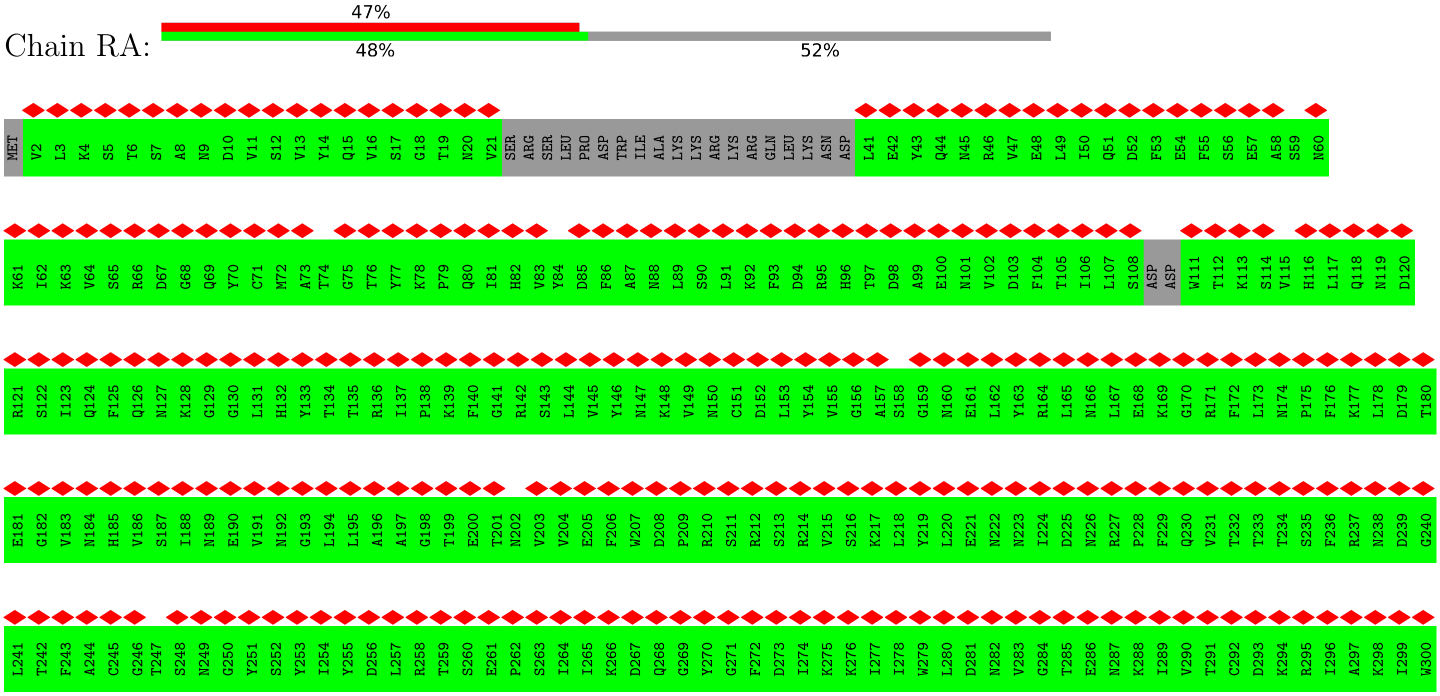
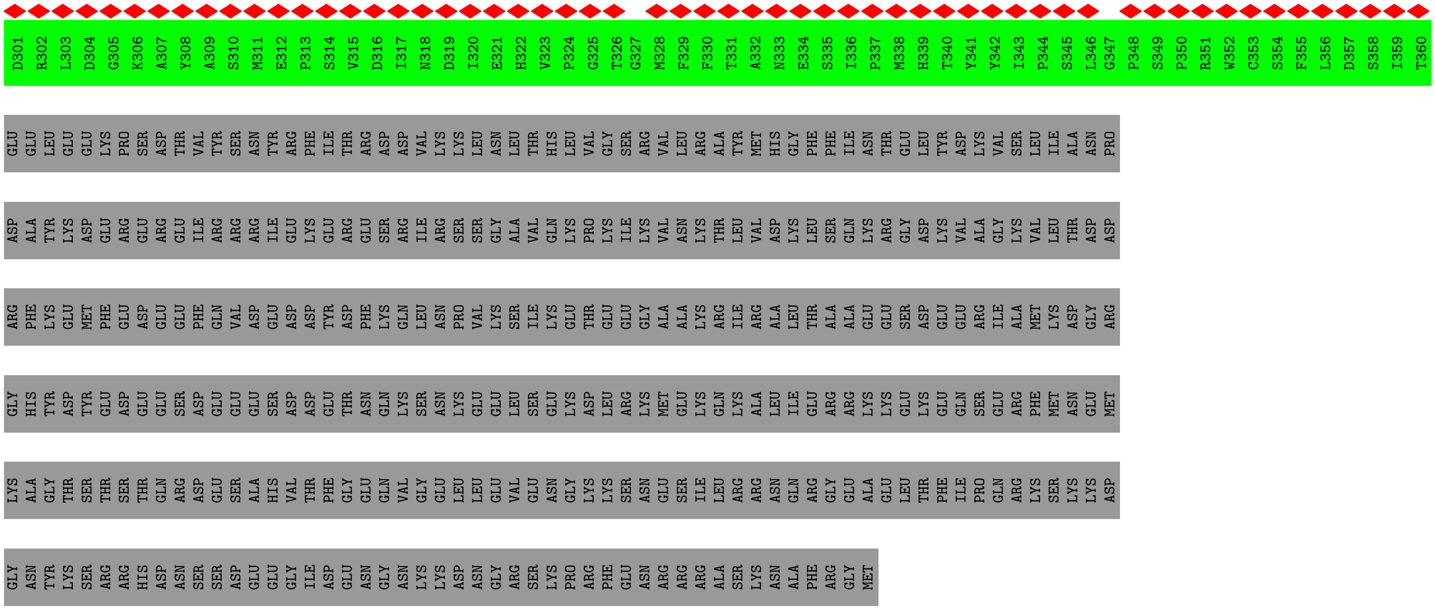


- Molecule 50: Ribosome biogenesis protein ENP2

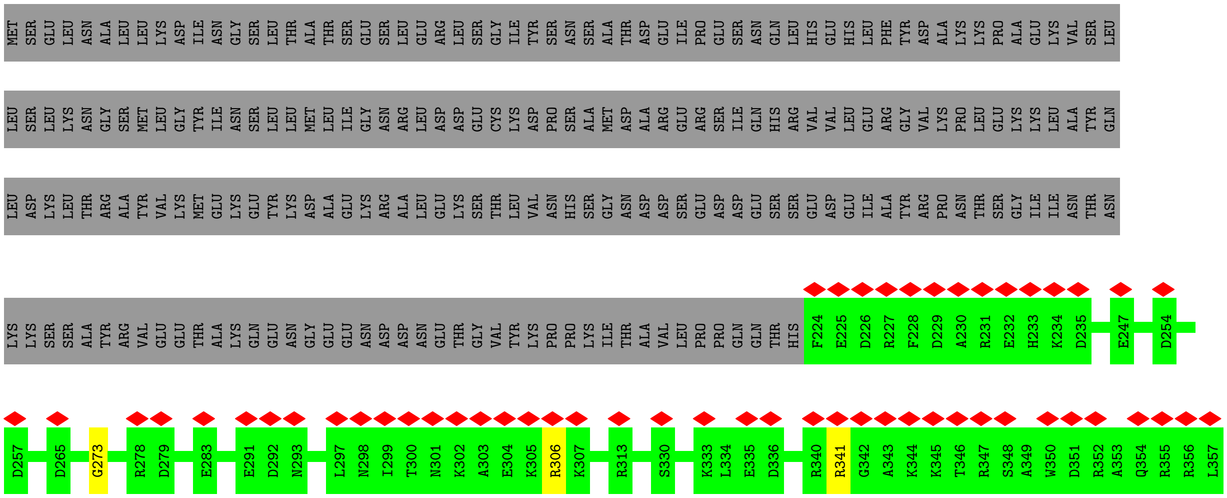
Chain RA:





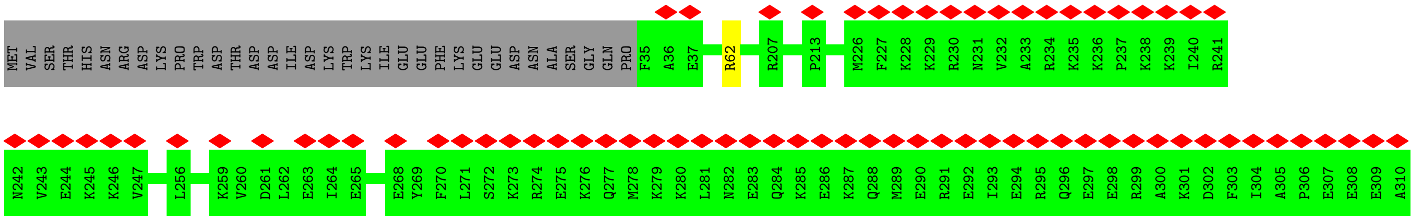
- Molecule 51: U3 small nucleolar ribonucleoprotein protein LCP5

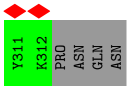
Chain RB:



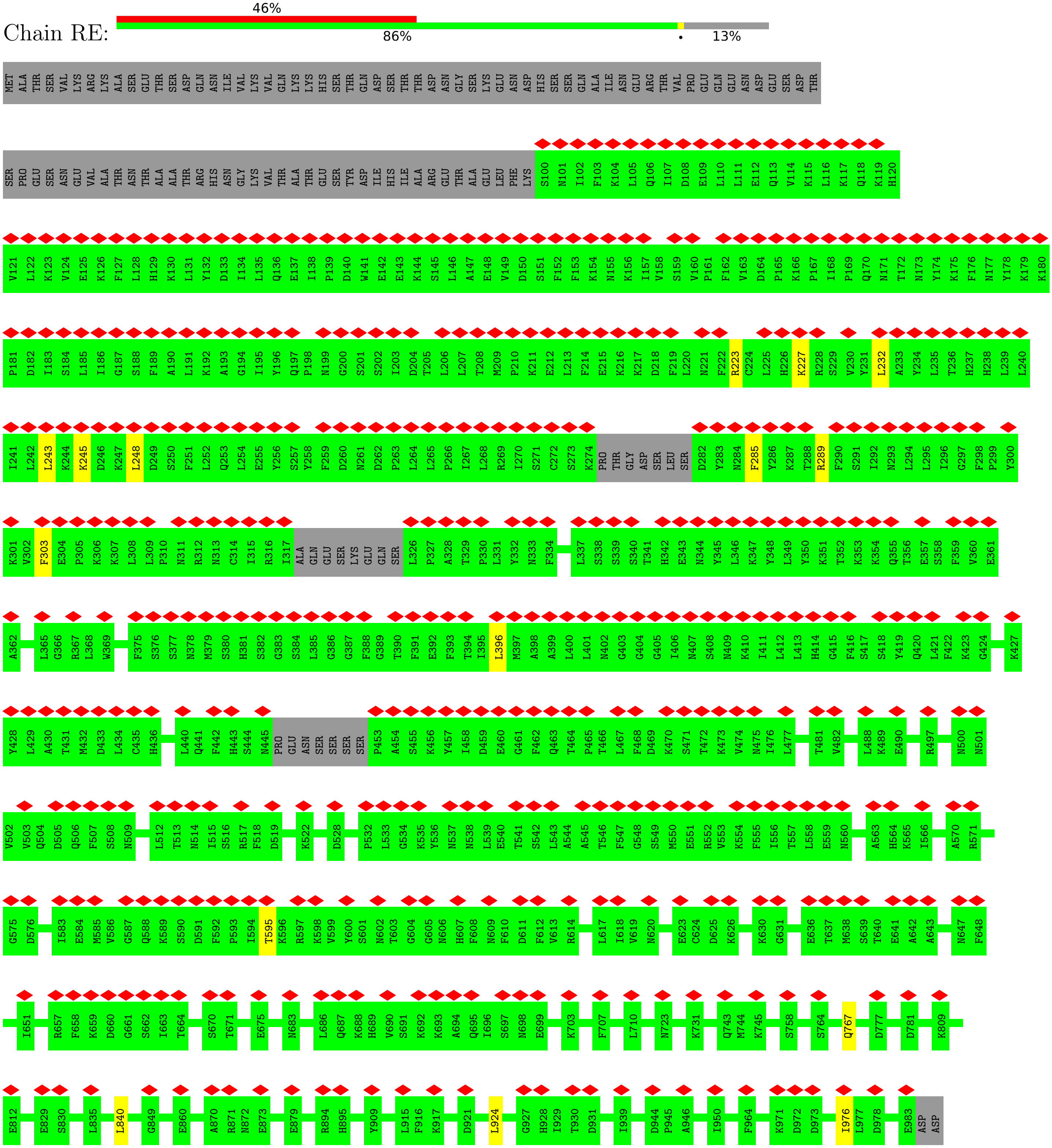
- Molecule 52: KRR1 small subunit processome component

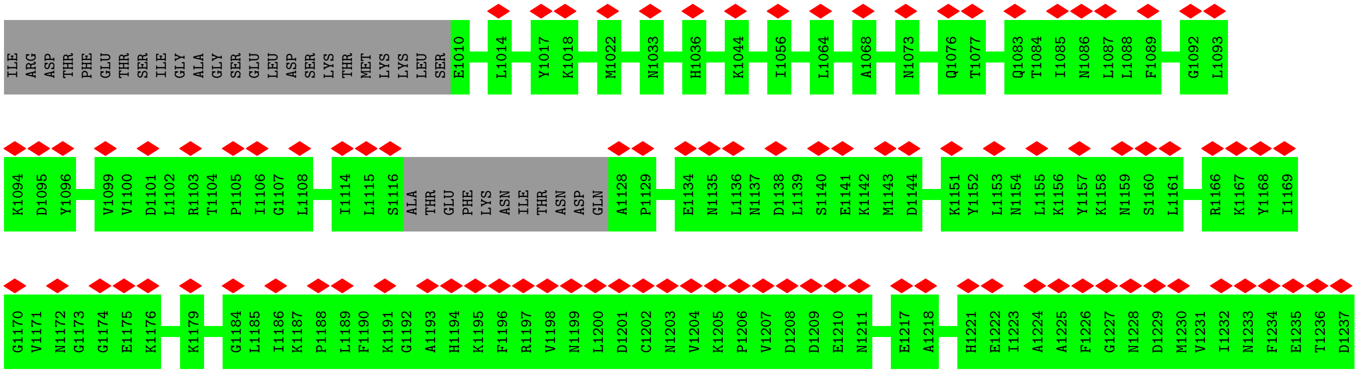
Chain RC:





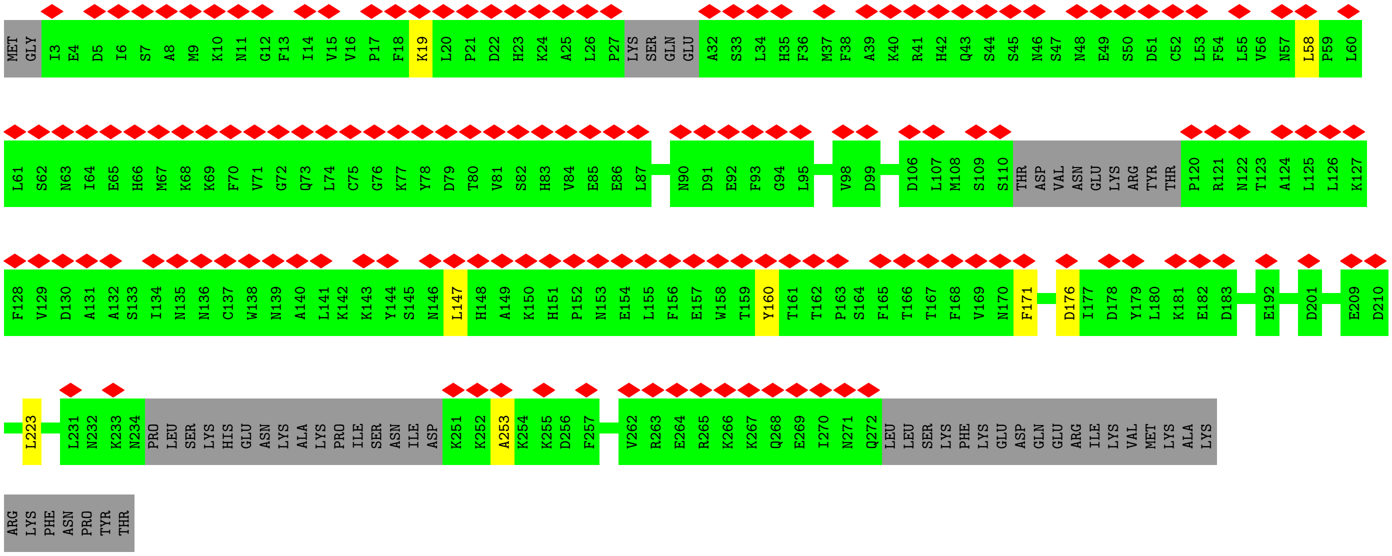
- Molecule 53: U3 small nucleolar RNA-associated protein 22





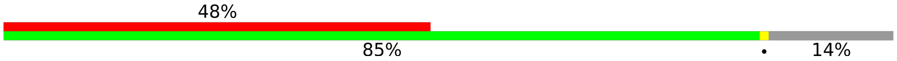
- Molecule 54: Ribosomal RNA-processing protein 7

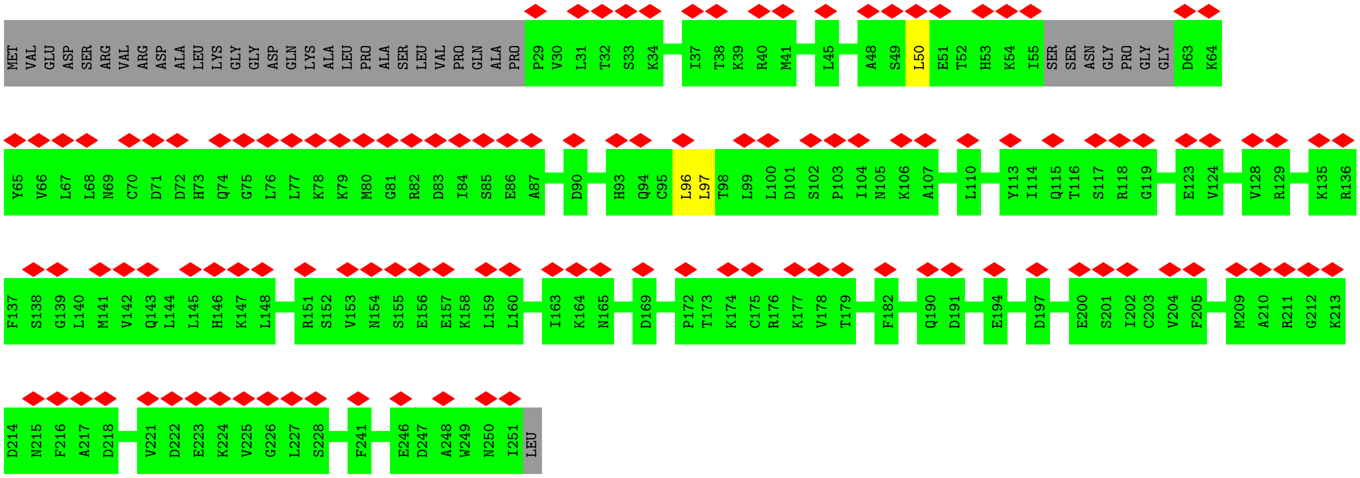
Chain RF:



- Molecule 55: Ribosomal RNA small subunit methyltransferase NEP1

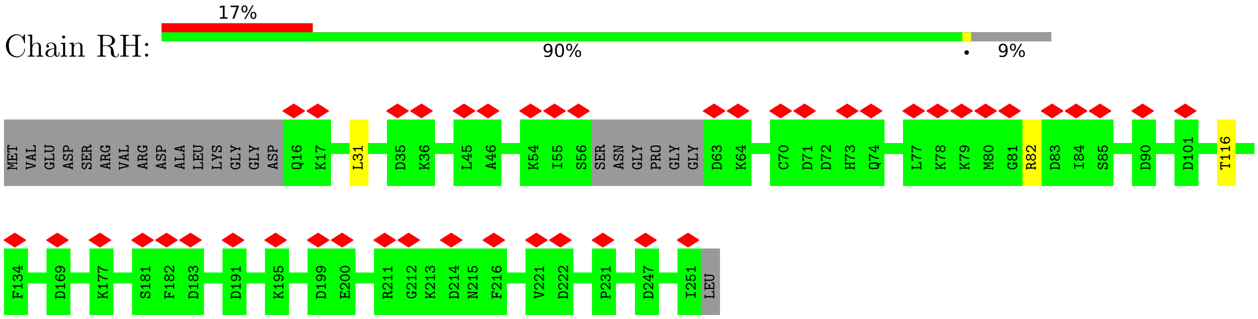
Chain RG:





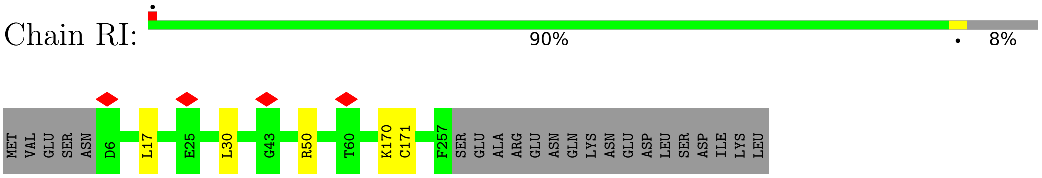
- Molecule 55: Ribosomal RNA small subunit methyltransferase NEP1

Chain RH:



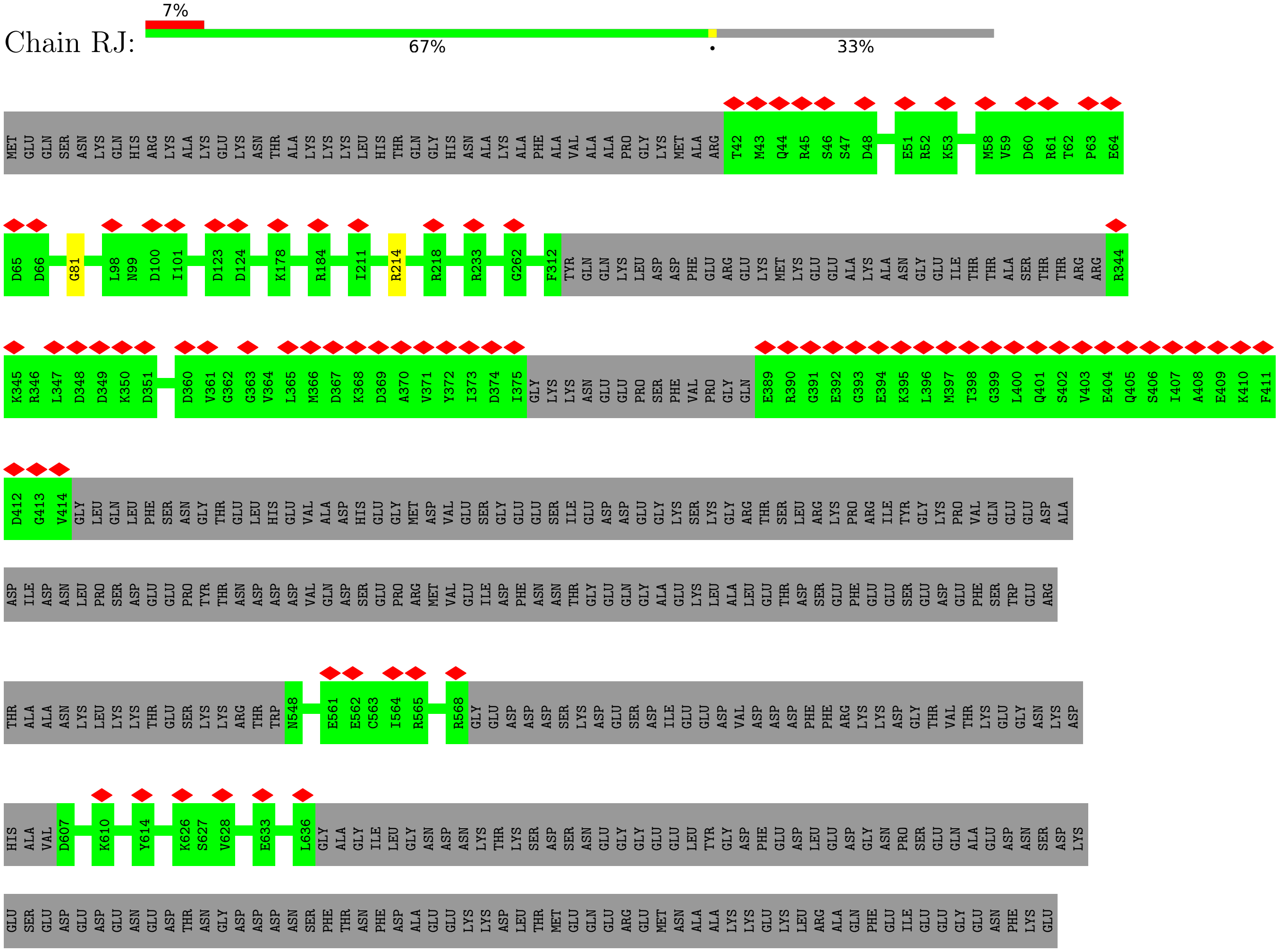
- Molecule 56: Ribosome biogenesis protein UTP30

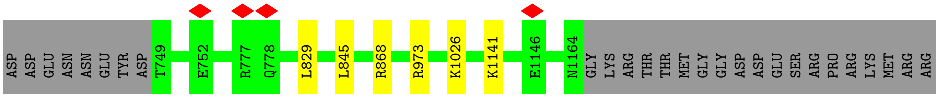
Chain RI:



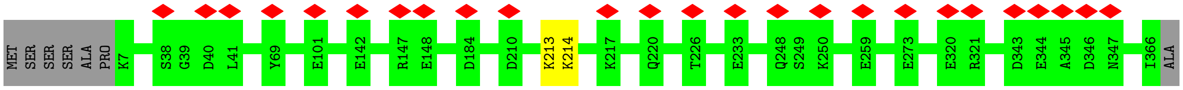
- Molecule 57: Ribosome biogenesis protein BMS1

Chain RJ:

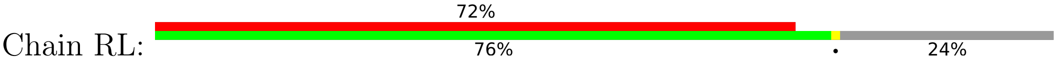


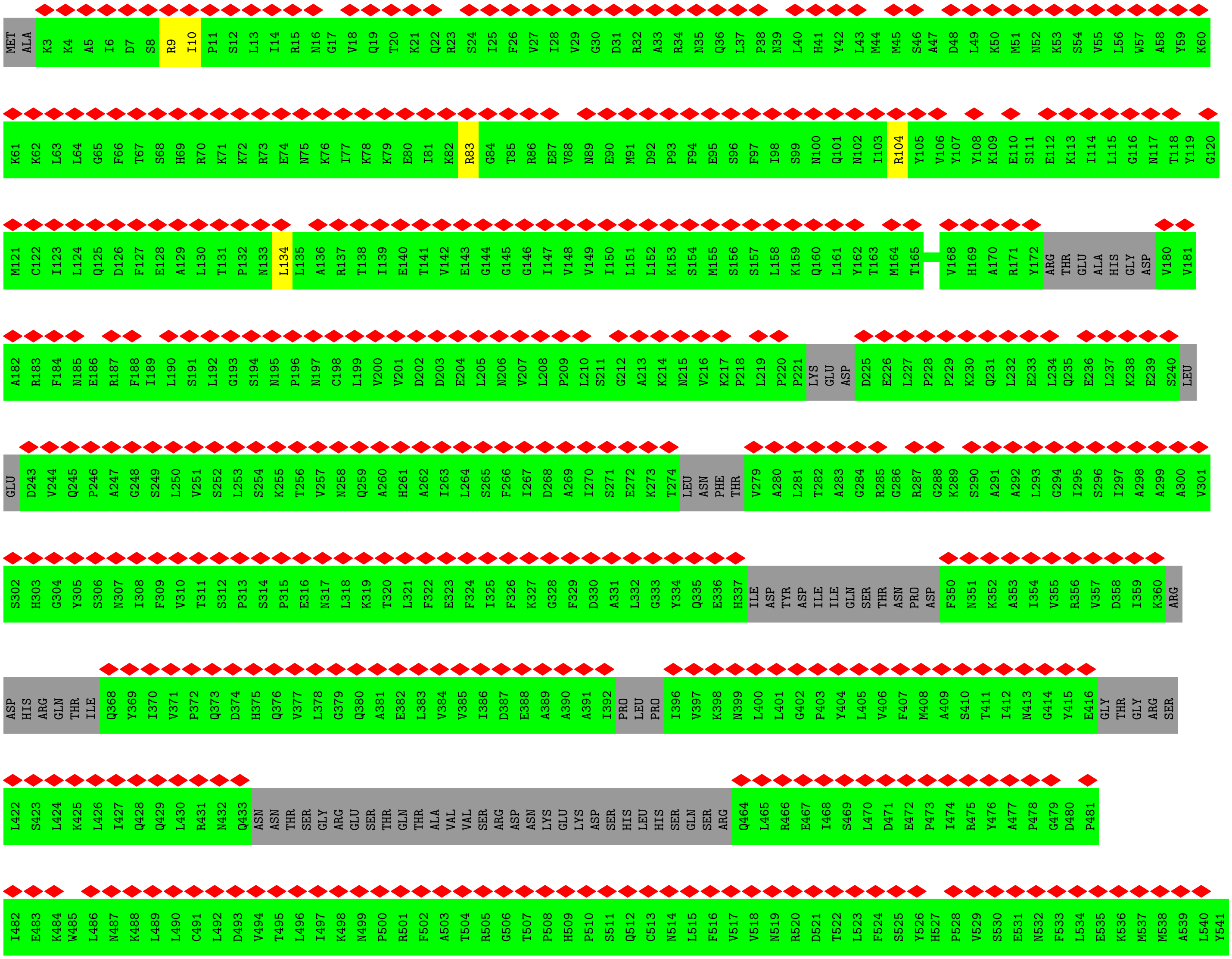


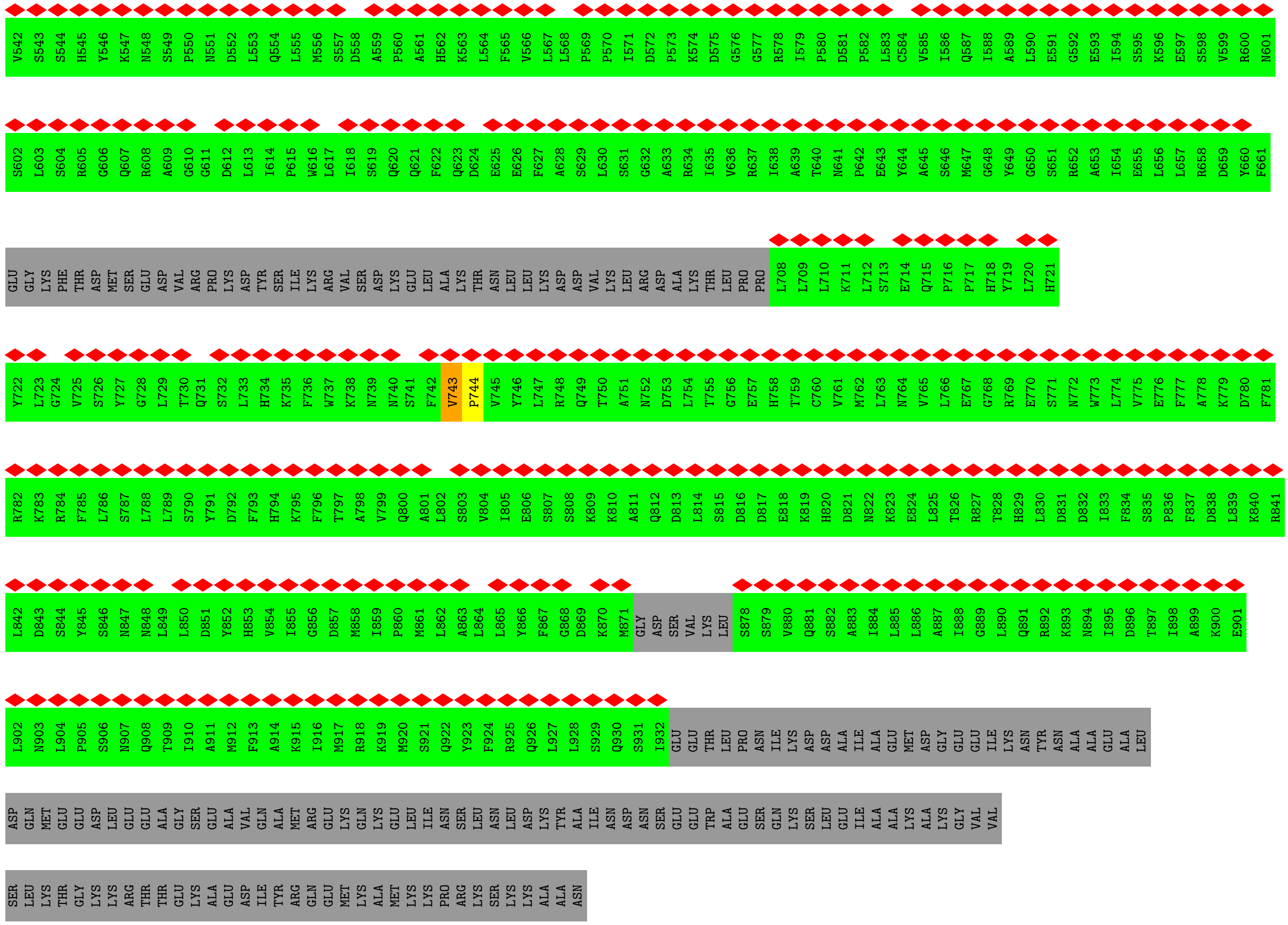
- Molecule 58: RNA 3'-terminal phosphate cyclase-like protein



- Molecule 59: RNA cytidine acetyltransferase

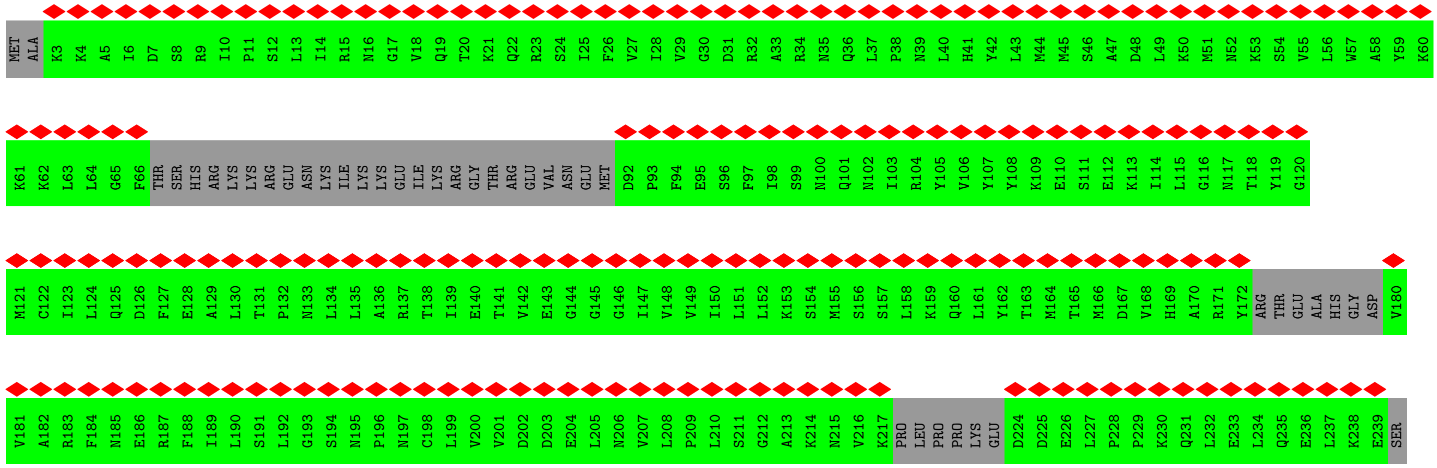


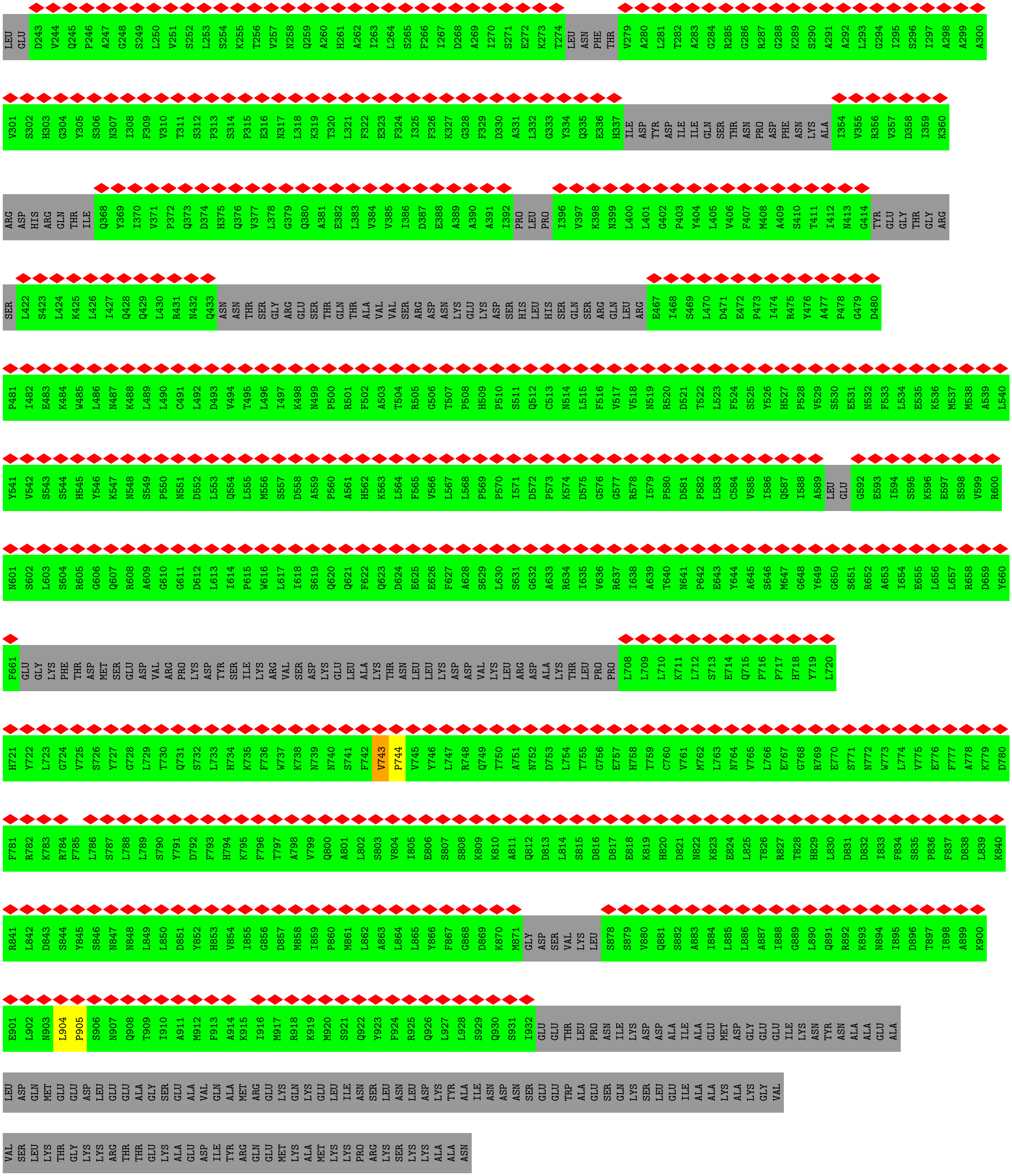




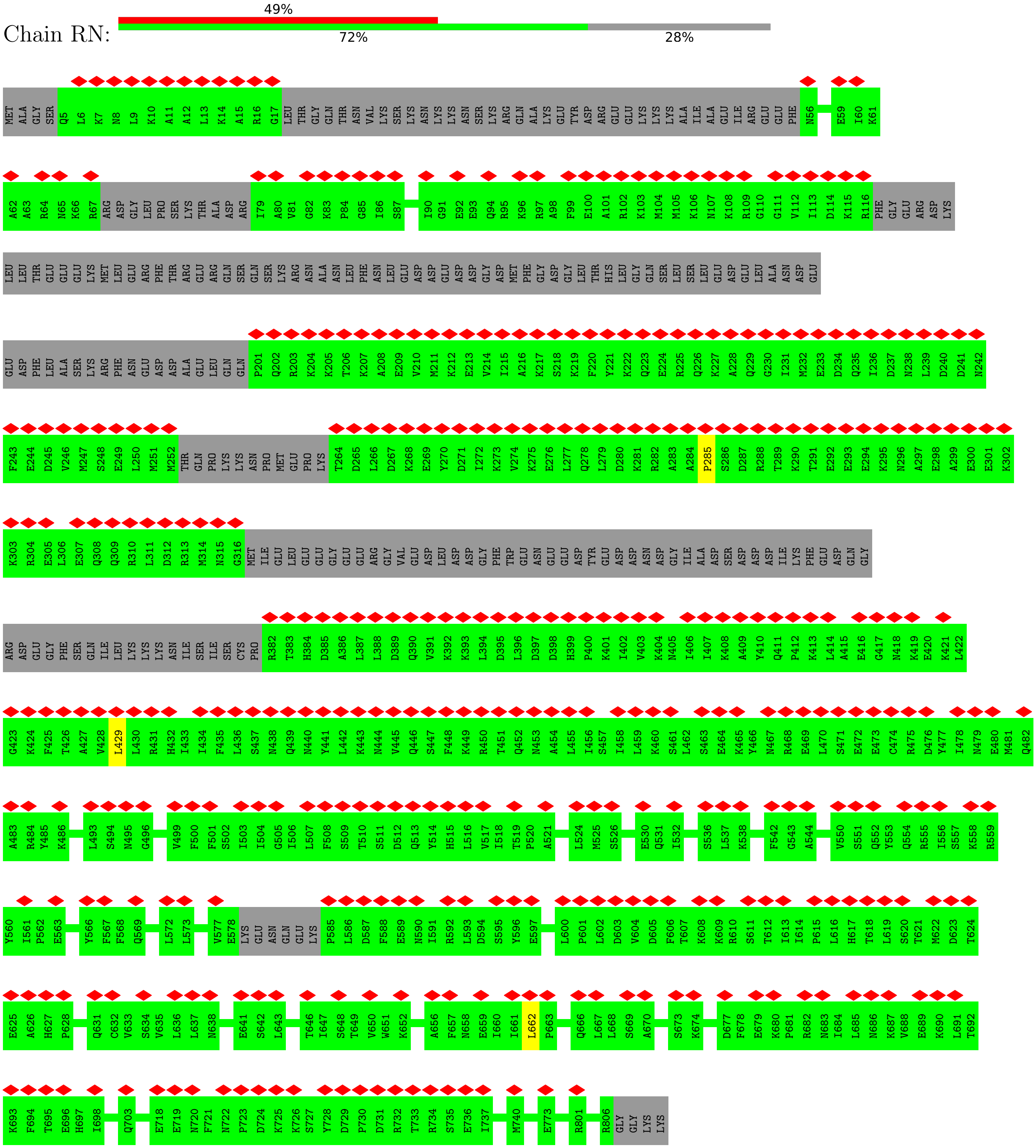
- Molecule 59: RNA cytidine acetyltransferase

Chain RM:

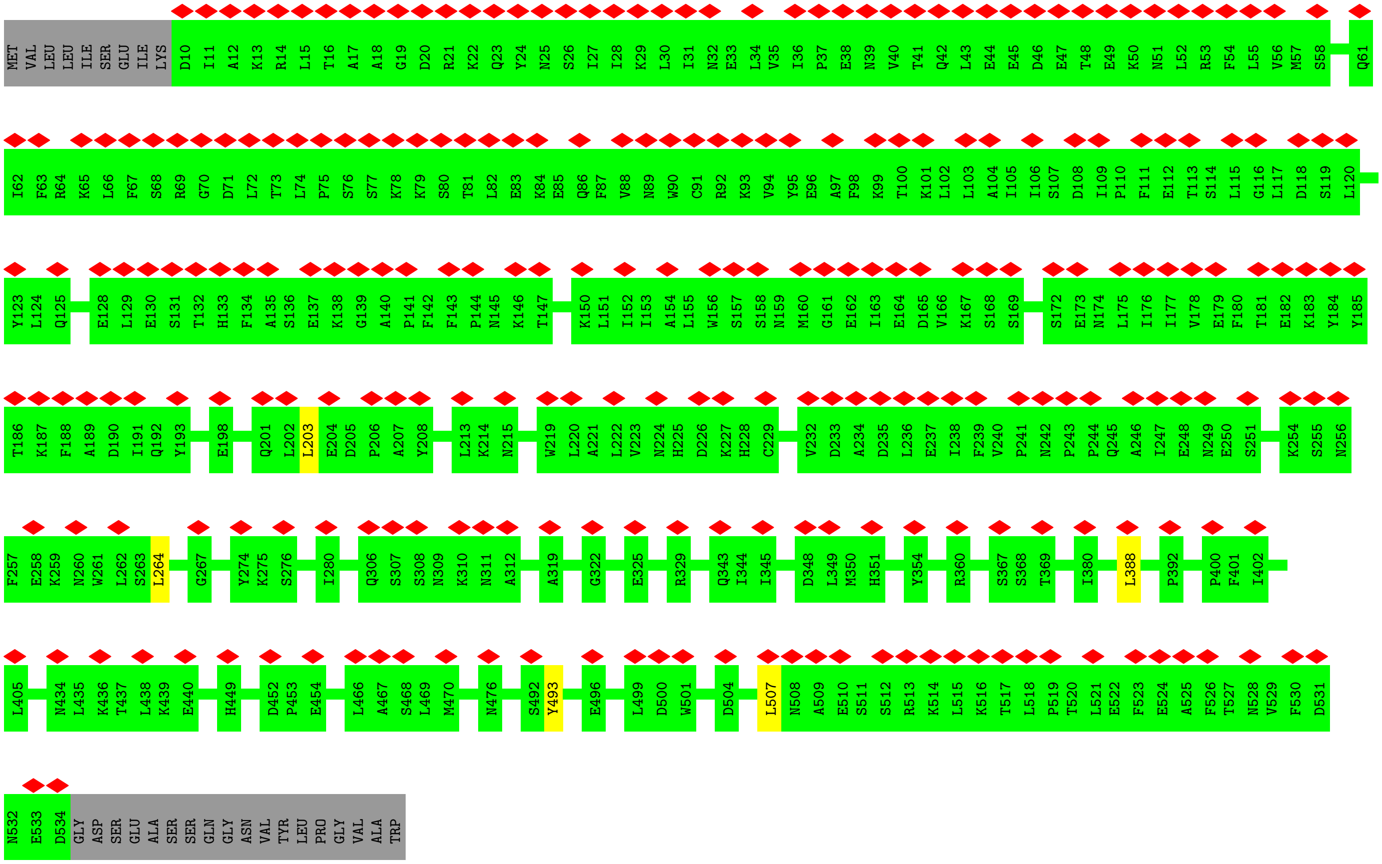




- Molecule 60: Nucleolar complex protein 14

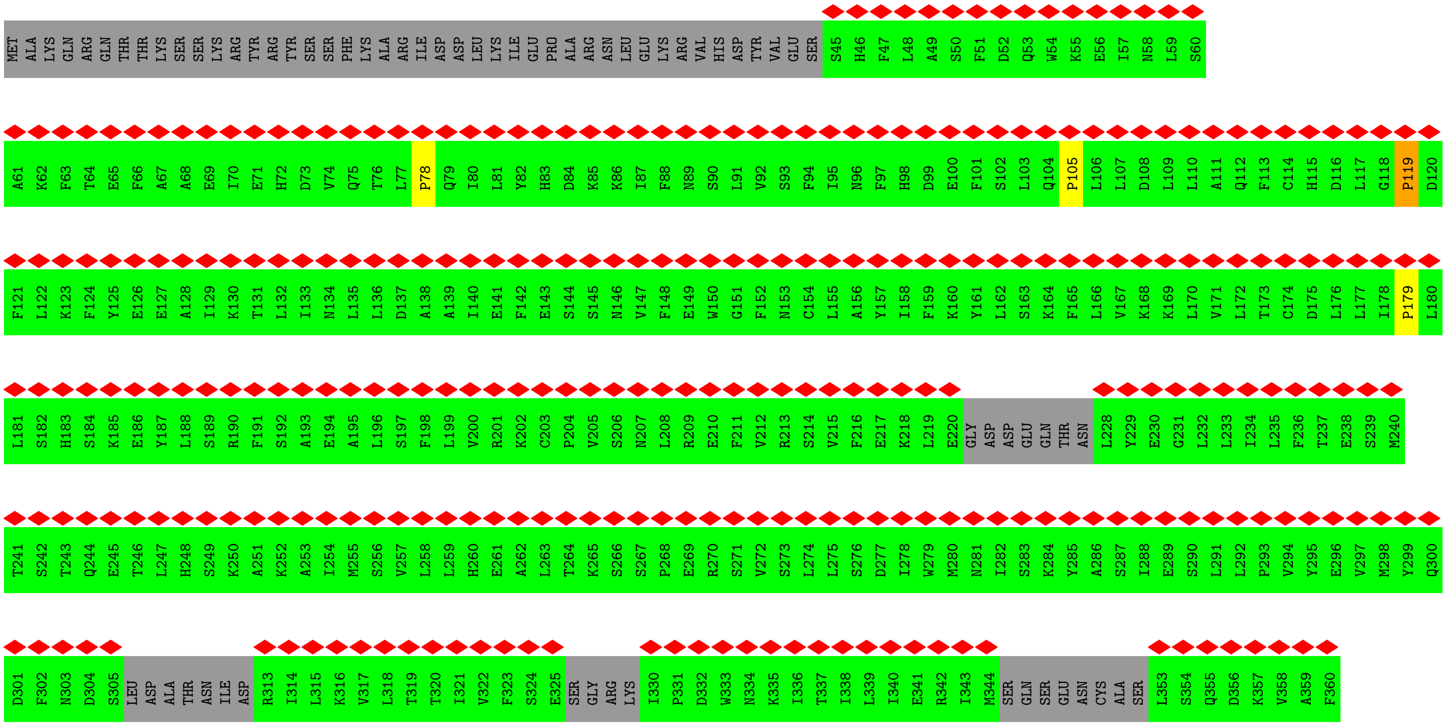


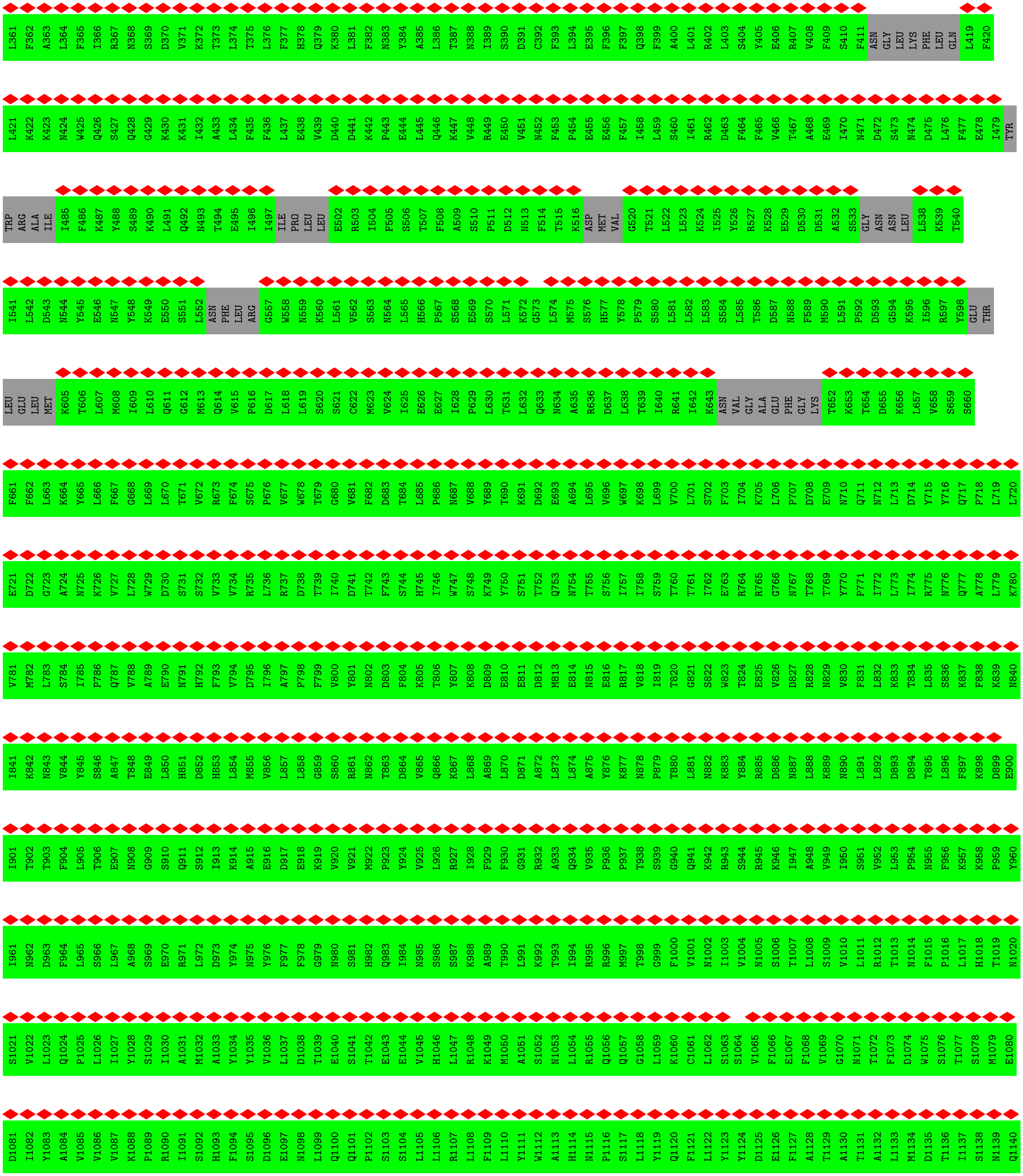
- Molecule 61: Nucleolar complex protein 4



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

Chain RP:

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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
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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
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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
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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
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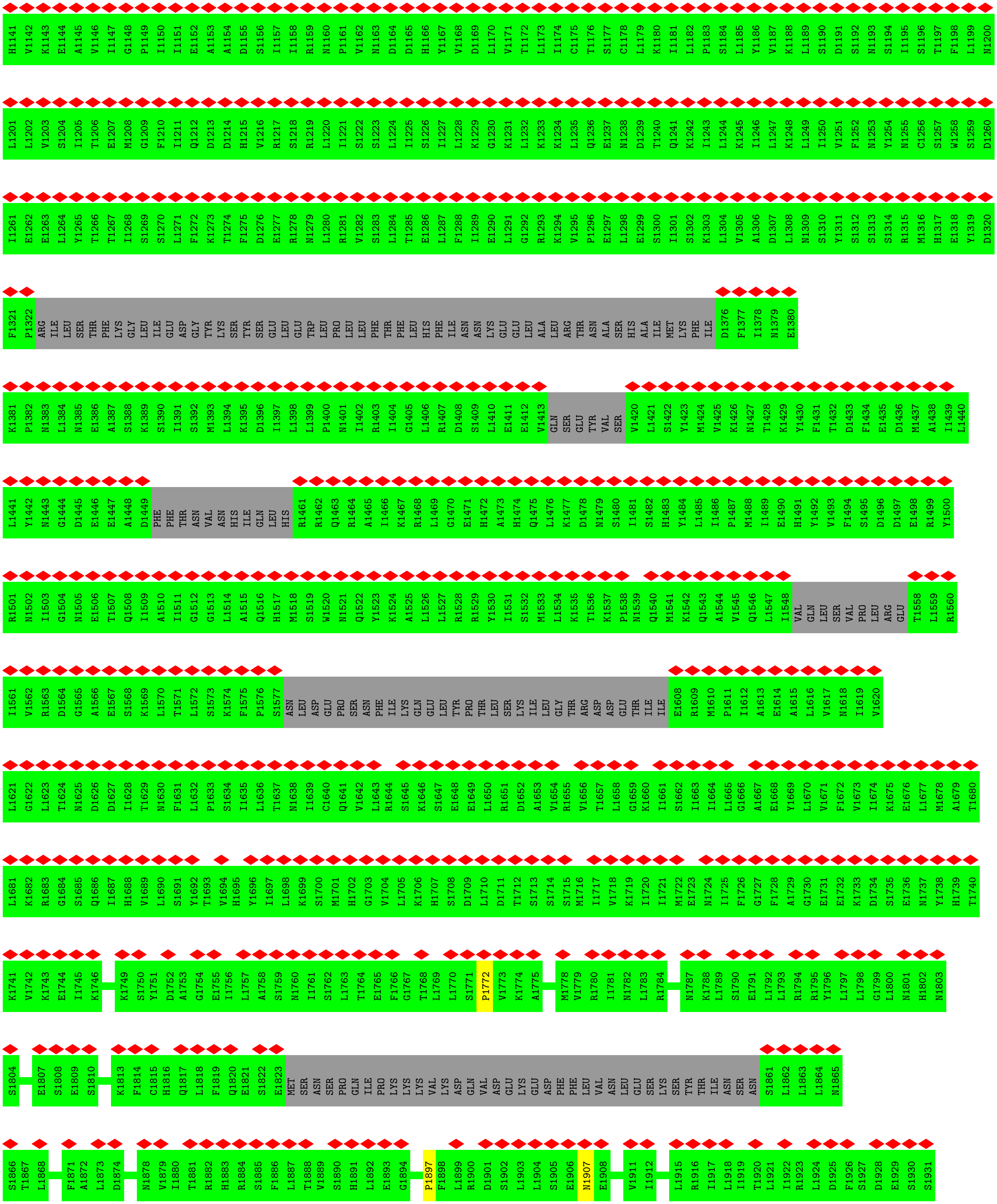
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I1261 E1262 E1263 L1264 Y1265 T1266 T1267 I1268 S1269 S1270 L1271 F1272 K1273 T1274 F1275 D1276 E1277 R1278 N1279 L1280 R1281 V1282 S1283 L1284 T1285 E1286 L1287 F1288 I1289 E1290 L1291 G1292 R1293 K1294 V1295 P1296 E1297 L1298 E1299 S1300 I1301 S1302 K1303 L1304 V1305 A1306 D1307 L1308 N1309 S1310 Y1311 S1312 S1313 S1314 R1315 M1316 H1317 E1318 Y1319 D1320
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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
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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 N1724 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
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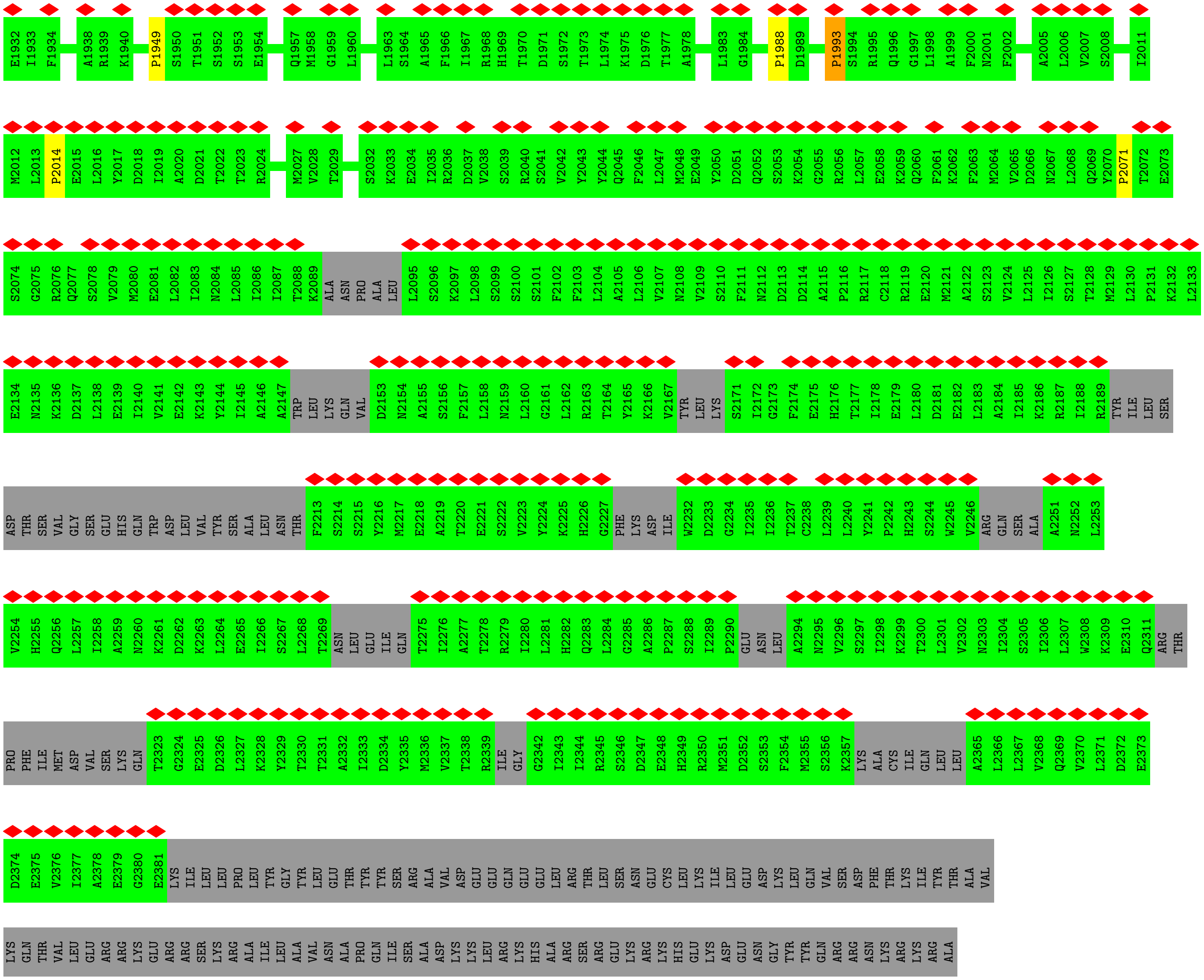
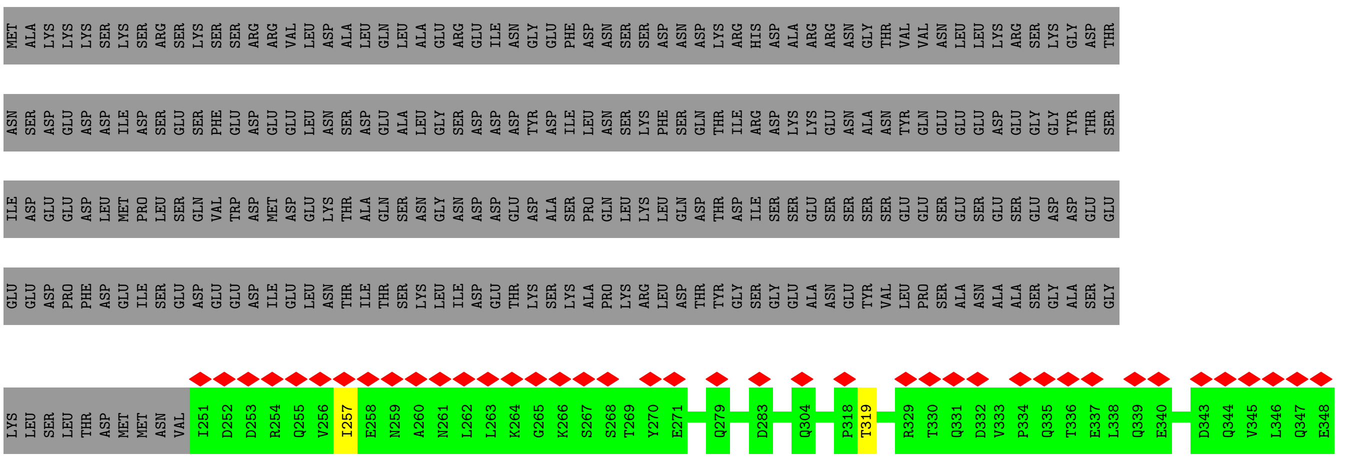
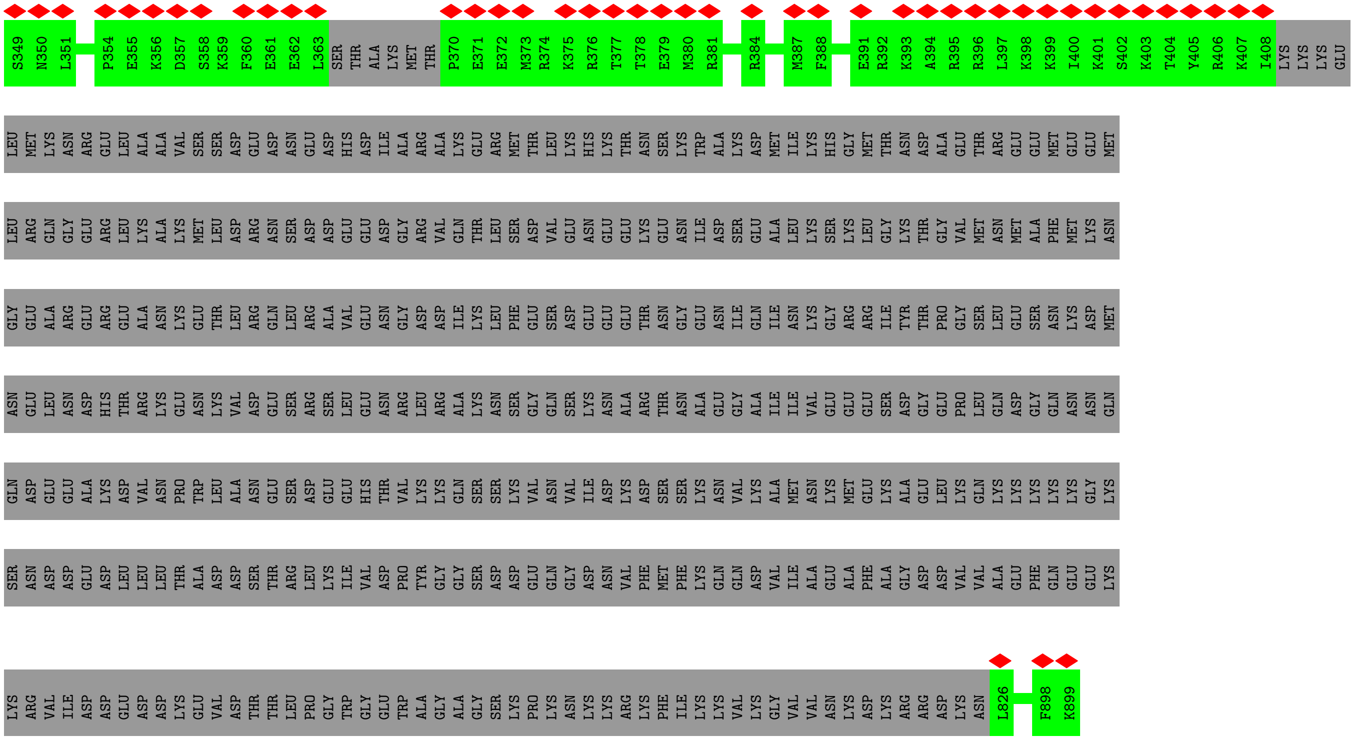
S1866 T1867 L1868 F1871 A1872 L1873 D1874 N1878 V1879 I1880 T1881 R1882 H1883 R1884 S1885 F1886 L1887 T1888 V1889 S1890 H1891 L1892 E1893 G1894 P1897 F1898 L1899 R1900 D1901 S1902 L1903 L1904 S1905 E1906 N1907 E1908 V1911 I1912 L1915 R1916 I1917 L1918 I1919 T1920 L1921 I1922 R1923 L1924 D1925 F1926 S1927 D1928 E1929 S1930 S1931



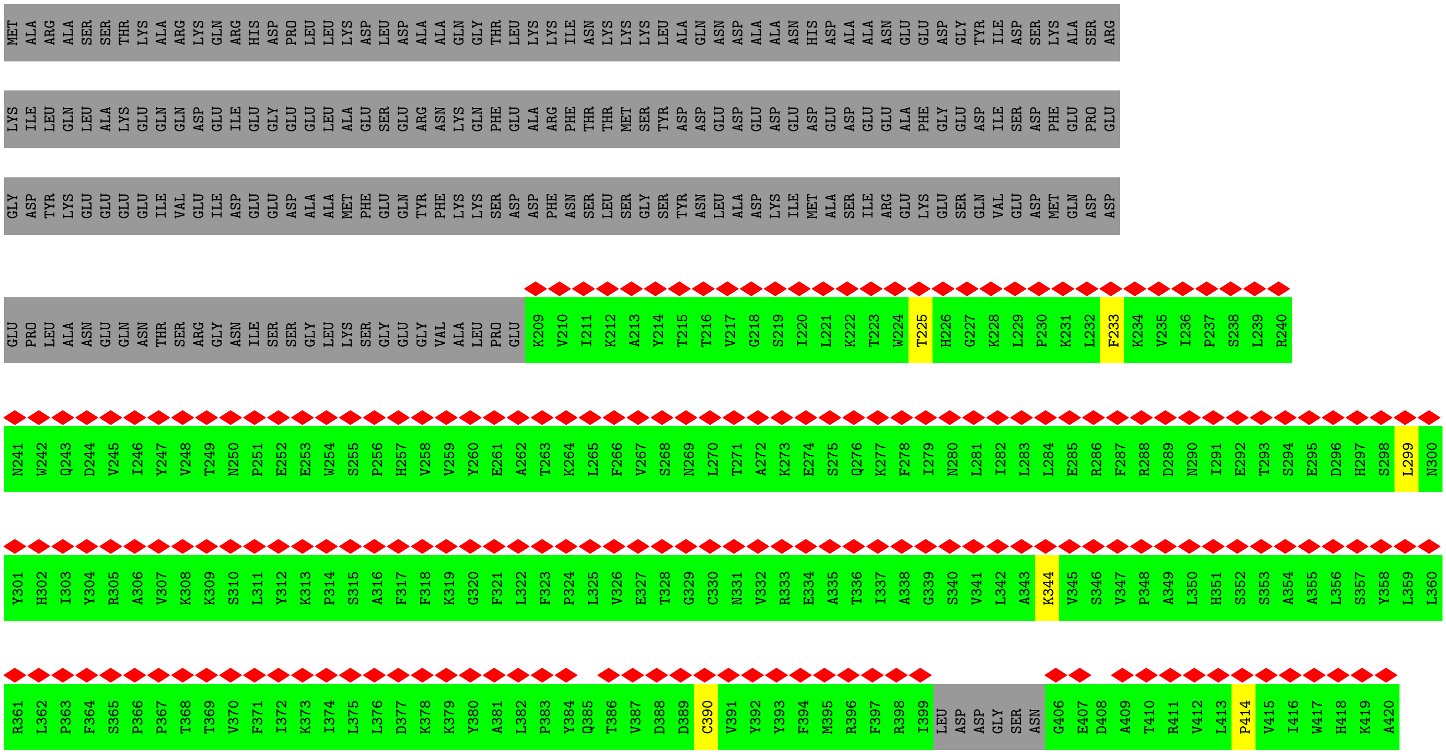
- Molecule 63: U3 small nucleolar RNA-associated protein 14

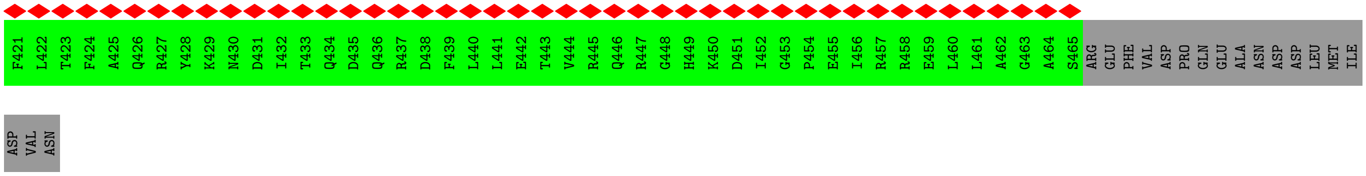
Chain RQ:



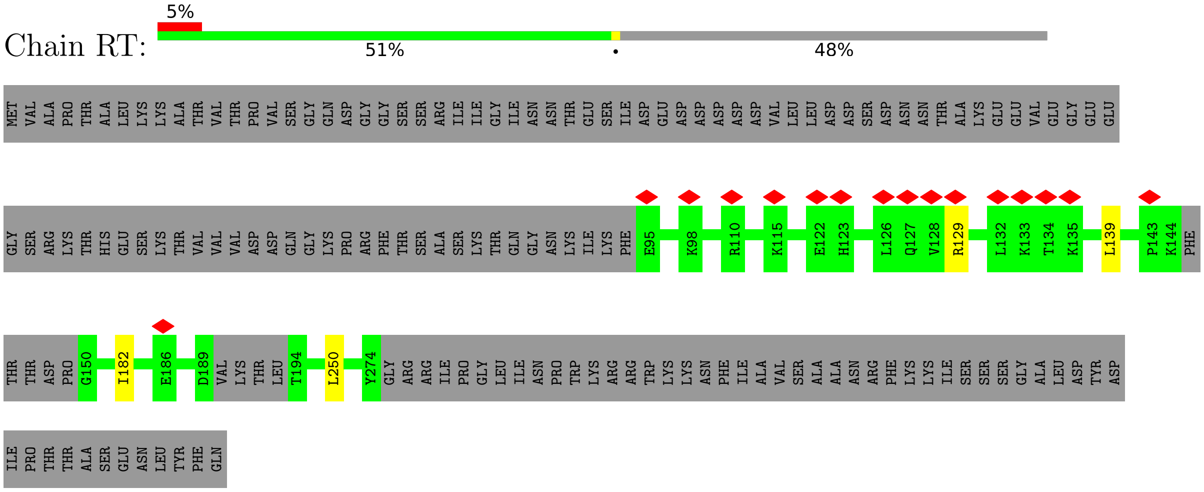


- Molecule 64: Essential nuclear protein 1

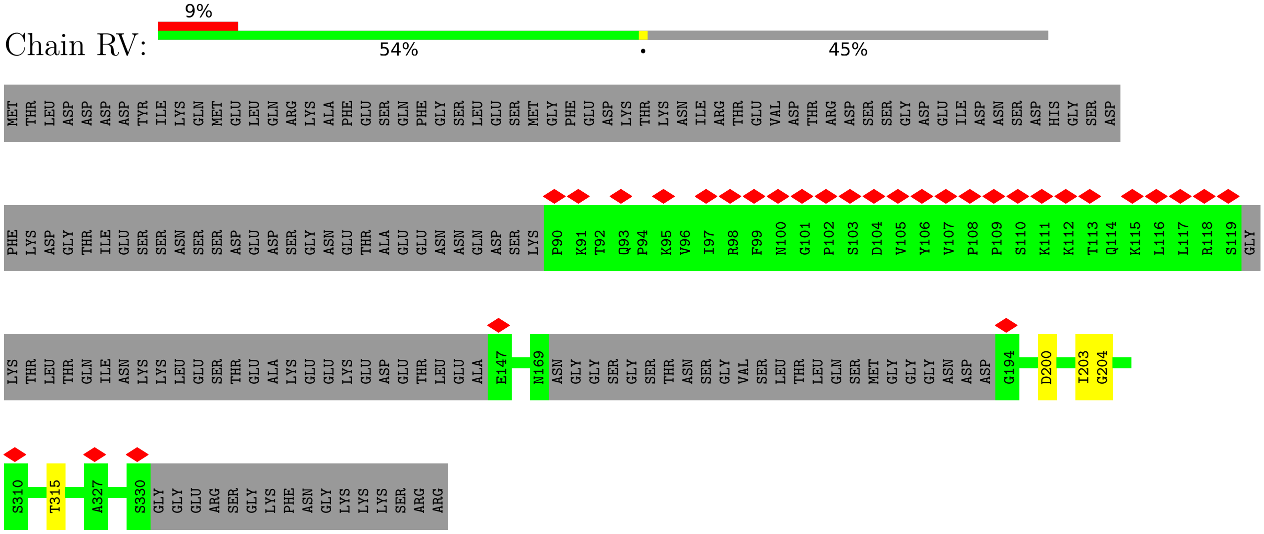




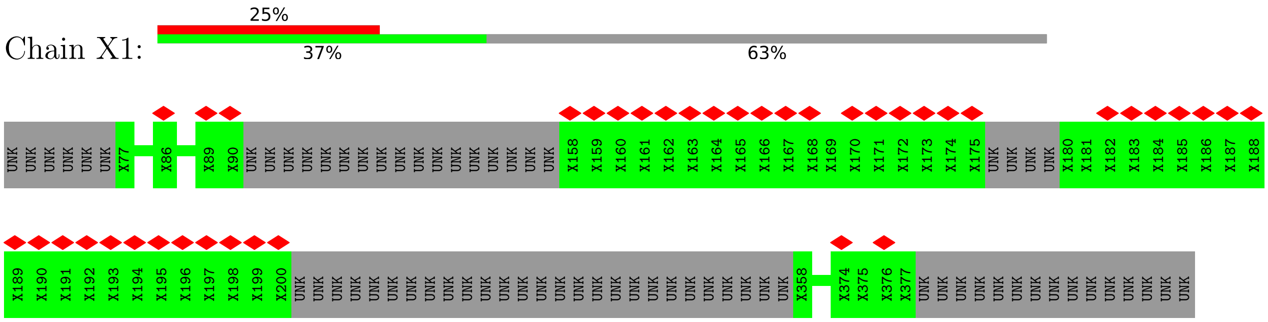
- Molecule 65: Pre-rRNA-processing protein PNO1

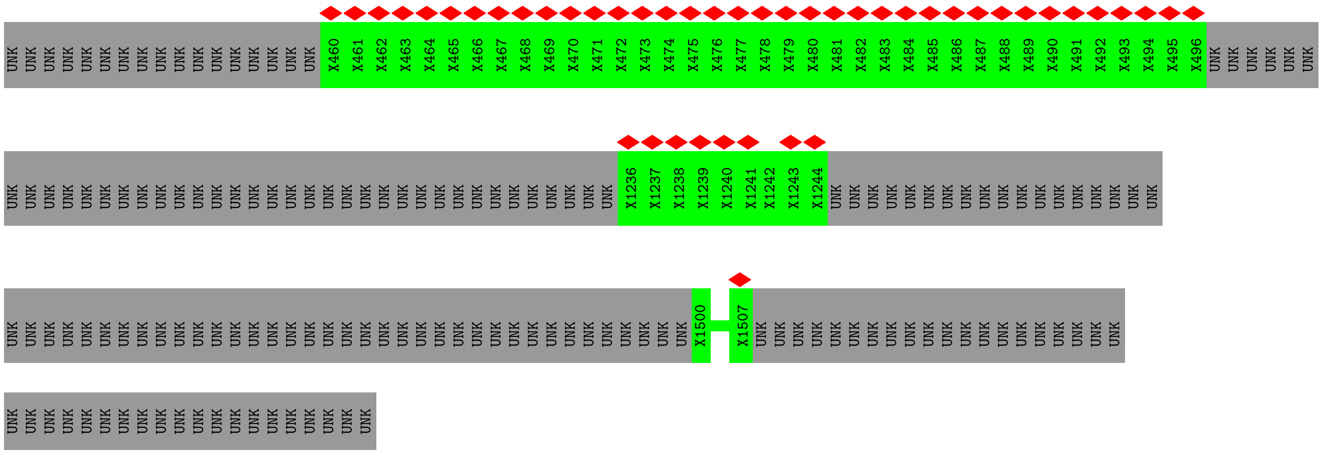


- Molecule 66: Protein FAF1



- Molecule 67: Unassigned helices

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X461
X462
X463
X464
X465
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X496
UNK
X1236
X1237
X1238
X1239
X1240
X1241
X1242
X1243
X1244
UNK
X1500
X1507
UNK

4 Experimental information ⓘ

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 $(e^-/\text{Å}^2)$	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 ⓘ

5.1 Standard geometry ⓘ

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.

All (494) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
3	SA	1451	C	N1-C2-O2	9.36	124.51	118.90
23	3D	283	ASP	CB-CG-OD1	9.26	126.64	118.30
3	SA	1451	C	N3-C2-O2	-9.26	115.42	121.90
2	5A	312	U	P-O3'-C3'	8.84	130.31	119.70
3	SA	1254	U	N1-C2-O2	8.78	128.95	122.80
3	SA	945	U	C5-C6-N1	8.63	127.01	122.70
3	SA	1174	C	N1-C2-O2	8.60	124.06	118.90
4	SC	54	LEU	CA-CB-CG	8.59	135.05	115.30
3	SA	864	U	N1-C2-O2	8.50	128.75	122.80
26	3G	65	LEU	CA-CB-CG	8.47	134.78	115.30
3	SA	864	U	N3-C2-O2	-8.37	116.34	122.20
53	RE	924	LEU	CA-CB-CG	8.35	134.51	115.30
3	SA	864	U	C2-N1-C1'	8.18	127.52	117.70
1	3A	72	C	C6-N1-C2	-8.18	117.03	120.30
1	3A	200	C	N1-C2-O2	8.10	123.76	118.90
2	5A	310	U	N1-C2-O2	8.00	128.40	122.80
3	SA	607	G	C4-N9-C1'	7.97	136.86	126.50
1	3A	89	C	C6-N1-C2	-7.95	117.12	120.30
3	SA	1034	C	C6-N1-C2	-7.91	117.14	120.30
2	5A	399	U	C5-C6-N1	7.91	126.65	122.70
3	SA	1518	C	N1-C2-O2	7.90	123.64	118.90
66	RV	200	ASP	CB-CG-OD1	7.86	125.37	118.30
3	SA	1269	U	N1-C2-O2	7.82	128.27	122.80
3	SA	1258	U	N1-C2-O2	7.77	128.24	122.80
1	3A	89	C	C2-N1-C1'	7.72	127.29	118.80
22	3B	306	LEU	CA-CB-CG	7.71	133.03	115.30
3	SA	172	C	N1-C2-O2	7.70	123.52	118.90
3	SA	354	C	C5-C6-N1	7.70	124.85	121.00
3	SA	1258	U	N3-C2-O2	-7.64	116.85	122.20
1	3A	72	C	C5-C6-N1	7.64	124.82	121.00
35	B2	757	ASP	CB-CG-OD1	7.63	125.17	118.30
3	SA	1177	C	C5-C6-N1	7.62	124.81	121.00
2	5A	523	U	C5-C6-N1	7.59	126.49	122.70
3	SA	1174	C	N3-C2-O2	-7.57	116.60	121.90
1	3A	75	C	C5-C6-N1	7.54	124.77	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	1665	U	N3-C2-O2	-7.52	116.94	122.20
2	5A	85	G	C5-C6-O6	-7.49	124.10	128.60
2	5A	173	G	P-O3'-C3'	7.49	128.69	119.70
3	SA	1441	C	C2-N1-C1'	7.49	127.04	118.80
2	5A	312	U	C2-N1-C1'	-7.48	108.72	117.70
3	SA	161	U	N3-C2-O2	-7.46	116.98	122.20
19	SZ	74	LEU	CA-CB-CG	7.45	132.43	115.30
3	SA	1760	G	N3-C4-N9	7.43	130.46	126.00
3	SA	405	C	C6-N1-C2	-7.42	117.33	120.30
3	SA	405	C	C2-N1-C1'	7.40	126.94	118.80
3	SA	1674	C	C5-C6-N1	7.35	124.67	121.00
3	SA	1174	C	C2-N1-C1'	7.34	126.87	118.80
15	SR	123	ARG	C-N-CD	-7.33	104.48	120.60
2	5A	219	U	C5-C6-N1	7.33	126.36	122.70
3	SA	172	C	N3-C2-O2	-7.31	116.78	121.90
3	SA	1175	U	N1-C2-O2	7.31	127.92	122.80
3	SA	1760	G	N3-C4-C5	-7.27	124.97	128.60
3	SA	1269	U	C2-N1-C1'	7.26	126.42	117.70
7	SH	68	LEU	CA-CB-CG	7.23	131.94	115.30
3	SA	883	C	C5-C6-N1	7.23	124.62	121.00
38	BE	536	LEU	CA-CB-CG	7.22	131.91	115.30
3	SA	644	C	C5-C6-N1	7.21	124.61	121.00
3	SA	1568	C	N1-C2-O2	7.20	123.22	118.90
60	RN	662	LEU	CA-CB-CG	7.19	131.84	115.30
3	SA	357	G	N3-C4-N9	-7.18	121.69	126.00
3	SA	381	C	N3-C2-O2	-7.17	116.89	121.90
3	SA	1440	C	N1-C2-O2	7.16	123.20	118.90
3	SA	1674	C	C6-N1-C2	-7.15	117.44	120.30
2	5A	111	C	C2-N1-C1'	7.15	126.67	118.80
3	SA	1254	U	C6-N1-C1'	-7.13	111.21	121.20
3	SA	1518	C	C2-N1-C1'	7.10	126.61	118.80
3	SA	258	C	N1-C2-O2	7.10	123.16	118.90
33	AG	601	LEU	CA-CB-CG	7.10	131.62	115.30
2	5A	111	C	C6-N1-C2	-7.08	117.47	120.30
2	5A	61	U	N3-C2-O2	-7.08	117.25	122.20
3	SA	1711	C	N3-C2-O2	-7.06	116.96	121.90
3	SA	405	C	C5-C6-N1	7.03	124.51	121.00
3	SA	1518	C	N3-C2-O2	-7.02	116.98	121.90
2	5A	91	U	C5-C6-N1	7.01	126.20	122.70
3	SA	381	C	N1-C2-O2	7.00	123.10	118.90
3	SA	883	C	C6-N1-C2	-6.98	117.51	120.30
3	SA	1126	G	C4-N9-C1'	6.97	135.56	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	3D	142	LEU	CA-CB-CG	6.96	131.30	115.30
3	SA	361	C	N1-C2-O2	6.94	123.06	118.90
3	SA	1254	U	N3-C2-O2	-6.93	117.35	122.20
3	SA	128	U	C2-N1-C1'	6.90	125.98	117.70
41	5C	74	LEU	CA-CB-CG	6.90	131.17	115.30
3	SA	272	U	P-O3'-C3'	6.88	127.96	119.70
3	SA	161	U	N1-C2-O2	6.88	127.61	122.80
1	3A	200	C	C2-N1-C1'	6.87	126.36	118.80
1	3A	201	C	N1-C2-O2	6.85	123.01	118.90
2	5A	219	U	C2-N1-C1'	6.85	125.92	117.70
28	A5	540	LEU	CA-CB-CG	6.83	131.02	115.30
3	SA	1584	G	C4-N9-C1'	-6.82	117.64	126.50
3	SA	579	A	P-O3'-C3'	6.82	127.88	119.70
3	SA	679	U	C5-C6-N1	6.80	126.10	122.70
41	5C	144	LEU	CA-CB-CG	6.79	130.93	115.30
34	B1	701	LEU	CA-CB-CG	6.79	130.92	115.30
3	SA	1175	U	N3-C2-O2	-6.79	117.45	122.20
3	SA	1053	G	O5'-P-OP1	-6.79	99.59	105.70
1	3A	43	C	C5-C6-N1	6.77	124.39	121.00
3	SA	298	C	C5-C6-N1	6.77	124.39	121.00
3	SA	1664	C	C5-C6-N1	6.76	124.38	121.00
2	5A	90	G	C8-N9-C1'	6.73	135.75	127.00
3	SA	607	G	C8-N9-C1'	-6.73	118.25	127.00
2	5A	358	G	P-O3'-C3'	6.72	127.77	119.70
24	3E	141	LEU	CA-CB-CG	6.72	130.75	115.30
2	5A	252	A	C2-N3-C4	6.72	113.96	110.60
2	5A	172	C	N1-C2-O2	6.69	122.91	118.90
2	5A	399	U	C2-N1-C1'	6.68	125.72	117.70
3	SA	1072	C	C5-C6-N1	6.68	124.34	121.00
3	SA	1258	U	C2-N1-C1'	6.65	125.68	117.70
3	SA	1664	C	C2-N1-C1'	6.64	126.11	118.80
3	SA	1646	C	N1-C2-O2	6.64	122.88	118.90
3	SA	1772	C	C2-N1-C1'	6.64	126.10	118.80
3	SA	258	C	C2-N1-C1'	6.63	126.10	118.80
3	SA	354	C	C6-N1-C2	-6.63	117.65	120.30
3	SA	368	U	C5-C6-N1	6.61	126.01	122.70
3	SA	1441	C	C5-C6-N1	6.61	124.30	121.00
3	SA	1451	C	C6-N1-C2	-6.60	117.66	120.30
2	5A	61	U	N1-C2-O2	6.58	127.41	122.80
44	5F	61	LEU	CA-CB-CG	6.57	130.41	115.30
3	SA	1664	C	C6-N1-C2	-6.57	117.67	120.30
3	SA	607	G	N3-C4-C5	-6.56	125.32	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	861	U	C2-N1-C1'	6.56	125.57	117.70
19	SZ	40	LEU	CB-CG-CD1	-6.54	99.87	111.00
3	SA	894	U	N1-C2-O2	6.54	127.38	122.80
3	SA	107	C	C6-N1-C2	-6.54	117.68	120.30
3	SA	64	U	C5-C6-N1	6.54	125.97	122.70
3	SA	514	G	N7-C8-N9	6.53	116.36	113.10
2	5A	90	G	C4-N9-C1'	-6.52	118.03	126.50
3	SA	1174	C	C6-N1-C2	-6.51	117.69	120.30
3	SA	1772	C	N1-C2-O2	6.51	122.81	118.90
3	SA	1441	C	C6-N1-C2	-6.51	117.70	120.30
2	5A	90	G	O4'-C1'-N9	6.50	113.40	108.20
3	SA	1126	G	N3-C4-N9	6.48	129.89	126.00
1	3A	63	C	C5-C6-N1	6.44	124.22	121.00
2	5A	85	G	C4-C5-N7	6.43	113.37	110.80
28	A5	457	LEU	CA-CB-CG	6.43	130.09	115.30
3	SA	1055	U	N1-C2-O2	6.42	127.30	122.80
3	SA	1254	U	C5-C6-N1	6.42	125.91	122.70
53	RE	303	PHE	C-N-CA	6.42	137.76	121.70
3	SA	401	A	P-O3'-C3'	6.42	127.40	119.70
3	SA	1084	A	P-O3'-C3'	6.42	127.40	119.70
3	SA	1760	G	C4-N9-C1'	6.42	134.84	126.50
62	RP	1949	PRO	N-CA-CB	6.40	110.98	103.30
55	RG	50	LEU	CA-CB-CG	6.39	130.00	115.30
26	3G	67	LEU	CA-CB-CG	6.39	130.00	115.30
24	3E	401	LEU	CA-CB-CG	6.37	129.95	115.30
3	SA	1031	U	P-O3'-C3'	6.36	127.33	119.70
37	B8	521	LEU	CA-CB-CG	6.36	129.92	115.30
3	SA	290	G	C4-N9-C1'	6.35	134.76	126.50
3	SA	1620	C	N3-C2-O2	-6.35	117.46	121.90
3	SA	1677	C	N1-C2-O2	6.34	122.71	118.90
3	SA	607	G	N3-C4-N9	6.34	129.80	126.00
3	SA	1585	U	C5-C6-N1	6.34	125.87	122.70
22	3C	306	LEU	CA-CB-CG	6.34	129.87	115.30
3	SA	56	U	P-O3'-C3'	6.33	127.30	119.70
1	3A	75	C	C6-N1-C2	-6.33	117.77	120.30
3	SA	657	U	N1-C2-O2	6.32	127.22	122.80
28	A5	151	LEU	CA-CB-CG	6.31	129.81	115.30
41	5C	148	LEU	CA-CB-CG	6.31	129.81	115.30
3	SA	514	G	C8-N9-C4	-6.30	103.88	106.40
3	SA	1056	U	N1-C2-O2	6.30	127.21	122.80
4	SC	172	LEU	CA-CB-CG	6.30	129.79	115.30
4	SC	120	LEU	CA-CB-CG	6.27	129.73	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5A	422	C	C2-N1-C1'	6.27	125.70	118.80
1	3A	198	U	P-O3'-C3'	6.25	127.20	119.70
3	SA	1126	G	C8-N9-C1'	-6.25	118.88	127.00
31	AE	315	LEU	CA-CB-CG	6.24	129.65	115.30
34	B1	717	LEU	CA-CB-CG	6.24	129.65	115.30
3	SA	373	G	C4-N9-C1'	6.23	134.60	126.50
1	3A	201	C	C5-C6-N1	6.23	124.11	121.00
3	SA	107	C	C5-C6-N1	6.22	124.11	121.00
2	5A	111	C	C5-C6-N1	6.21	124.10	121.00
3	SA	357	G	C5-C6-O6	6.20	132.32	128.60
48	5J	81	VAL	C-N-CA	6.20	137.20	121.70
3	SA	1033	C	O4'-C1'-N1	6.19	113.15	108.20
3	SA	1665	U	N1-C2-O2	6.19	127.13	122.80
2	5A	390	C	C5-C6-N1	6.18	124.09	121.00
3	SA	1055	U	C2-N1-C1'	6.18	125.11	117.70
27	A4	563	LEU	CA-CB-CG	6.17	129.50	115.30
45	5G	152	LEU	CA-CB-CG	6.16	129.47	115.30
1	3A	102	U	N3-C2-O2	-6.15	117.89	122.20
3	SA	873	U	N3-C2-O2	-6.15	117.89	122.20
3	SA	368	U	C5-C4-O4	-6.15	122.21	125.90
37	B8	22	LEU	CA-CB-CG	6.14	129.43	115.30
3	SA	1584	G	C8-N9-C1'	6.14	134.98	127.00
1	3A	248	G	P-O3'-C3'	6.14	127.07	119.70
3	SA	1052	U	O4'-C1'-N1	6.13	113.11	108.20
3	SA	417	A	P-O3'-C3'	6.12	127.04	119.70
2	5A	263	C	C5-C6-N1	6.11	124.06	121.00
3	SA	1269	U	N3-C2-O2	-6.11	117.93	122.20
2	5A	312	U	OP1-P-O3'	6.08	118.59	105.20
42	5D	224	LEU	CB-CG-CD2	-6.08	100.67	111.00
3	SA	648	G	C4-N9-C1'	6.06	134.38	126.50
3	SA	1760	G	C2-N3-C4	6.05	114.93	111.90
3	SA	530	C	N1-C2-O2	6.04	122.53	118.90
38	BE	522	LEU	CA-CB-CG	6.04	129.20	115.30
33	AG	323	LEU	CA-CB-CG	6.04	129.19	115.30
3	SA	1711	C	N1-C2-O2	6.03	122.52	118.90
38	BE	614	LEU	CA-CB-CG	6.03	129.17	115.30
2	5A	368	U	P-O3'-C3'	6.02	126.93	119.70
2	5A	7	A	O4'-C1'-N9	6.01	113.01	108.20
9	SJ	29	LEU	CA-CB-CG	5.99	129.08	115.30
23	3D	292	LEU	CA-CB-CG	5.99	129.07	115.30
1	3A	248	G	OP1-P-O3'	5.98	118.37	105.20
3	SA	1620	C	N1-C2-O2	5.97	122.48	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	1568	C	N3-C2-O2	-5.97	117.72	121.90
2	5A	312	U	N1-C1'-C2'	5.97	121.75	114.00
34	B1	603	LEU	CA-CB-CG	5.96	129.02	115.30
3	SA	1072	C	C6-N1-C2	-5.95	117.92	120.30
2	5A	172	C	P-O3'-C3'	5.93	126.82	119.70
18	SY	132	LEU	CA-CB-CG	5.93	128.95	115.30
3	SA	290	G	N3-C4-N9	5.93	129.56	126.00
3	SA	1439	C	C5-C6-N1	5.93	123.97	121.00
3	SA	311	U	C2-N1-C1'	5.93	124.81	117.70
27	A4	611	LEU	CA-CB-CG	5.92	128.93	115.30
1	3A	201	C	C2-N1-C1'	5.92	125.31	118.80
2	5A	219	U	N1-C2-O2	5.90	126.93	122.80
61	RO	388	LEU	CA-CB-CG	5.90	128.87	115.30
2	5A	393	C	O5'-P-OP1	-5.89	100.40	105.70
3	SA	1078	C	C5-C6-N1	5.88	123.94	121.00
3	SA	1080	U	N3-C2-O2	-5.87	118.09	122.20
25	3F	348	LEU	CA-CB-CG	5.87	128.80	115.30
2	5A	369	G	O5'-P-OP1	-5.86	100.43	105.70
38	BE	417	LEU	CA-CB-CG	5.86	128.77	115.30
1	3A	89	C	C5-C6-N1	5.85	123.93	121.00
3	SA	1769	U	N3-C2-O2	-5.85	118.10	122.20
3	SA	361	C	C2-N1-C1'	5.85	125.24	118.80
1	3A	102	U	N1-C2-O2	5.85	126.89	122.80
3	SA	280	U	N1-C2-O2	5.85	126.89	122.80
3	SA	280	U	C2-N1-C1'	5.84	124.71	117.70
3	SA	1177	C	C6-N1-C2	-5.84	117.97	120.30
34	B1	69	LEU	CA-CB-CG	5.83	128.72	115.30
2	5A	90	G	N9-C4-C5	5.82	107.73	105.40
3	SA	298	C	C6-N1-C2	-5.82	117.97	120.30
1	3A	61	G	C2-N3-C4	5.82	114.81	111.90
2	5A	311	C	O4'-C1'-N1	5.80	112.84	108.20
3	SA	1760	G	P-O3'-C3'	5.80	126.66	119.70
27	A4	416	LEU	CA-CB-CG	5.80	128.64	115.30
65	RT	250	LEU	CA-CB-CG	5.80	128.64	115.30
3	SA	657	U	C2-N1-C1'	5.80	124.66	117.70
1	3A	201	C	C6-N1-C2	-5.79	117.98	120.30
36	B3	620	LEU	CA-CB-CG	5.79	128.62	115.30
3	SA	1439	C	C6-N1-C2	-5.77	117.99	120.30
5	SF	42	LEU	CA-CB-CG	5.76	128.56	115.30
3	SA	1585	U	C2-N1-C1'	5.76	124.61	117.70
3	SA	1521	G	P-O3'-C3'	5.76	126.61	119.70
3	SA	1594	G	O4'-C1'-N9	5.76	112.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	909	U	N3-C2-O2	-5.75	118.17	122.20
1	3A	203	U	N1-C2-O2	5.75	126.82	122.80
3	SA	290	G	N3-C4-C5	-5.74	125.73	128.60
3	SA	545	A	O4'-C1'-N9	5.74	112.79	108.20
3	SA	1646	C	C5-C6-N1	5.74	123.87	121.00
27	A4	225	LEU	CA-CB-CG	5.74	128.50	115.30
3	SA	1191	U	N1-C2-O2	5.74	126.82	122.80
3	SA	1083	G	C4-N9-C1'	5.74	133.96	126.50
2	5A	65	U	N3-C2-O2	-5.72	118.20	122.20
62	RP	2071	PRO	N-CA-CB	5.72	110.16	103.30
45	5G	13	LEU	CA-CB-CG	5.72	128.45	115.30
62	RP	78	PRO	N-CA-CB	5.71	110.16	103.30
3	SA	1037	C	C6-N1-C2	-5.71	118.02	120.30
3	SA	965	U	C2-N1-C1'	5.71	124.55	117.70
44	5F	67	THR	C-N-CA	-5.70	107.45	121.70
3	SA	1769	U	N1-C2-O2	5.70	126.79	122.80
3	SA	1675	C	N1-C2-O2	5.69	122.32	118.90
2	5A	390	C	C6-N1-C2	-5.68	118.03	120.30
3	SA	1759	C	C6-N1-C2	-5.68	118.03	120.30
3	SA	1760	G	C8-N9-C1'	-5.68	119.61	127.00
3	SA	657	U	N3-C2-O2	-5.68	118.22	122.20
3	SA	945	U	C6-N1-C2	-5.67	117.60	121.00
3	SA	1594	G	P-O3'-C3'	5.67	126.51	119.70
2	5A	543	C	C6-N1-C2	-5.67	118.03	120.30
3	SA	542	A	P-O3'-C3'	5.67	126.50	119.70
3	SA	1053	G	C8-N9-C4	-5.67	104.13	106.40
3	SA	1440	C	C2-N1-C1'	5.66	125.03	118.80
57	RJ	845	LEU	CA-CB-CG	5.66	128.31	115.30
2	5A	312	U	C6-N1-C1'	5.66	129.12	121.20
54	RF	58	LEU	CA-CB-CG	5.65	128.30	115.30
3	SA	870	C	C6-N1-C2	-5.65	118.04	120.30
3	SA	1222	C	C5-C6-N1	5.65	123.82	121.00
3	SA	1743	U	C2-N1-C1'	5.64	124.47	117.70
3	SA	1078	C	C6-N1-C2	-5.64	118.05	120.30
62	RP	2014	PRO	N-CA-CB	5.63	110.06	103.30
2	5A	537	G	N3-C4-N9	5.63	129.38	126.00
3	SA	1275	A	C2-N3-C4	5.63	113.42	110.60
62	RP	179	PRO	N-CA-CB	5.63	110.06	103.30
39	B6	18	LEU	CA-CB-CG	5.63	128.25	115.30
3	SA	128	U	N1-C2-O2	5.62	126.74	122.80
3	SA	1665	U	C2-N1-C1'	5.62	124.44	117.70
62	RP	119	PRO	N-CA-CB	5.62	110.04	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	1734	U	N3-C2-O2	-5.62	118.27	122.20
34	B1	29	LEU	CA-CB-CG	5.62	128.22	115.30
37	B8	164	LEU	CA-CB-CG	5.61	128.21	115.30
32	AF	195	LEU	CA-CB-CG	5.61	128.20	115.30
3	SA	1037	C	N1-C2-O2	5.61	122.26	118.90
62	RP	1988	PRO	N-CA-CB	5.61	110.03	103.30
1	3A	89	C	N1-C2-O2	5.60	122.26	118.90
3	SA	405	C	N1-C2-O2	5.60	122.26	118.90
3	SA	894	U	N3-C2-O2	-5.60	118.28	122.20
43	5E	314	LEU	CA-CB-CG	5.60	128.17	115.30
3	SA	311	U	N1-C2-O2	5.59	126.71	122.80
3	SA	607	G	C2-N3-C4	5.59	114.69	111.90
2	5A	492	G	P-O3'-C3'	5.58	126.39	119.70
2	5A	7	A	C8-N9-C4	-5.57	103.57	105.80
3	SA	373	G	N3-C4-C5	-5.57	125.82	128.60
62	RP	105	PRO	N-CA-CB	5.56	109.98	103.30
1	3A	203	U	N3-C2-O2	-5.56	118.31	122.20
3	SA	1440	C	N3-C2-O2	-5.56	118.01	121.90
3	SA	0	U	P-O3'-C3'	5.56	126.37	119.70
3	SA	302	U	N3-C2-O2	-5.56	118.31	122.20
3	SA	1595	U	O5'-P-OP1	-5.55	100.70	105.70
1	3A	200	C	C6-N1-C1'	-5.55	114.14	120.80
3	SA	655	G	N3-C4-N9	-5.55	122.67	126.00
3	SA	1585	U	N1-C2-O2	5.55	126.69	122.80
3	SA	411	C	C6-N1-C2	-5.55	118.08	120.30
3	SA	161	U	C2-N1-C1'	5.54	124.35	117.70
3	SA	1067	C	C6-N1-C2	-5.54	118.08	120.30
34	B1	585	TYR	CB-CG-CD2	-5.54	117.67	121.00
3	SA	1584	G	N3-C4-N9	-5.54	122.68	126.00
3	SA	1772	C	C5-C6-N1	5.54	123.77	121.00
3	SA	50	C	C2-N1-C1'	5.53	124.88	118.80
38	BE	557	LEU	CA-CB-CG	5.53	128.02	115.30
2	5A	263	C	C6-N1-C2	-5.53	118.09	120.30
54	RF	147	LEU	CA-CB-CG	5.53	128.01	115.30
37	B8	328	LEU	CA-CB-CG	5.52	128.00	115.30
2	5A	491	U	N1-C2-O2	5.52	126.67	122.80
3	SA	1034	C	C2-N1-C1'	5.52	124.88	118.80
3	SA	35	U	N1-C2-O2	5.52	126.66	122.80
3	SA	908	U	N3-C2-O2	-5.52	118.34	122.20
3	SA	1717	G	C4-N9-C1'	5.52	133.68	126.50
2	5A	585	C	C6-N1-C2	-5.52	118.09	120.30
3	SA	692	C	N1-C2-O2	5.51	122.21	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5A	252	A	N7-C8-N9	5.51	116.56	113.80
10	SK	105	LEU	CA-CB-CG	5.51	127.97	115.30
23	3D	152	LEU	CA-CB-CG	5.51	127.97	115.30
2	5A	537	G	C4-N9-C1’	5.50	133.66	126.50
3	SA	1191	U	C2-N1-C1’	5.50	124.31	117.70
3	SA	361	C	C6-N1-C2	-5.50	118.10	120.30
3	SA	194	U	C2-N1-C1’	5.50	124.30	117.70
3	SA	1083	G	N7-C8-N9	5.50	115.85	113.10
31	AE	94	LEU	CA-CB-CG	5.49	127.93	115.30
3	SA	894	U	C5-C6-N1	5.49	125.44	122.70
3	SA	1055	U	N3-C2-O2	-5.49	118.36	122.20
2	5A	263	C	C2-N1-C1’	5.47	124.82	118.80
3	SA	1053	G	N9-C4-C5	5.47	107.59	105.40
2	5A	252	A	C4-N9-C1’	5.46	136.13	126.30
3	SA	373	G	N3-C4-N9	5.45	129.27	126.00
3	SA	1779	U	N3-C2-O2	-5.45	118.39	122.20
3	SA	194	U	N1-C2-O2	5.44	126.61	122.80
3	SA	147	A	C2-N3-C4	5.43	113.32	110.60
62	RP	1772	PRO	N-CA-CB	5.43	109.82	103.30
3	SA	413	U	C5-C6-N1	5.43	125.41	122.70
29	A8	563	LEU	CA-CB-CG	5.42	127.77	115.30
35	B2	914	LEU	CA-CB-CG	5.42	127.77	115.30
3	SA	280	U	N3-C2-O2	-5.41	118.41	122.20
3	SA	361	C	C5-C6-N1	5.41	123.71	121.00
3	SA	150	U	N3-C2-O2	-5.41	118.41	122.20
3	SA	1476	C	C2-N1-C1’	5.41	124.75	118.80
3	SA	1109	G	C8-N9-C4	5.40	108.56	106.40
1	3A	6	C	C6-N1-C2	-5.40	118.14	120.30
3	SA	1034	C	N1-C2-O2	5.40	122.14	118.90
36	B3	471	PRO	C-N-CA	5.40	135.20	121.70
3	SA	1032	G	N3-C4-N9	5.40	129.24	126.00
2	5A	252	A	N3-C4-N9	5.40	131.72	127.40
2	5A	381	G	C4-C5-N7	5.39	112.96	110.80
62	RP	1993	PRO	N-CA-CB	5.39	109.77	103.30
3	SA	1056	U	N3-C2-O2	-5.38	118.43	122.20
3	SA	864	U	C6-N1-C1’	-5.38	113.67	121.20
3	SA	530	C	N3-C2-O2	-5.38	118.14	121.90
2	5A	85	G	N1-C6-O6	5.38	123.12	119.90
33	AG	373	LEU	CA-CB-CG	5.37	127.64	115.30
3	SA	682	C	N1-C2-O2	5.36	122.12	118.90
3	SA	873	U	N1-C2-O2	5.36	126.55	122.80
32	AF	118	LEU	CA-CB-CG	5.36	127.63	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	32	U	N3-C2-O2	-5.36	118.45	122.20
3	SA	1646	C	C2-N1-C1’	5.35	124.69	118.80
3	SA	357	G	N9-C4-C5	5.35	107.54	105.40
2	5A	523	U	C6-N1-C2	-5.35	117.79	121.00
2	5A	363	A	P-O3’-C3’	5.34	126.11	119.70
3	SA	1704	U	N1-C2-O2	5.34	126.53	122.80
2	5A	84	G	C4-N9-C1’	5.33	133.43	126.50
2	5A	65	U	N1-C2-O2	5.33	126.53	122.80
1	3A	43	C	C6-N1-C2	-5.32	118.17	120.30
2	5A	6	A	O4’-C1’-N9	5.32	112.46	108.20
2	5A	543	C	C5-C6-N1	5.32	123.66	121.00
3	SA	644	C	C6-N1-C2	-5.32	118.17	120.30
3	SA	1231	U	N3-C2-O2	-5.32	118.48	122.20
2	5A	90	G	N3-C4-N9	-5.32	122.81	126.00
3	SA	346	G	N3-C4-N9	5.31	129.19	126.00
3	SA	1476	C	N1-C2-O2	5.30	122.08	118.90
3	SA	1747	G	C4-N9-C1’	5.30	133.39	126.50
38	BE	834	LEU	CA-CB-CG	-5.30	103.11	115.30
62	RP	1897	PRO	N-CA-CB	5.30	109.66	103.30
57	RJ	829	LEU	CA-CB-CG	5.29	127.46	115.30
3	SA	290	G	C8-N9-C1’	-5.28	120.13	127.00
64	RS	299	LEU	CA-CB-CG	5.28	127.45	115.30
3	SA	1269	U	C6-N1-C1’	-5.28	113.81	121.20
66	RV	204	GLY	N-CA-C	5.28	126.29	113.10
2	5A	85	G	C6-C5-N7	-5.27	127.24	130.40
3	SA	311	U	N3-C2-O2	-5.27	118.51	122.20
2	5A	173	G	OP1-P-O3’	5.26	116.78	105.20
2	5A	169	A	P-O3’-C3’	5.26	126.01	119.70
3	SA	894	U	C2-N1-C1’	5.26	124.01	117.70
49	5K	146	LEU	CA-CB-CG	5.26	127.40	115.30
54	RF	223	LEU	CA-CB-CG	5.26	127.39	115.30
3	SA	1174	C	C5-C6-N1	5.26	123.63	121.00
4	SC	188	LEU	CA-CB-CG	5.26	127.39	115.30
3	SA	648	G	C8-N9-C1’	-5.26	120.17	127.00
53	RE	248	LEU	CA-CB-CG	5.25	127.38	115.30
42	5D	225	LEU	CA-CB-CG	5.25	127.37	115.30
2	5A	98	G	C4-N9-C1’	5.24	133.31	126.50
53	RE	396	LEU	CA-CB-CG	5.24	127.36	115.30
23	3D	184	LEU	CA-CB-CG	5.24	127.35	115.30
3	SA	1759	C	C5-C6-N1	5.23	123.62	121.00
3	SA	1040	G	N9-C4-C5	-5.23	103.31	105.40
3	SA	1451	C	C5-C6-N1	5.23	123.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3F	318	LEU	CA-CB-CG	5.23	127.33	115.30
28	A5	63	LEU	CA-CB-CG	5.23	127.33	115.30
31	AE	756	LEU	CA-CB-CG	5.23	127.32	115.30
2	5A	61	U	C2-N1-C1'	5.22	123.97	117.70
33	AG	208	LEU	CA-CB-CG	5.22	127.31	115.30
36	B3	237	LEU	CB-CG-CD2	-5.22	102.12	111.00
3	SA	209	U	N3-C2-O2	-5.22	118.55	122.20
3	SA	121	U	N3-C2-O2	-5.21	118.55	122.20
47	5I	298	LEU	CA-CB-CG	5.21	127.29	115.30
3	SA	1492	A	C4-N9-C1'	5.21	135.68	126.30
2	5A	90	G	C6-C5-N7	5.20	133.52	130.40
2	5A	223	C	N1-C2-O2	5.20	122.02	118.90
3	SA	130	C	N1-C2-O2	5.20	122.02	118.90
3	SA	258	C	N3-C2-O2	-5.20	118.26	121.90
39	B6	23	LEU	CA-CB-CG	5.19	127.24	115.30
3	SA	1779	U	N1-C2-O2	5.19	126.43	122.80
3	SA	908	U	N1-C2-O2	5.18	126.43	122.80
45	5G	209	LEU	CA-CB-CG	5.18	127.22	115.30
3	SA	1518	C	C6-N1-C1'	-5.17	114.59	120.80
1	3A	89	C	N3-C2-O2	-5.17	118.28	121.90
2	5A	536	A	P-O3'-C3'	5.17	125.91	119.70
61	RO	264	LEU	CA-CB-CG	5.17	127.19	115.30
3	SA	146	U	O4'-C1'-N1	5.16	112.33	108.20
32	AF	285	ASP	CB-CG-OD1	5.16	122.94	118.30
3	SA	1461	C	C5-C6-N1	5.16	123.58	121.00
3	SA	357	G	C8-N9-C1'	5.16	133.70	127.00
2	5A	64	U	N3-C2-O2	-5.15	118.59	122.20
2	5A	537	G	C8-N9-C1'	-5.15	120.31	127.00
60	RN	429	LEU	CA-CB-CG	5.14	127.13	115.30
3	SA	692	C	N3-C2-O2	-5.14	118.30	121.90
3	SA	68	A	OP2-P-O3'	5.14	116.50	105.20
3	SA	1161	C	C2-N1-C1'	5.13	124.45	118.80
3	SA	1084	A	OP1-P-O3'	5.13	116.49	105.20
1	3A	61	G	C5-C6-N1	5.12	114.06	111.50
1	3A	250	C	N1-C2-O2	5.12	121.97	118.90
5	SF	87	MET	CA-CB-CG	5.12	122.01	113.30
2	5A	121	G	N7-C8-N9	5.12	115.66	113.10
1	3A	80	U	C2-N1-C1'	5.11	123.84	117.70
3	SA	302	U	C2-N1-C1'	5.11	123.83	117.70
3	SA	1743	U	C6-N1-C1'	-5.10	114.06	121.20
2	5A	252	A	N3-C4-C5	-5.10	123.23	126.80
3	SA	353	A	N1-C6-N6	-5.10	115.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3A	8	U	N3-C2-O2	-5.09	118.64	122.20
3	SA	1585	U	N3-C2-O2	-5.09	118.64	122.20
2	5A	310	U	C6-N1-C2	-5.08	117.95	121.00
3	SA	1623	C	C6-N1-C2	-5.07	118.27	120.30
3	SA	275	C	N1-C2-O2	5.07	121.94	118.90
2	5A	224	G	P-O3'-C3'	5.07	125.78	119.70
3	SA	376	C	N1-C2-O2	5.07	121.94	118.90
3	SA	258	C	C5-C6-N1	5.07	123.53	121.00
15	SR	123	ARG	C-N-CA	5.07	143.27	122.00
2	5A	90	G	N1-C6-O6	-5.06	116.86	119.90
3	SA	945	U	C2-N1-C1'	5.06	123.77	117.70
1	3A	41	C	C5-C6-N1	5.06	123.53	121.00
3	SA	909	U	N1-C2-O2	5.06	126.34	122.80
3	SA	1646	C	C6-N1-C2	-5.06	118.28	120.30
3	SA	25	C	N1-C2-O2	5.05	121.93	118.90
3	SA	297	U	N3-C2-O2	-5.05	118.66	122.20
3	SA	150	U	N1-C2-O2	5.05	126.34	122.80
2	5A	585	C	C2-N1-C1'	5.05	124.36	118.80
53	RE	243	LEU	CA-CB-CG	5.05	126.92	115.30
3	SA	363	G	N3-C2-N2	5.04	123.43	119.90
3	SA	1727	G	N3-C4-N9	-5.04	122.97	126.00
38	BE	121	LEU	CA-CB-CG	5.03	126.88	115.30
3	SA	346	G	C4-N9-C1'	5.03	133.04	126.50
36	B3	390	LEU	CA-CB-CG	5.03	126.87	115.30
36	B3	237	LEU	CA-CB-CG	5.03	126.87	115.30
55	RG	96	LEU	CA-CB-CG	5.03	126.86	115.30
3	SA	373	G	C8-N9-C1'	-5.02	120.47	127.00
1	3A	265	C	N1-C2-O2	5.02	121.91	118.90
3	SA	357	G	N1-C6-O6	-5.02	116.89	119.90
3	SA	1568	C	C2-N1-C1'	5.02	124.32	118.80
33	AG	79	LEU	CA-CB-CG	5.01	126.83	115.30
3	SA	186	C	C5-C6-N1	5.01	123.51	121.00
3	SA	130	C	C2-N1-C1'	5.01	124.31	118.80
3	SA	1448	G	N3-C4-N9	-5.01	122.99	126.00

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	3B	176	ALA	Peptide
23	3D	142	LEU	Peptide
24	3E	228	PRO	Peptide

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Mol	Chain	Res	Type	Group
24	3E	36	ASP	Peptide
26	3G	59	GLU	Peptide
26	3G	64	LEU	Peptide
26	3G	9	PHE	Peptide
26	3H	59	GLU	Peptide
41	5C	111	PHE	Peptide
41	5C	140	ARG	Peptide
41	5C	540	GLU	Peptide
42	5D	84	GLY	Peptide
43	5E	453	SER	Peptide
44	5F	101	VAL	Peptide
47	5I	141	ASP	Peptide
49	5K	25	LEU	Peptide
49	5K	51	LEU	Peptide
28	A5	167	SER	Peptide
28	A5	457	LEU	Peptide
29	A8	257	SER	Peptide
29	A8	266	ILE	Peptide
29	A8	529	HIS	Peptide
29	A8	599	MET	Peptide
33	AG	178	PHE	Peptide
33	AG	769	ASN	Peptide
33	AG	780	GLU	Peptide
34	B1	288	ASP	Peptide
34	B1	661	LEU	Peptide
34	B1	733	LYS	Peptide
35	B2	131	GLY	Peptide
35	B2	266	SER	Peptide
35	B2	267	ASP	Peptide
35	B2	359	SER	Peptide
35	B2	52	TRP	Peptide
35	B2	575	PRO	Peptide
35	B2	613	ALA	Peptide
35	B2	653	LEU	Peptide
35	B2	916	HIS	Peptide
36	B3	35	PRO	Peptide
36	B3	473	ALA	Peptide
36	B3	480	ILE	Peptide
36	B3	530	ALA	Peptide
36	B3	593	CYS	Peptide
36	B3	594	GLY	Peptide
36	B3	785	ILE	Peptide

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Mol	Chain	Res	Type	Group
36	B3	90	LEU	Peptide
39	B6	354	ASP	Peptide
37	B8	366	SER	Peptide
37	B8	438	ASN	Peptide
37	B8	501	THR	Peptide
38	BE	173	LEU	Peptide
38	BE	899	ASN	Peptide
38	BE	94	TYR	Peptide
51	RB	273	GLY	Peptide
53	RE	767	GLN	Peptide
54	RF	253	ALA	Peptide
56	RI	50	ARG	Peptide
57	RJ	1026	LYS	Peptide
57	RJ	81	GLY	Peptide
59	RL	743	VAL	Peptide
59	RM	743	VAL	Peptide
62	RP	1907	ASN	Peptide
63	RQ	257	ILE	Peptide
66	RV	203	ILE	Peptide
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
8	SI	64	VAL	Peptide
11	SM	128	CYS	Peptide
12	SN	99	GLU	Peptide
13	SO	24	ALA	Peptide
14	SP	90	ARG	Peptide
19	SZ	76	TYR	Peptide
20	Sc	74	SER	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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

All (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
36	B3	91	LYS
59	RM	905	PRO
62	RP	1993	PRO
34	B1	670	LEU
43	5E	460	PRO
59	RM	904	LEU
60	RN	285	PRO
25	3F	552	TRP
29	A8	308	PHE
34	B1	442	GLY
35	B2	132	THR
41	5C	492	GLY
36	B3	71	PRO
59	RL	743	VAL
59	RM	743	VAL
32	AF	49	PRO
64	RS	414	PRO
4	SC	221	PRO
7	SH	70	PRO
26	3G	10	PRO
29	A8	267	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	SC	92	GLN
4	SC	162	ARG
4	SC	205	PHE
5	SF	181	VAL
5	SF	200	ARG
5	SF	207	LEU
5	SF	211	LYS
5	SF	233	LYS
6	SG	123	VAL
7	SH	92	ARG
8	SI	159	VAL
8	SI	189	THR
9	SJ	43	ILE
10	SK	57	ARG
10	SK	74	ASN
10	SK	87	SER
11	SM	69	LYS
13	SO	58	HIS
13	SO	135	LEU
14	SP	86	THR
14	SP	117	ASP
19	SZ	74	LEU
22	3B	120	GLU
23	3D	10	GLU
23	3D	48	ILE
23	3D	103	LYS

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Mol	Chain	Res	Type
23	3D	285	ARG
24	3E	265	PHE
24	3E	371	LEU
25	3F	223	THR
25	3F	293	ASP
25	3F	370	ARG
25	3F	418	ASP
25	3F	506	ARG
26	3G	67	LEU
27	A4	33	VAL
27	A4	130	THR
27	A4	282	ASP
27	A4	579	ARG
27	A4	648	PHE
27	A4	745	ASP
27	A4	775	VAL
27	A4	776	PHE
28	A5	139	HIS
28	A5	235	LEU
28	A5	310	THR
29	A8	576	ARG
31	AE	147	VAL
31	AE	253	CYS
31	AE	264	PHE
31	AE	366	ILE
31	AE	396	ASP
31	AE	485	THR
31	AE	515	PHE
31	AE	713	PHE
32	AF	20	THR
32	AF	149	THR
32	AF	199	ARG
32	AF	236	VAL
32	AF	255	VAL
33	AG	109	VAL
33	AG	131	HIS
33	AG	271	LEU
33	AG	336	ARG
33	AG	421	LYS
33	AG	606	HIS
33	AG	716	ARG
34	B1	76	ASP

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Mol	Chain	Res	Type
34	B1	167	ASP
34	B1	173	TRP
34	B1	215	VAL
34	B1	321	SER
34	B1	351	LEU
34	B1	519	LEU
34	B1	526	ASP
34	B1	574	SER
34	B1	603	LEU
34	B1	698	THR
35	B2	159	LEU
35	B2	331	THR
35	B2	343	TRP
35	B2	450	ARG
35	B2	576	VAL
35	B2	579	ILE
35	B2	663	LEU
36	B3	24	THR
36	B3	32	LEU
36	B3	51	LYS
36	B3	97	ARG
36	B3	100	LYS
36	B3	222	LEU
36	B3	482	VAL
36	B3	520	LEU
36	B3	533	LYS
36	B3	534	ARG
36	B3	539	VAL
37	B8	272	LEU
37	B8	344	ARG
37	B8	406	ASP
37	B8	546	LEU
38	BE	207	ASP
38	BE	209	ILE
38	BE	312	THR
38	BE	470	GLN
38	BE	494	LEU
38	BE	570	ILE
38	BE	713	LEU
38	BE	813	PHE
38	BE	899	ASN
39	B6	23	LEU

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Mol	Chain	Res	Type
39	B6	34	LYS
39	B6	67	ARG
39	B6	133	TYR
39	B6	297	ASP
40	5B	168	LYS
41	5C	153	THR
41	5C	253	ASN
41	5C	291	THR
41	5C	296	ARG
41	5C	347	LEU
41	5C	392	VAL
41	5C	505	THR
41	5C	544	ASP
42	5D	91	LEU
42	5D	161	ARG
43	5E	297	LEU
43	5E	330	VAL
45	5G	176	ILE
45	5G	223	THR
46	5H	579	VAL
47	5I	91	VAL
47	5I	119	THR
47	5I	124	HIS
47	5I	214	ASP
47	5I	232	THR
47	5I	250	ARG
47	5I	261	THR
47	5I	356	TYR
47	5I	410	ILE
49	5K	17	LEU
49	5K	41	THR
51	RB	306	ARG
51	RB	341	ARG
52	RC	62	ARG
53	RE	223	ARG
53	RE	227	LYS
53	RE	232	LEU
53	RE	245	LYS
53	RE	285	PHE
53	RE	289	ARG
53	RE	595	THR
53	RE	840	LEU

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Mol	Chain	Res	Type
53	RE	976	ILE
54	RF	19	LYS
54	RF	160	TYR
54	RF	171	PHE
54	RF	176	ASP
55	RG	97	LEU
55	RH	31	LEU
55	RH	82	ARG
55	RH	116	THR
56	RI	17	LEU
56	RI	30	LEU
56	RI	170	LYS
56	RI	171	CYS
57	RJ	214	ARG
57	RJ	868	ARG
57	RJ	973	ARG
57	RJ	1141	LYS
58	RK	213	LYS
58	RK	214	LYS
59	RL	9	ARG
59	RL	10	ILE
59	RL	83	ARG
59	RL	104	ARG
59	RL	134	LEU
61	RO	203	LEU
61	RO	493	TYR
61	RO	507	LEU
63	RQ	319	THR
64	RS	225	THR
64	RS	233	PHE
64	RS	344	LYS
64	RS	390	CYS
65	RT	129	ARG
65	RT	139	LEU
65	RT	182	ILE
66	RV	315	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (285) such sidechains are listed below:

Mol	Chain	Res	Type
4	SC	101	HIS
4	SC	118	GLN

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Mol	Chain	Res	Type
4	SC	183	GLN
5	SF	153	ASN
5	SF	188	ASN
5	SF	224	ASN
6	SG	86	GLN
6	SG	104	ASN
6	SG	127	GLN
6	SG	131	GLN
6	SG	169	ASN
6	SG	186	ASN
7	SH	59	GLN
8	SI	74	GLN
9	SJ	64	ASN
9	SJ	103	GLN
11	SM	92	HIS
11	SM	98	ASN
11	SM	106	ASN
12	SN	38	HIS
12	SN	96	GLN
13	SO	49	GLN
13	SO	58	HIS
15	SR	74	HIS
16	ST	21	ASN
16	ST	44	ASN
17	SX	16	ASN
19	SZ	29	HIS
19	SZ	77	ASN
22	3B	258	HIS
22	3C	145	ASN
23	3D	172	ASN
23	3D	183	GLN
23	3D	302	ASN
23	3D	381	ASN
24	3E	191	HIS
24	3E	254	ASN
24	3E	256	ASN
24	3E	286	ASN
24	3E	289	GLN
24	3E	396	ASN
24	3E	400	GLN
25	3F	226	HIS
25	3F	485	ASN

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Mol	Chain	Res	Type
25	3F	525	GLN
26	3G	29	ASN
26	3G	38	ASN
26	3H	18	GLN
26	3H	45	ASN
26	3H	66	HIS
27	A4	53	HIS
27	A4	140	ASN
27	A4	273	ASN
27	A4	274	GLN
27	A4	279	HIS
27	A4	292	ASN
27	A4	317	ASN
27	A4	452	HIS
27	A4	529	ASN
27	A4	589	ASN
27	A4	621	ASN
27	A4	632	ASN
27	A4	642	ASN
28	A5	103	ASN
28	A5	133	GLN
28	A5	213	ASN
28	A5	302	ASN
28	A5	308	ASN
28	A5	316	ASN
28	A5	324	ASN
28	A5	509	HIS
29	A8	553	GLN
29	A8	609	ASN
30	A9	443	GLN
30	A9	444	ASN
30	A9	474	HIS
30	A9	478	ASN
31	AE	7	GLN
31	AE	51	ASN
31	AE	141	ASN
31	AE	166	ASN
31	AE	202	HIS
31	AE	219	ASN
31	AE	224	ASN
31	AE	309	GLN
31	AE	480	ASN

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Mol	Chain	Res	Type
31	AE	559	ASN
31	AE	709	ASN
31	AE	773	GLN
31	AE	774	ASN
32	AF	24	GLN
32	AF	44	HIS
32	AF	48	ASN
32	AF	64	GLN
32	AF	72	GLN
32	AF	133	HIS
32	AF	217	ASN
32	AF	250	ASN
32	AF	280	HIS
32	AF	289	ASN
32	AF	391	ASN
32	AF	403	ASN
32	AF	481	GLN
32	AF	502	GLN
33	AG	9	GLN
33	AG	169	GLN
33	AG	190	GLN
33	AG	398	HIS
33	AG	424	GLN
33	AG	489	ASN
33	AG	535	ASN
33	AG	624	HIS
33	AG	660	GLN
33	AG	669	ASN
33	AG	759	HIS
33	AG	760	HIS
34	B1	91	HIS
34	B1	142	HIS
34	B1	190	HIS
34	B1	201	HIS
34	B1	302	GLN
34	B1	303	ASN
34	B1	349	ASN
34	B1	386	HIS
34	B1	452	ASN
34	B1	456	HIS
34	B1	650	ASN
34	B1	691	ASN

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Mol	Chain	Res	Type
34	B1	795	ASN
34	B1	813	HIS
34	B1	837	ASN
34	B1	842	ASN
35	B2	128	GLN
35	B2	172	GLN
35	B2	264	ASN
35	B2	276	ASN
35	B2	524	HIS
35	B2	596	ASN
35	B2	657	GLN
35	B2	677	HIS
35	B2	770	ASN
35	B2	798	ASN
35	B2	856	ASN
35	B2	879	GLN
36	B3	143	HIS
36	B3	301	GLN
36	B3	328	GLN
36	B3	392	ASN
36	B3	502	ASN
36	B3	519	ASN
36	B3	616	HIS
36	B3	767	HIS
36	B3	792	HIS
36	B3	802	GLN
37	B8	41	ASN
37	B8	159	HIS
37	B8	162	ASN
37	B8	282	ASN
37	B8	283	HIS
37	B8	308	ASN
37	B8	352	GLN
37	B8	472	GLN
37	B8	492	ASN
38	BE	20	ASN
38	BE	67	HIS
38	BE	203	ASN
38	BE	447	ASN
38	BE	481	ASN
38	BE	501	HIS
38	BE	903	GLN

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Mol	Chain	Res	Type
39	B6	90	GLN
39	B6	115	ASN
40	5B	207	ASN
41	5C	101	ASN
41	5C	124	HIS
41	5C	133	HIS
41	5C	164	GLN
41	5C	170	GLN
41	5C	400	ASN
41	5C	468	GLN
41	5C	480	ASN
41	5C	507	ASN
42	5D	144	ASN
42	5D	221	GLN
43	5E	526	ASN
44	5F	27	HIS
44	5F	39	GLN
44	5F	59	ASN
44	5F	135	HIS
45	5G	18	GLN
45	5G	143	HIS
45	5G	159	HIS
45	5G	208	HIS
46	5H	515	ASN
47	5I	46	ASN
47	5I	76	ASN
47	5I	202	HIS
47	5I	207	ASN
47	5I	260	GLN
47	5I	284	HIS
47	5I	371	ASN
47	5I	392	ASN
47	5I	406	HIS
48	5J	126	HIS
48	5J	184	ASN
48	5J	192	ASN
48	5J	195	GLN
49	5K	43	ASN
50	RA	101	ASN
50	RA	118	GLN
51	RB	301	ASN
51	RB	314	ASN

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Mol	Chain	Res	Type
52	RC	149	ASN
52	RC	151	ASN
52	RC	284	GLN
53	RE	197	GLN
53	RE	221	ASN
53	RE	293	ASN
53	RE	371	GLN
53	RE	414	HIS
53	RE	439	HIS
53	RE	520	ASN
53	RE	607	HIS
53	RE	634	HIS
53	RE	665	HIS
53	RE	834	ASN
53	RE	841	ASN
53	RE	901	ASN
53	RE	1159	ASN
53	RE	1180	ASN
54	RF	23	HIS
55	RG	105	ASN
55	RG	125	ASN
55	RG	170	HIS
55	RG	190	GLN
55	RG	215	ASN
55	RH	69	ASN
56	RI	52	ASN
56	RI	186	ASN
56	RI	192	ASN
56	RI	221	ASN
57	RJ	126	ASN
57	RJ	162	HIS
57	RJ	239	ASN
57	RJ	289	HIS
57	RJ	776	GLN
57	RJ	778	GLN
57	RJ	944	ASN
58	RK	16	ASN
58	RK	88	HIS
58	RK	167	HIS
58	RK	317	GLN
59	RL	16	ASN
59	RL	75	ASN

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Mol	Chain	Res	Type
59	RL	89	ASN
60	RN	452	GLN
60	RN	482	GLN
60	RN	527	GLN
60	RN	569	GLN
60	RN	738	ASN
60	RN	771	ASN
60	RN	797	ASN
61	RO	228	HIS
61	RO	256	ASN
61	RO	268	GLN
61	RO	273	GLN
61	RO	290	HIS
61	RO	304	ASN
61	RO	309	ASN
61	RO	343	GLN
61	RO	346	ASN
61	RO	370	HIS
61	RO	472	HIS
63	RQ	310	HIS
63	RQ	321	HIS
63	RQ	331	GLN
63	RQ	832	ASN
63	RQ	839	ASN
64	RS	302	HIS
64	RS	385	GLN
65	RT	111	ASN
65	RT	218	ASN
65	RT	232	HIS
66	RV	224	HIS
66	RV	225	GLN

5.3.3 RNA ⓘ

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%)

All (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
1	3A	25	U
1	3A	28	A
1	3A	30	A
1	3A	33	A
1	3A	35	U
1	3A	56	A
1	3A	60	A
1	3A	61	G
1	3A	82	G
1	3A	87	G
1	3A	88	U
1	3A	89	C
1	3A	90	C
1	3A	91	C
1	3A	102	U
1	3A	104	C
1	3A	111	G
1	3A	114	A
1	3A	115	G
1	3A	198	U
1	3A	199	G
1	3A	200	C
1	3A	201	C
1	3A	204	U
1	3A	205	G
1	3A	206	C
1	3A	246	A
1	3A	248	G
1	3A	249	G
1	3A	252	C
1	3A	265	C
1	3A	266	C
1	3A	305	G
1	3A	309	G
1	3A	310	G
1	3A	313	A
1	3A	314	C
1	3A	322	A

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Mol	Chain	Res	Type
1	3A	324	U
1	3A	325	C
1	3A	329	C
2	5A	5	G
2	5A	6	A
2	5A	7	A
2	5A	8	A
2	5A	13	U
2	5A	62	C
2	5A	63	G
2	5A	64	U
2	5A	70	A
2	5A	82	A
2	5A	83	U
2	5A	85	G
2	5A	86	C
2	5A	87	C
2	5A	103	G
2	5A	104	A
2	5A	109	C
2	5A	110	G
2	5A	114	G
2	5A	124	A
2	5A	125	G
2	5A	126	A
2	5A	127	U
2	5A	128	C
2	5A	129	U
2	5A	130	G
2	5A	140	U
2	5A	142	U
2	5A	144	C
2	5A	148	G
2	5A	150	G
2	5A	151	U
2	5A	156	U
2	5A	161	A
2	5A	163	G
2	5A	169	A
2	5A	170	U
2	5A	171	G
2	5A	172	C

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Mol	Chain	Res	Type
2	5A	173	G
2	5A	174	U
2	5A	177	U
2	5A	185	A
2	5A	190	U
2	5A	200	A
2	5A	201	U
2	5A	211	G
2	5A	219	U
2	5A	220	U
2	5A	223	C
2	5A	224	G
2	5A	225	U
2	5A	226	U
2	5A	227	U
2	5A	235	A
2	5A	240	C
2	5A	256	U
2	5A	259	G
2	5A	260	A
2	5A	261	U
2	5A	266	U
2	5A	267	U
2	5A	268	G
2	5A	271	G
2	5A	279	A
2	5A	280	A
2	5A	281	G
2	5A	304	U
2	5A	305	A
2	5A	309	A
2	5A	310	U
2	5A	311	C
2	5A	312	U
2	5A	313	A
2	5A	316	U
2	5A	324	U
2	5A	325	U
2	5A	326	C
2	5A	327	A
2	5A	328	A
2	5A	337	G

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Mol	Chain	Res	Type
2	5A	339	A
2	5A	353	A
2	5A	354	G
2	5A	359	U
2	5A	360	C
2	5A	363	A
2	5A	364	A
2	5A	365	G
2	5A	368	U
2	5A	369	G
2	5A	370	U
2	5A	371	G
2	5A	372	A
2	5A	373	U
2	5A	381	G
2	5A	385	A
2	5A	386	A
2	5A	393	C
2	5A	395	C
2	5A	407	A
2	5A	419	A
2	5A	427	A
2	5A	428	A
2	5A	429	A
2	5A	430	C
2	5A	431	A
2	5A	432	C
2	5A	433	C
2	5A	440	U
2	5A	443	G
2	5A	461	A
2	5A	462	G
2	5A	464	G
2	5A	468	A
2	5A	469	C
2	5A	472	A
2	5A	474	A
2	5A	481	U
2	5A	482	A
2	5A	485	G
2	5A	487	A
2	5A	488	U

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Mol	Chain	Res	Type
2	5A	489	G
2	5A	490	G
2	5A	491	U
2	5A	493	A
2	5A	517	A
2	5A	519	A
2	5A	525	U
2	5A	526	U
2	5A	533	G
2	5A	536	A
2	5A	537	G
2	5A	539	A
2	5A	540	U
2	5A	541	U
2	5A	542	U
2	5A	547	C
2	5A	549	G
2	5A	555	A
2	5A	585	C
2	5A	586	A
2	5A	587	G
2	5A	589	U
2	5A	590	G
3	SA	-5	G
3	SA	-4	A
3	SA	-1	G
3	SA	0	U
3	SA	1	U
3	SA	6	G
3	SA	10	G
3	SA	17	C
3	SA	18	C
3	SA	21	U
3	SA	24	U
3	SA	25	C
3	SA	26	A
3	SA	36	C
3	SA	37	U
3	SA	51	A
3	SA	53	G
3	SA	54	C
3	SA	55	A

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Mol	Chain	Res	Type
3	SA	56	U
3	SA	57	G
3	SA	59	C
3	SA	61	A
3	SA	63	G
3	SA	65	A
3	SA	66	U
3	SA	67	A
3	SA	68	A
3	SA	69	G
3	SA	72	A
3	SA	73	U
3	SA	74	U
3	SA	77	U
3	SA	80	A
3	SA	81	G
3	SA	85	A
3	SA	89	G
3	SA	92	A
3	SA	93	A
3	SA	96	G
3	SA	97	C
3	SA	100	A
3	SA	102	U
3	SA	104	A
3	SA	105	A
3	SA	114	C
3	SA	115	G
3	SA	126	A
3	SA	127	G
3	SA	128	U
3	SA	129	U
3	SA	130	C
3	SA	131	C
3	SA	141	U
3	SA	145	A
3	SA	146	U
3	SA	153	G
3	SA	159	U
3	SA	160	C
3	SA	163	G
3	SA	168	A

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Mol	Chain	Res	Type
3	SA	170	U
3	SA	174	U
3	SA	176	C
3	SA	177	U
3	SA	182	A
3	SA	183	U
3	SA	184	C
3	SA	187	G
3	SA	188	A
3	SA	190	C
3	SA	191	C
3	SA	192	U
3	SA	193	U
3	SA	194	U
3	SA	195	G
3	SA	197	A
3	SA	203	U
3	SA	211	U
3	SA	214	G
3	SA	228	G
3	SA	231	U
3	SA	233	C
3	SA	234	G
3	SA	236	A
3	SA	237	C
3	SA	238	U
3	SA	239	C
3	SA	241	U
3	SA	242	U
3	SA	246	G
3	SA	254	A
3	SA	255	U
3	SA	256	A
3	SA	261	U
3	SA	262	U
3	SA	265	A
3	SA	266	A
3	SA	267	U
3	SA	272	U
3	SA	273	G
3	SA	276	C
3	SA	277	U

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Mol	Chain	Res	Type
3	SA	278	U
3	SA	279	G
3	SA	280	U
3	SA	281	G
3	SA	283	U
3	SA	288	A
3	SA	290	G
3	SA	311	U
3	SA	313	U
3	SA	315	A
3	SA	316	A
3	SA	319	U
3	SA	320	U
3	SA	321	C
3	SA	322	G
3	SA	333	A
3	SA	334	G
3	SA	337	G
3	SA	339	C
3	SA	350	U
3	SA	351	C
3	SA	352	A
3	SA	356	G
3	SA	359	A
3	SA	360	A
3	SA	361	C
3	SA	362	G
3	SA	365	G
3	SA	366	A
3	SA	369	A
3	SA	371	G
3	SA	373	G
3	SA	374	U
3	SA	375	U
3	SA	376	C
3	SA	379	U
3	SA	382	C
3	SA	383	G
3	SA	386	G
3	SA	387	A
3	SA	390	G
3	SA	400	A

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Mol	Chain	Res	Type
3	SA	401	A
3	SA	402	C
3	SA	403	G
3	SA	404	G
3	SA	405	C
3	SA	407	A
3	SA	410	A
3	SA	411	C
3	SA	416	A
3	SA	418	G
3	SA	420	A
3	SA	421	A
3	SA	422	G
3	SA	423	G
3	SA	424	C
3	SA	425	A
3	SA	426	G
3	SA	428	A
3	SA	431	C
3	SA	436	A
3	SA	437	A
3	SA	439	U
3	SA	440	U
3	SA	441	A
3	SA	444	C
3	SA	445	A
3	SA	452	A
3	SA	454	U
3	SA	455	C
3	SA	456	A
3	SA	468	A
3	SA	469	C
3	SA	470	A
3	SA	471	A
3	SA	473	A
3	SA	477	A
3	SA	480	G
3	SA	485	A
3	SA	486	G
3	SA	487	G
3	SA	493	U
3	SA	496	G

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Mol	Chain	Res	Type
3	SA	501	U
3	SA	502	U
3	SA	505	A
3	SA	506	A
3	SA	507	U
3	SA	520	A
3	SA	534	A
3	SA	538	A
3	SA	539	G
3	SA	541	A
3	SA	542	A
3	SA	543	C
3	SA	545	A
3	SA	551	G
3	SA	557	G
3	SA	563	U
3	SA	564	G
3	SA	570	A
3	SA	572	C
3	SA	575	C
3	SA	579	A
3	SA	580	A
3	SA	583	C
3	SA	584	C
3	SA	585	A
3	SA	586	G
3	SA	587	C
3	SA	594	A
3	SA	595	G
3	SA	603	U
3	SA	604	A
3	SA	606	A
3	SA	608	U
3	SA	609	U
3	SA	610	G
3	SA	612	U
3	SA	613	G
3	SA	614	C
3	SA	615	A
3	SA	616	G
3	SA	635	A
3	SA	636	A

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Mol	Chain	Res	Type
3	SA	638	U
3	SA	644	C
3	SA	648	G
3	SA	649	U
3	SA	652	G
3	SA	654	C
3	SA	656	G
3	SA	657	U
3	SA	658	C
3	SA	659	C
3	SA	677	G
3	SA	678	A
3	SA	680	U
3	SA	682	C
3	SA	687	G
3	SA	689	G
3	SA	691	C
3	SA	692	C
3	SA	859	A
3	SA	860	U
3	SA	861	U
3	SA	863	A
3	SA	864	U
3	SA	865	A
3	SA	876	G
3	SA	894	U
3	SA	901	G
3	SA	906	A
3	SA	913	G
3	SA	914	G
3	SA	932	U
3	SA	933	A
3	SA	935	U
3	SA	940	A
3	SA	945	U
3	SA	951	A
3	SA	960	U
3	SA	966	A
3	SA	969	C
3	SA	970	A
3	SA	1021	C
3	SA	1022	C

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Mol	Chain	Res	Type
3	SA	1023	A
3	SA	1024	U
3	SA	1025	A
3	SA	1026	A
3	SA	1027	A
3	SA	1031	U
3	SA	1032	G
3	SA	1036	A
3	SA	1037	C
3	SA	1039	A
3	SA	1040	G
3	SA	1052	U
3	SA	1053	G
3	SA	1056	U
3	SA	1058	U
3	SA	1059	U
3	SA	1060	U
3	SA	1062	A
3	SA	1063	U
3	SA	1064	G
3	SA	1075	C
3	SA	1076	A
3	SA	1081	A
3	SA	1082	C
3	SA	1084	A
3	SA	1085	G
3	SA	1086	A
3	SA	1106	U
3	SA	1107	G
3	SA	1108	G
3	SA	1109	G
3	SA	1110	G
3	SA	1111	G
3	SA	1118	G
3	SA	1119	G
3	SA	1122	G
3	SA	1125	A
3	SA	1127	G
3	SA	1128	C
3	SA	1131	A
3	SA	1132	A
3	SA	1145	U

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Mol	Chain	Res	Type
3	SA	1146	G
3	SA	1147	A
3	SA	1158	C
3	SA	1164	G
3	SA	1191	U
3	SA	1192	C
3	SA	1193	A
3	SA	1196	A
3	SA	1197	C
3	SA	1198	G
3	SA	1199	G
3	SA	1200	G
3	SA	1201	G
3	SA	1202	A
3	SA	1205	C
3	SA	1207	C
3	SA	1208	A
3	SA	1210	C
3	SA	1213	G
3	SA	1217	A
3	SA	1218	G
3	SA	1219	A
3	SA	1226	A
3	SA	1227	A
3	SA	1228	G
3	SA	1229	G
3	SA	1232	U
3	SA	1235	C
3	SA	1236	A
3	SA	1253	U
3	SA	1255	G
3	SA	1258	U
3	SA	1259	U
3	SA	1266	U
3	SA	1268	G
3	SA	1271	G
3	SA	1272	U
3	SA	1273	G
3	SA	1274	C
3	SA	1275	A
3	SA	1436	A
3	SA	1437	U

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Mol	Chain	Res	Type
3	SA	1440	C
3	SA	1443	U
3	SA	1450	U
3	SA	1457	C
3	SA	1461	C
3	SA	1469	A
3	SA	1472	C
3	SA	1473	U
3	SA	1474	G
3	SA	1475	A
3	SA	1477	G
3	SA	1485	C
3	SA	1488	G
3	SA	1489	U
3	SA	1492	A
3	SA	1493	A
3	SA	1496	U
3	SA	1498	G
3	SA	1506	G
3	SA	1517	U
3	SA	1518	C
3	SA	1520	U
3	SA	1521	G
3	SA	1522	U
3	SA	1523	G
3	SA	1524	A
3	SA	1531	G
3	SA	1535	U
3	SA	1536	G
3	SA	1539	G
3	SA	1541	G
3	SA	1543	A
3	SA	1544	U
3	SA	1567	U
3	SA	1568	C
3	SA	1569	A
3	SA	1570	A
3	SA	1573	A
3	SA	1584	G
3	SA	1590	G
3	SA	1594	G
3	SA	1595	U

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Mol	Chain	Res	Type
3	SA	1601	G
3	SA	1602	C
3	SA	1607	G
3	SA	1614	A
3	SA	1618	C
3	SA	1628	U
3	SA	1629	G
3	SA	1630	U
3	SA	1631	A
3	SA	1639	C
3	SA	1651	A
3	SA	1658	G
3	SA	1659	A
3	SA	1664	C
3	SA	1670	G
3	SA	1671	A
3	SA	1672	G
3	SA	1677	C
3	SA	1678	A
3	SA	1679	G
3	SA	1680	G
3	SA	1681	A
3	SA	1682	U
3	SA	1683	C
3	SA	1684	U
3	SA	1685	G
3	SA	1690	G
3	SA	1695	G
3	SA	1700	C
3	SA	1702	A
3	SA	1707	A
3	SA	1710	U
3	SA	1711	C
3	SA	1713	G
3	SA	1717	G
3	SA	1718	G
3	SA	1719	A
3	SA	1724	U
3	SA	1725	U
3	SA	1727	G
3	SA	1731	A
3	SA	1732	A

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Mol	Chain	Res	Type
3	SA	1736	G
3	SA	1737	G
3	SA	1742	U
3	SA	1743	U
3	SA	1745	G
3	SA	1747	G
3	SA	1749	A
3	SA	1751	C
3	SA	1756	A
3	SA	1757	G
3	SA	1758	U
3	SA	1759	C
3	SA	1761	U
3	SA	1764	C
3	SA	1765	A
3	SA	1766	A
3	SA	1768	G
3	SA	1772	C
3	SA	1779	U
3	SA	1780	G
3	SA	1781	A
3	SA	1782	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3A	198	U
1	3A	248	G
2	5A	169	A
2	5A	172	C
2	5A	173	G
2	5A	224	G
2	5A	312	U
2	5A	358	G
2	5A	363	A
2	5A	368	U
2	5A	492	G
2	5A	536	A
3	SA	0	U
3	SA	56	U
3	SA	68	A
3	SA	272	U

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Mol	Chain	Res	Type
3	SA	372	G
3	SA	401	A
3	SA	417	A
3	SA	538	A
3	SA	542	A
3	SA	579	A
3	SA	602	U
3	SA	1031	U
3	SA	1052	U
3	SA	1084	A
3	SA	1521	G
3	SA	1594	G

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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

All (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
69	RJ	1201	GTP	O6-C6-C5	-2.05	120.36	124.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

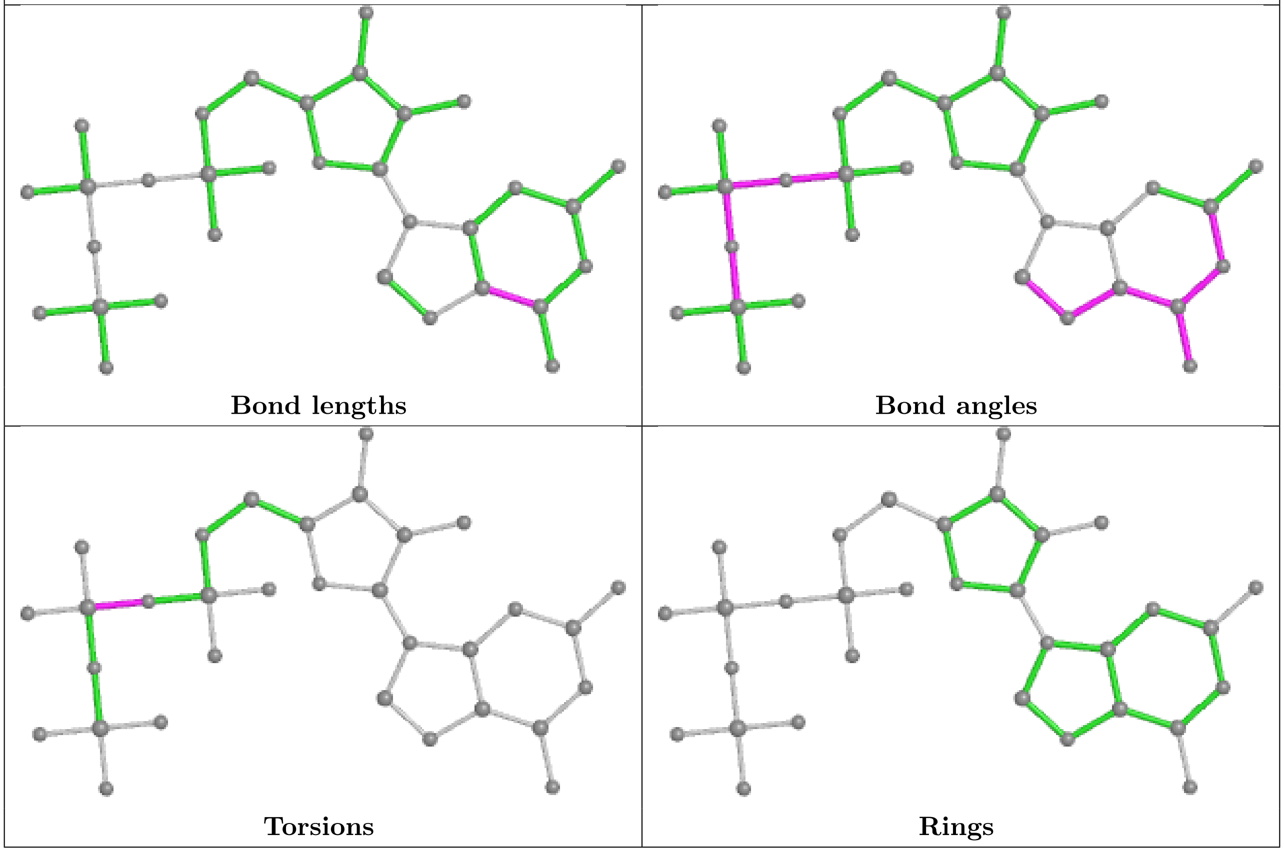
Mol	Chain	Res	Type	Atoms
69	RJ	1201	GTP	PA-O3A-PB-O2B
69	RJ	1201	GTP	PA-O3A-PB-O1B

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

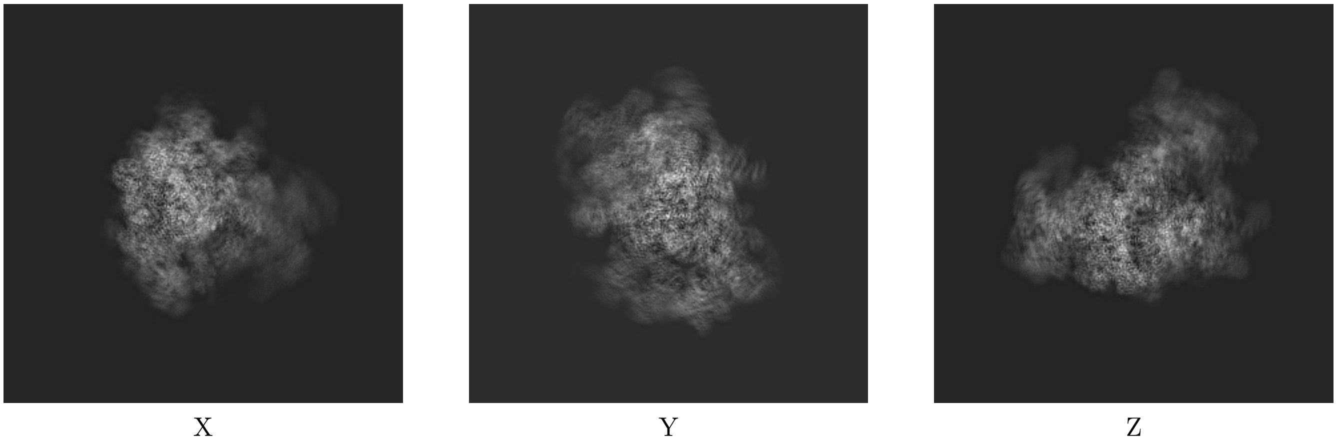
6 Map visualisation ⓘ

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 ⓘ

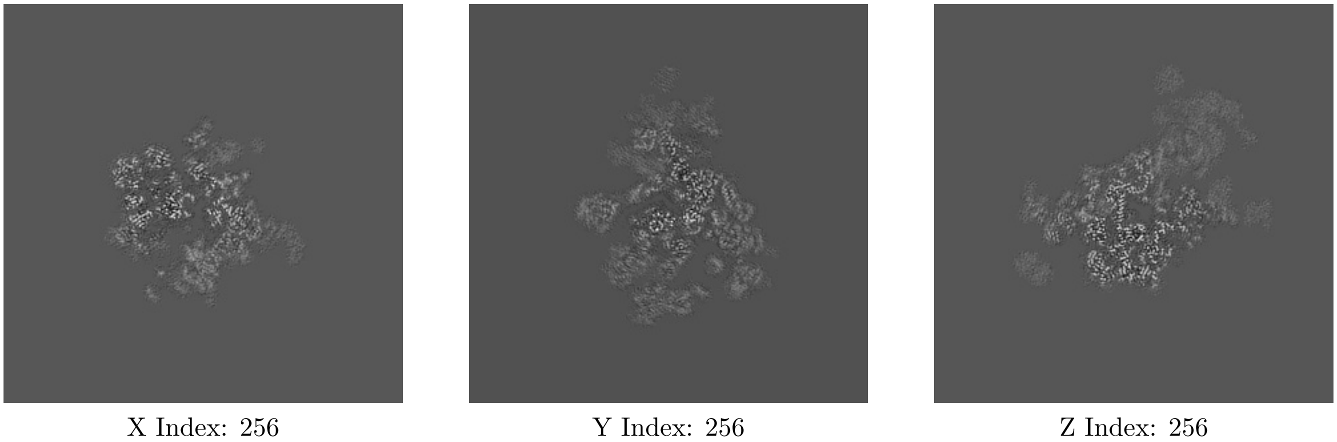
6.1.1 Primary map


X Y Z

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

6.2 Central slices ⓘ

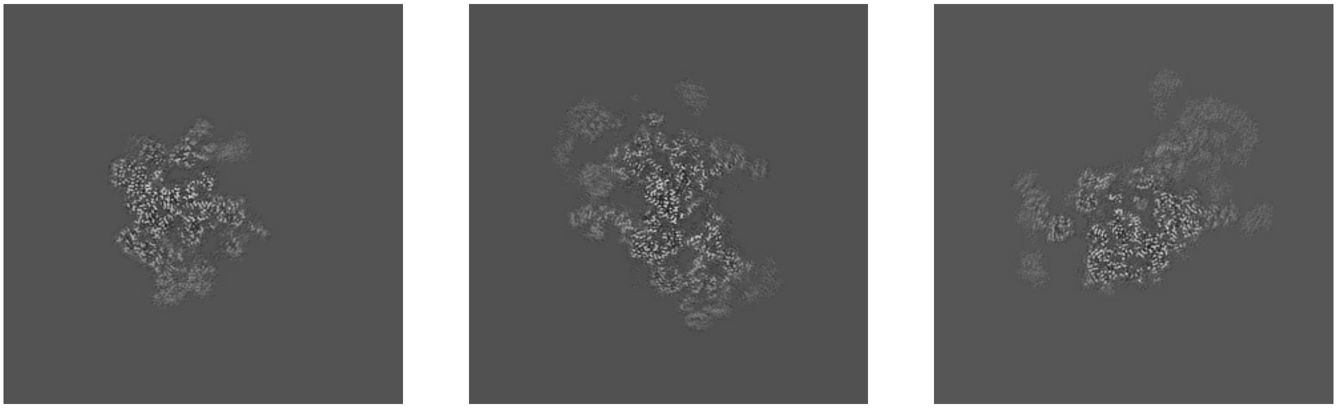
6.2.1 Primary map


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

6.3.1 Primary map

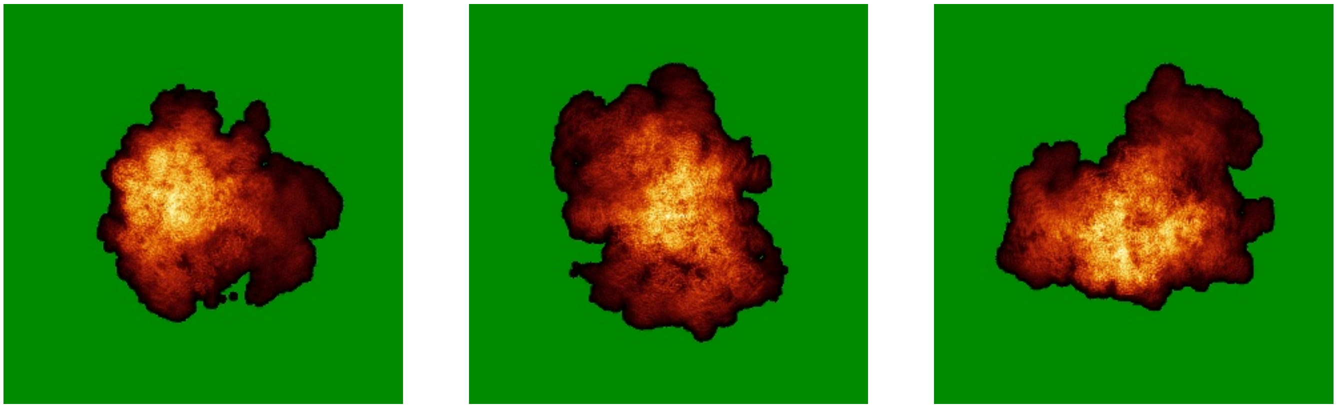


X Index: 240 Y Index: 216 Z Index: 267

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

6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

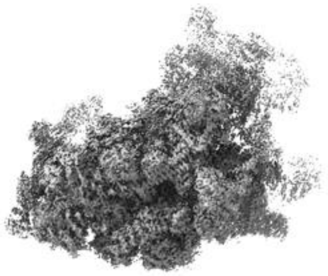
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

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.

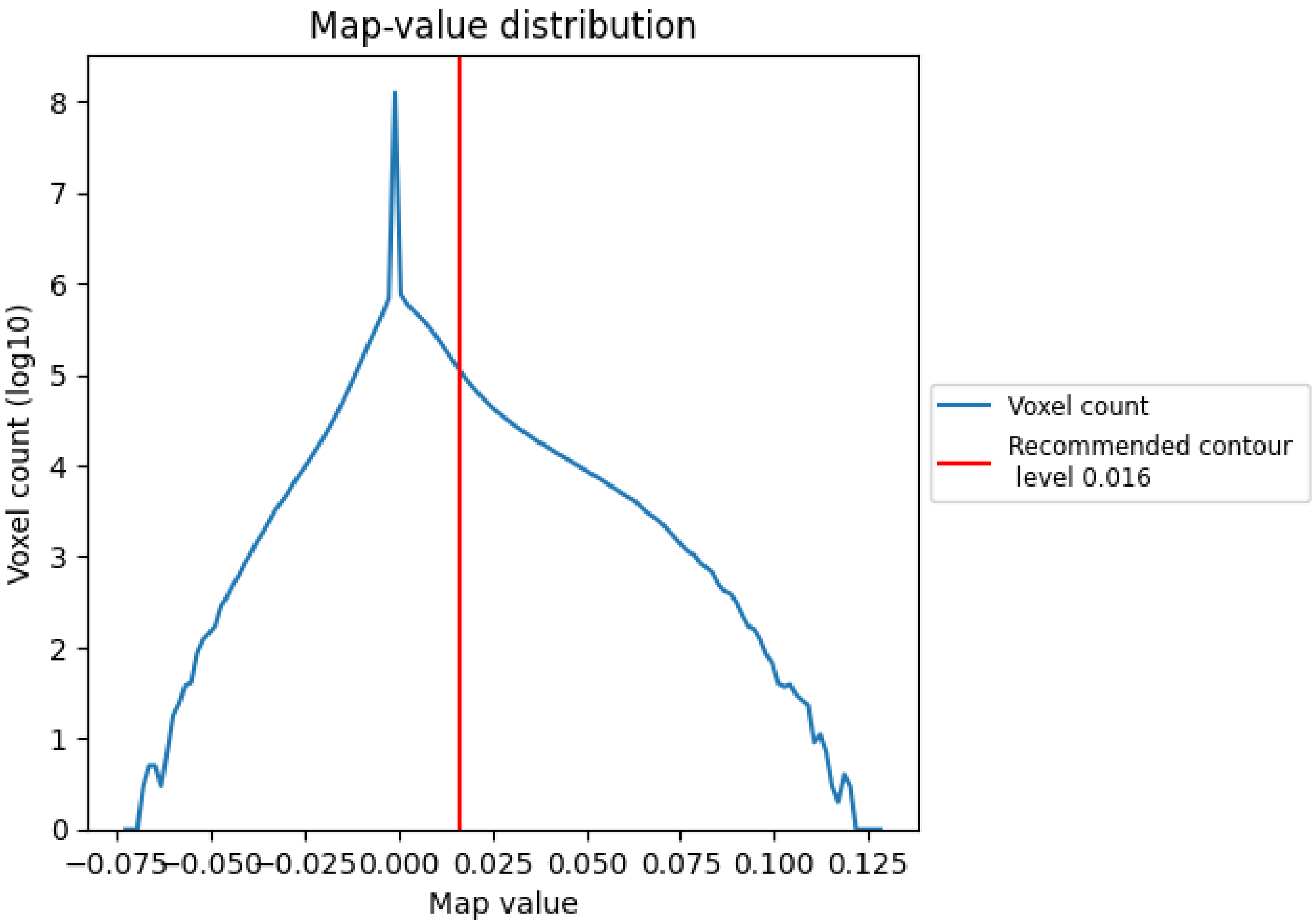
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

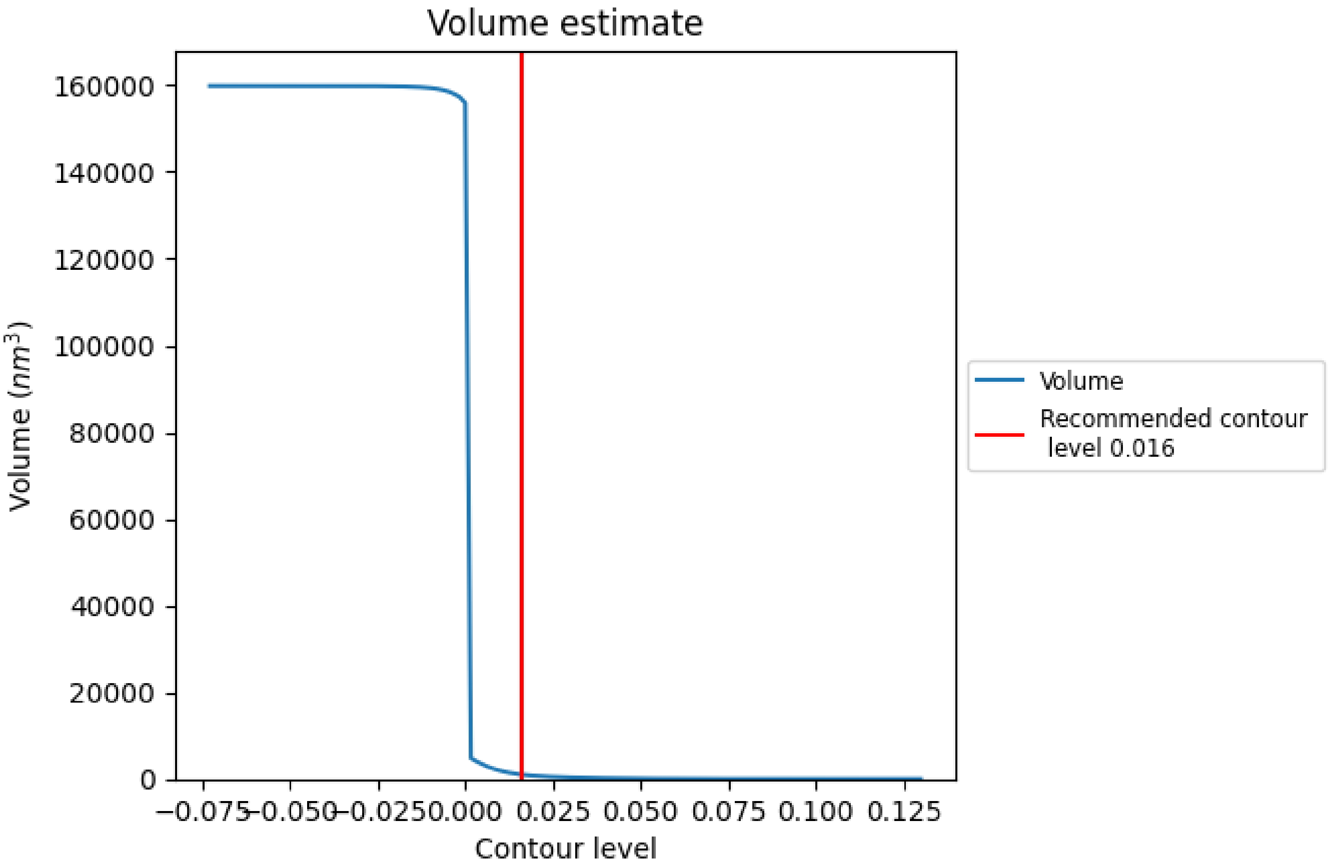
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

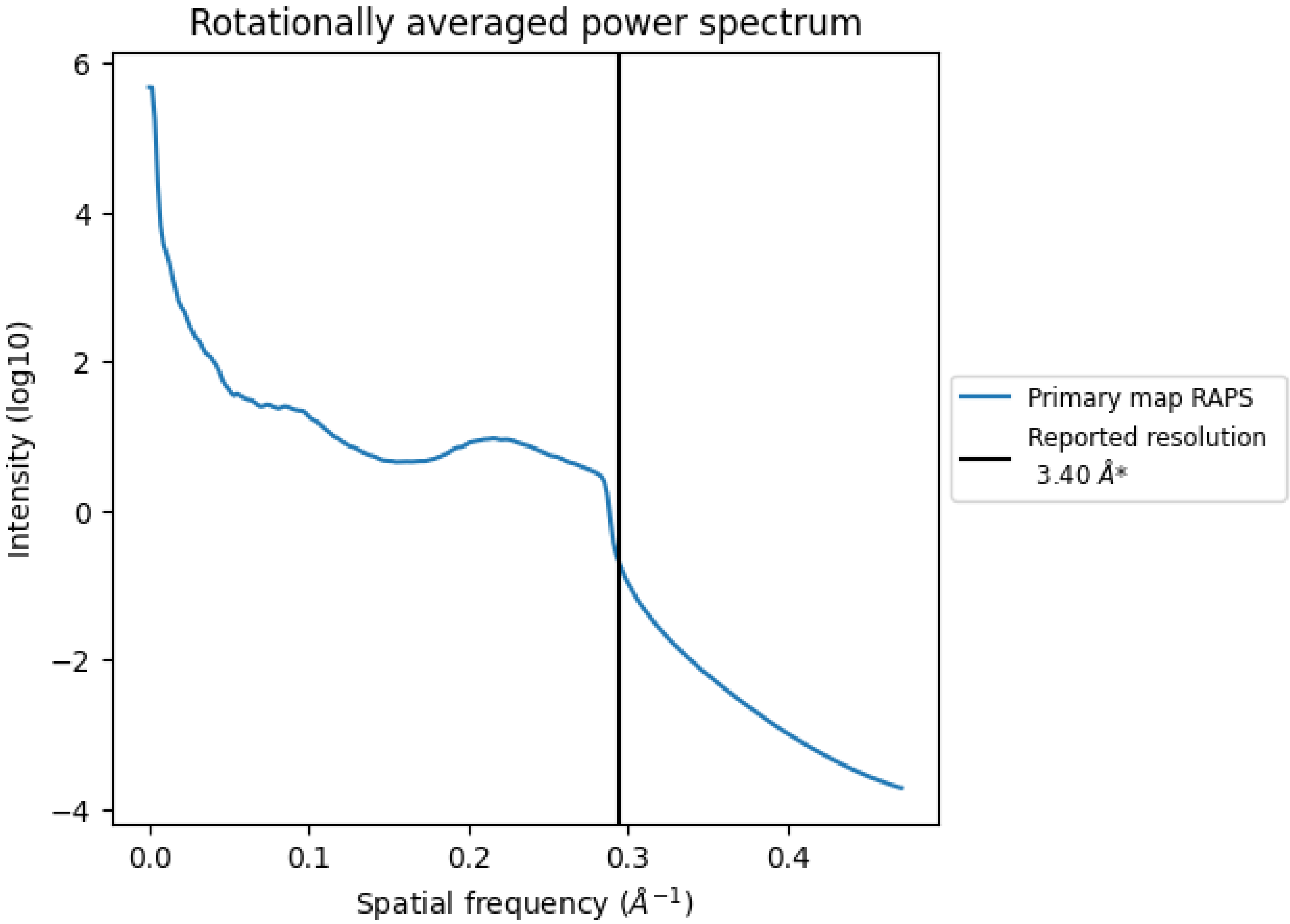
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 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 ⓘ

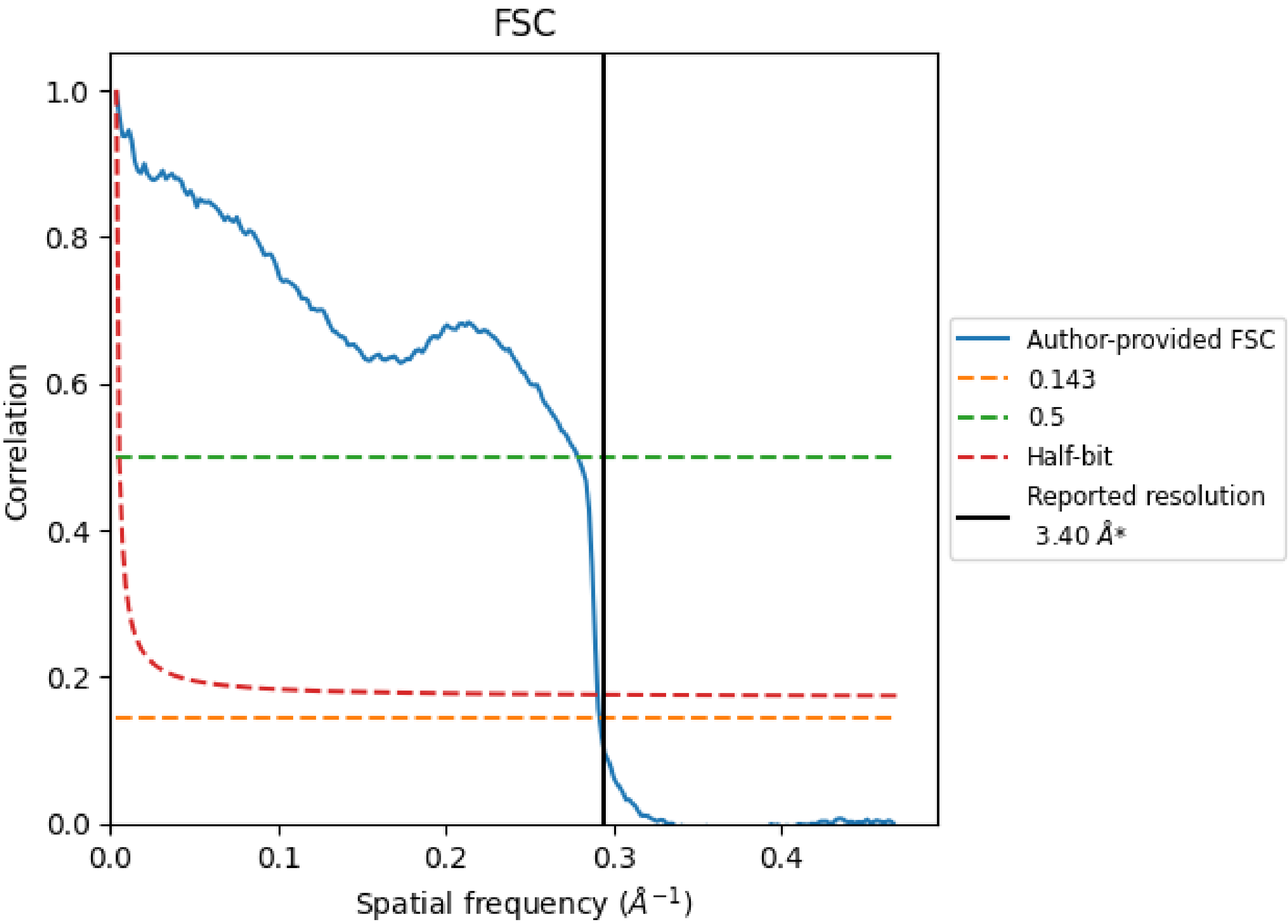


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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)

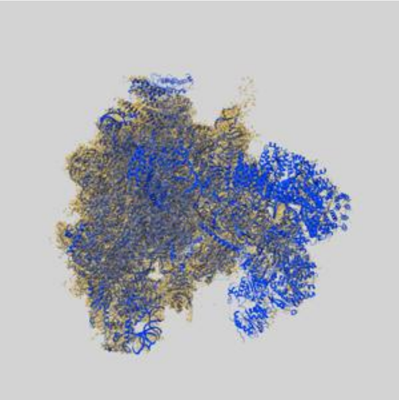
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	3.59	3.44
Unmasked-calculated*	-	-	-

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

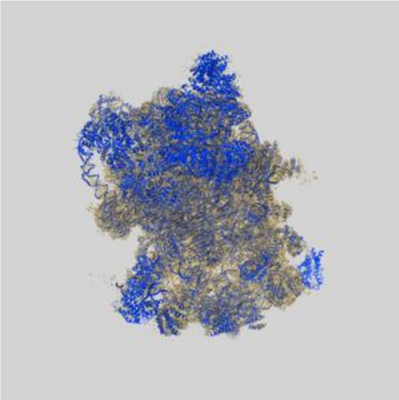
9 Map-model fit ⓘ

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.

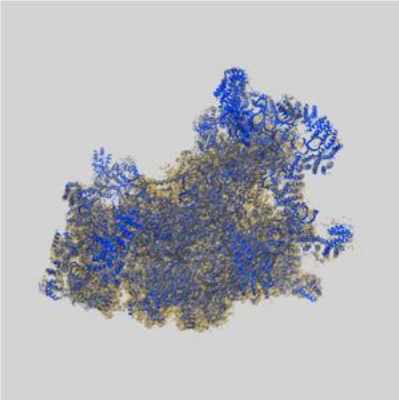
9.1 Map-model overlay ⓘ



X



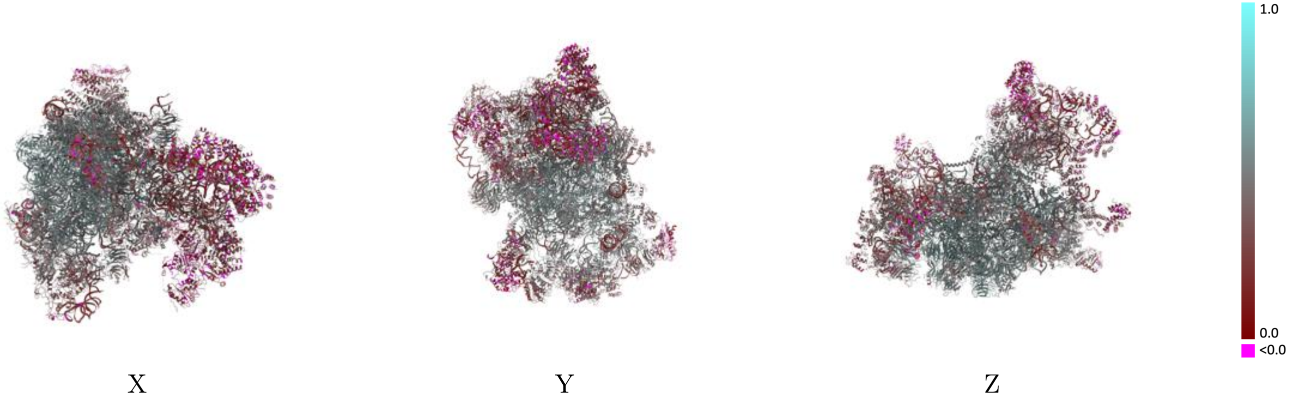
Y



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.

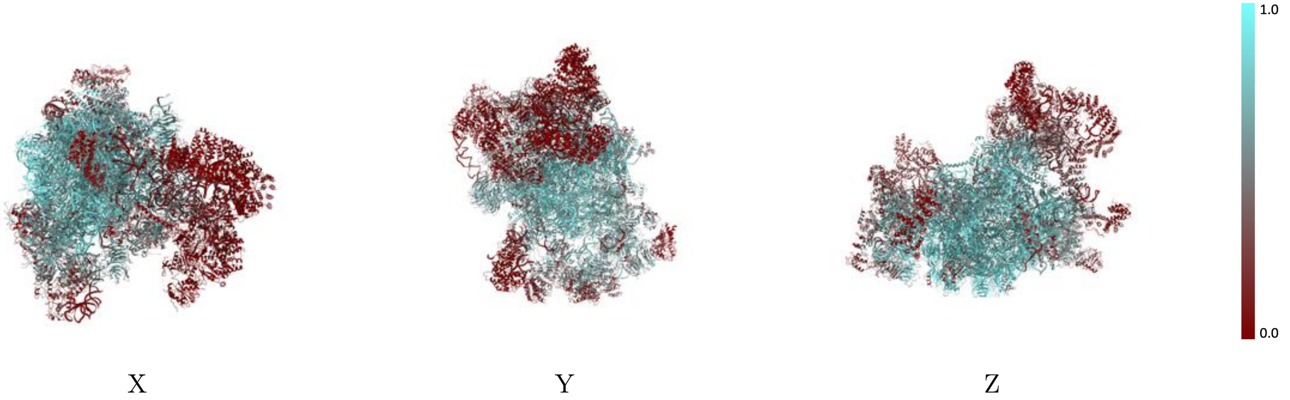
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

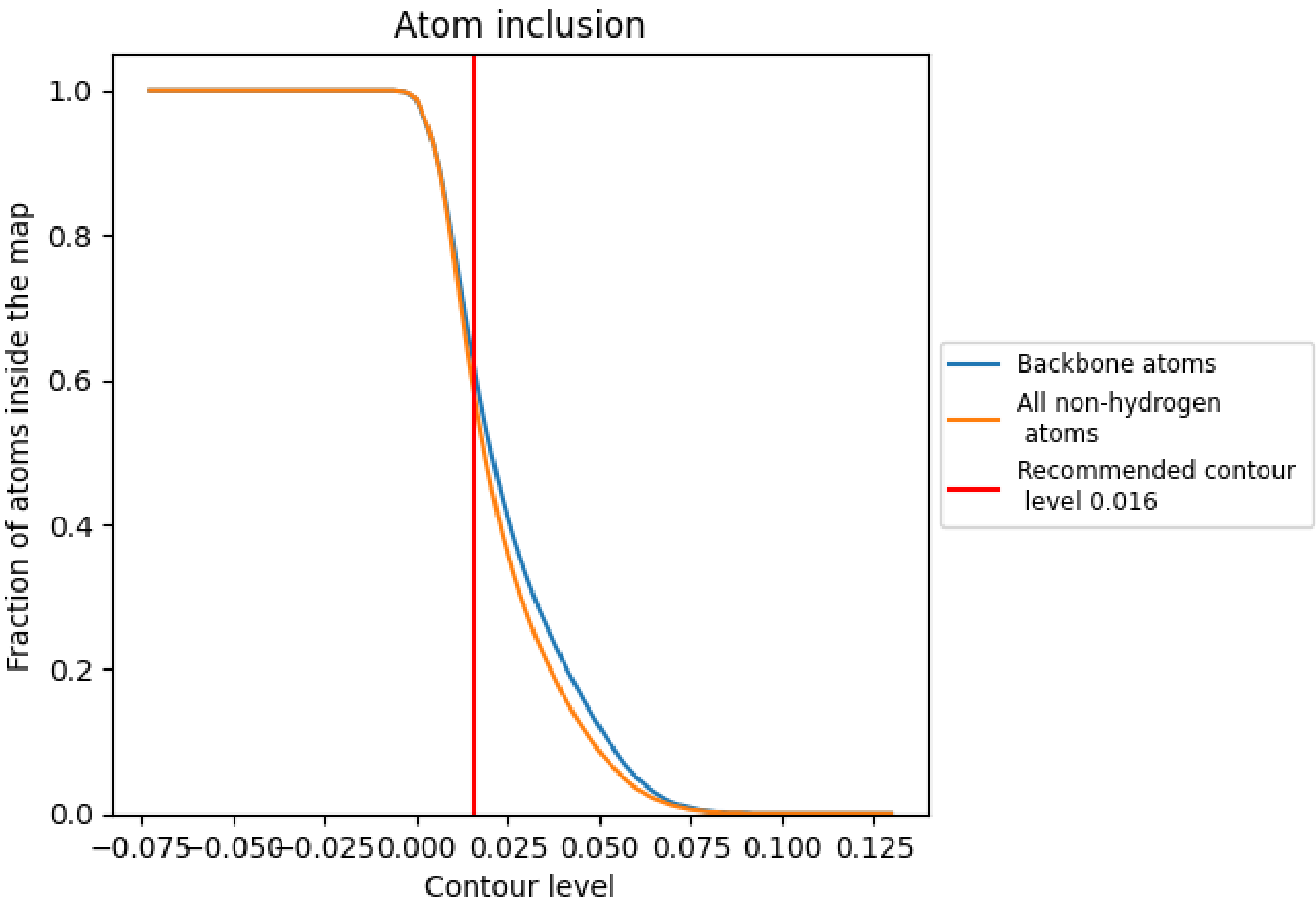
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

9.4 Atom inclusion ⓘ



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

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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