Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 05:39 PM JST

PDB ID	:	7D4I
EMDB ID	:	EMD-30574
Title	:	Cryo-EM structure of 90S small ribosomal precursors complex with the DEAH-box RNA helicase Dhr1 (State F)
Authors	:	Du, Y.; Zhang, J.; An, W.; Ye, K.
Deposited on	:	2020-09-24
Resolution	:	4.00 Å(reported)
Based on initial model	:	6LQS

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

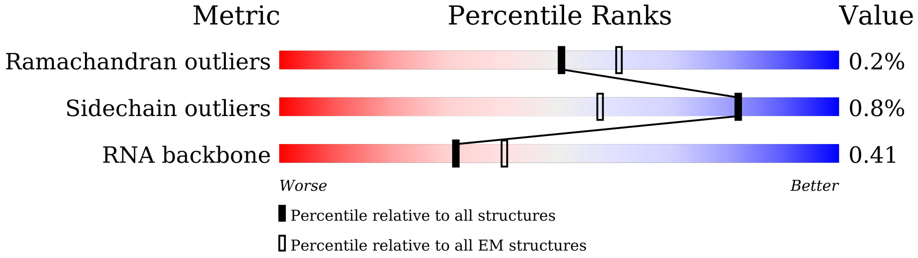
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

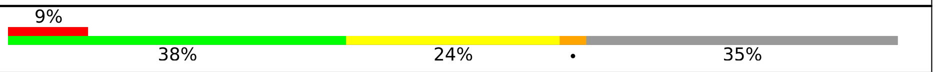
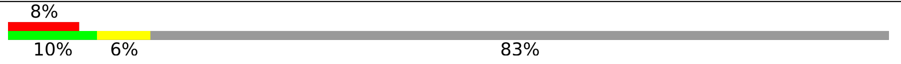
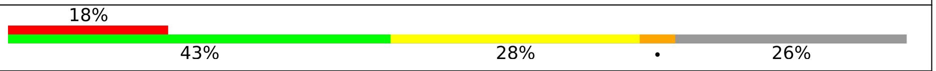
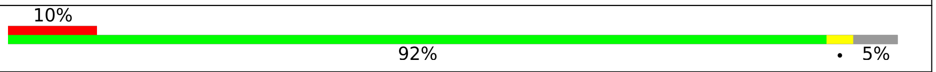
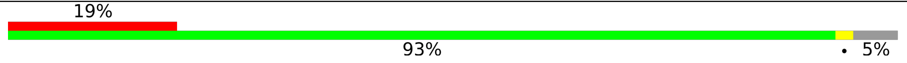
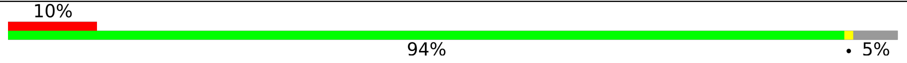
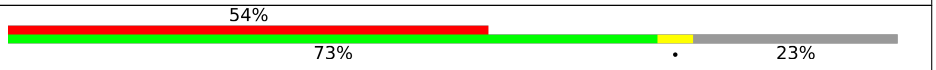
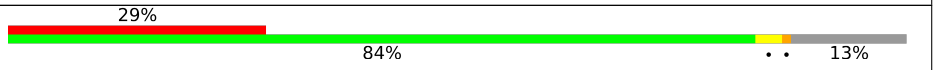
The reported resolution of this entry is 4.00 Å.

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	1812	
4	SC	255	
5	SF	261	
6	SG	225	
7	SH	236	
8	SI	190	

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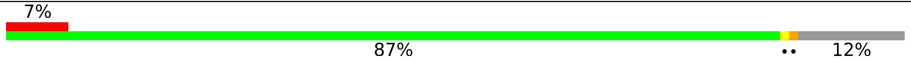
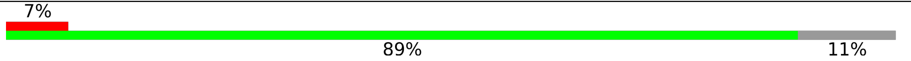
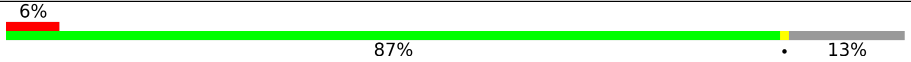
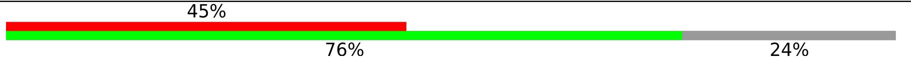
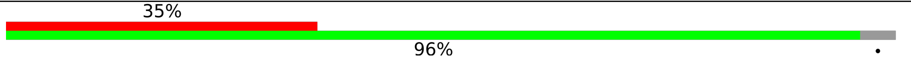
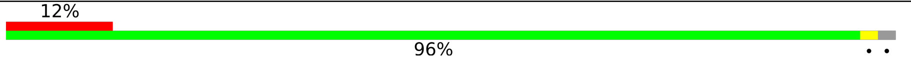
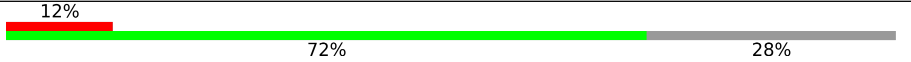
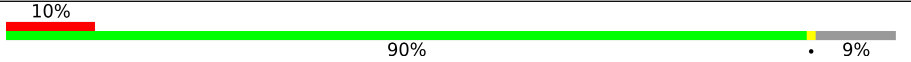
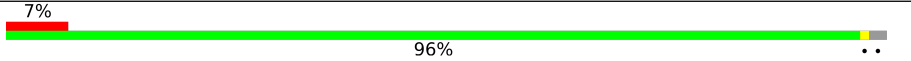
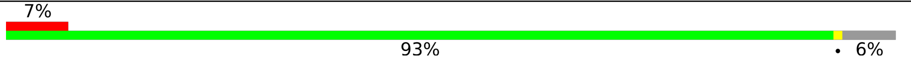
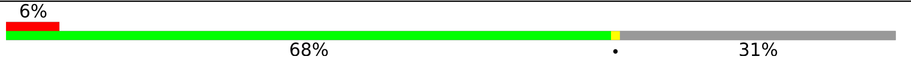
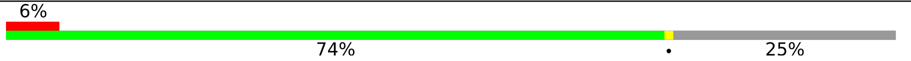
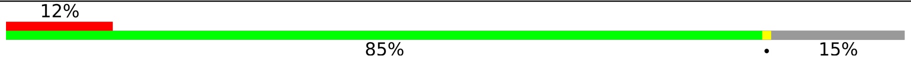
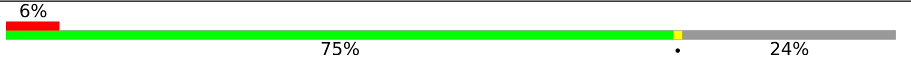
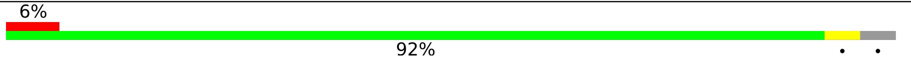
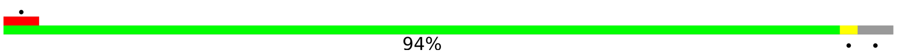
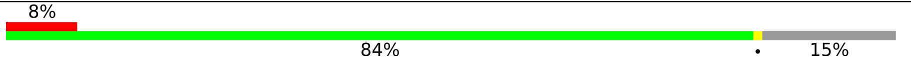
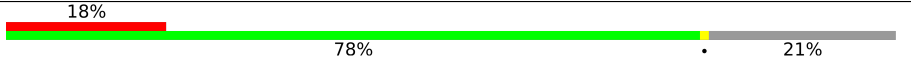
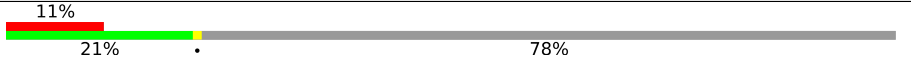
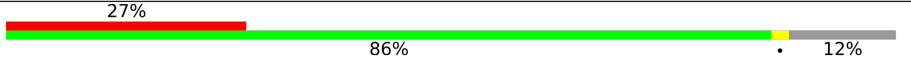
Mol	Chain	Length	Quality of chain
9	SJ	200	
10	SK	197	
11	SM	156	
12	SO	151	
13	SP	137	
14	SR	143	
15	ST	146	
16	SU	144	
17	SX	130	
18	SY	145	
19	SZ	135	
20	Sc	82	
21	Sd	67	
22	3B	327	
22	3C	327	
23	3D	504	
24	3E	511	
25	3F	573	
26	3G	126	
26	3H	126	
27	A4	776	
28	A5	643	
29	A8	713	
30	A9	575	
31	AE	1769	

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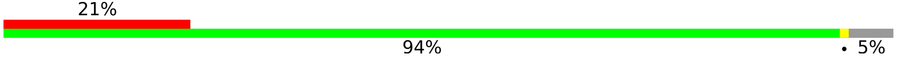
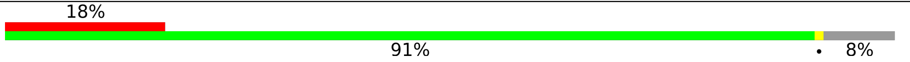
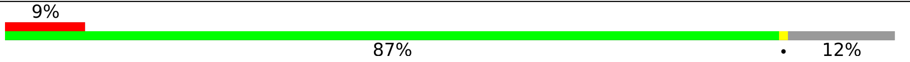
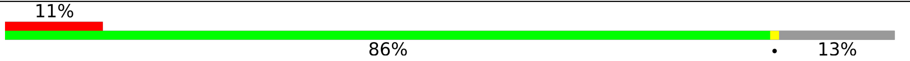
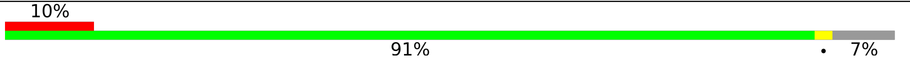
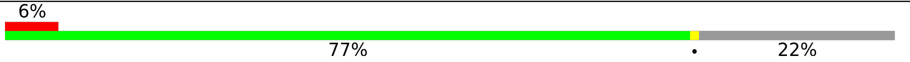
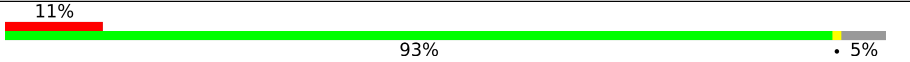
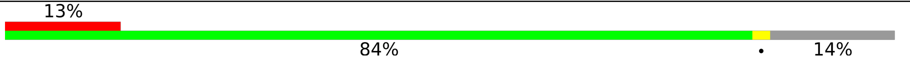
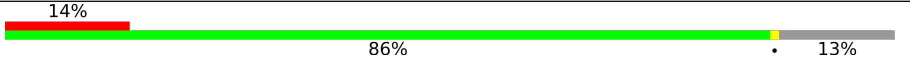
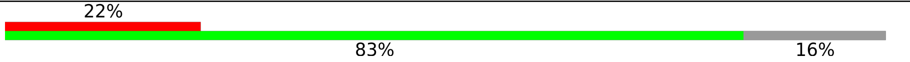
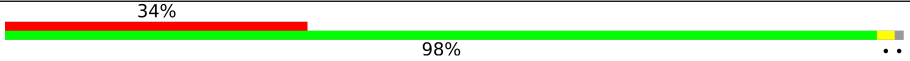
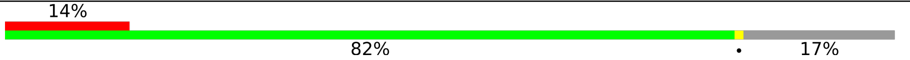
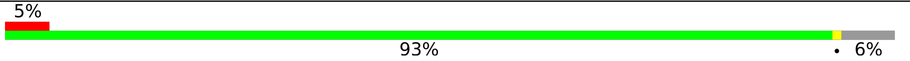
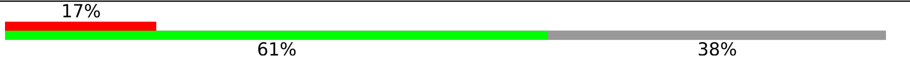
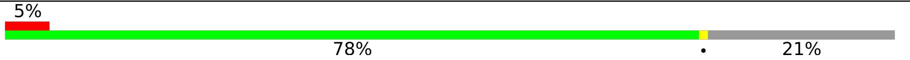
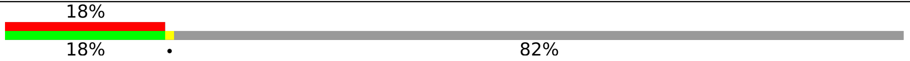
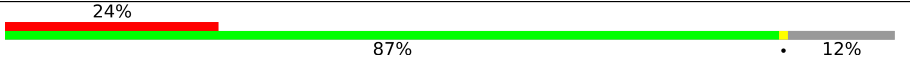
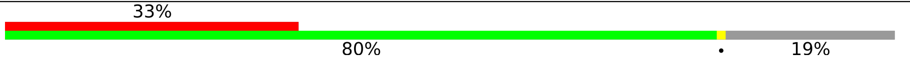
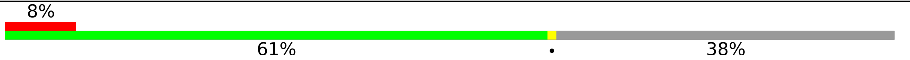
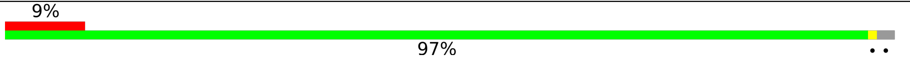
Mol	Chain	Length	Quality of chain
32	AF	513	 21% 94% • 5%
33	AG	896	 18% 91% • 8%
34	B1	900	 9% 87% • 12%
35	B2	943	 11% 86% • 13%
36	B3	817	 10% 91% • 7%
37	B8	594	 6% 77% • 22%
38	BE	939	 11% 93% • 5%
39	B6	440	 13% 84% • 14%
40	5B	214	 10% 26% • 73%
41	5C	554	 14% 86% • 13%
42	5D	250	 22% 83% 16%
43	5E	593	 8% 36% 64%
44	5F	183	 34% 98% • •
45	5G	290	 14% 82% • 17%
46	5H	610	 • 15% 84%
47	5I	489	 5% 93% • 6%
48	5J	217	 17% 61% 38%
49	5K	189	 5% 78% • 21%
50	RD	1729	 18% 18% • 82%
51	RE	1237	 24% 87% • 12%
52	RF	297	 33% 80% • 19%
53	RG	252	 73% 84% • 14%
53	RH	252	 64% 90% • 9%
54	RJ	1183	 8% 61% • 38%
55	RK	367	 9% 97% • •

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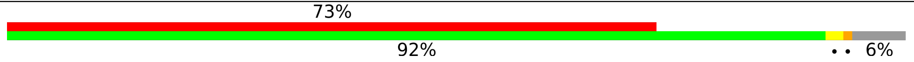
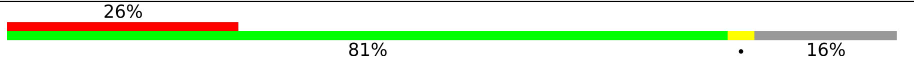
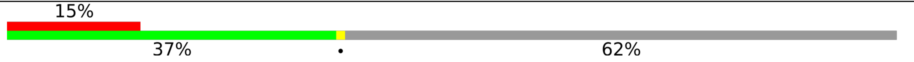
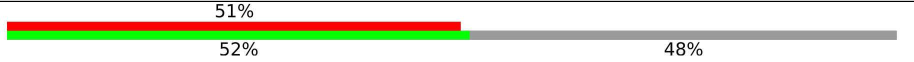
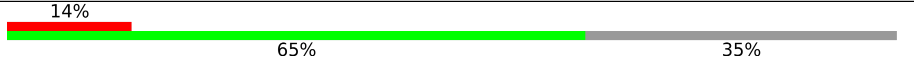
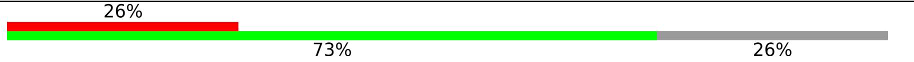
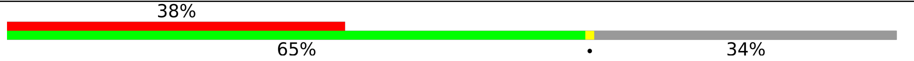
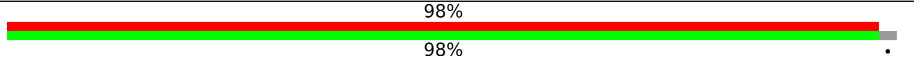
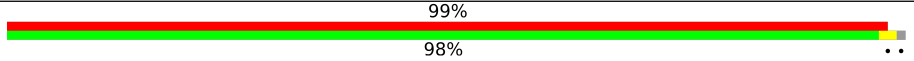
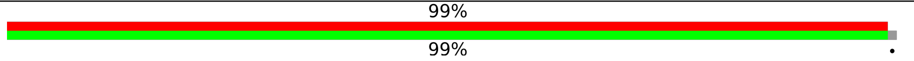
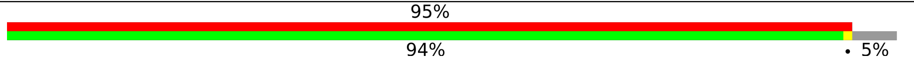
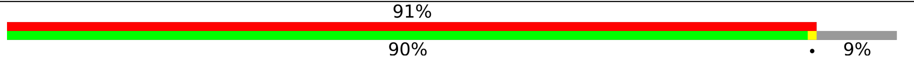
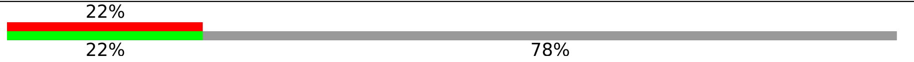
Mol	Chain	Length	Quality of chain
56	RN	810	
57	RO	552	
58	RP	2493	
59	RQ	899	
60	RS	480	
61	RT	326	
62	RW	206	
63	RZ	1267	
64	X1	611	
65	X2	694	
66	R5	305	
67	R1	246	
68	R3	394	
69	R6	223	
70	R2	265	
71	M3	250	
72	R0	240	
73	r4	359	
74	C4	292	
75	R4	1001	
76	r6	733	
77	R7	184	
78	M4	1073	
79	M6	186	

2 Entry composition

There are 83 unique types of molecules in this entry. The entry contains 253642 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	216	4570	2044	784	1526	216	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5A	118	2536	1131	467	820	118	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	SA	1337	28478	12732	5036	9373	1337	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	242	1923	1214	356	349	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	247	1915	1223	351	338	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	182	1456	916	273	266	1	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	148	1181	739	228	212	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	174	1410	892	272	245	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	137	1113	715	212	183	3	0	0

- Molecule 12 is a protein called 40S ribosomal protein S13.

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

- Molecule 13 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SP	116	848	524	158	163	3	0	0

- Molecule 14 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 15 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	ST	111	902	568	171	161	2	0	0

- Molecule 16 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	SU	138	1075	673	203	197	2	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	SY	104	792	506	145	139	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	SZ	123	986	626	188	172	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3B	242	Total 1878	C 1190	N 338	O 340	S 10	0	0
22	3C	224	Total 1754	C 1114	N 314	O 316	S 10	0	0

- Molecule 23 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3D	378	Total 2974	C 1886	N 511	O 568	S 9	0	0

- Molecule 24 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3E	435	Total 3056	C 1904	N 548	O 595	S 9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3F	437	Total 3498	C 2227	N 609	O 652	S 10	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A4	657	Total 5187	C 3286	N 902	O 978	S 21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A5	511	Total 3953	C 2507	N 682	O 751	S 13	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AE	1552	Total 10262	C 6453	N 1810	O 1979	S 20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AF	487	Total 3860	C 2431	N 692	O 725	S 12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AG	825	Total 6565	C 4178	N 1110	O 1258	S 19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B1	791	Total 6316	C 4037	N 1082	O 1179	S 18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	B2	824	Total 6497	C 4153	N 1095	O 1222	S 27	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B3	757	Total 5906	C 3763	N 993	O 1123	S 27	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B8	463	Total 3648	C 2314	N 640	O 684	S 10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BE	890	Total 6876	C 4356	N 1191	O 1308	S 21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B6	377	Total 3077	C 1984	N 529	O 549	S 15	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
40	5B	58	Total 482	C 302	N 98	O 82	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	5C	482	Total 3825	C 2409	N 684	O 721	S 11	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	209	1778	1111	344	317	6	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	213	1728	1072	304	348	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	241	1956	1228	368	353	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	95	700	435	143	122	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	134	1127	712	205	207	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	5K	150	1190	765	212	203	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5K	138	ASN	ASP	variant	UNP Q05498

- Molecule 50 is a protein called rRNA biogenesis protein RRP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	RD	316	2413	1541	415	452	5	0	0

- Molecule 51 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	RE	1090	8805	5720	1452	1609	24	0	0

- Molecule 52 is a protein called Ribosomal RNA-processing protein 7.

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

- Molecule 53 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

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

- Molecule 54 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	RJ	738	5994	3851	1063	1054	26	0	0

- Molecule 55 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 56 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	RN	584	4459	2819	800	827	13	0	0

- Molecule 57 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	RO	520	3741	2397	641	691	12	0	0

- Molecule 58 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	RP	2084	12263	7556	2298	2392	17	0	0

- Molecule 59 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	RQ	339	2408	1484	456	466	2	0	0

- Molecule 60 is a protein called Essential nuclear protein 1.

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

- Molecule 61 is a protein called Pno1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	RT	213	1652	1051	300	297	4	0	0

- Molecule 62 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	RW	153	Total 762	C 456	N 153	O 153	0	0

- Molecule 63 is a protein called Probable ATP-dependent RNA helicase DHR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	RZ	838	Total 6598	C 4212	N 1145	O 1206	S 35	1	0

- Molecule 64 is a protein called Unassigned peptides 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	X1	221	Total 1105	C 663	N 221	O 221	0	0

- Molecule 65 is a protein called Unassigned peptides 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	X2	141	Total 705	C 423	N 141	O 141	0	0

- Molecule 66 is a protein called Exosome complex component RRP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	R5	299	Total 2304	C 1444	N 393	O 451	S 16	0	0

- Molecule 67 is a protein called Exosome complex component SKI6.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	R1	244	Total 1886	C 1177	N 335	O 366	S 8	0	0

- Molecule 68 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	R3	339	Total 2588	C 1640	N 441	O 497	S 10	1	0

- Molecule 69 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	R6	223	Total 1701	C 1072	N 285	O 334	S 10	1	0

- Molecule 70 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	R2	265	Total 2035	C 1299	N 334	O 397	S 5	1	0

- Molecule 71 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	M3	215	Total 1639	C 1024	N 273	O 332	S 10	0	0

- Molecule 72 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	R0	237	Total 1792	C 1143	N 295	O 344	S 10	0	0

- Molecule 73 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	r4	293	Total 2236	C 1393	N 403	O 428	S 12	0	0

- Molecule 74 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	C4	222	Total 1653	C 1034	N 287	O 325	S 7	0	0

- Molecule 75 is a protein called Exosome complex exonuclease DIS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	R4	948	Total 7430	C 4693	N 1308	O 1394	S 35	0	0

- Molecule 76 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	r6	414	2517	1544	469	498	6	0	0

- Molecule 77 is a protein called Exosome complex protein LRP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	R7	113	894	565	151	174	4	0	0

- Molecule 78 is a protein called ATP-dependent RNA helicase DOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	M4	978	7626	4871	1294	1419	42	0	0

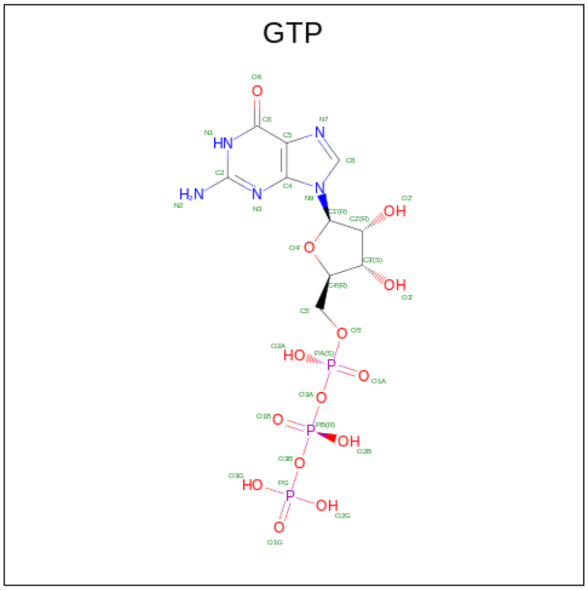
- Molecule 79 is a protein called M-phase phosphoprotein 6 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
79	M6	40	275	170	51	54	0	0

- Molecule 80 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
80	Sc	1	1	1	0
80	5K	1	1	1	0

- Molecule 81 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

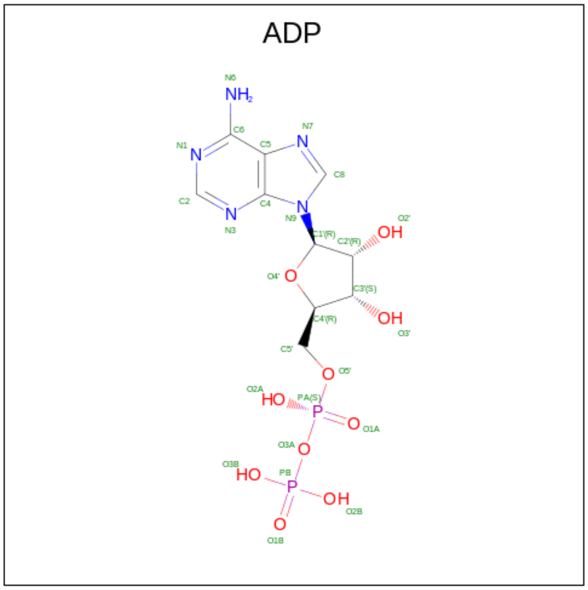


Mol	Chain	Residues	Atoms					AltConf
81	RJ	1	Total 32	C 10	N 5	O 14	P 3	0

- Molecule 82 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 83 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

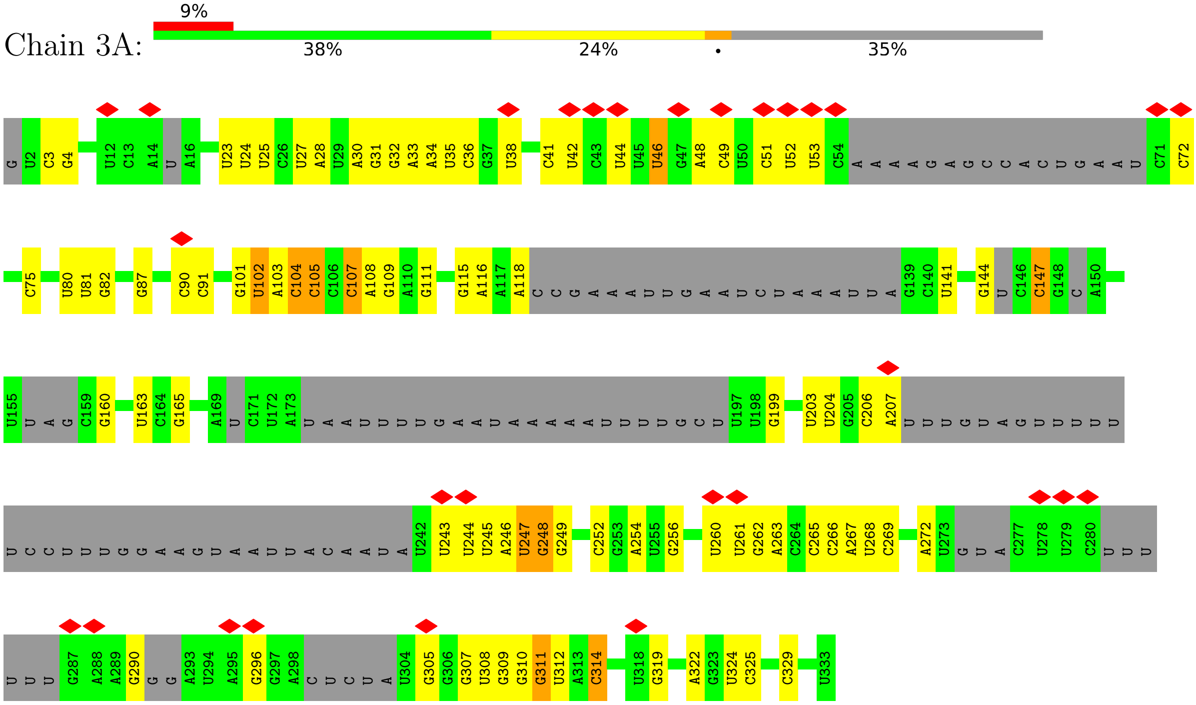


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
83	RZ	1	27	10	5	10	2	0

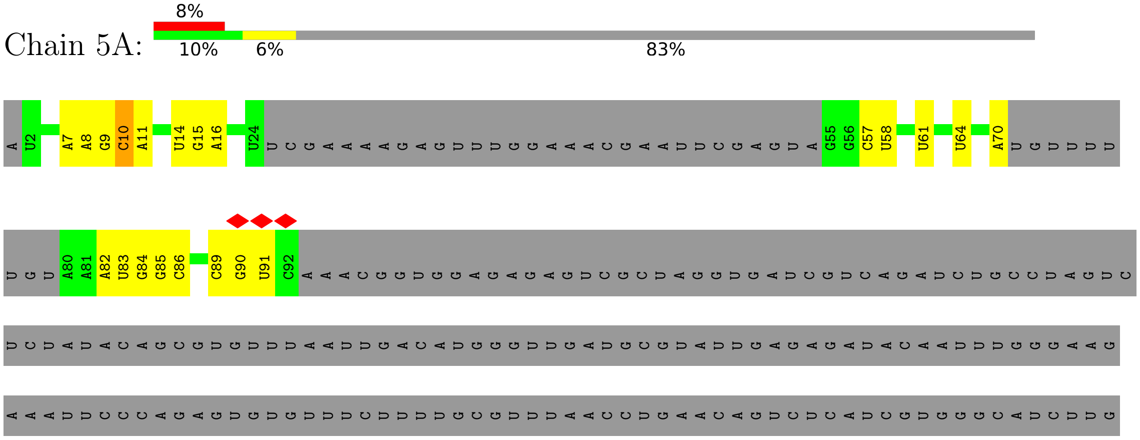
3 Residue-property plots (i)

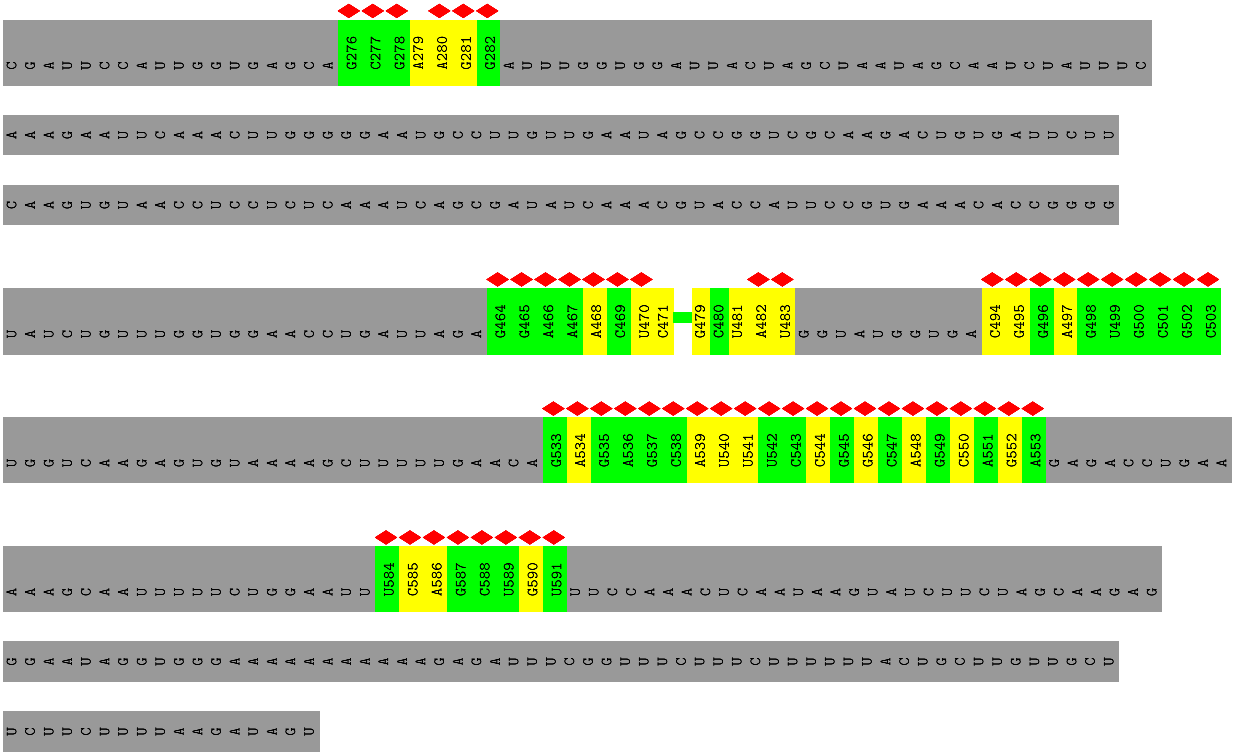
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: U3 snoRNA



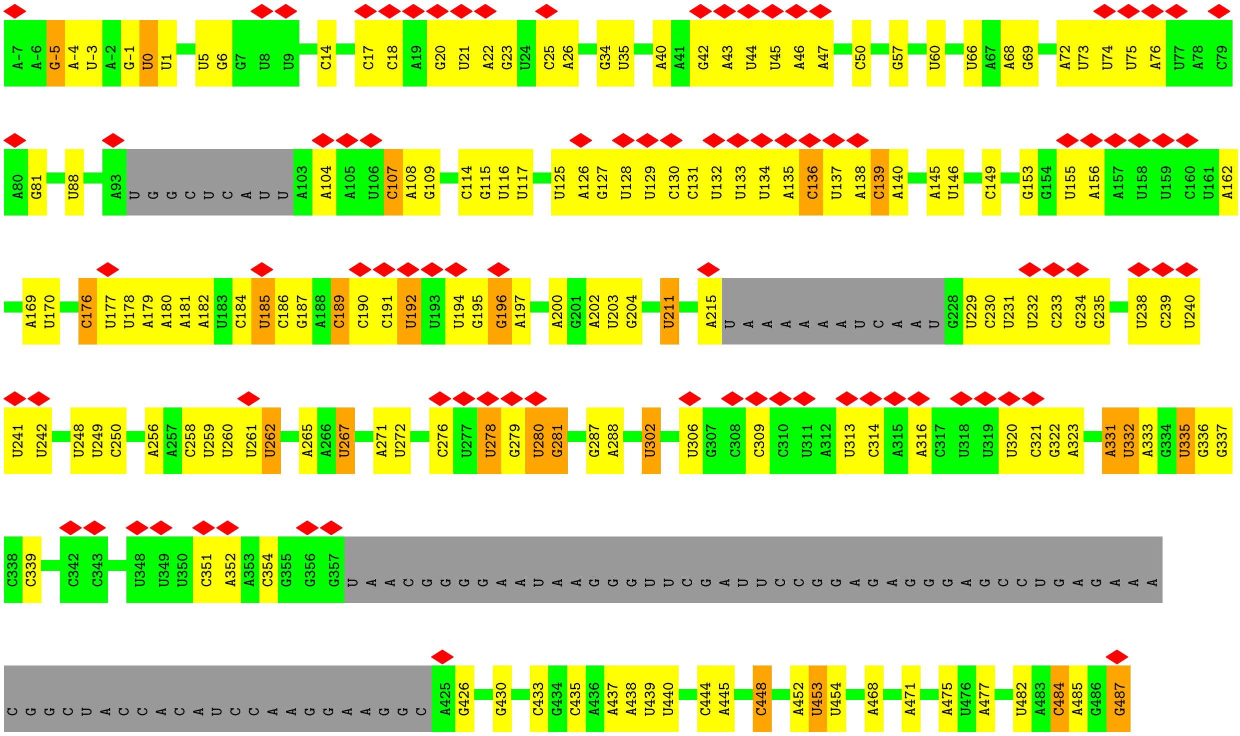
- Molecule 2: 5’ ETS

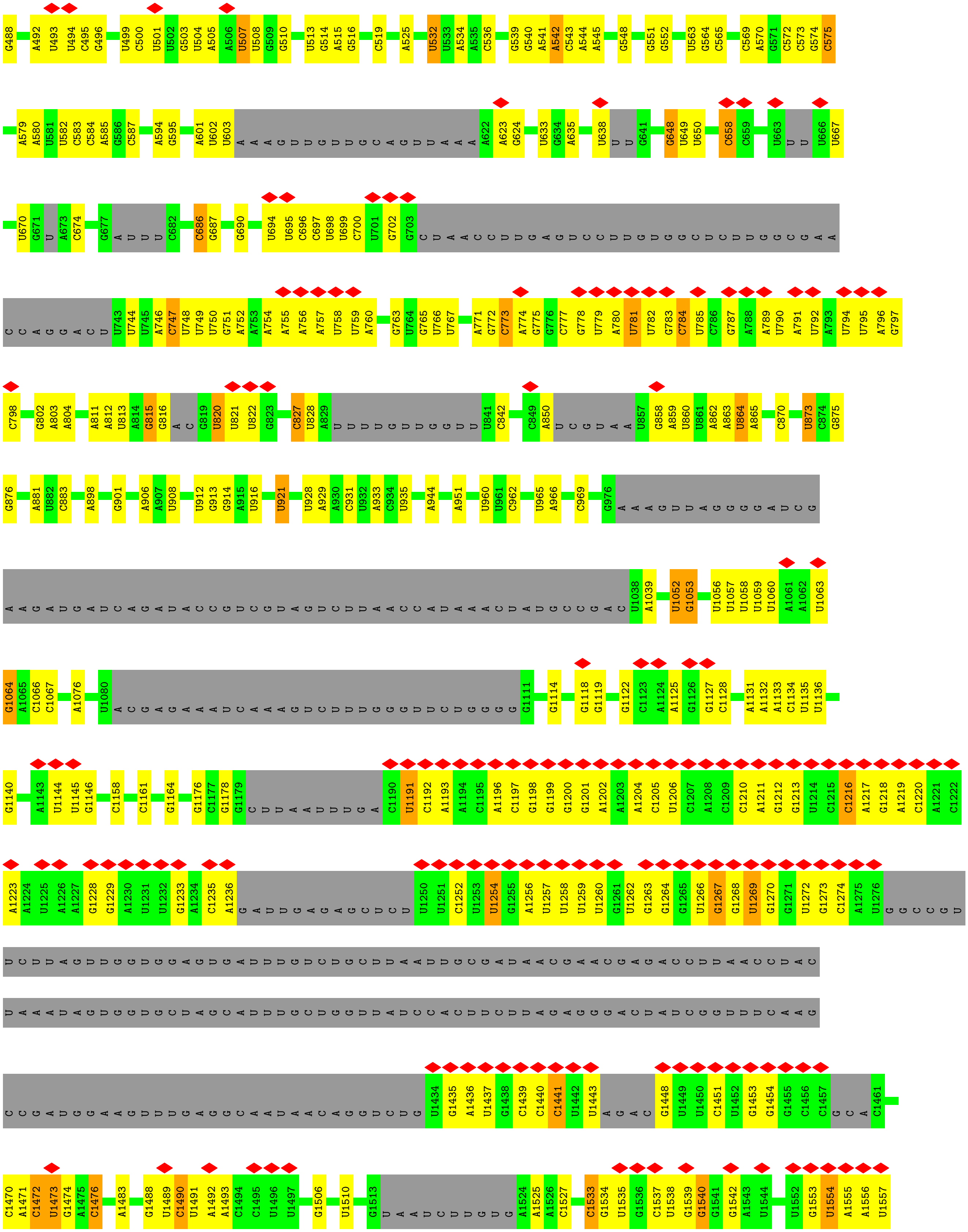




- Molecule 3: 18S rRNA

Chain SA:

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A579 A580 U581 U582 C583 C584 A585 G586 C587 A594 G595 A601 U602 U603 A A A G U U G U U G C A G U U A A A A622 A623 G624 U633 G634 A635 U638 U U G641 G648 U649 U650 C658 C659 U663 U U U666 U667
U670 G671 U A673 C674 G677 A U U U C682 C686 G687 G690 U694 U695 C696 C697 U698 U699 C700 U701 G702 G703 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 U743 U744 U745 A746 C747 U748 U749 U750 G751 A752 A753 A754 A755 A756 A757 U758 U759 A760 G763 U764 G765 U766 U767 A771 G772 C773 A774 G775 G776 C777 G778 U779 A780 U781 U782 G783 C784 U785 C786 G787 A788 A789 U790 A791 U792 A793 U794 U795 A796 G797
C798 G802 A803 A804 A811 A812 U813 A814 G815 G816 A C G819 U820 U821 U822 G823 C827 U828 A829 U U U U G U U G G U U U841 C842 C849 A850 U C G U A A U857 G858 A859 U860 U861 A862 A863 U864 A865 C870 U873 C874 G875
G876 A881 U882 C883 A898 G901 A906 A907 U908 U912 G913 G914 A915 U916 U921 U928 A929 A930 C931 U932 A933 C934 U935 A944 A951 U960 U961 C962 U965 A966 C969 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 C G U C G U A G U C U U A A C C A U A A A C U A U G C C G A C U1038 A1039 U1052 G1053 U1056 U1057 U1058 U1059 U1060 A1061 A1062 U1063
G1064 A1065 C1066 C1067 A1076 U1080 A C G A G A A A U C A A A G U C U U U G G G U U C U G G G G G1111 G1114 G1118 G1119 G1122 C1123 A1124 A1125 G1126 G1127 C1128 A1131 A1132 A1133 C1134 U1135 U1136
G1140 A1143 U1144 U1145 G1146 C1158 C1161 G1164 G1176 C1177 G1178 G1179 C U U A A U 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 U G U C U G C U U A A U U G C G A U A A C G A A C G A G A C C U U A A C C U A C
U A A A U A G U U G G U G C U A G C A U U U G C U G G U U A U C C 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
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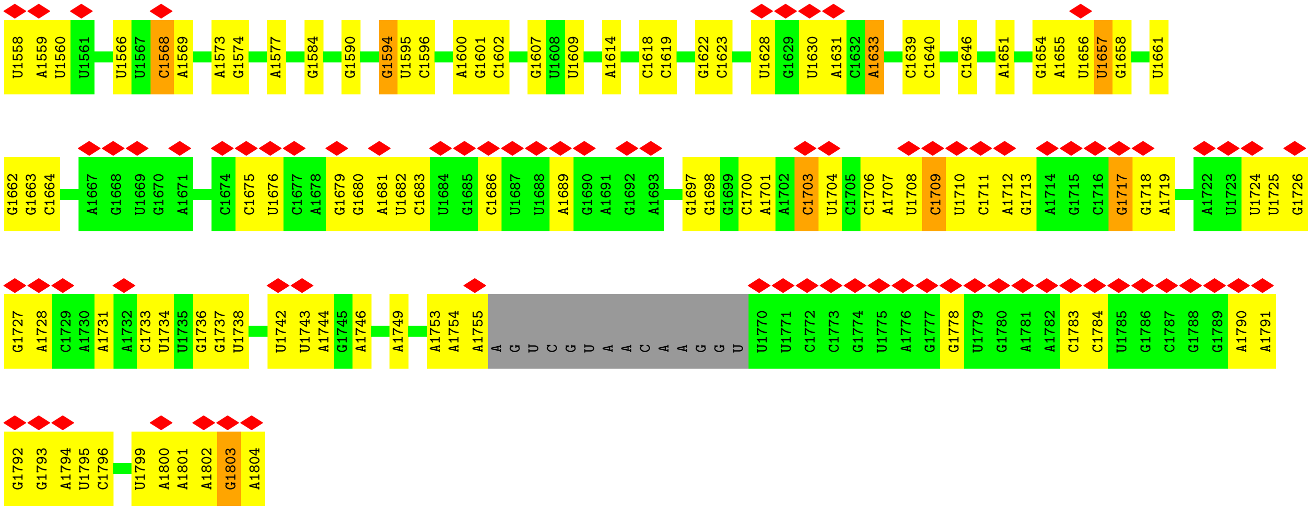
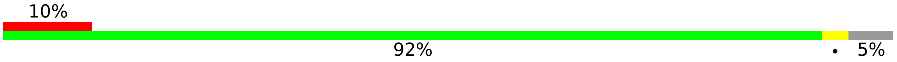
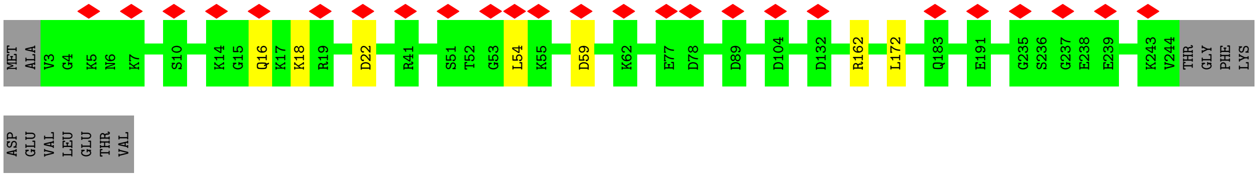


- Molecule 4: 40S ribosomal protein S1-A

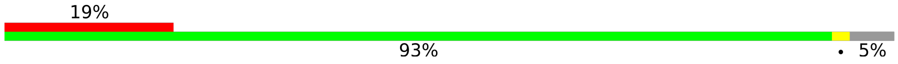
Chain SC:

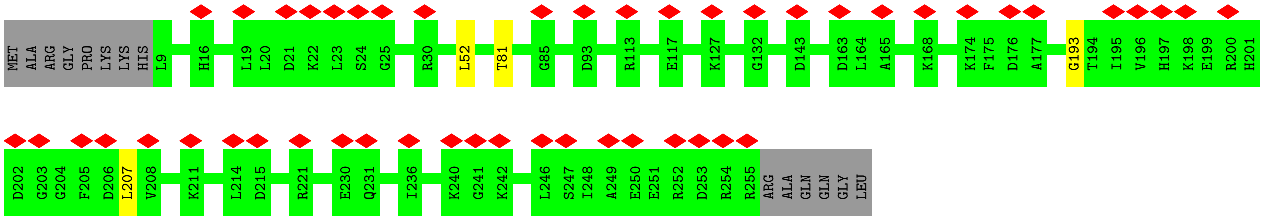




- Molecule 5: 40S ribosomal protein S4-A

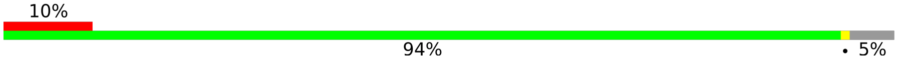
Chain SF:

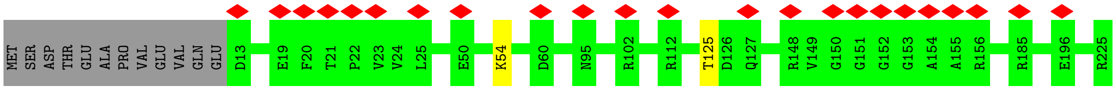




- Molecule 6: 40S ribosomal protein S5

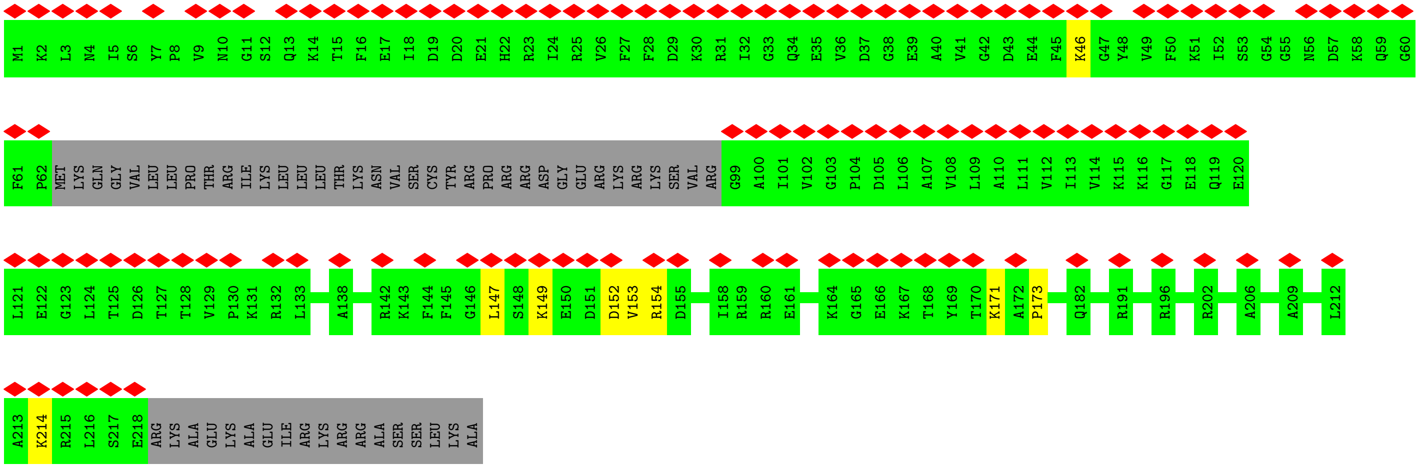
Chain SG:





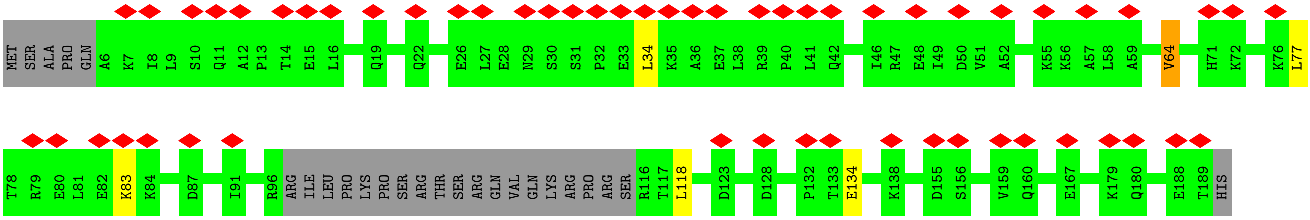
- Molecule 7: 40S ribosomal protein S6-A

Chain SH:



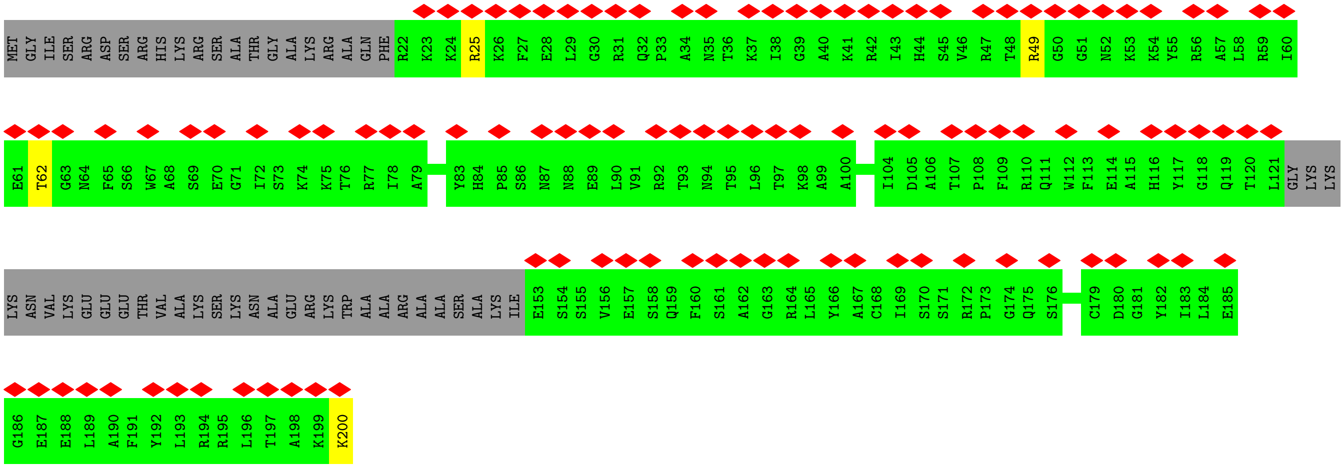
- Molecule 8: 40S ribosomal protein S7-A

Chain SI:



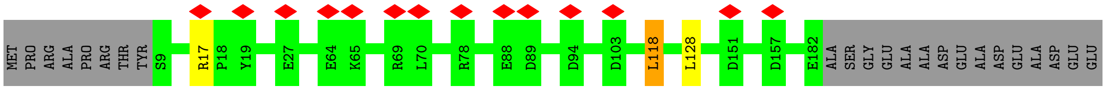
- Molecule 9: 40S ribosomal protein S8-A

Chain SJ:

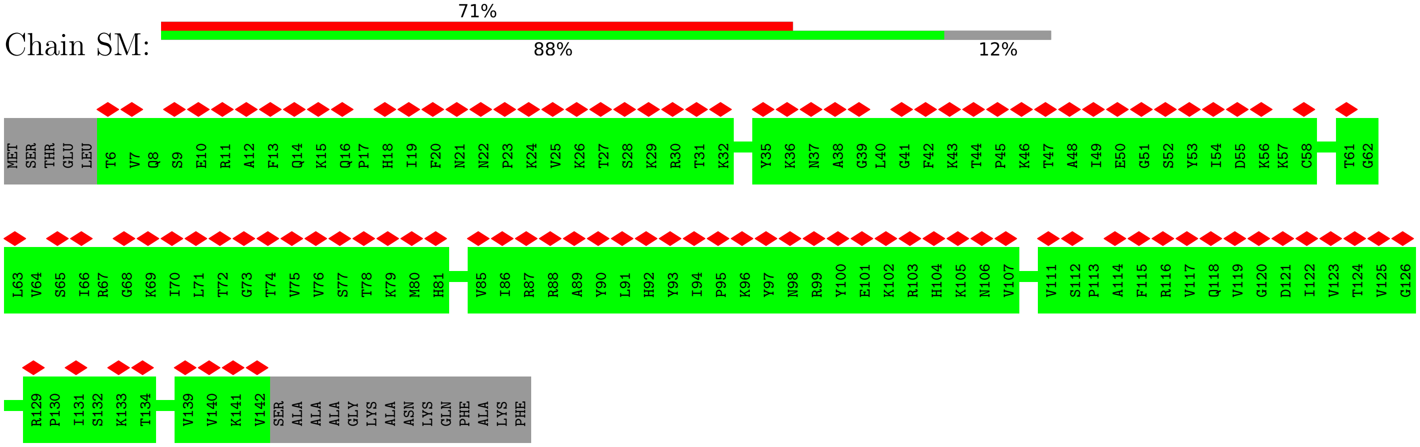


- Molecule 10: 40S ribosomal protein S9-A

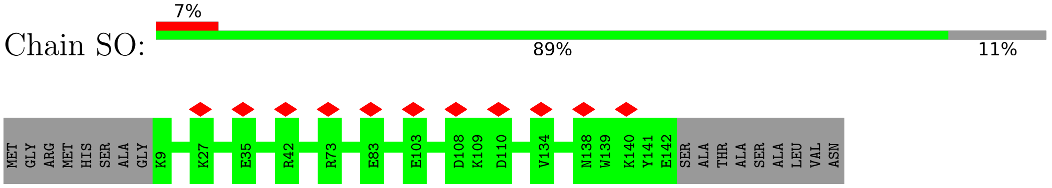
Chain SK:



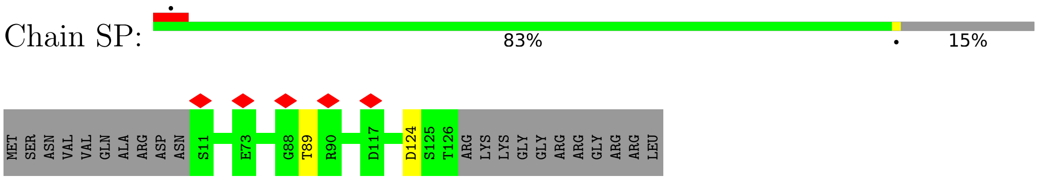
- Molecule 11: 40S ribosomal protein S11-A



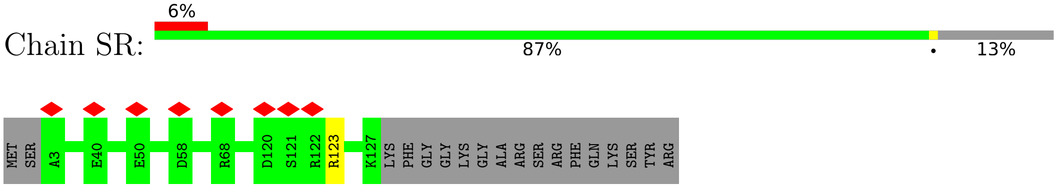
- Molecule 12: 40S ribosomal protein S13



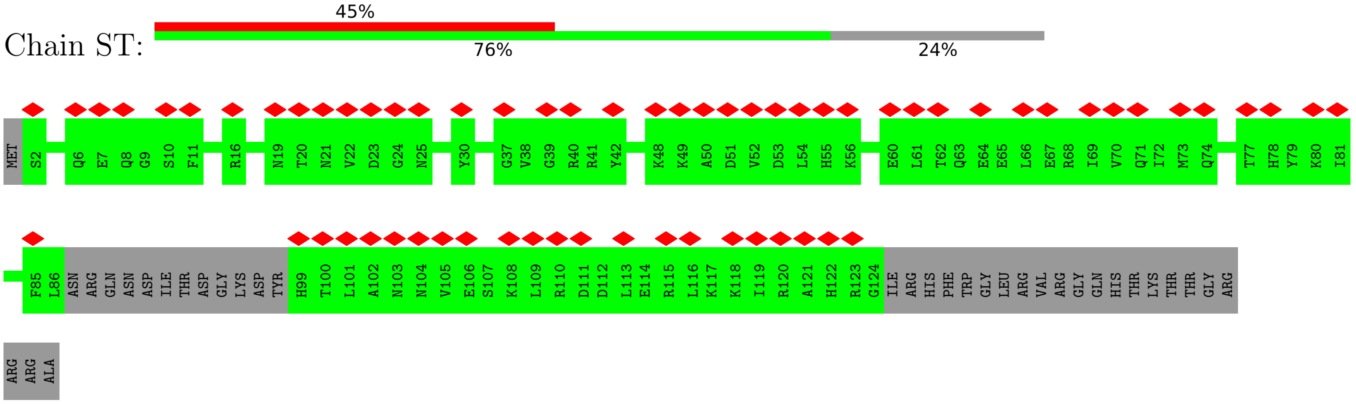
- Molecule 13: 40S ribosomal protein S14-A



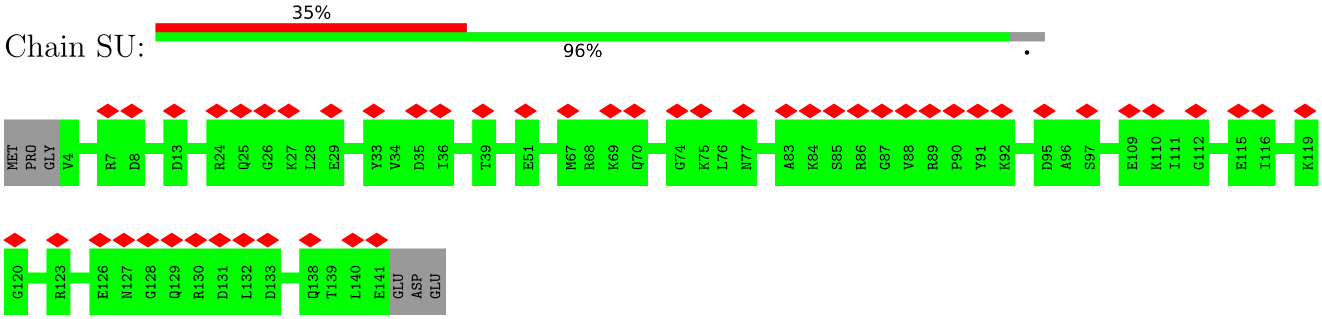
- Molecule 14: 40S ribosomal protein S16-A



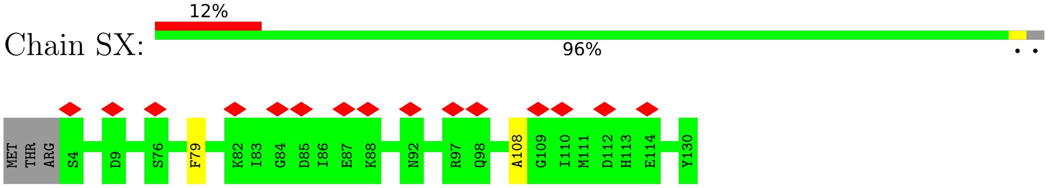
- Molecule 15: 40S ribosomal protein S18-A



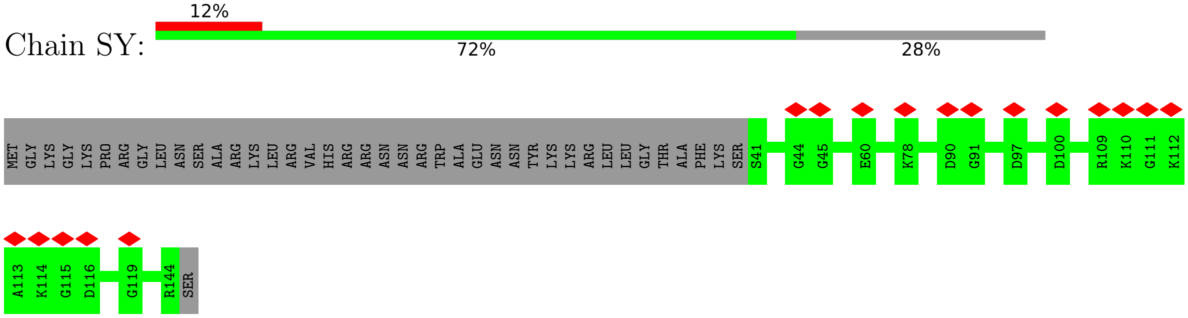
- Molecule 16: 40S ribosomal protein S19-A



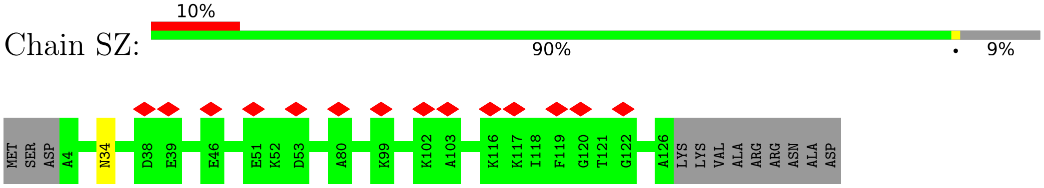
- Molecule 17: 40S ribosomal protein S22-B



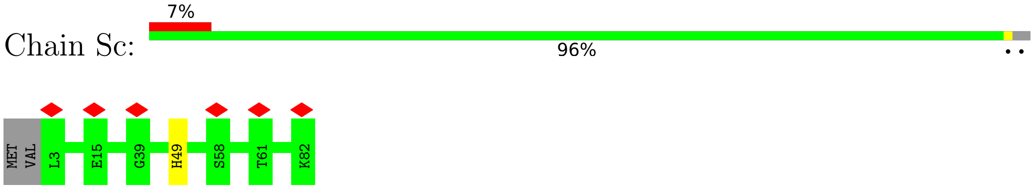
- Molecule 18: 40S ribosomal protein S23-A



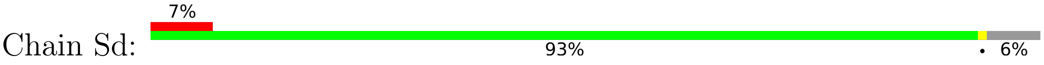
- Molecule 19: 40S ribosomal protein S24-A

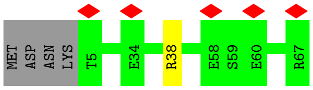


- Molecule 20: 40S ribosomal protein S27-A



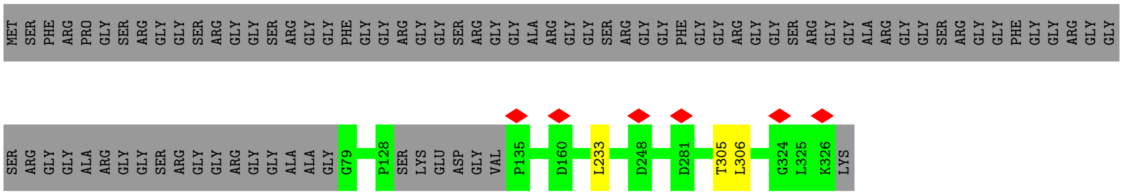
- Molecule 21: 40S ribosomal protein S28-A





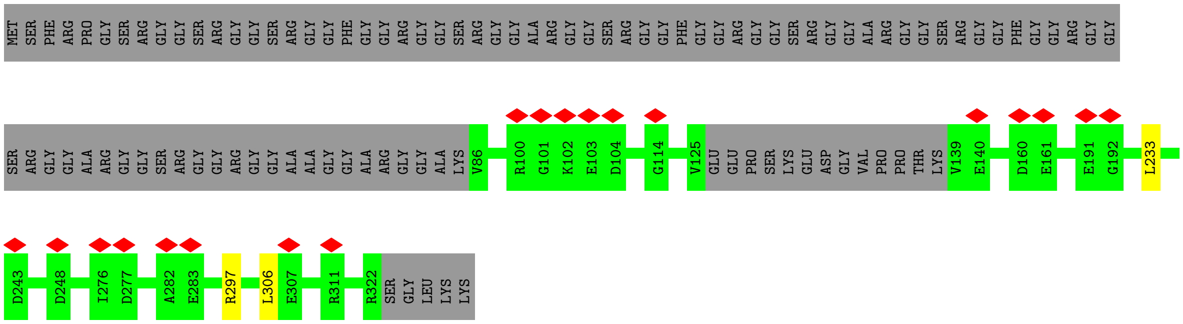
- Molecule 22: rRNA 2'-O-methyltransferase fibrillarin

Chain 3B:



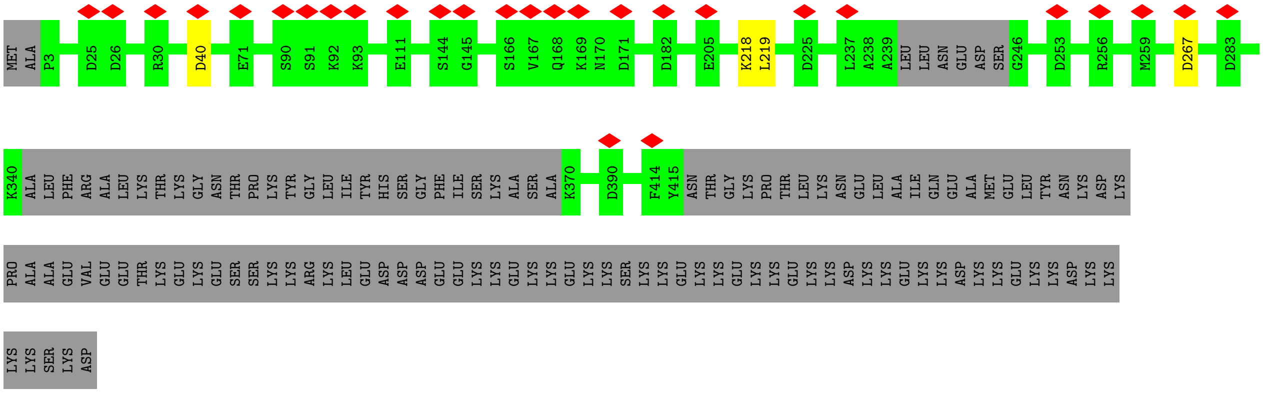
- Molecule 22: rRNA 2'-O-methyltransferase fibrillarin

Chain 3C:



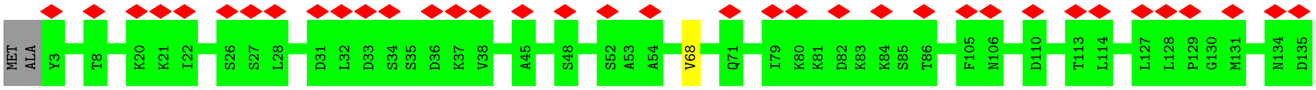
- Molecule 23: Nucleolar protein 56

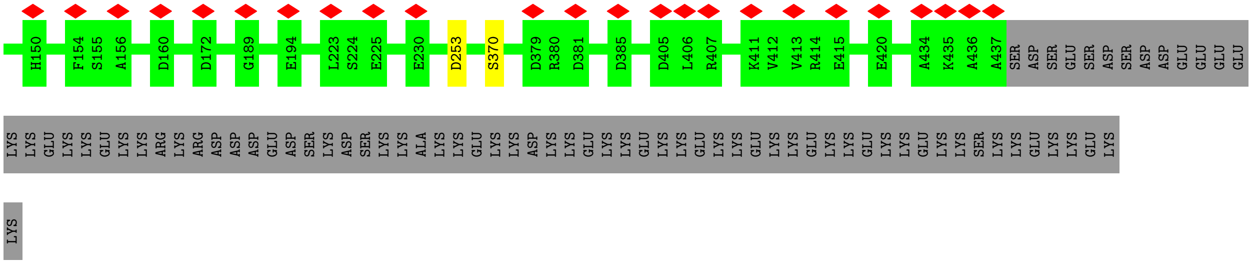
Chain 3D:



- Molecule 24: Nucleolar protein 58

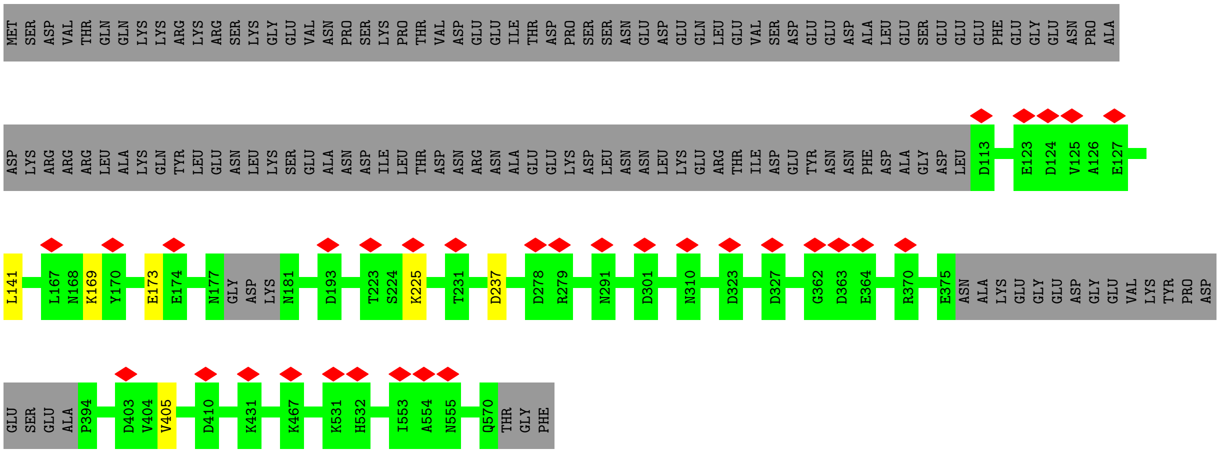
Chain 3E:





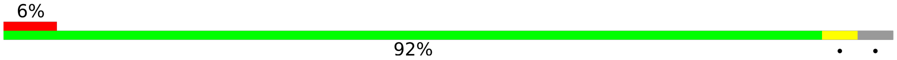
- Molecule 25: Ribosomal RNA-processing protein 9

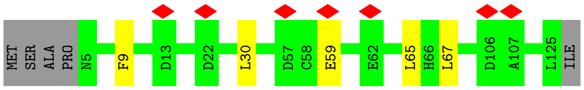
Chain 3F:



- Molecule 26: 13 kDa ribonucleoprotein-associated protein

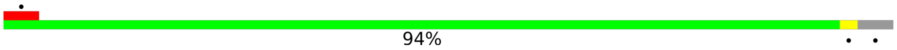
Chain 3G:

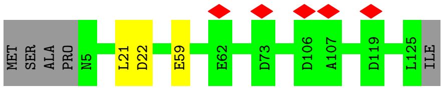




- Molecule 26: 13 kDa ribonucleoprotein-associated protein

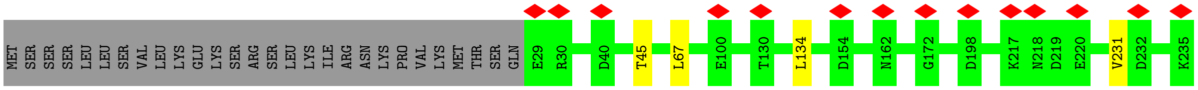
Chain 3H:

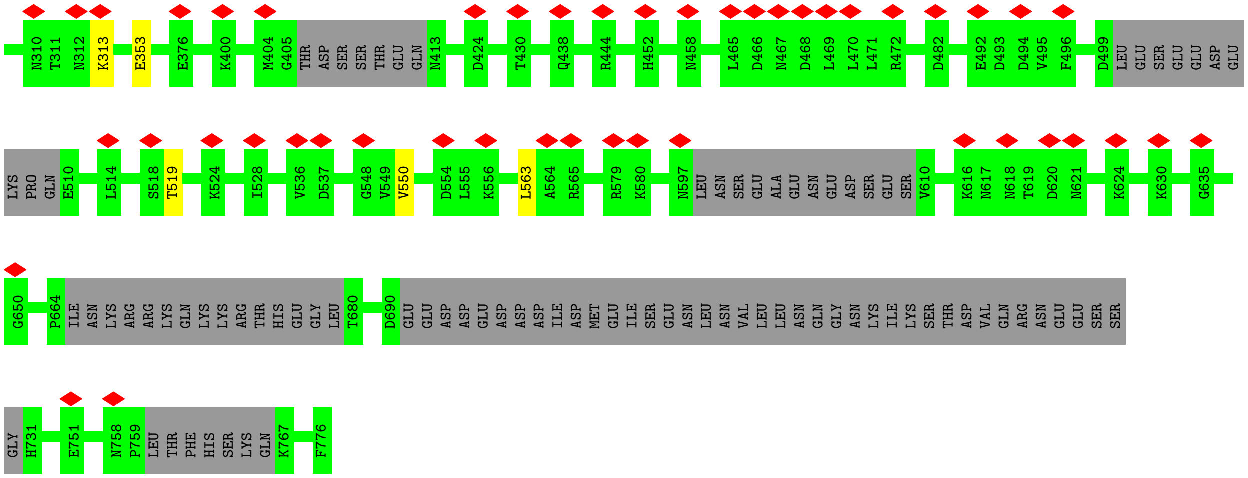




- Molecule 27: U3 small nucleolar RNA-associated protein 4

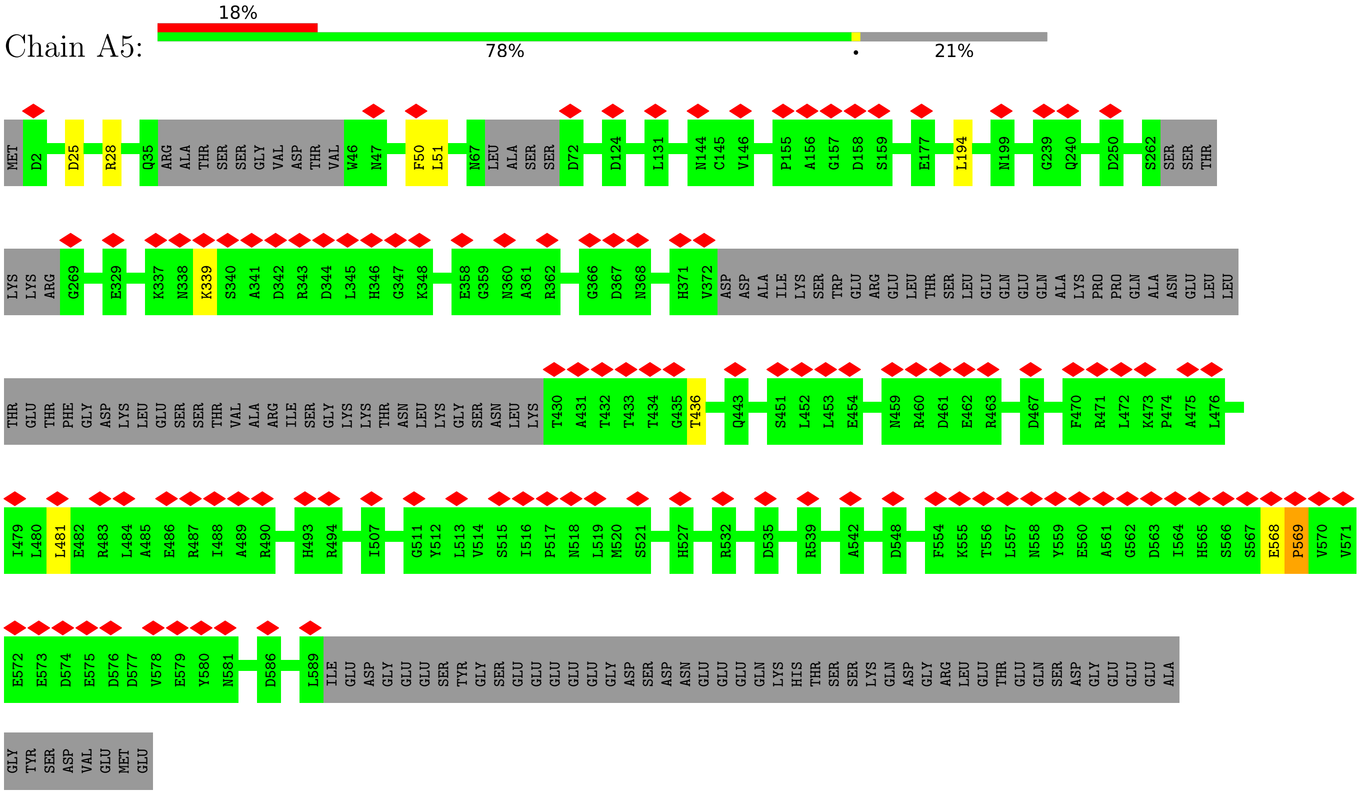
Chain A4:





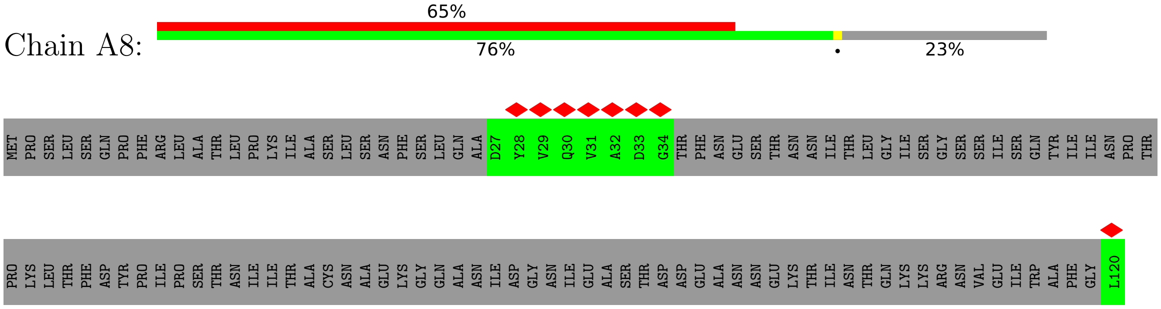
• Molecule 28: U3 small nucleolar RNA-associated protein 5

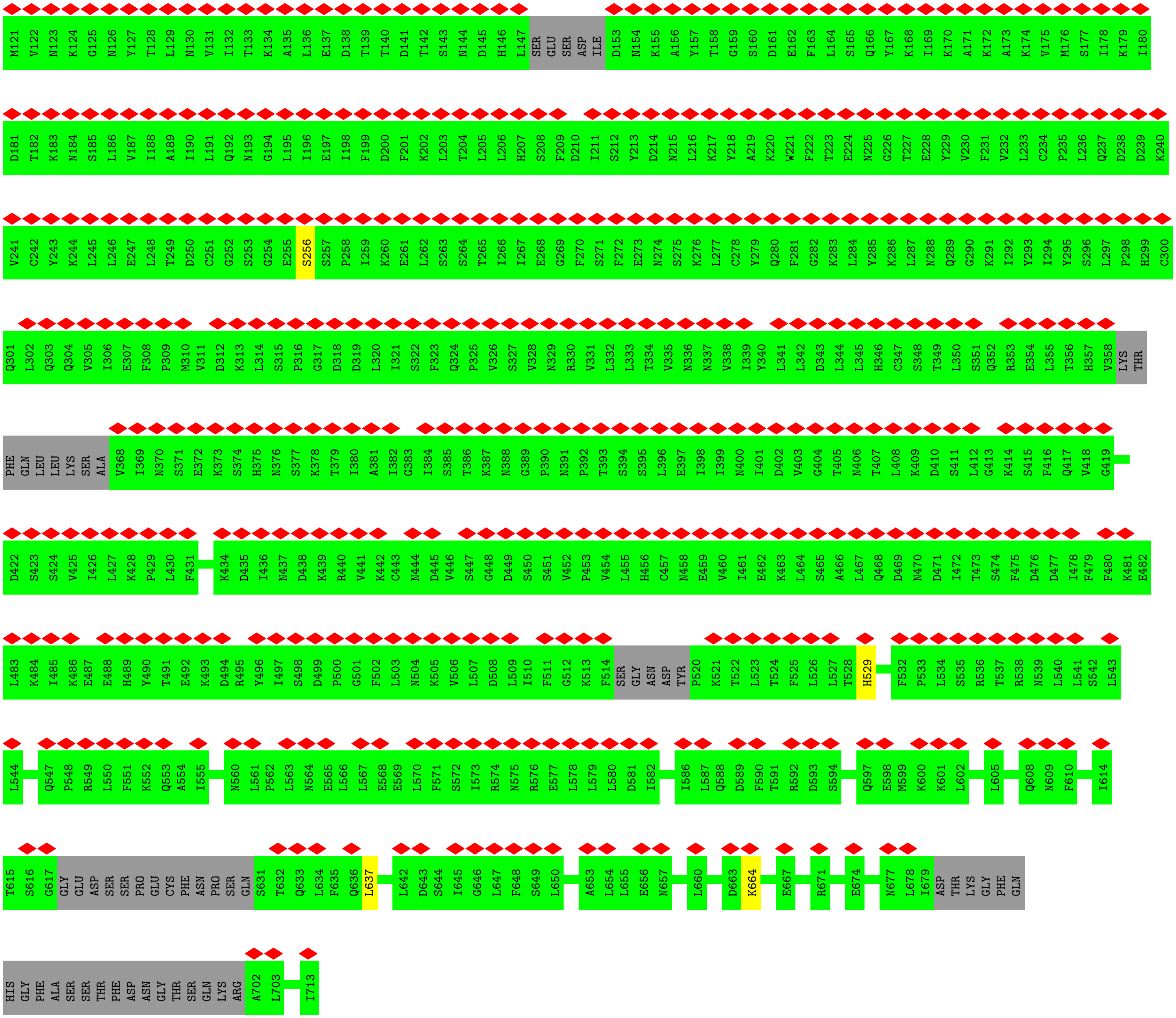
Chain A5:



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

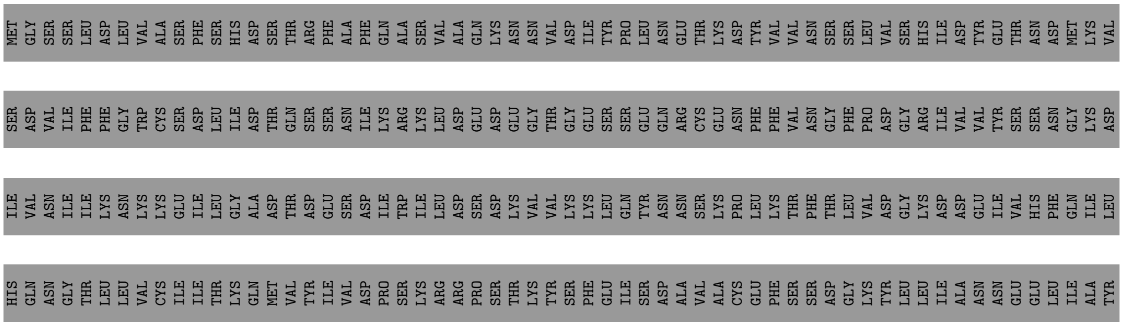
Chain A8:

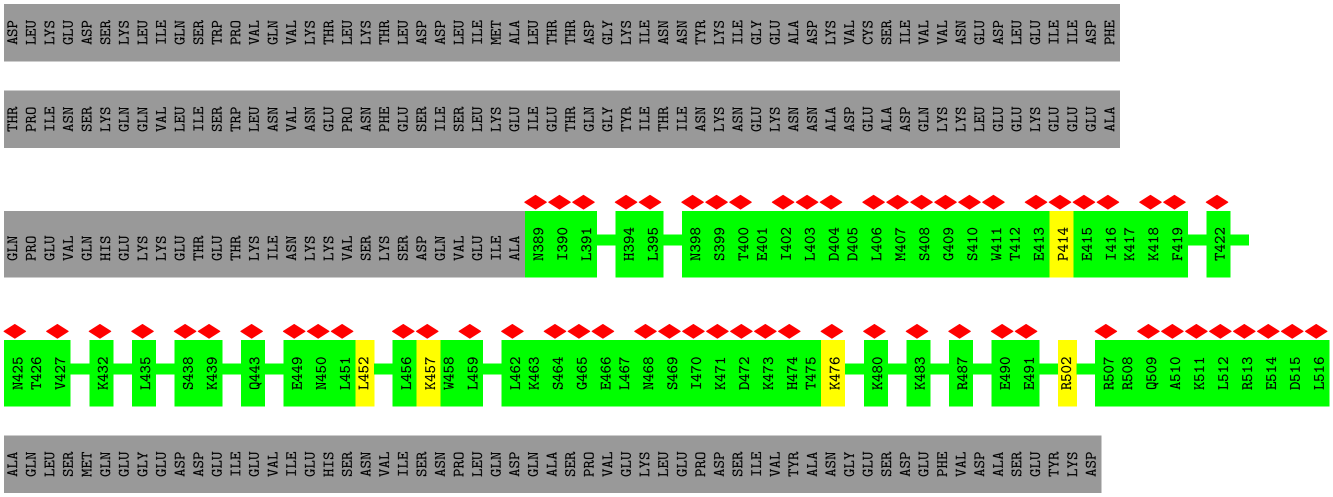




- Molecule 30: U3 small nucleolar RNA-associated protein 9

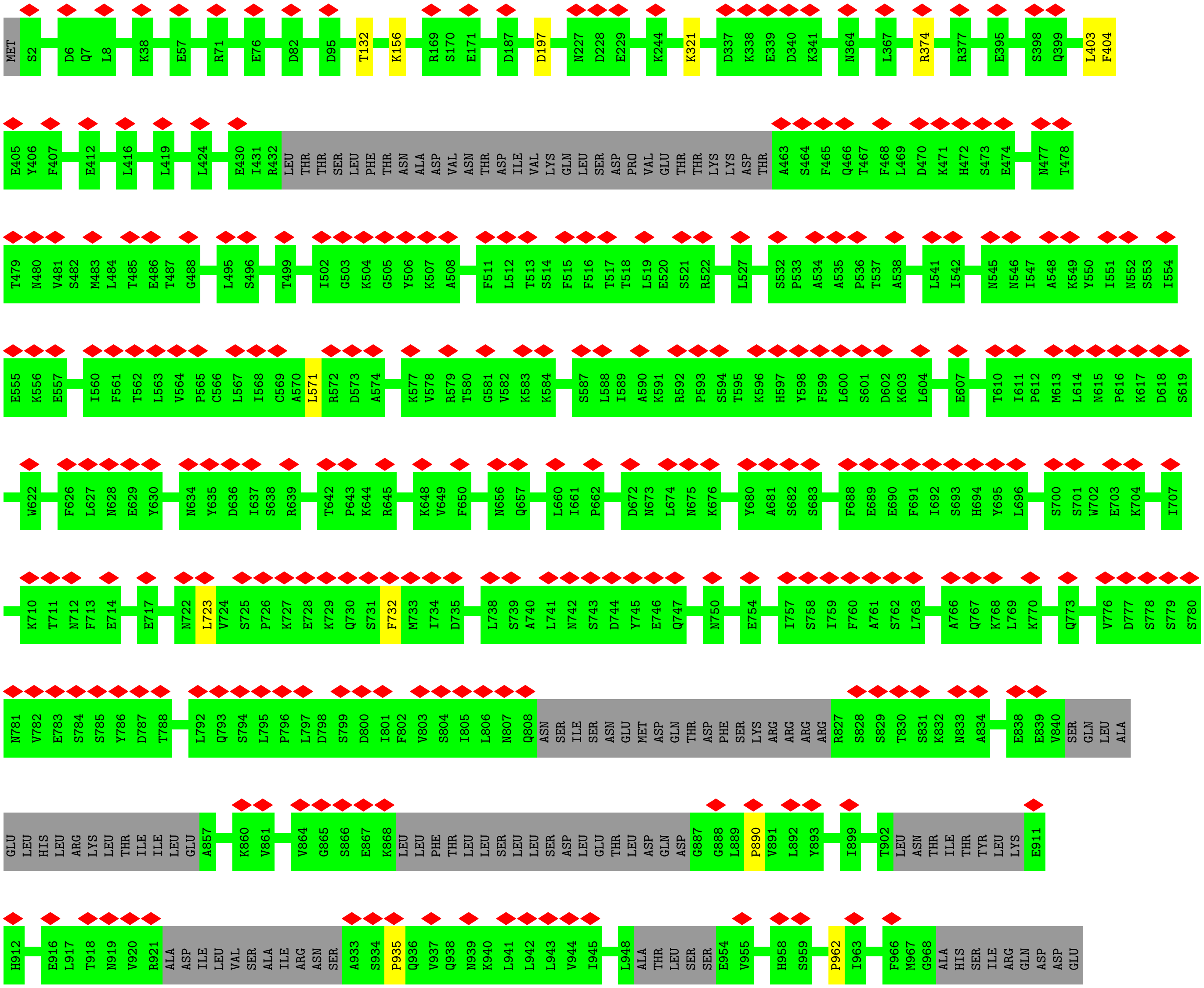
Chain A9:

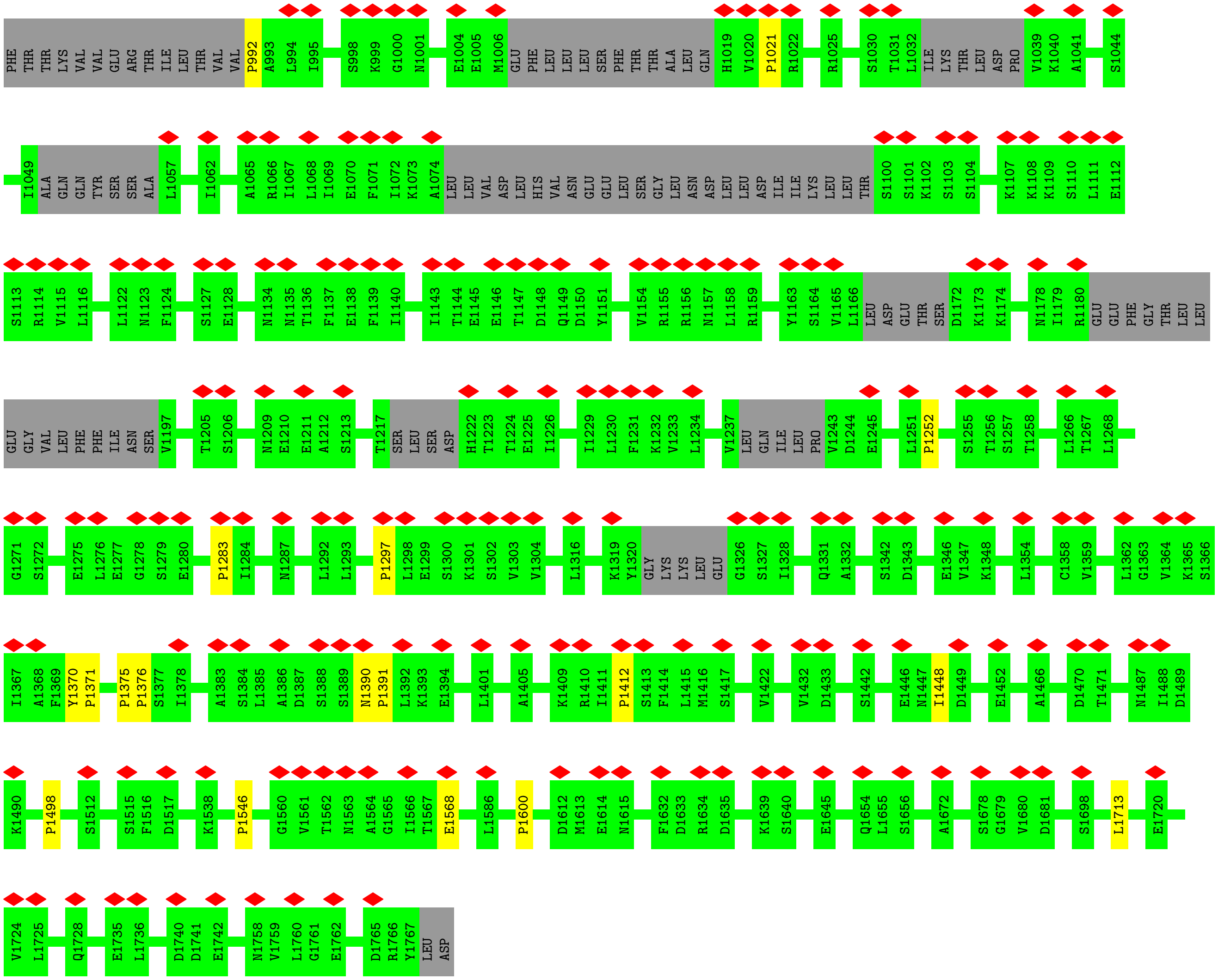




- Molecule 31: U3 small nucleolar RNA-associated protein 10

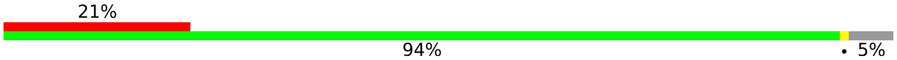
Chain AE:

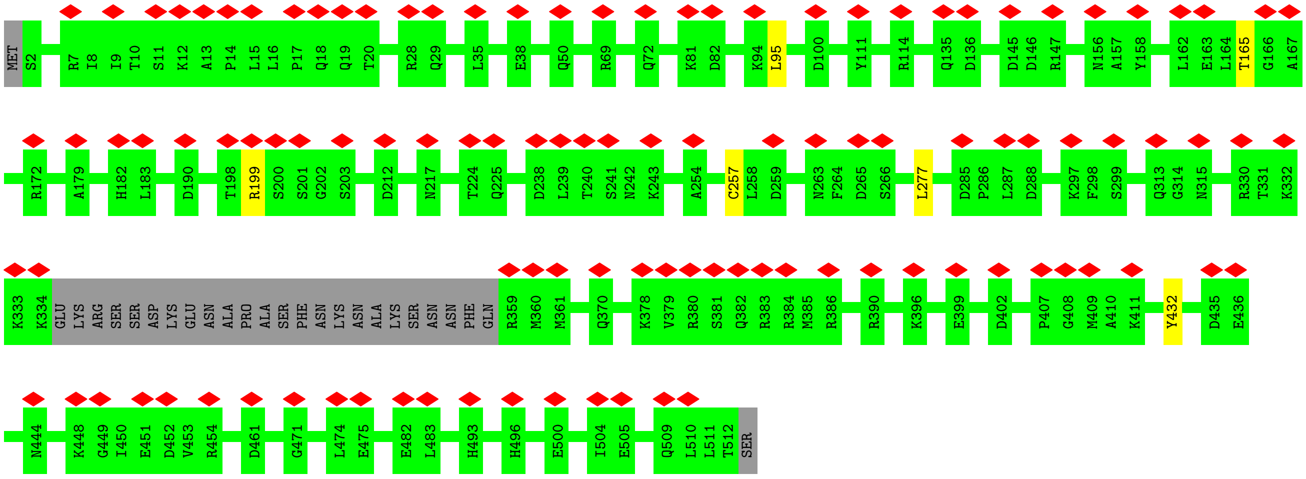




- Molecule 32: U3 small nucleolar RNA-associated protein 15

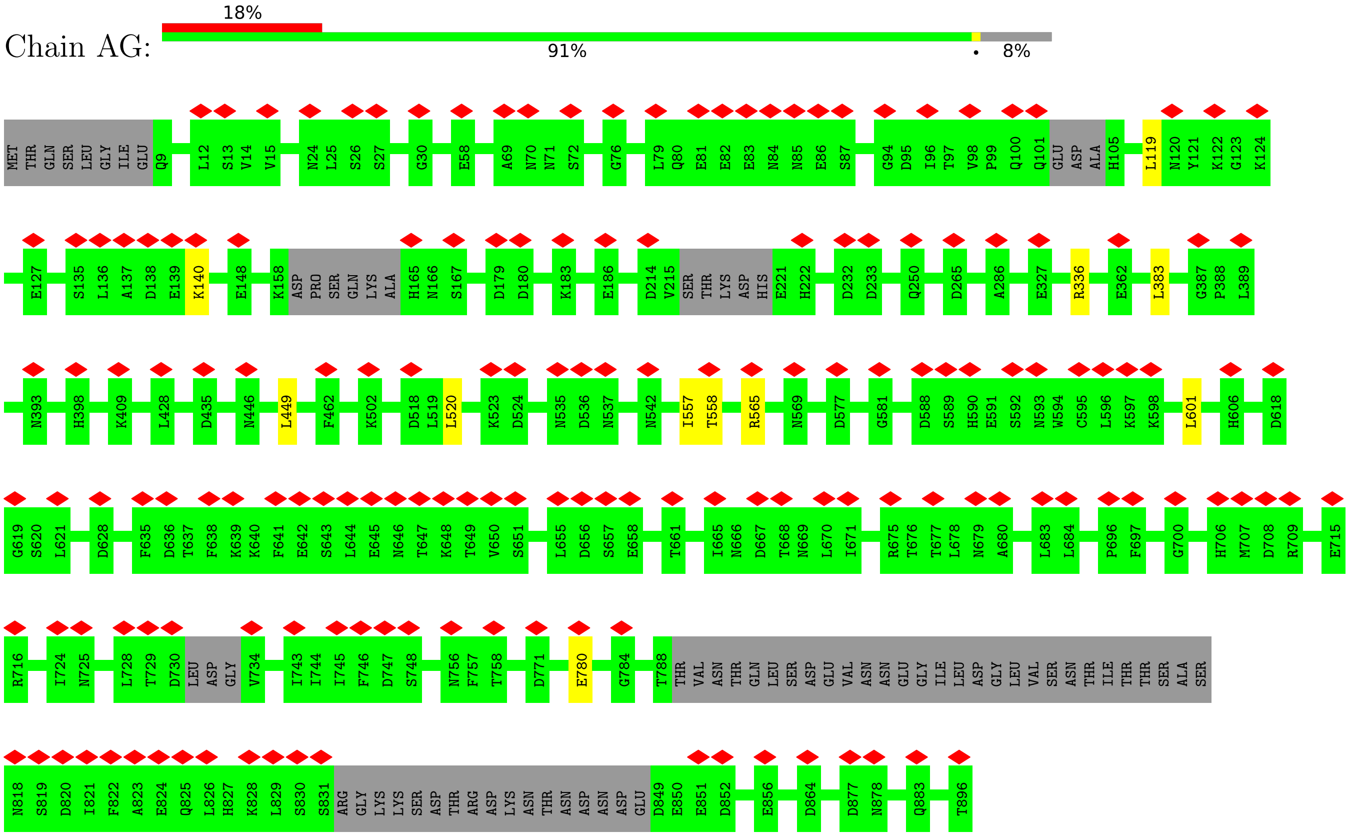
Chain AF:





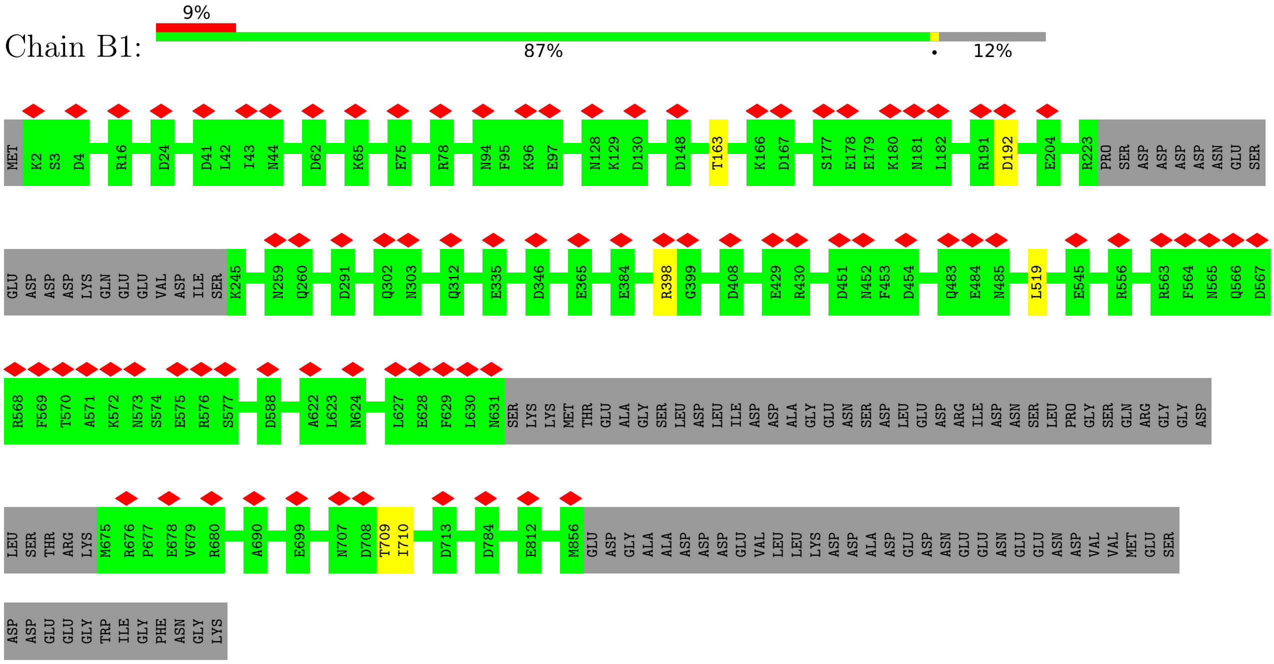
- Molecule 33: NET1-associated nuclear protein 1

Chain AG:



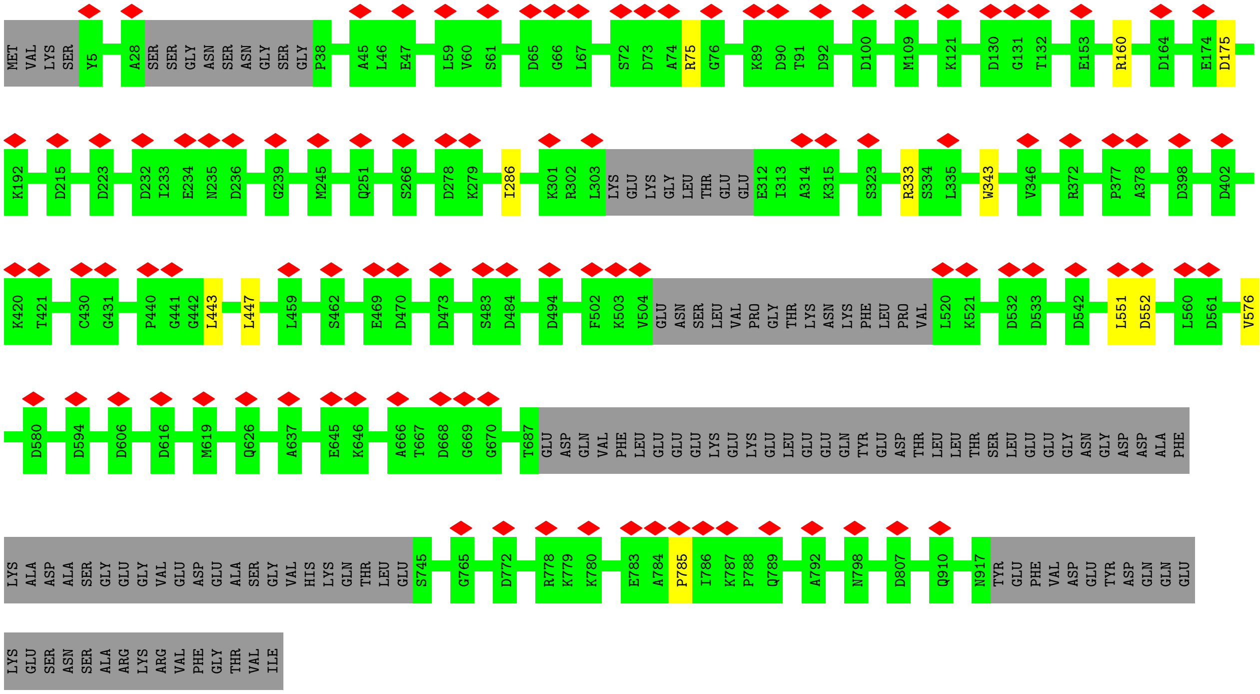
- Molecule 34: Periodic tryptophan protein 2

Chain B1:



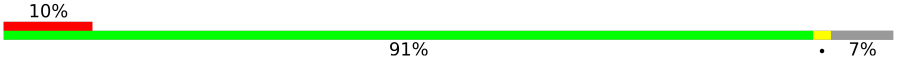
- Molecule 35: U3 small nucleolar RNA-associated protein 12

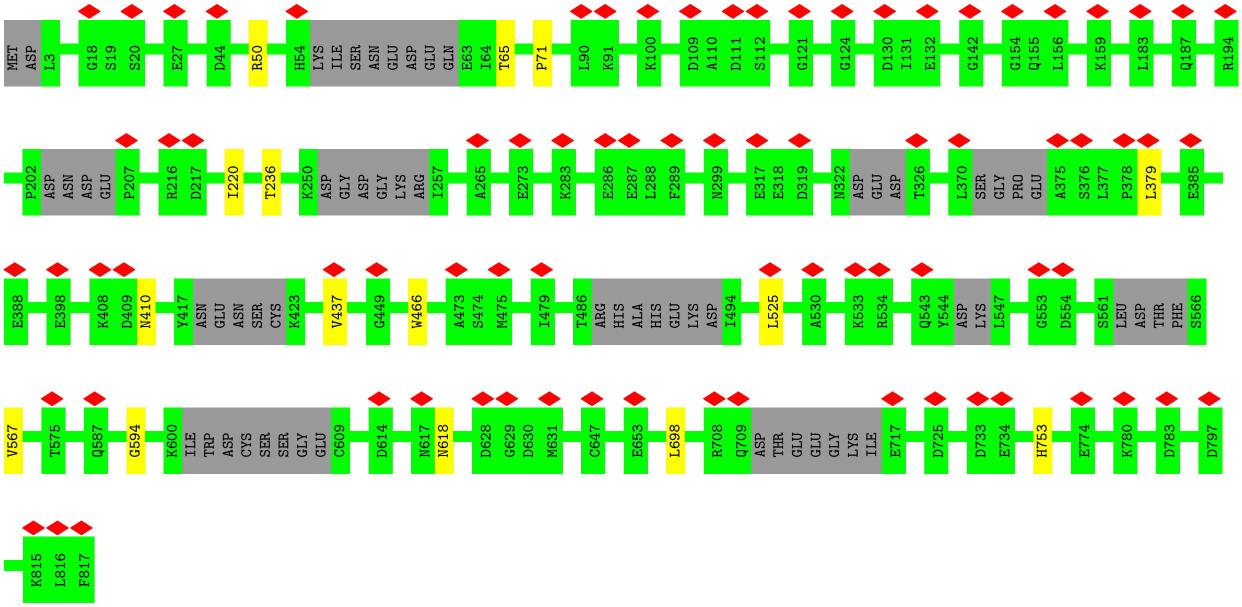
Chain B2:



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

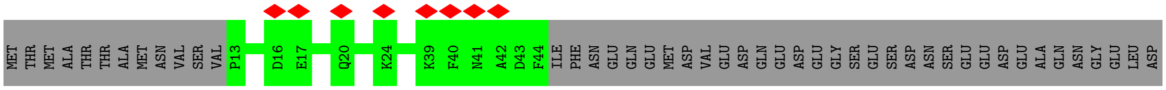
Chain B3:

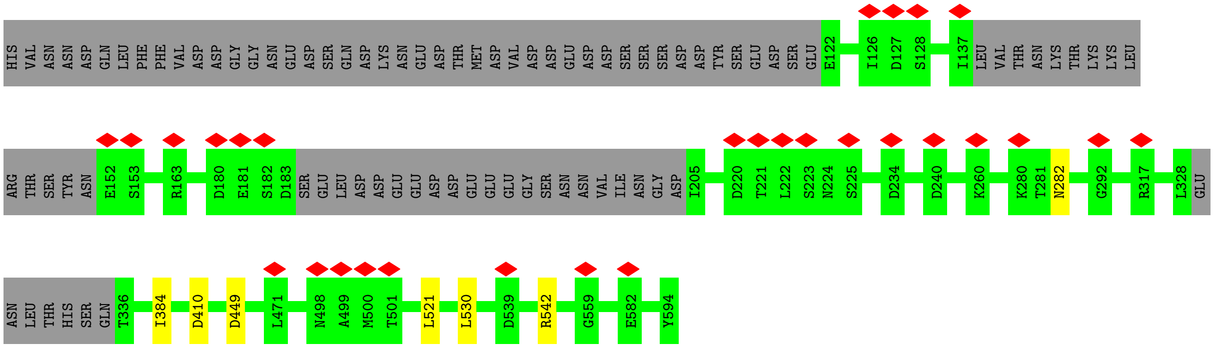




- Molecule 37: U3 small nucleolar RNA-associated protein 18

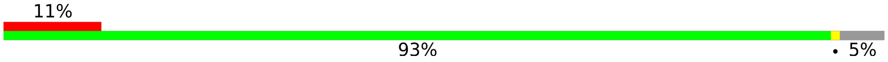
Chain B8:

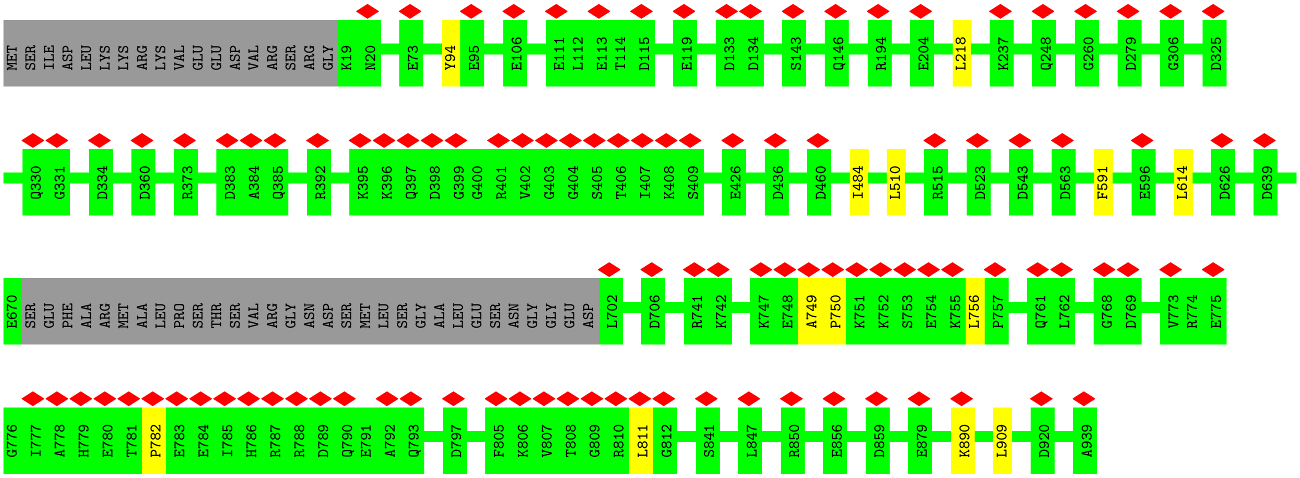




- Molecule 38: U3 small nucleolar RNA-associated protein 21

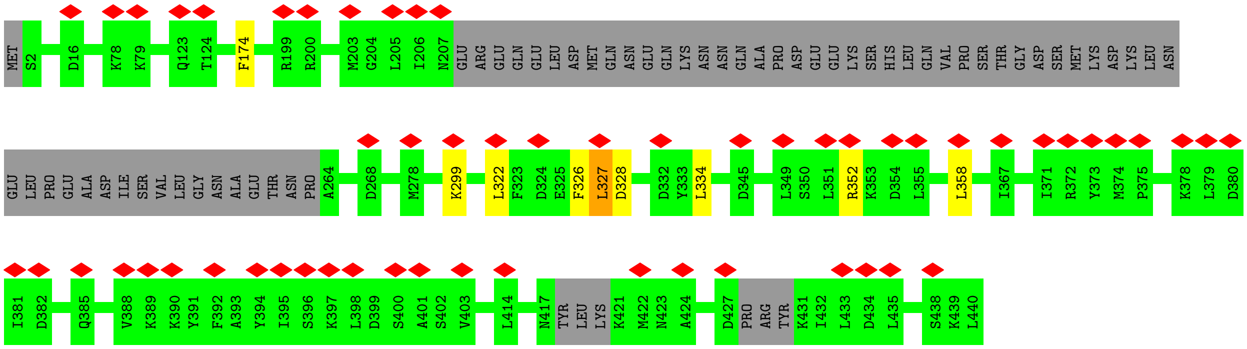
Chain BE:





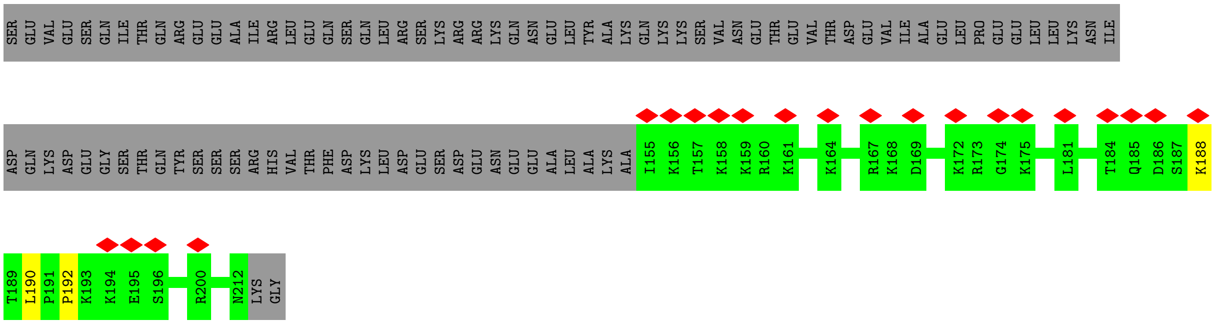
- Molecule 39: U3 small nucleolar RNA-associated protein 6

Chain B6:



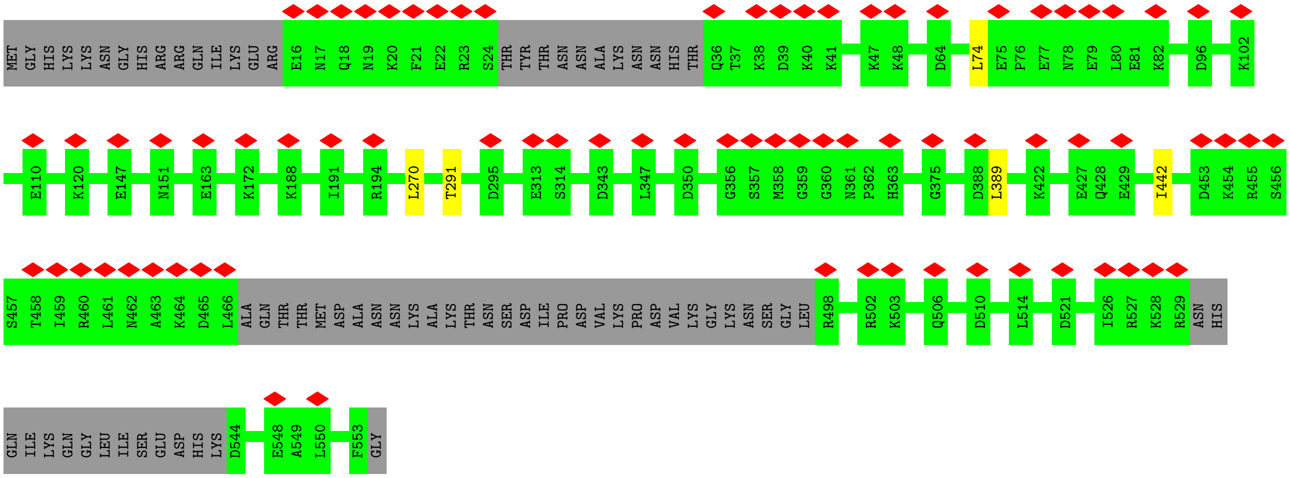
- Molecule 40: Bud site selection protein 21

Chain 5B:



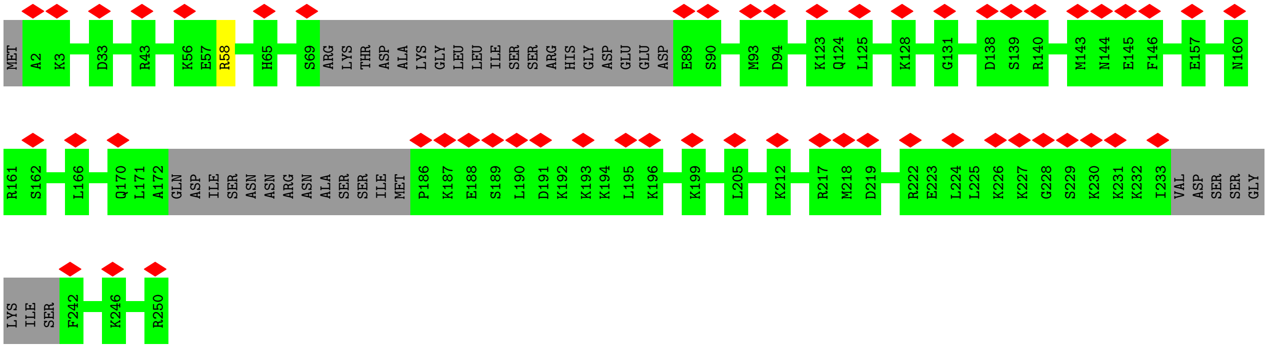
- Molecule 41: U3 small nucleolar RNA-associated protein 7

Chain 5C:



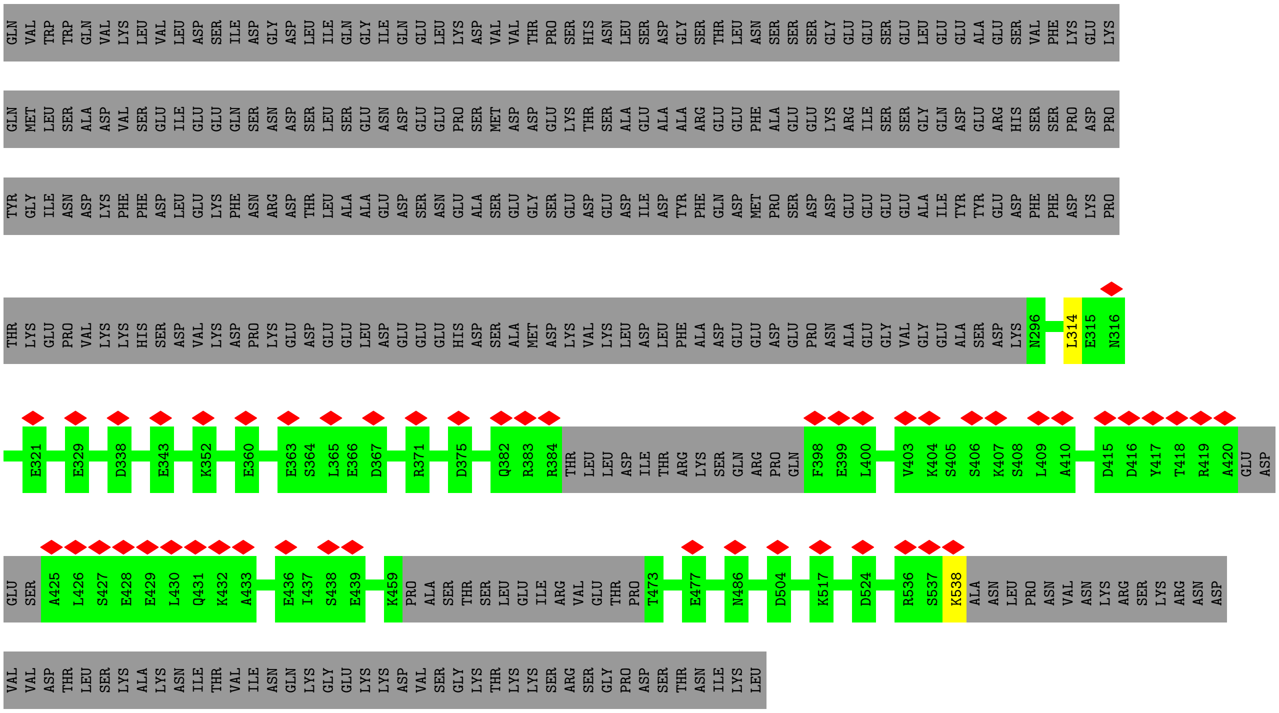
- Molecule 42: U3 small nucleolar RNA-associated protein 11

Chain 5D:

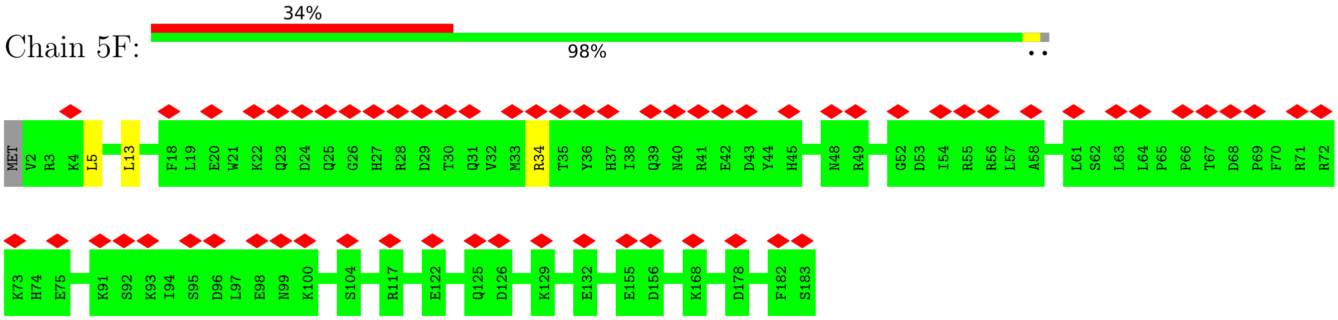


- Molecule 43: U3 small nucleolar RNA-associated protein MPP10

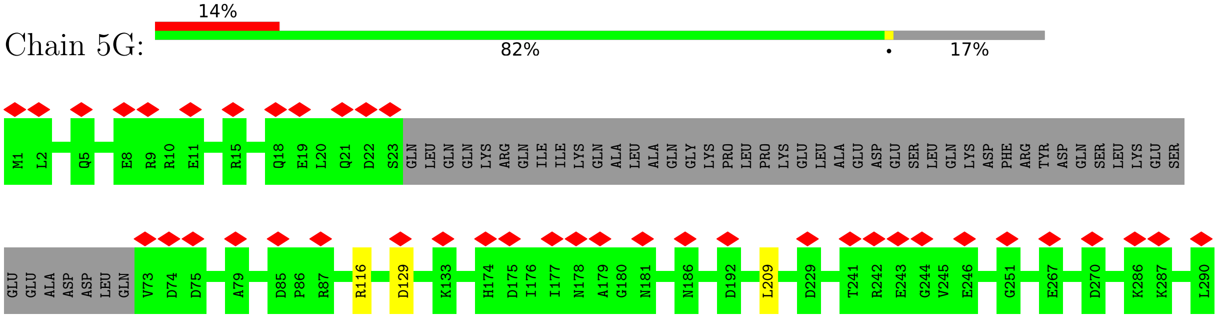
Chain 5E:



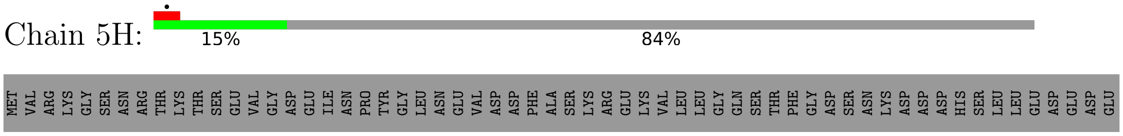
- Molecule 44: U3 small nucleolar ribonucleoprotein protein IMP3

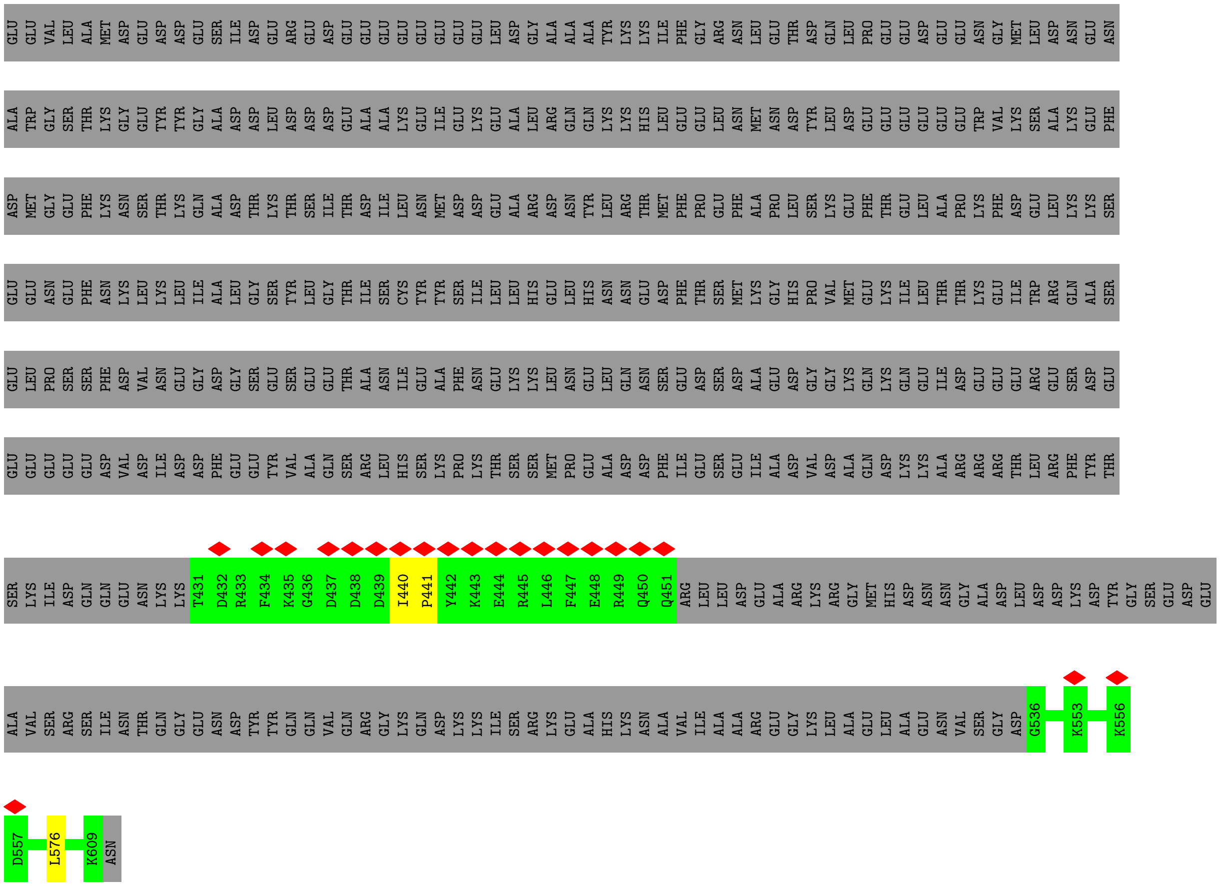


- Molecule 45: U3 small nucleolar ribonucleoprotein protein IMP4



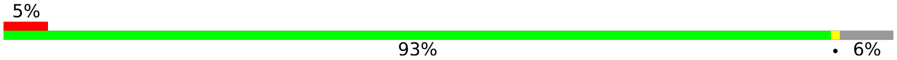
- Molecule 46: Something about silencing protein 10

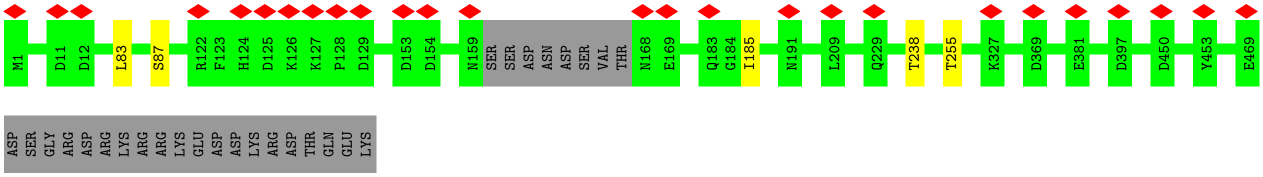




- Molecule 47: Protein SOF1

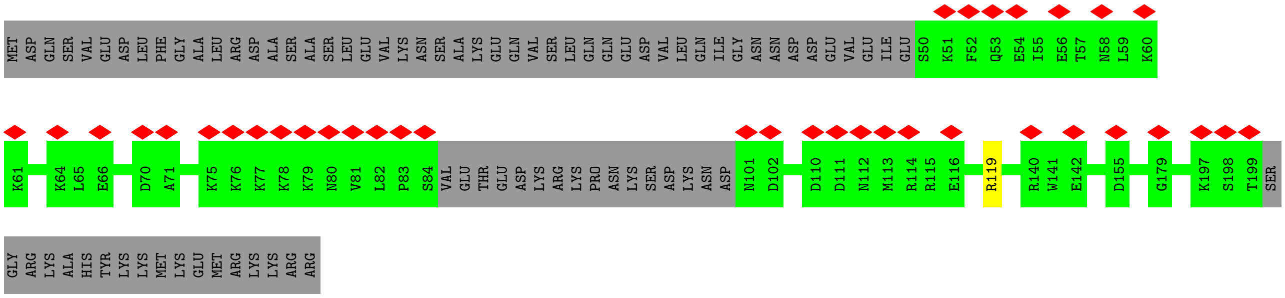
Chain 5I:





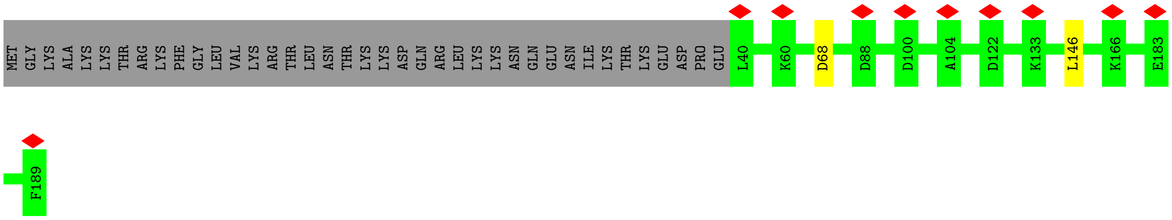
- Molecule 48: rRNA-processing protein FCF2

Chain 5J:



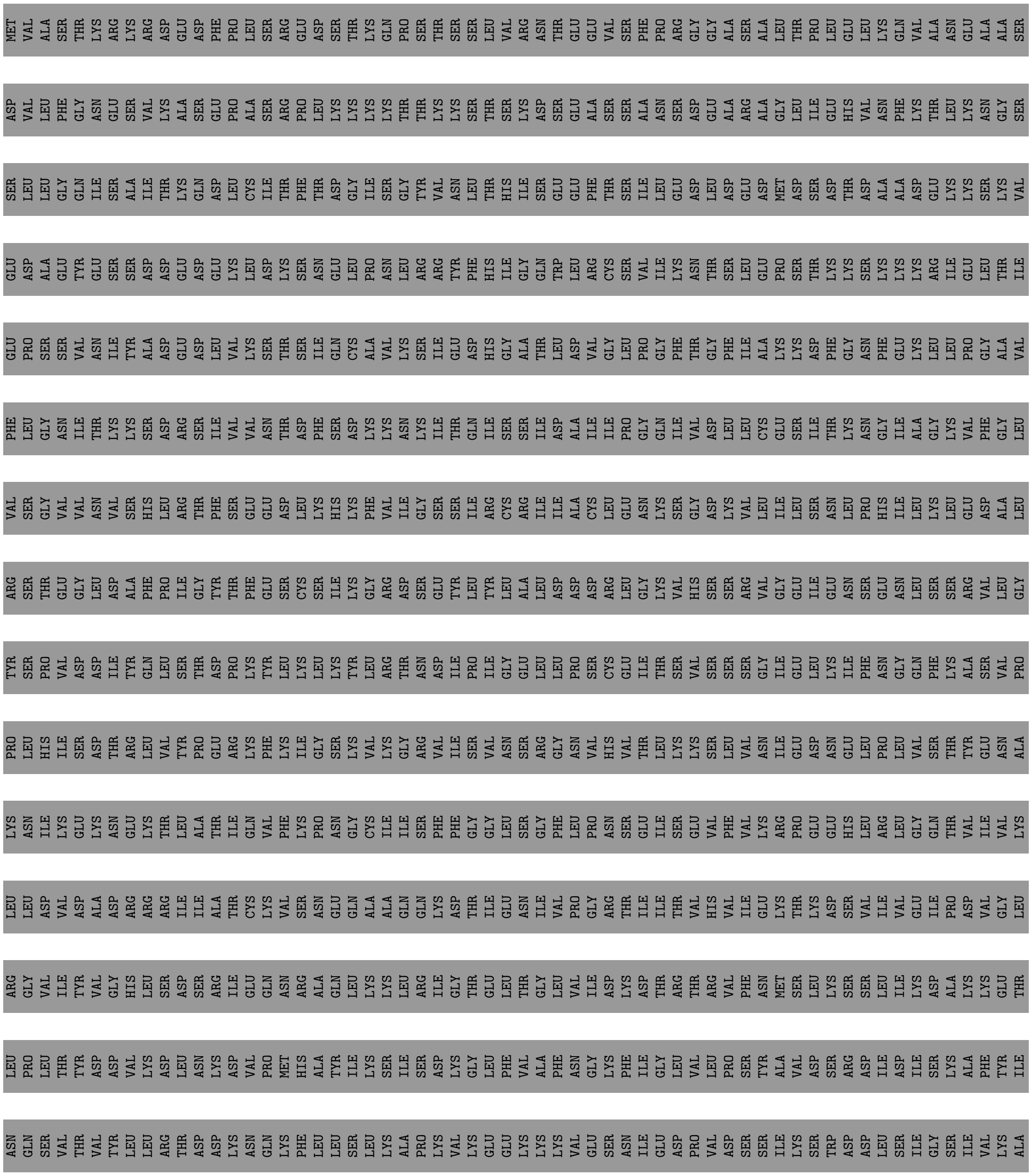
- Molecule 49: rRNA-processing protein FCF1

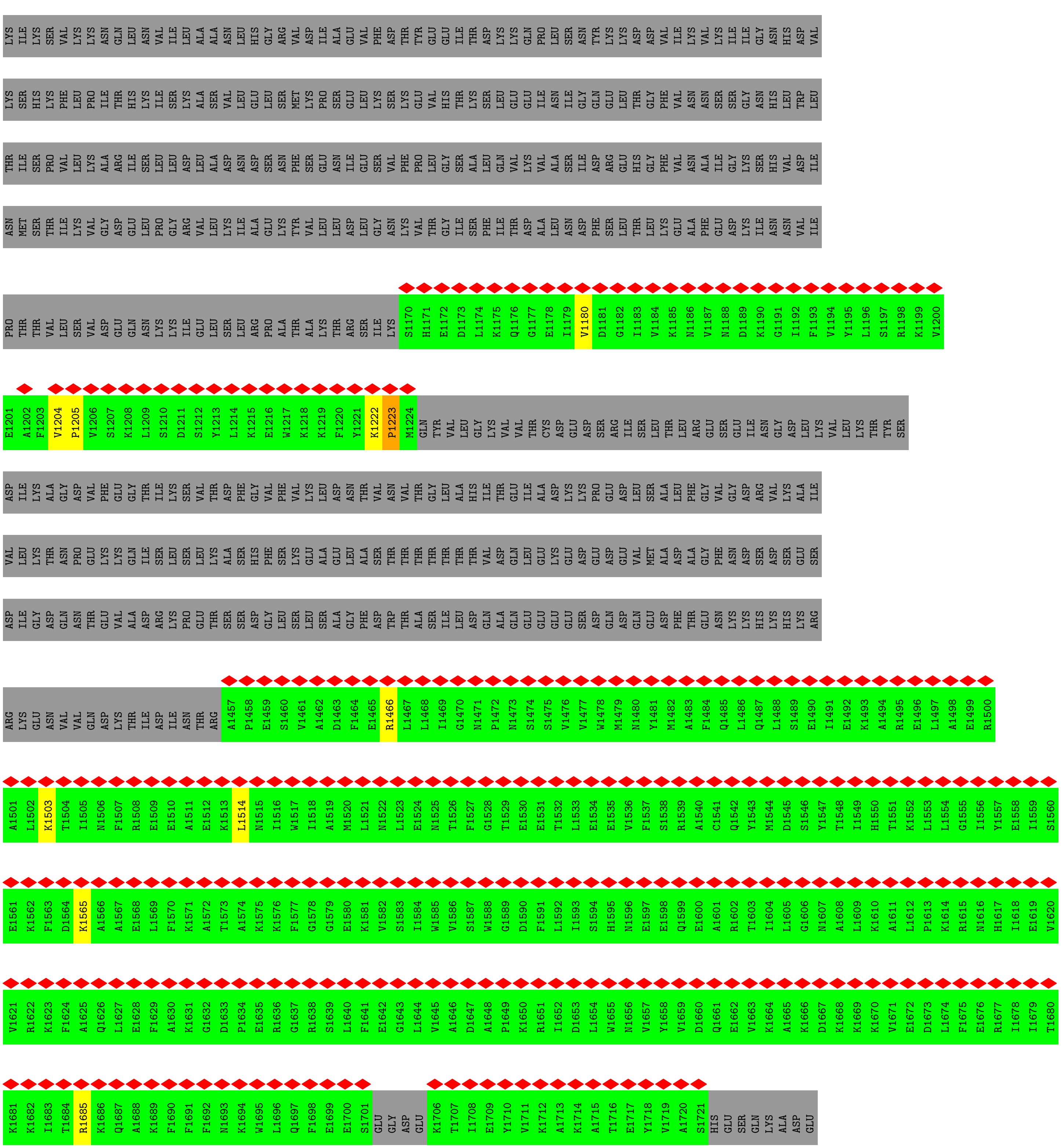
Chain 5K:



- Molecule 50: rRNA biogenesis protein RRP5

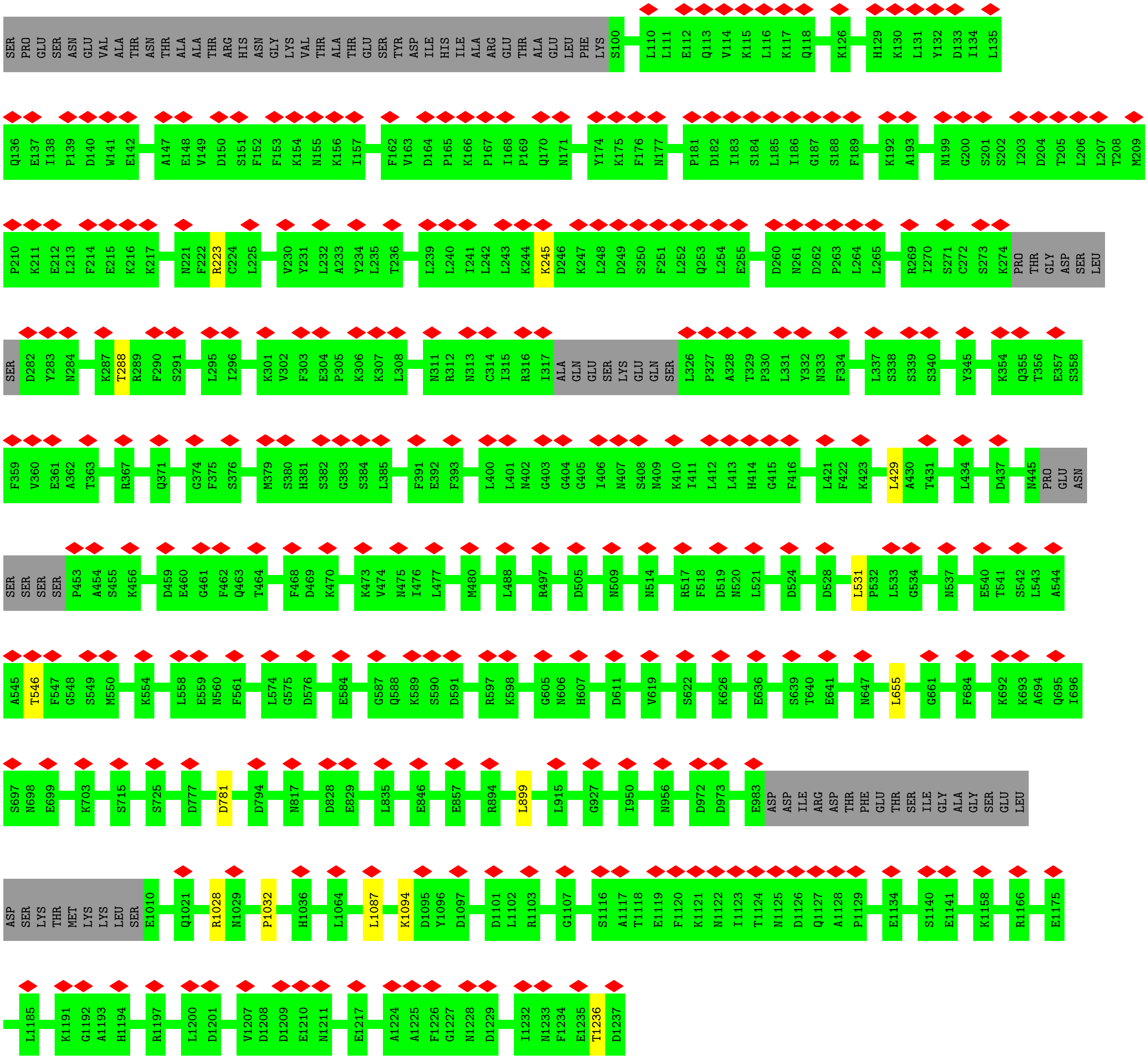
Chain RD:



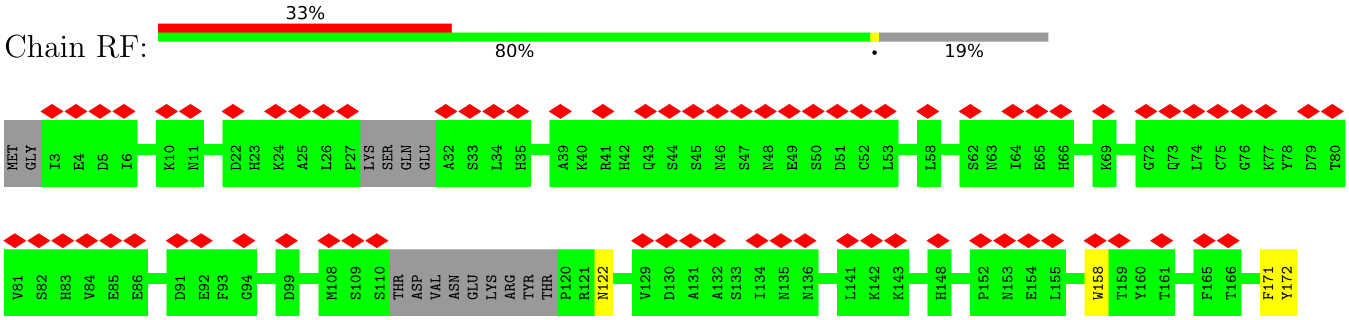


- Molecule 51: U3 small nucleolar RNA-associated protein 22

Chain RE:

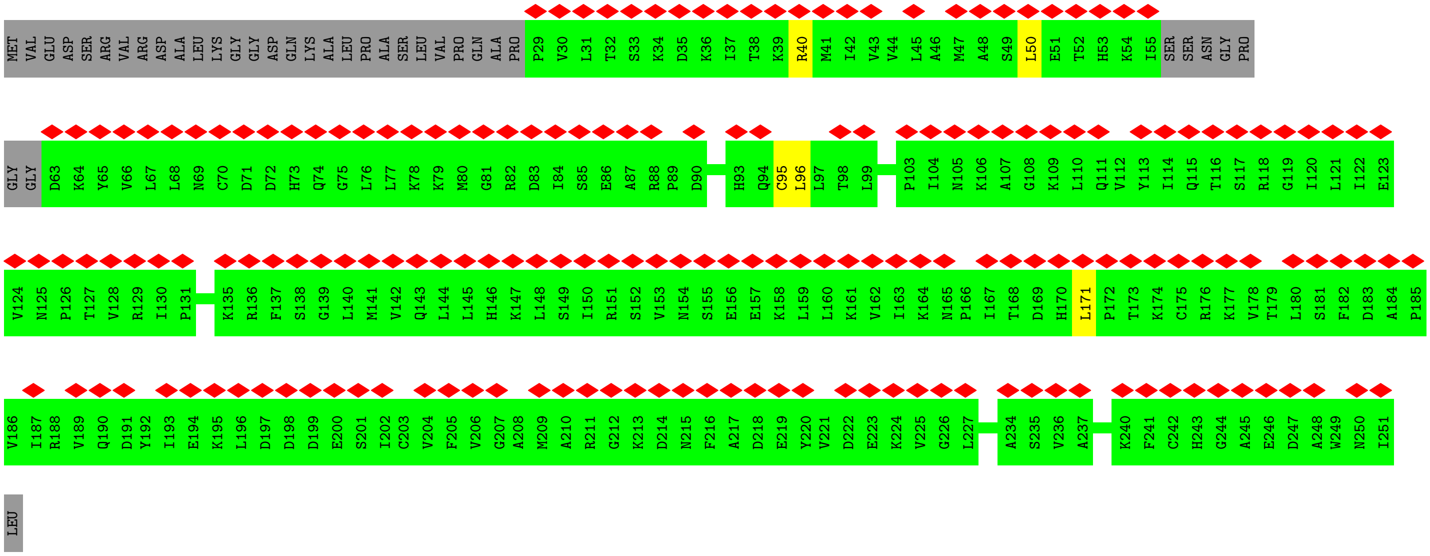


- Molecule 52: Ribosomal RNA-processing protein 7



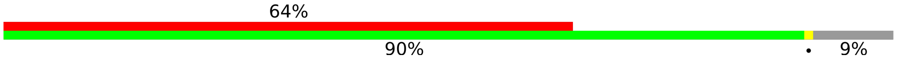
- Molecule 53: Ribosomal RNA small subunit methyltransferase NEP1

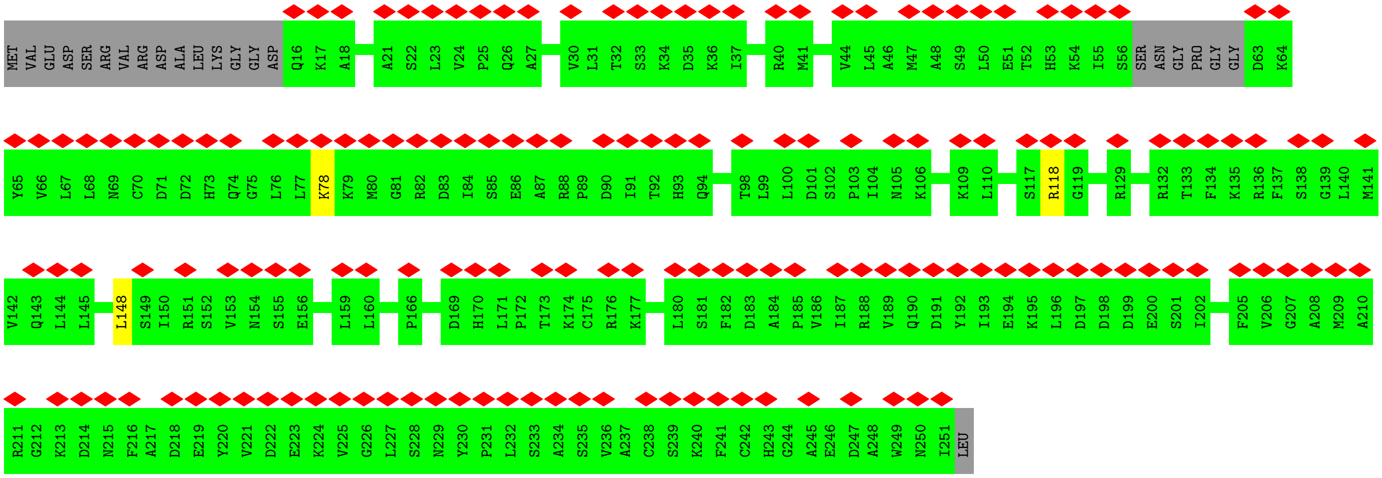
Chain RG:



- Molecule 53: Ribosomal RNA small subunit methyltransferase NEP1

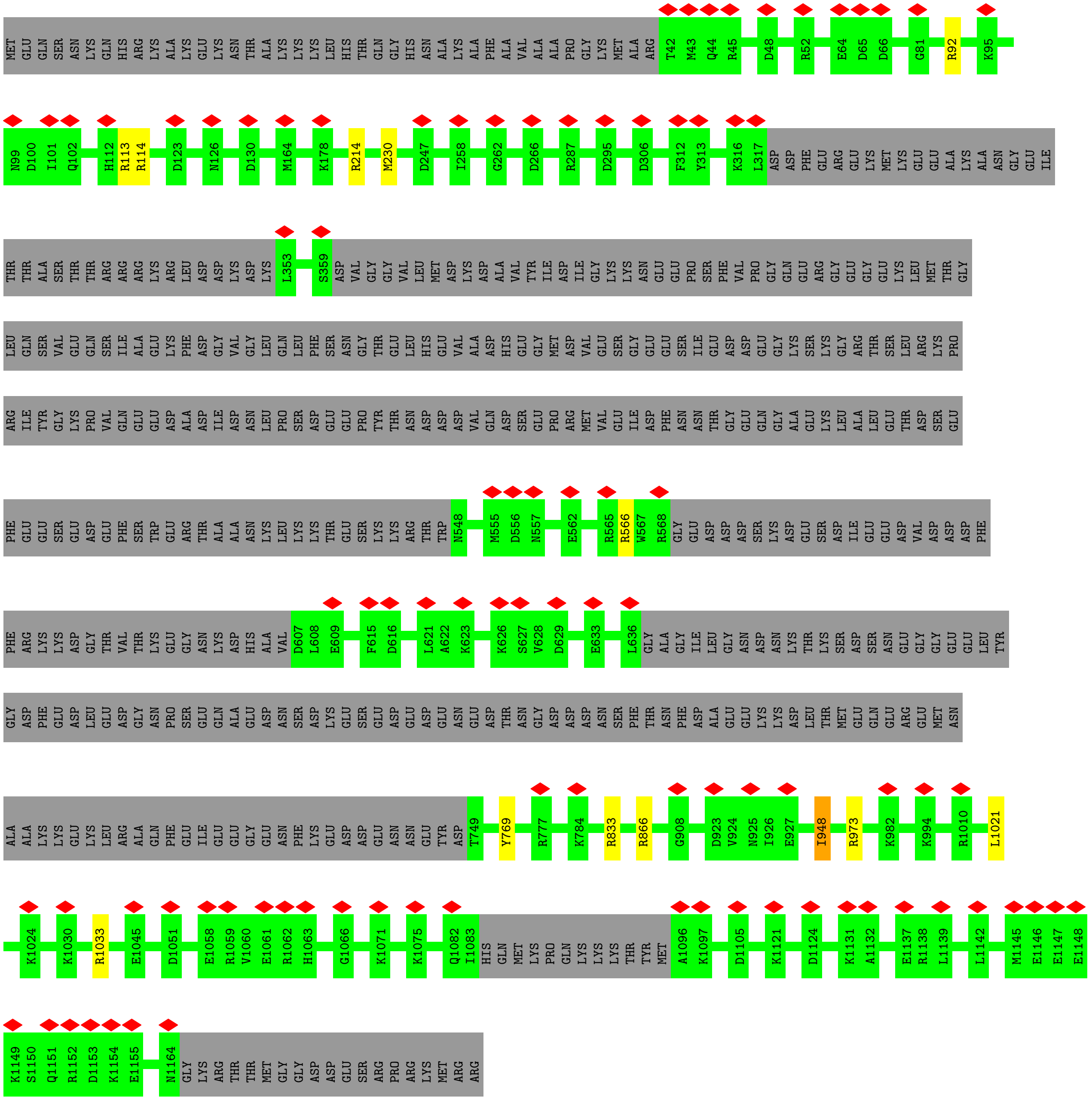
Chain RH:





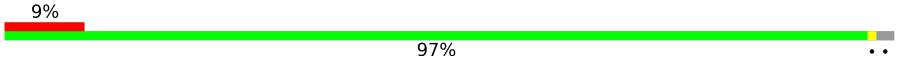
- Molecule 54: Ribosome biogenesis protein BMS1

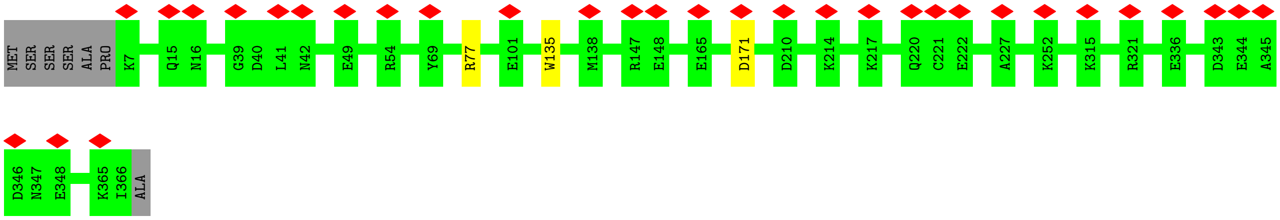
Chain RJ:



- Molecule 55: RNA 3'-terminal phosphate cyclase-like protein

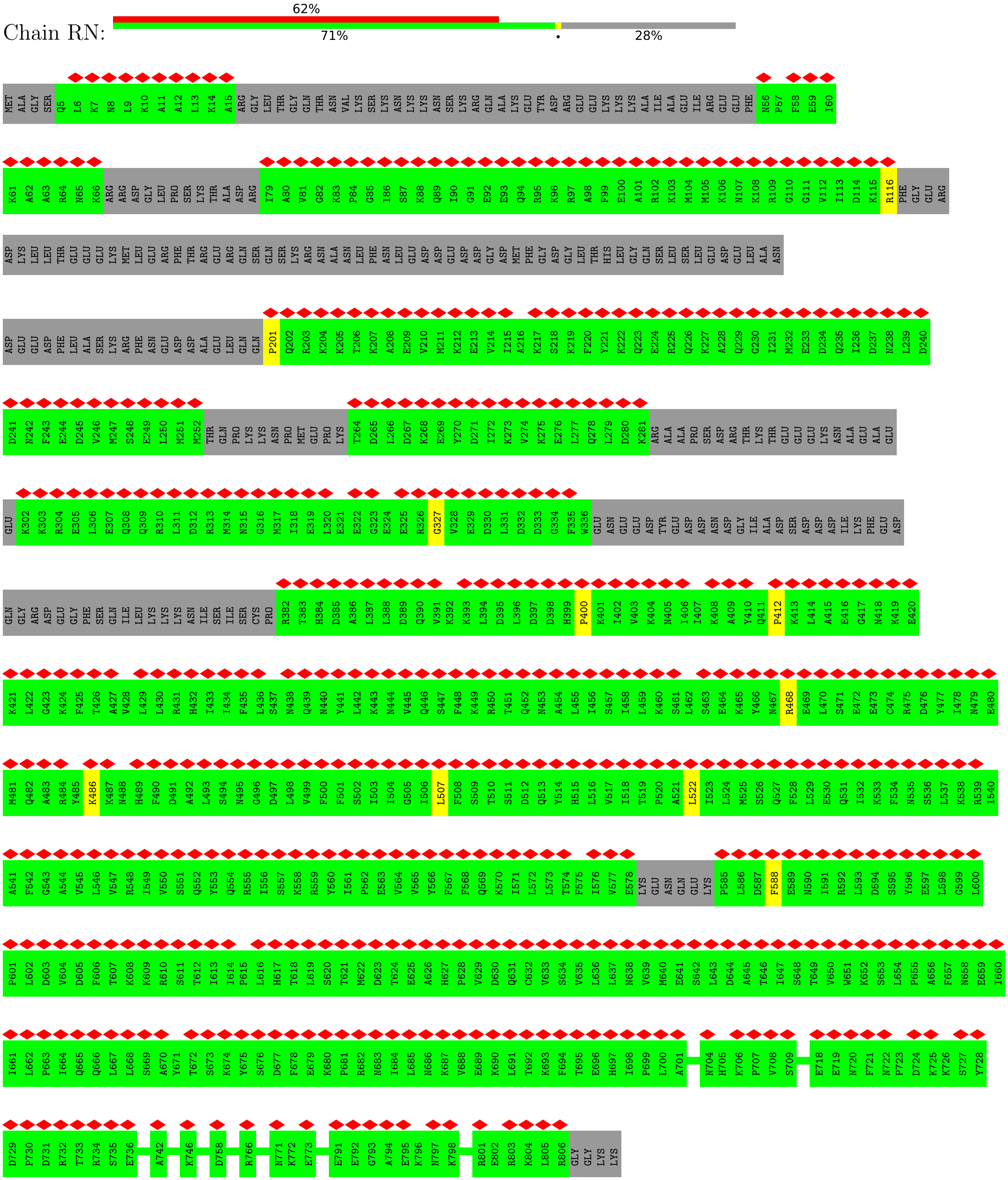
Chain RK:



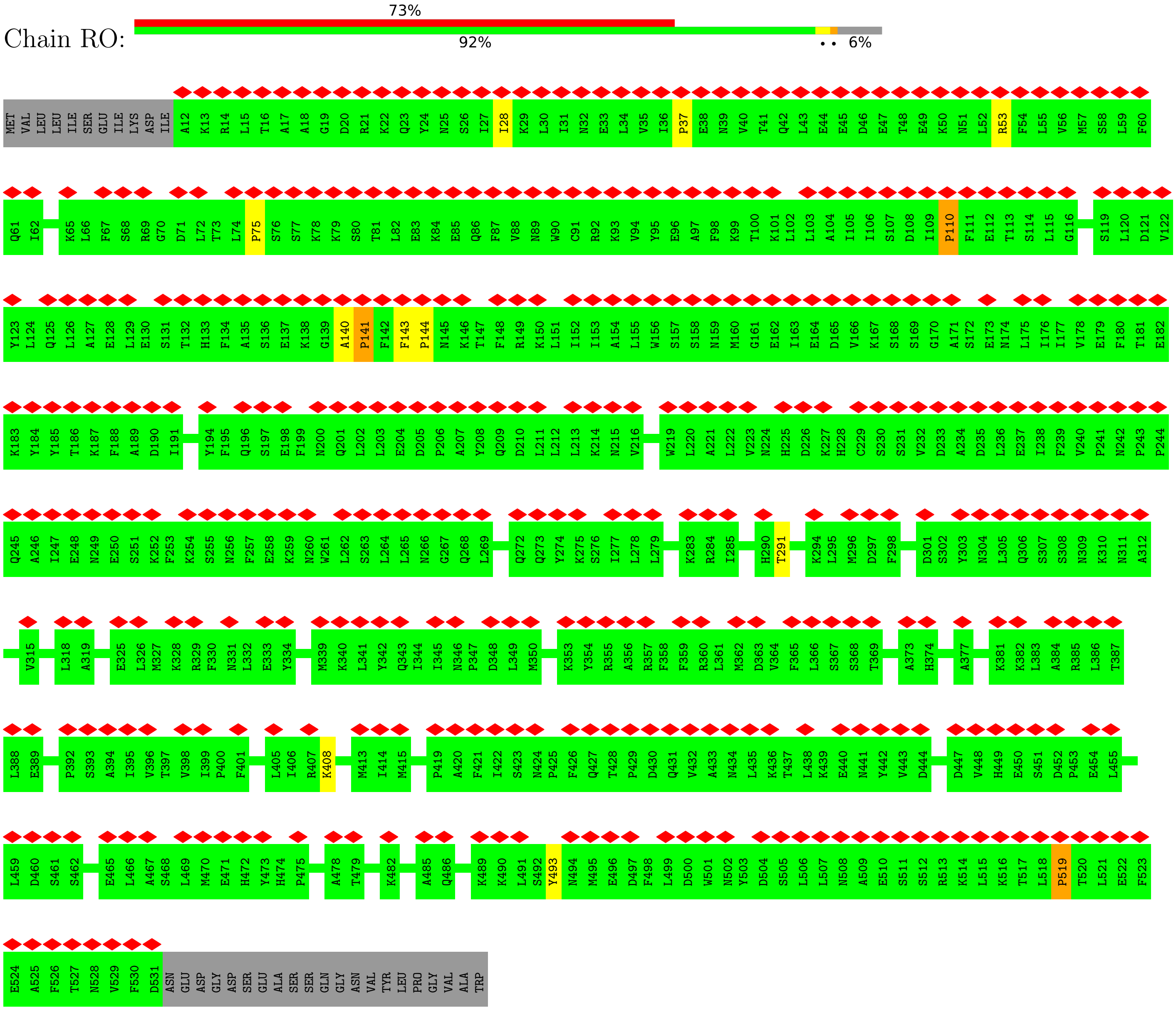


- Molecule 56: Nucleolar complex protein 14

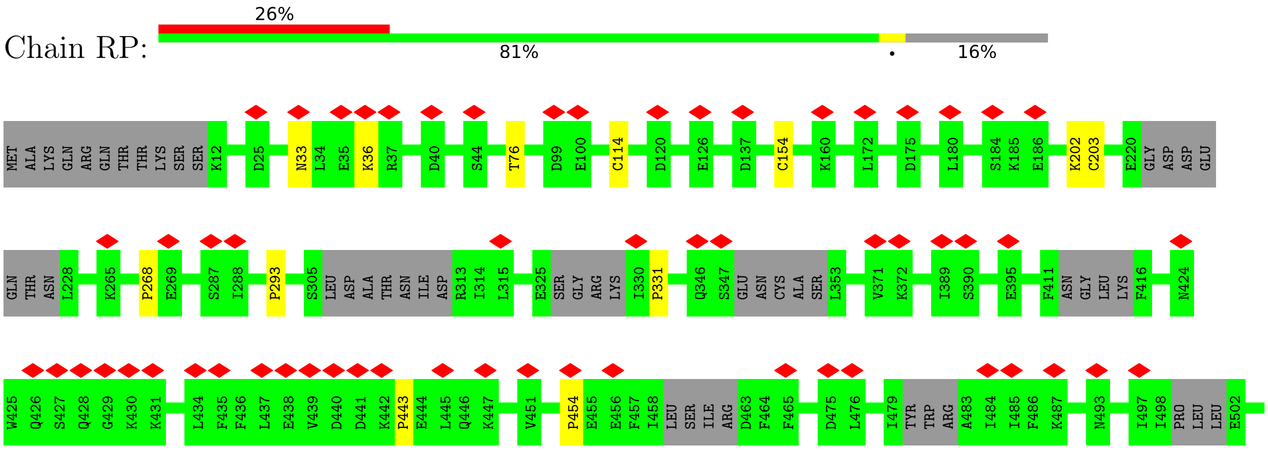
Chain RN:

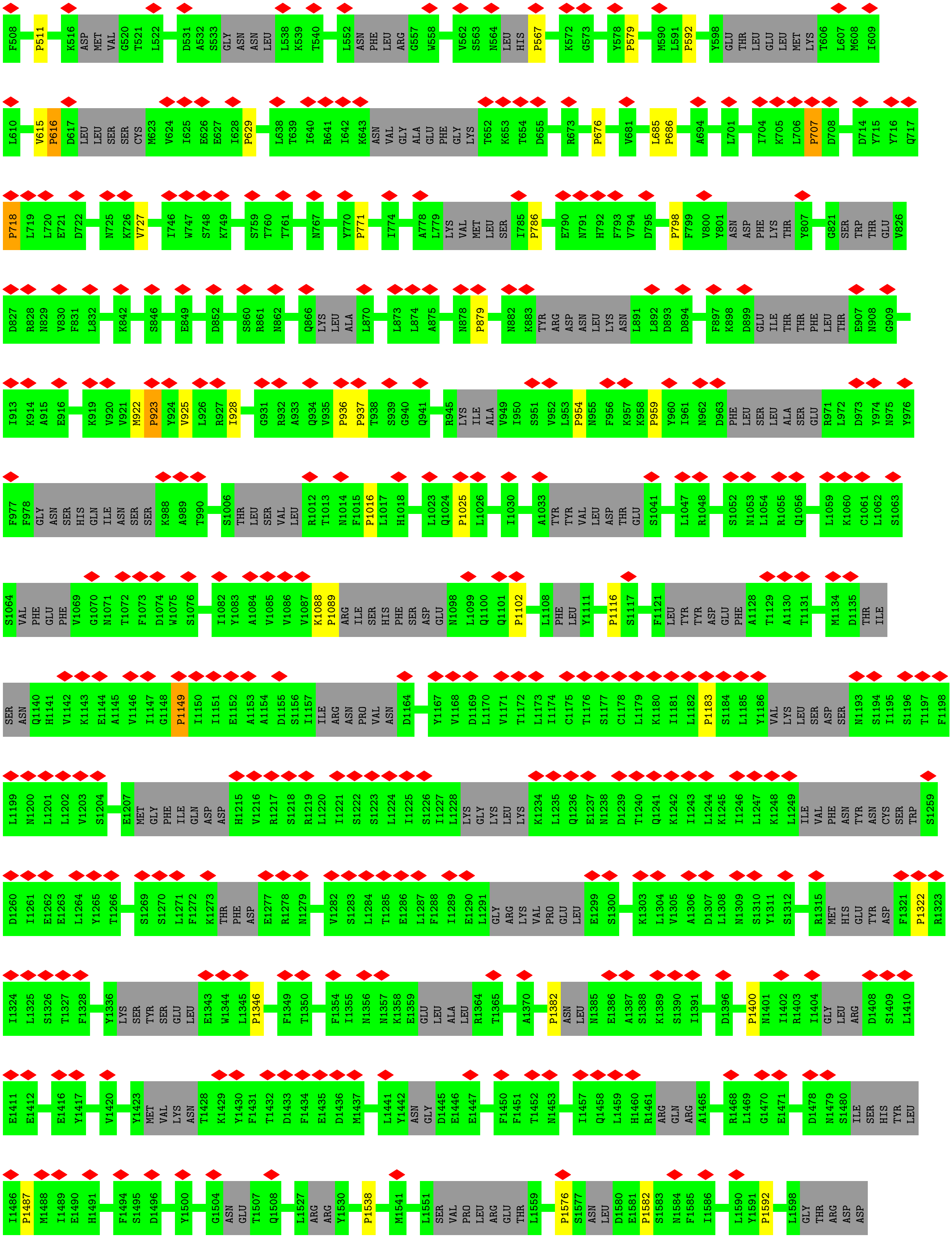


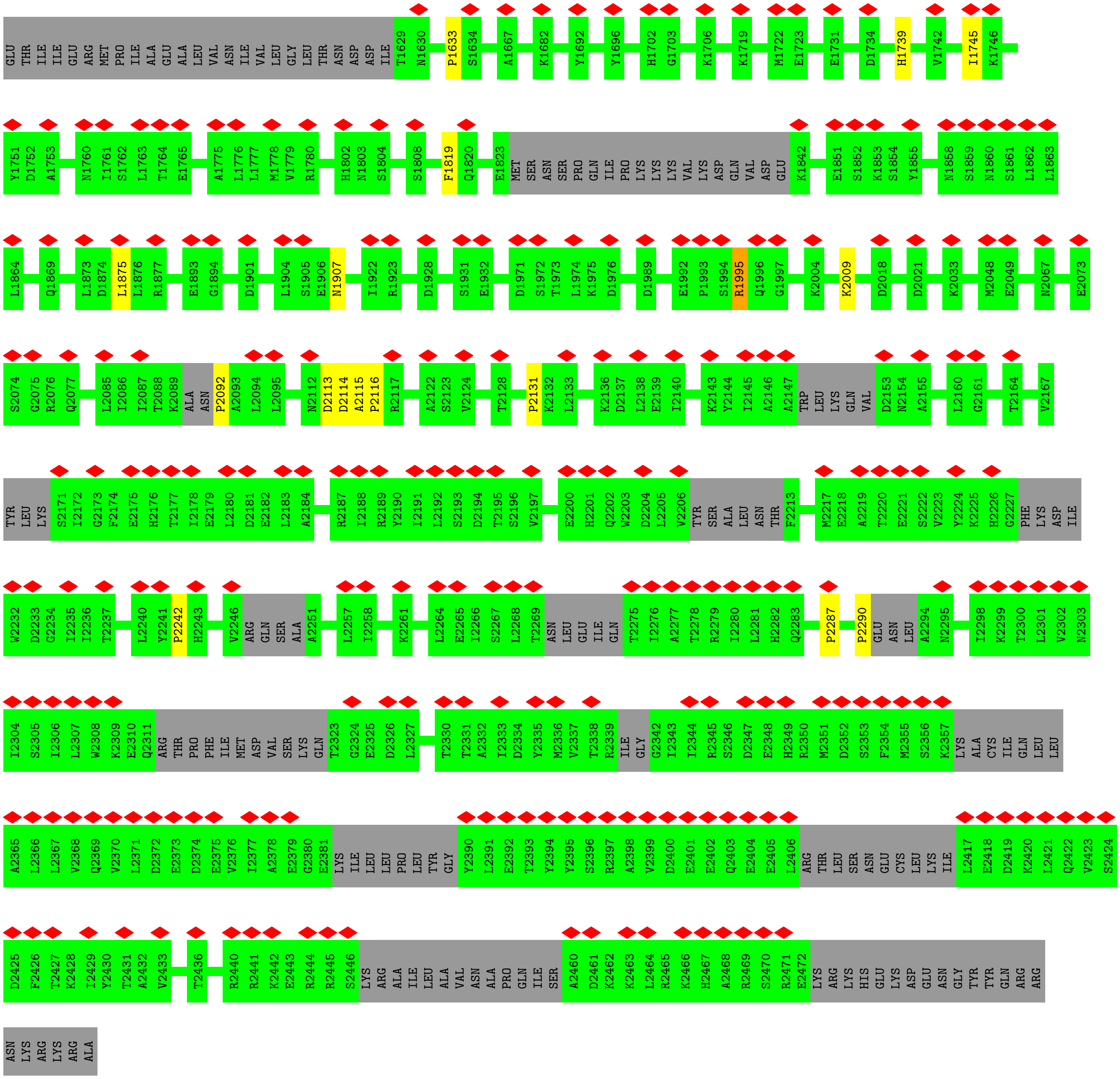
- Molecule 57: Nucleolar complex protein 4



- Molecule 58: U3 small nucleolar RNA-associated protein 20

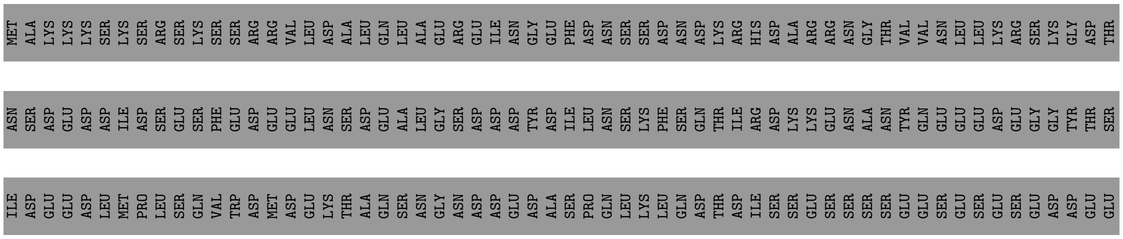


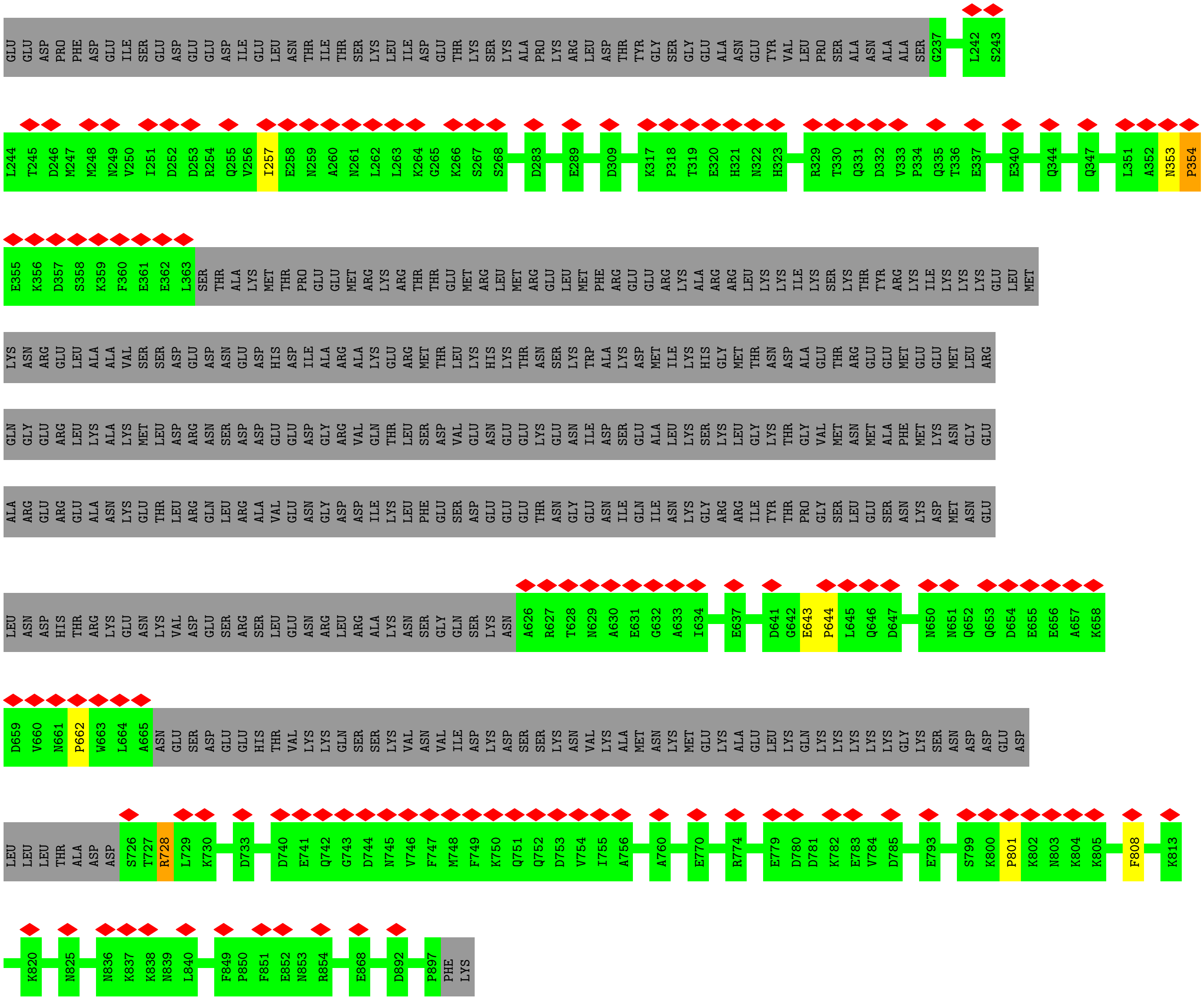

F508 P511 K516 ASP MET VAL G520 T521 L522 D531 A532 S533 GLY ASN ASN LEU L538 K539 T540 L552 ASN PHE LEU ARG G557 W558 V562 S563 N564 LEU HIS P567 K572 G573 Y578 P579 M590 L591 P592 Y598 GLU THR LEU GLU LEU MET LYS T606 L607 M608 I609
L610 V615 P616 D617 LEU LEU SER SER CYS M623 V624 I625 E626 E627 I628 P629 L638 T639 I640 R641 I642 K643 ASN VAL GLY ALA GLU PHE GLY LYS T652 K653 T654 D655 R673 P676 V681 L685 P686 A694 L701 I704 K705 L706 P707 D708 D714 Y715 Y716 Q717
P718 L719 L720 E721 D722 N725 K726 V727 I746 W747 S748 K749 S759 T760 T761 N767 Y770 P771 I774 A778 L779 LYS VAL MET LEU SER I785 P786 E790 N791 H792 F793 V794 D795 P798 F799 V800 Y801 ASN ASP PHE LYS THR Y807 G821 SER TRP THR GLU V826
D827 R828 N829 V830 F831 L832 K842 S846 E849 D852 S860 R861 N862 Q866 LYS LEU ALA L870 L873 L874 A875 N878 P879 N882 K883 TYR ARG ASP ASN LEU LYS ASN L891 L892 D893 D894 F897 K898 D899 GLU ILE THR THR PHE LEU THR E907 N908 G909
I913 K914 A915 E916 K919 V920 V921 M922 P923 Y924 V925 L926 R927 I928 G931 R932 A933 Q934 V935 P936 P937 T938 S939 G940 Q941 R945 LYS ILE ALA V949 I950 S951 V952 L953 P954 N955 F956 K957 K958 P959 Y960 I961 N962 D963 PHE LEU SER LEU ALA SER GLU R971 L972 D973 Y974 N975 Y976
F977 F978 GLY ASN SER HIS GLN ILE ASN SER SER K988 A989 T990 S1006 THR LEU SER VAL LEU R1012 T1013 N1014 F1015 P1016 L1017 H1018 L1023 Q1024 P1025 L1026 I1030 A1033 TYR TYR VAL LEU ASP THR GLU S1041 L1047 R1048 S1052 N1053 L1054 R1055 Q1056 L1059 K1060 C1061 L1062 S1063
S1064 VAL PHE GLU PHE V1069 G1070 N1071 T1072 F1073 D1074 W1075 S1076 I1082 Y1083 A1084 V1085 V1086 V1087 K1088 P1089 ARG ILE SER HIS PHE SER ASP GLU N1098 L1099 Q1100 Q1101 P1102 L1108 PHE LEU Y1111 P1116 S1117 F1121 LEU TYR TYR ASP GLU PHE A1128 T1129 A1130 T1131 M1134 D1135 THR ILE
SER ASN Q1140 H1141 V1142 K1143 E1144 A1145 V1146 I1147 G1148 P1149 I1150 I1151 E1152 A1153 A1154 D1155 S1156 I1157 ILE ARG ASN PRO VAL ASN D1164 Y1167 V1168 D1169 L1170 V1171 T1172 L1173 I1174 C1175 T1176 S1177 C1178 L1179 K1180 I1181 L1182 P1183 S1184 L1185 Y1186 VAL LYS LEU SER ASP SER N1193 S1194 I1195 S1196 T1197 F1198
L1199 N1200 L1201 L1202 V1203 S1204 E1207 MET GLY PHE ILE GLN ASP ASP H1215 V1216 R1217 S1218 R1219 L1220 I1221 S1222 S1223 L1224 I1225 S1226 I1227 L1228 LYS GLY LYS LEU LYS K1234 L1235 Q1236 E1237 N1238 D1239 T1240 Q1241 K1242 I1243 L1244 K1245 I1246 L1247 K1248 L1249 ILE VAL PHE ASN TYR ASN CYS SER TRP S1259
D1260 I1261 E1262 E1263 L1264 Y1265 T1266 S1269 S1270 L1271 F1272 K1273 THR PHE ASP E1277 R1278 N1279 V1282 S1283 L1284 T1285 E1286 L1287 F1288 I1289 E1290 L1291 GLY ARG LYS VAL PRO GLU LEU E1299 S1300 K1303 L1304 V1305 A1306 D1307 L1308 N1309 S1310 Y1311 S1312 R1315 MET HIS GLU TYR ASP F1321 P1322 R1323
I1324 L1325 S1326 T1327 F1328 Y1336 LYS SER TYR SER GLU LEU E1343 W1344 L1345 P1346 F1349 T1350 F1354 I1355 N1356 N1357 K1358 E1359 GLU LEU ALA LEU R1364 T1365 A1370 P1382 ASN LEU N1385 E1386 A1387 S1388 K1389 S1390 I1391 D1396 P1400 N1401 I1402 R1403 I1404 GLY LEU ARG D1408 S1409 L1410
E1411 E1412 E1416 Y1417 V1420 Y1423 MET VAL LYS ASN T1428 K1429 Y1430 F1431 T1432 D1433 F1434 E1435 D1436 M1437 L1441 Y1442 ASN GLY D1445 E1446 E1447 F1450 F1451 T1452 N1453 I1457 Q1458 L1459 H1460 R1461 ARG GLN ARG A1465 R1468 L1469 G1470 E1471 D1478 N1479 S1480 ILE SER HIS TYR LEU
I1486 P1487 M1488 I1489 E1490 H1491 F1494 S1495 D1496 Y1500 G1504 ASN GLU T1507 Q1508 L1527 ARG ARG Y1530 P1538 M1541 L1551 SER VAL PRO LEU ARG GLU THR L1559 P1576 S1577 ASN LEU D1580 E1581 P1582 S1583 N1584 F1585 I1586 L1590 Y1591 P1592 L1598 GLY THR ARG ASP ASP



- Molecule 59: U3 small nucleolar RNA-associated protein 14

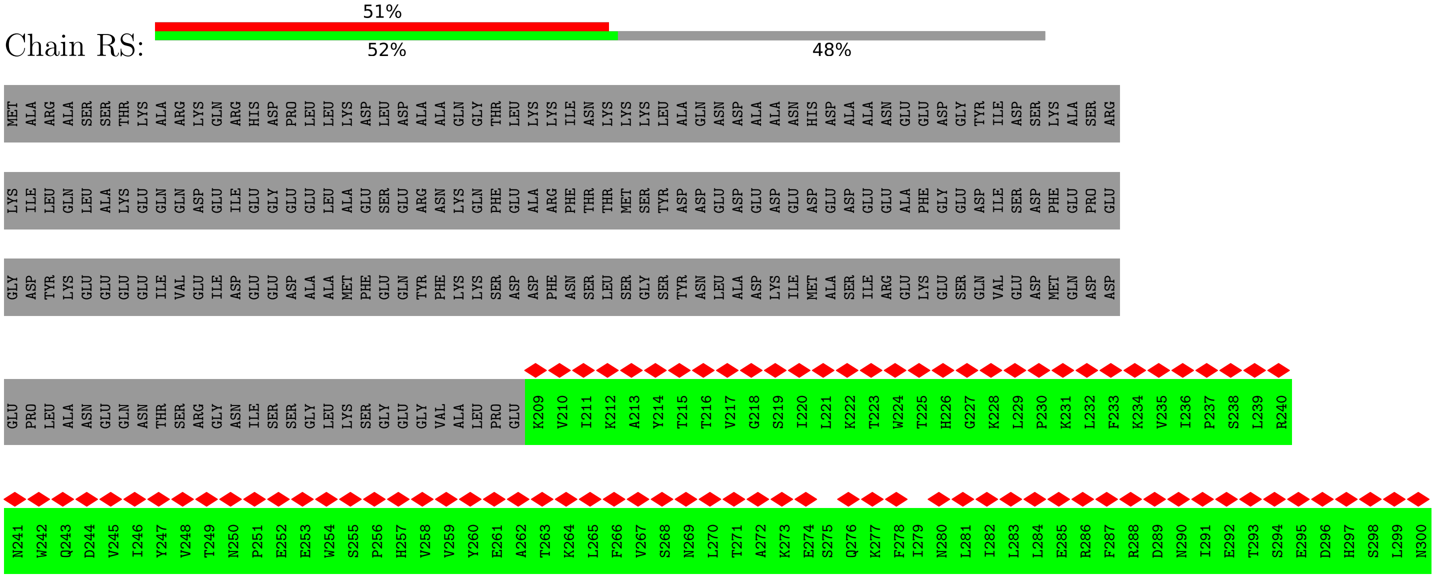
Chain RQ:

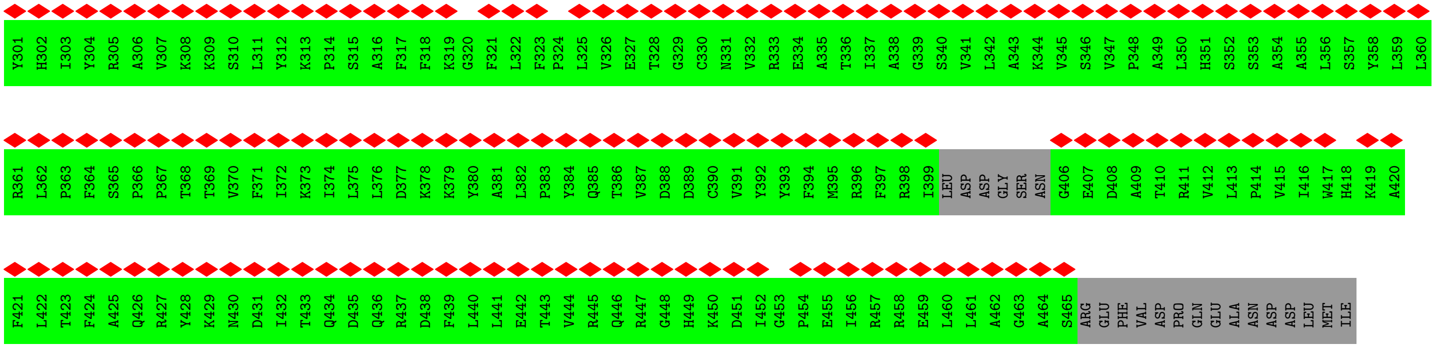




- Molecule 60: Essential nuclear protein 1

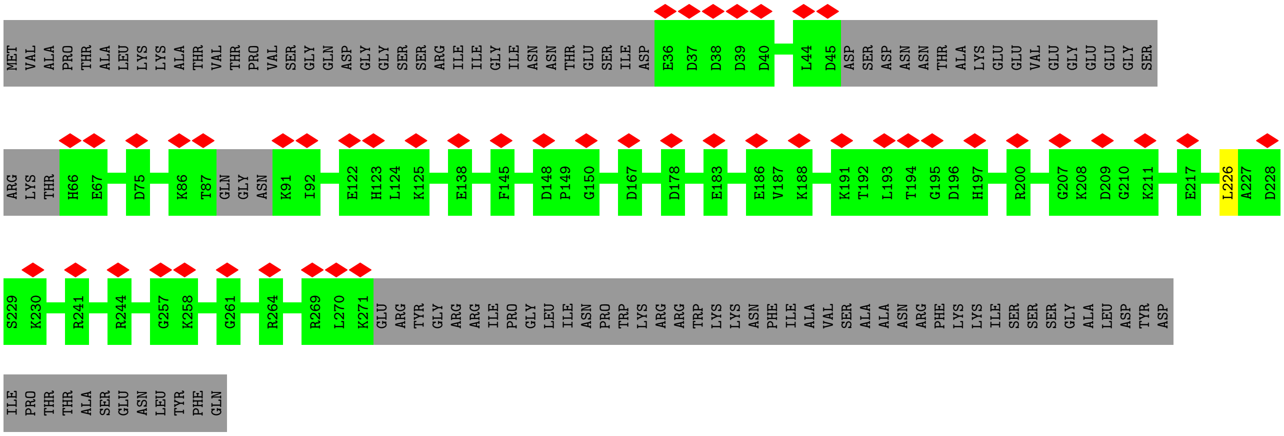
Chain RS:





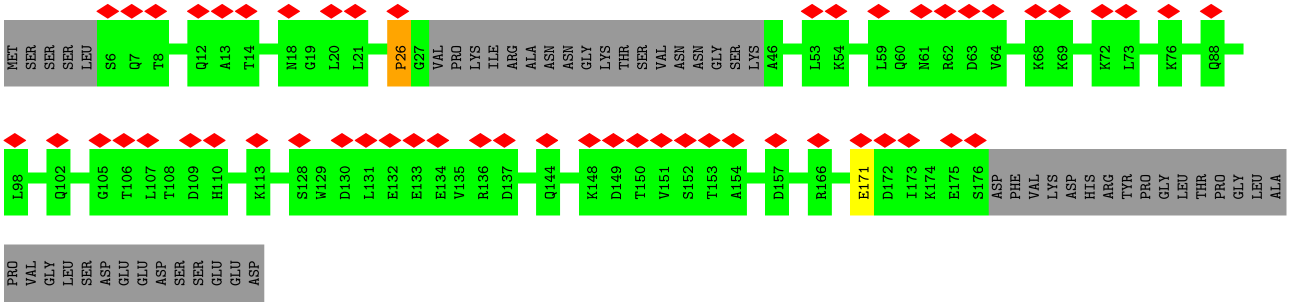
- Molecule 61: Pno1

Chain RT:



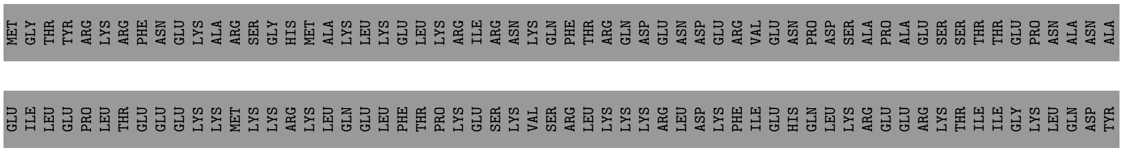
- Molecule 62: Regulator of rDNA transcription protein 14

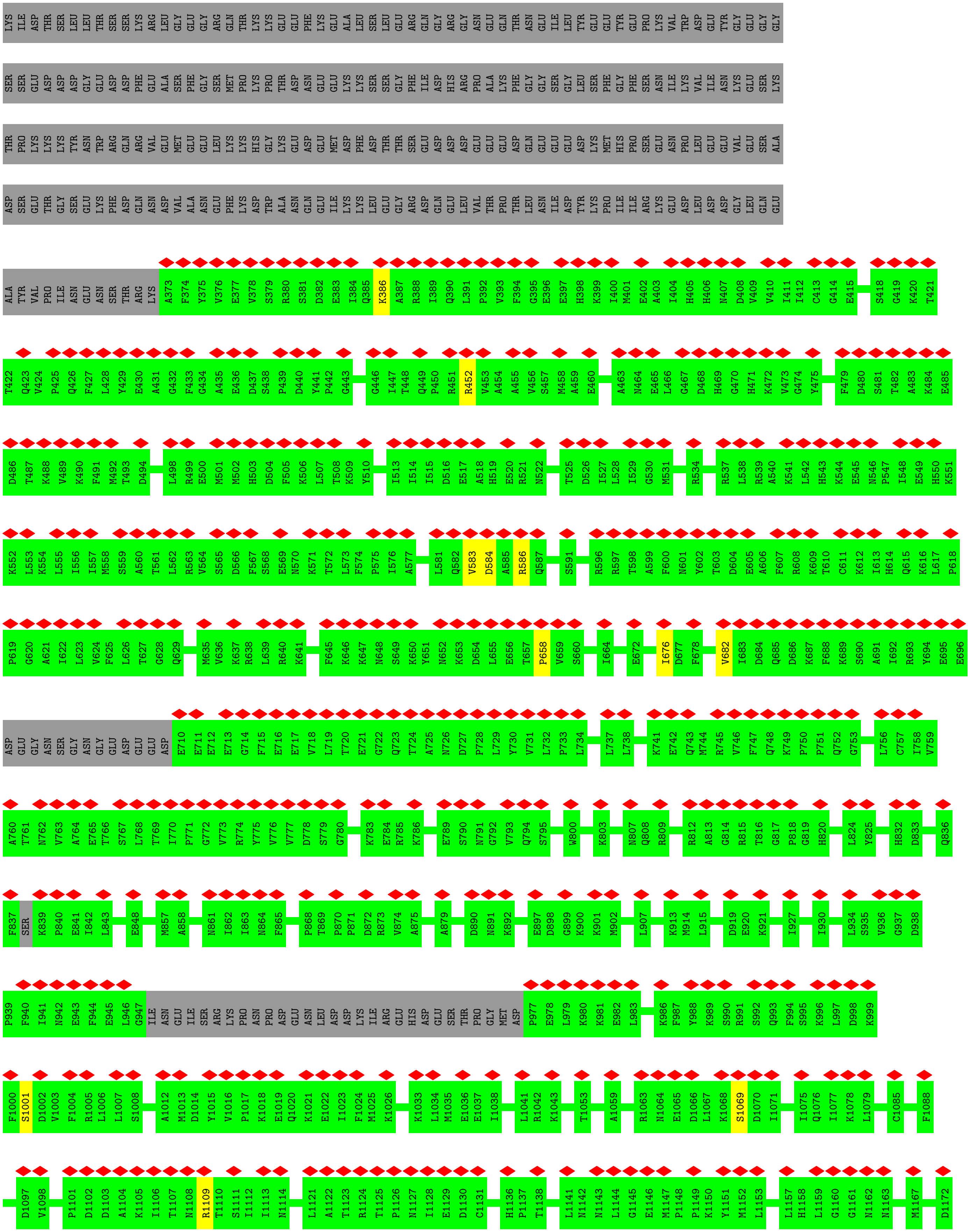
Chain RW:

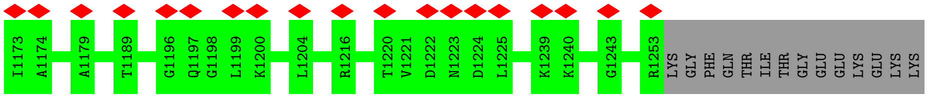


- Molecule 63: Probable ATP-dependent RNA helicase DHR1

Chain RZ:

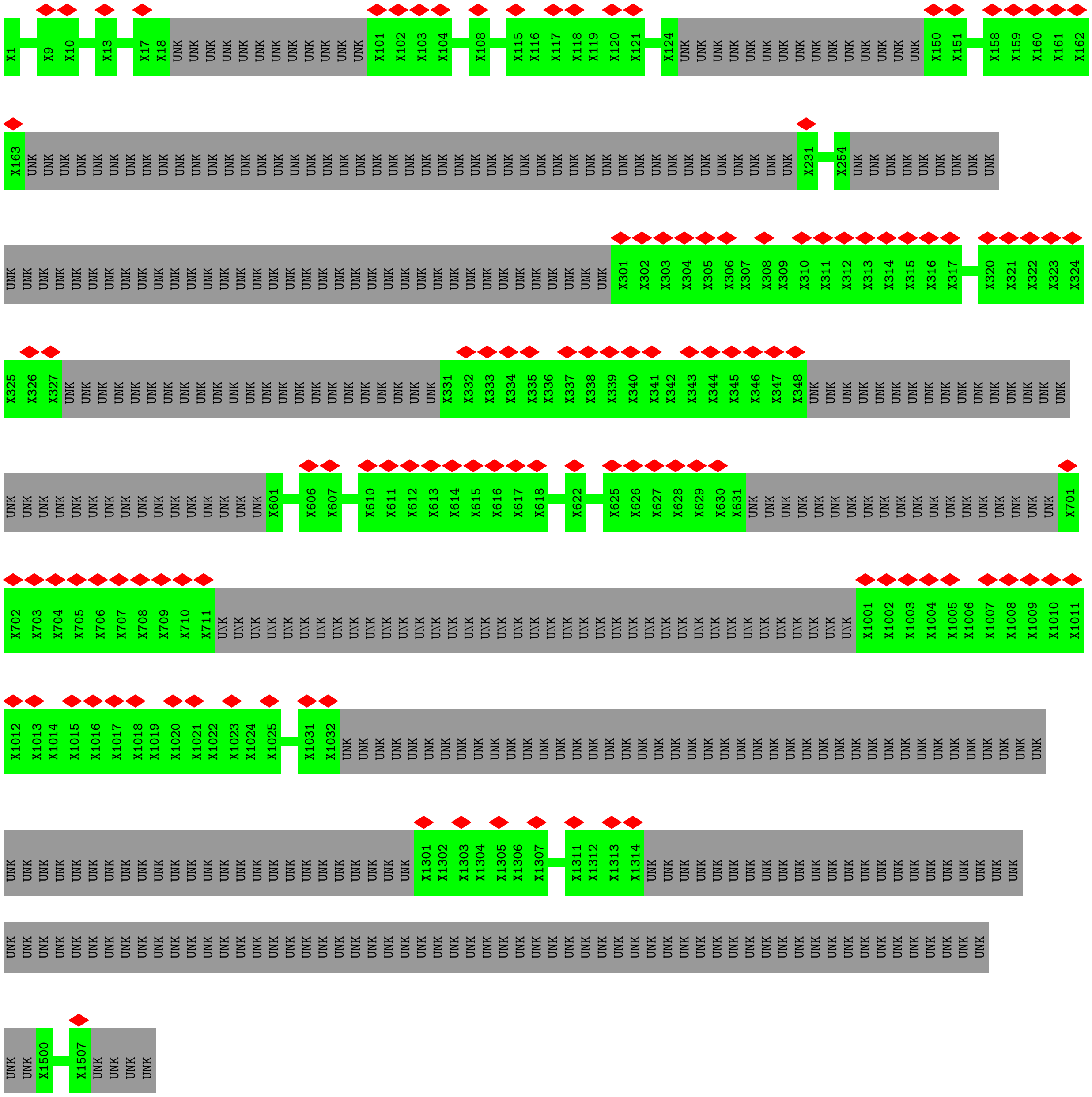



LYS ILE ASP THR SER LEU LEU THR SER SER LYS ARG LEU GLY GLU GLY ARG GLN THR LYS LYS GLU GLU PHE LYS GLU ALA LEU SER LEU GLU ARG GLN GLY ARG GLY ASN GLU GLN THR ASN GLU ILE LEU TYR GLU GLU TYR GLU PRO LYS VAL TRP ASP GLU TYR GLY GLU GLY GLY
SER SER GLU ASP ASP ASP GLY GLU ASP ASP PHE GLU ALA SER PHE GLY SER MET PRO LYS PRO THR ASP ASN GLU GLU LYS LYS SER SER GLY PHE ILE ASP HIS ARG PRO ALA LYS PHE GLY GLY SER GLY LEU SER PHE GLY PHE SER ASN ILE LYS VAL ILE ASN LYS GLU SER LYS
THR PRO LYS LYS TYR ASN TRP ARG GLN ARG VAL GLU MET GLU GLU LEU LYS LYS HIS GLY LYS GLU ASP GLU MET ASP PHE ASP THR THR SER GLU ASP ASP GLU GLU GLU ASP GLN GLU GLU GLU ASP LYS MET HIS PRO SER GLU ASN PRO LEU GLU GLU VAL GLU SER ALA
ASP SER GLU THR GLY SER GLU LYS PHE ASP GLN ASN ASP VAL ALA ASN GLU PHE LYS ASP TRP ALA ASN GLN GLU ILE LYS LYS LEU GLU GLY ARG ASP GLN ASP LEU VAL THR PRO THR LEU ASN ASN ASP TYR LYS PRO ILE ILE ARG LYS GLU ASP LEU ASP ASP GLY LEU GLN GLU
ALA TYR VAL PRO ILE ASN GLU ASN SER THR ARG LYS A373 F374 Y375 V376 E377 V378 S379 R380 S381 D382 E383 I384 Q385 K386 A387 R388 I389 Q390 L391 P392 V393 F394 G395 E396 E397 H398 K399 I400 M401 E402 A403 I404 H405 H406 N407 D408 V409 V410 I411 I412 G413 G414 E415 S418 G419 K420 T421
T422 Q423 V424 P425 Q426 F427 L428 Y429 E430 A431 G432 F433 G434 A435 E436 D437 S438 P439 D440 Y441 P442 G443 G446 I447 T448 Q449 P450 R451 R452 V453 A454 A455 V456 S457 M458 A459 E460 A463 N464 E465 L466 G467 D468 H469 G470 H471 K472 V473 G474 Y475 F479 D480 S481 T482 A483 K484 E485
D486 T487 K488 V489 K490 F491 M492 T493 D494 L498 R499 E500 M501 M502 H503 D504 F505 K506 L507 T508 K509 Y510 I513 I514 I515 D516 E517 A518 H519 E520 R521 N522 T525 D526 I527 L528 I529 G530 M531 R534 R537 L538 R539 A540 K541 L542 H543 K544 E545 N546 P547 I548 E549 H550 K551
K552 L553 K554 L555 I556 I557 M558 S559 A560 T561 L562 R563 V564 S565 D566 F567 S568 E569 N570 K571 T572 L573 F574 P575 I576 A577 L581 Q582 V583 D584 A585 R586 Q587 S591 R596 R597 T598 A599 F600 N601 Y602 T603 D604 E605 A606 F607 R608 K609 T610 C611 K612 I613 H614 Q615 K616 L617 P618
P619 G620 A621 I622 L623 V624 F625 L626 T627 G628 Q629 M635 V636 K637 R638 L639 R640 K641 F645 K646 K647 N648 S649 K650 Y651 N652 K653 D654 L655 E656 T657 P658 V659 S660 I664 E672 I676 D677 F678 V682 I683 D684 Q685 D686 K687 F688 K689 S690 A691 I692 R693 Y694 E695 E696
ASP GLU GLY ASN SER GLY ASN GLY GLU ASP GLU ASP E710 E711 E712 E713 G714 F715 E716 E717 V718 L719 T720 E721 G722 Q723 T724 A725 N726 D727 P728 L729 Y730 V731 L732 P733 L734 L737 L738 K741 E742 Q743 M744 R745 V746 F747 Q748 K749 P750 P751 Q752 G753 L756 C757 I758 V759
A760 T761 N762 V763 A764 E765 T766 S767 L768 T769 I770 P771 G772 V773 R774 Y775 V776 V777 D778 S779 G780 K783 E784 R785 K786 E789 S790 N791 G792 V793 Q794 S795 W800 K803 N807 Q808 R809 R812 A813 G814 R815 T816 G817 P818 G819 H820 L824 Y825 H832 D833 Q836
F837 SER K839 P840 E841 I842 L843 E848 M857 A858 N861 I862 S863 N864 F865 P868 T869 P870 P871 D872 R873 V874 A875 A879 D890 N891 K892 E897 D898 G899 K900 K901 M902 L907 K913 M914 L915 D919 E920 K921 I927 I930 L934 S935 V936 G937 D938
P939 F940 I941 N942 E943 F944 E945 L946 G947 ILE ASN GLU ILE SER ARG LYS PRO ASN PRO ASP GLU ASN LEU ASP LYS ILE ARG GLU HIS ASP GLU SER THR PRO GLY MET ASP P977 E978 L979 K980 K981 E982 L983 K986 F987 Y988 K989 S990 R991 S992 Q993 F994 S995 K996 L997 D998 K999
F1000 S1001 D1002 V1003 F1004 R1005 L1006 L1007 S1008 A1012 M1013 D1014 Y1015 V1016 P1017 K1018 E1019 Q1020 K1021 E1022 I1023 F1024 M1025 K1026 K1033 L1034 M1035 E1036 E1037 I1038 L1041 R1042 K1043 T1053 A1059 R1063 N1064 E1065 D1066 L1067 K1068 S1069 D1070 I1071 I1075 Q1076 I1077 K1078 L1079 C1085 F1088
D1097 V1098 P1101 D1102 D1103 A1104 K1105 I1106 T1107 N1108 R1109 T1110 S1111 I1112 I1113 N1114 L1121 A1122 T1123 R1124 T1125 P1126 N1127 I1128 E1129 D1130 C1131 H1136 P1137 T1138 L1141 N1142 N1143 L1144 G1145 E1146 M1147 P1148 P1149 K1150 Y1151 M1152 L1153 L1157 H1158 L1159 G1160 G1161 N1162 N1163 M1167 D1172



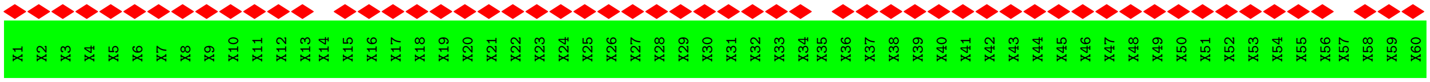
- Molecule 64: Unassigned peptides 1

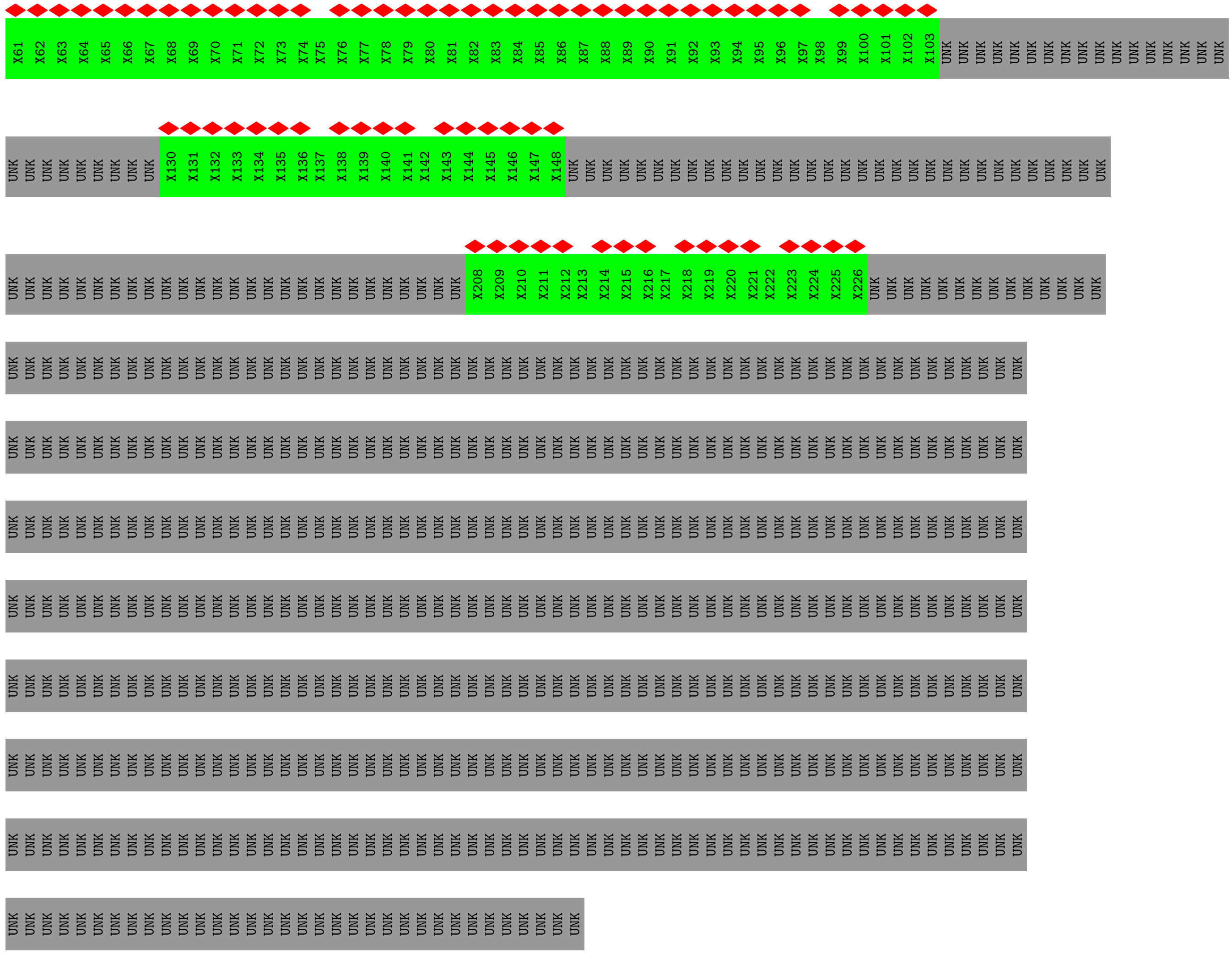
Chain X1:



- Molecule 65: Unassigned peptides 2

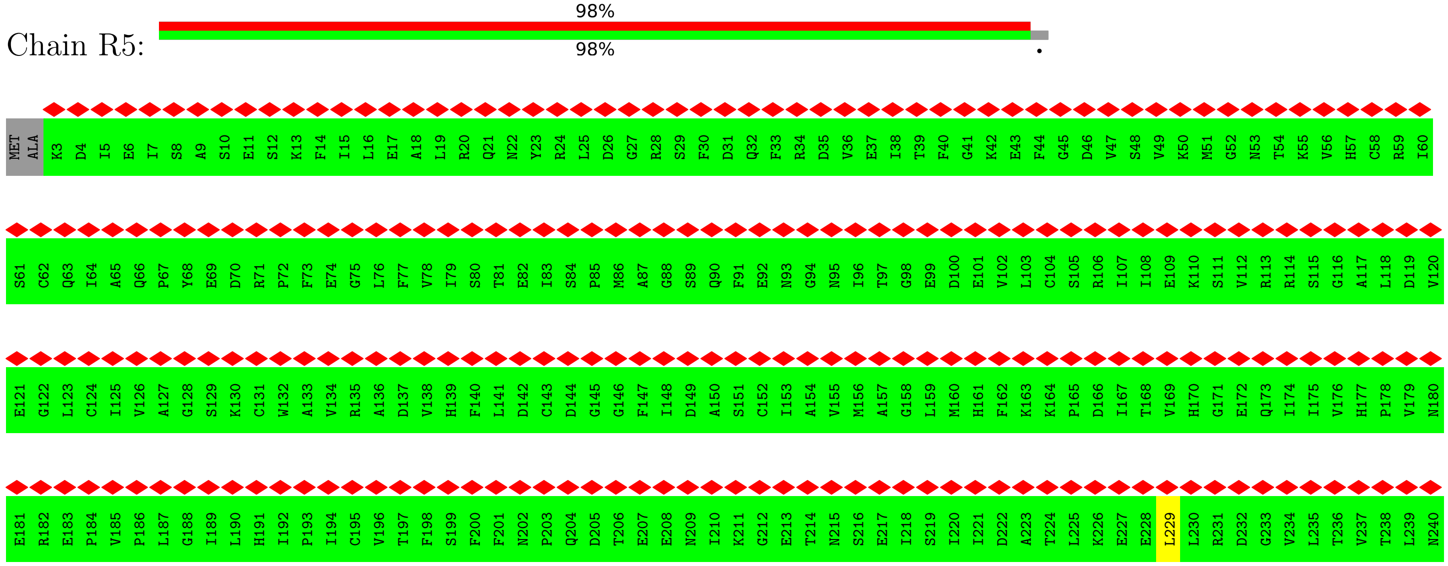
Chain X2:





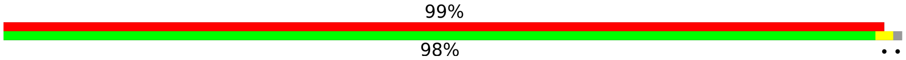
- Molecule 66: Exosome complex component RRP45

Chain R5:



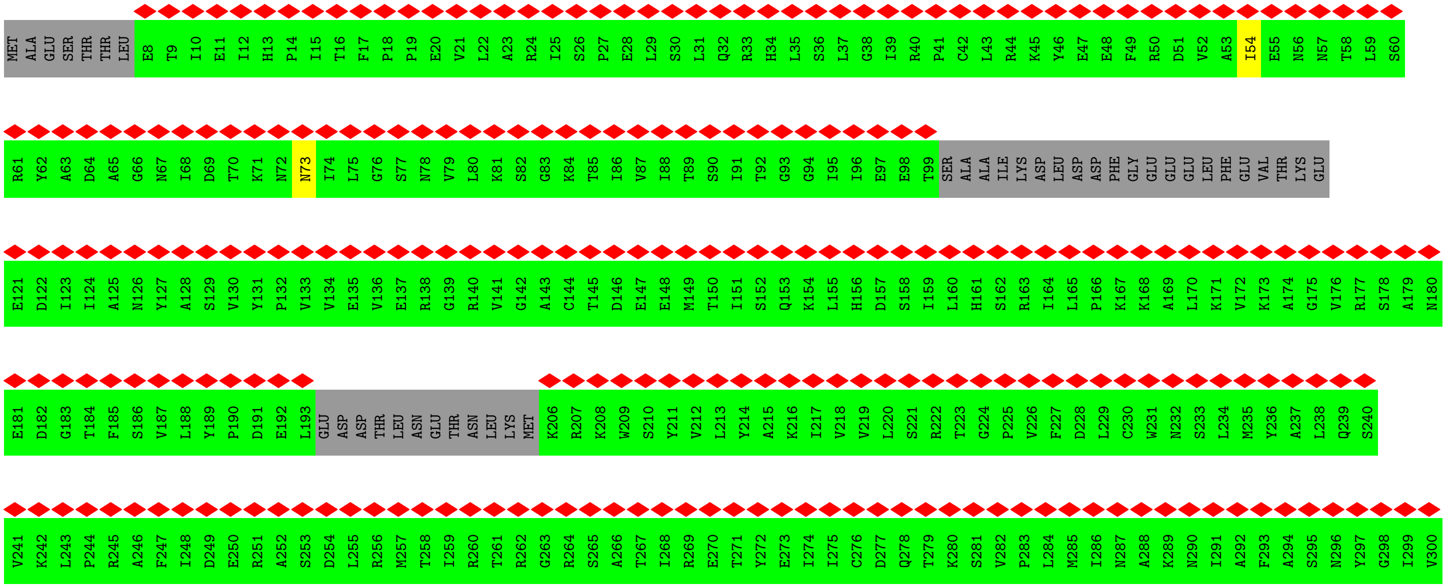
- Molecule 67: Exosome complex component SKI6

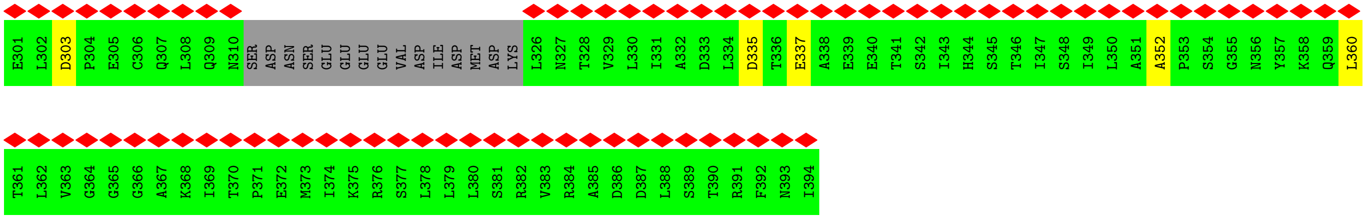
Chain R1:



- Molecule 68: Exosome complex component RRP43

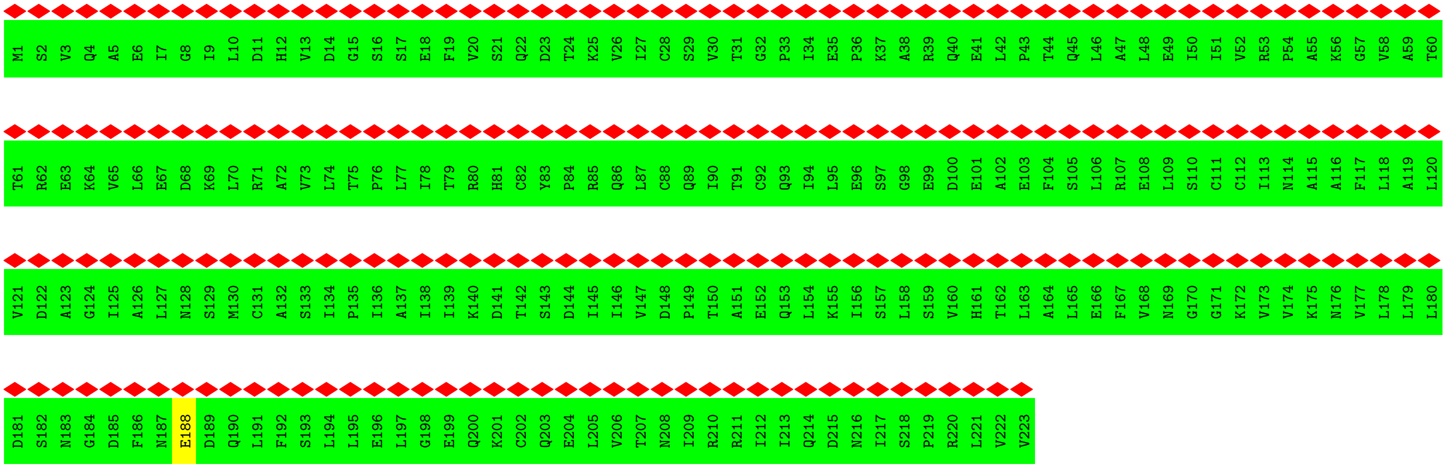
Chain R3:





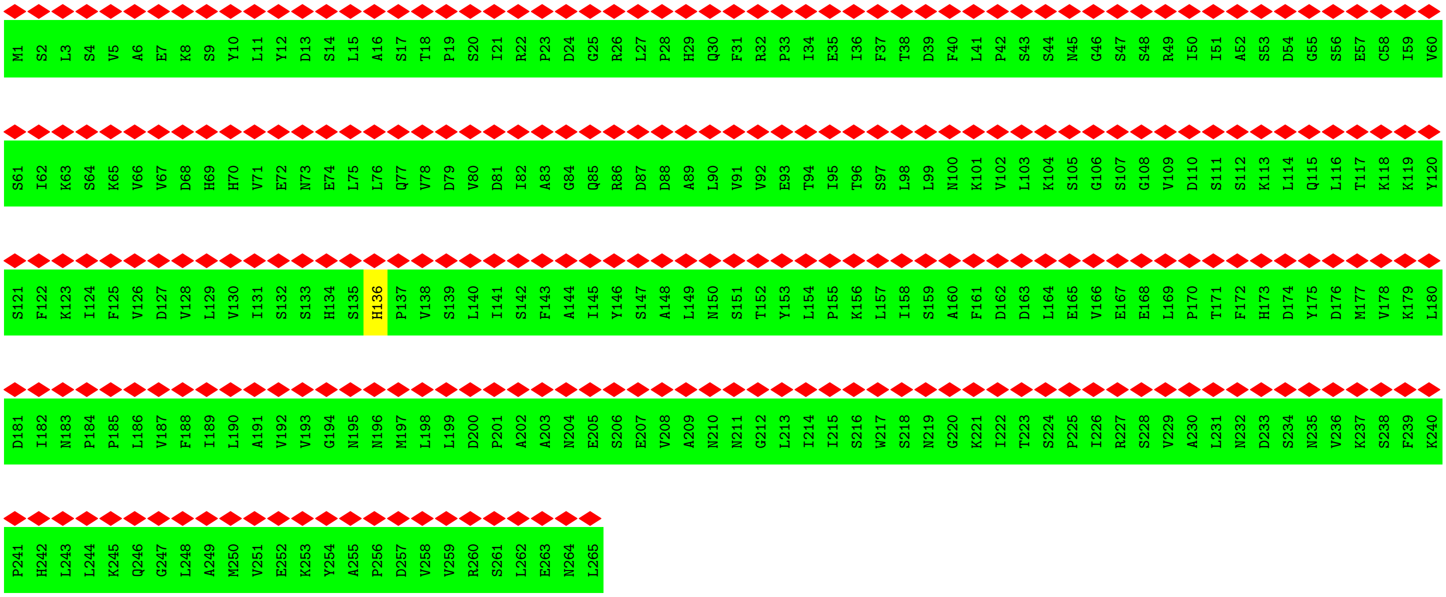
- Molecule 69: Exosome complex component RRP46

Chain R6:



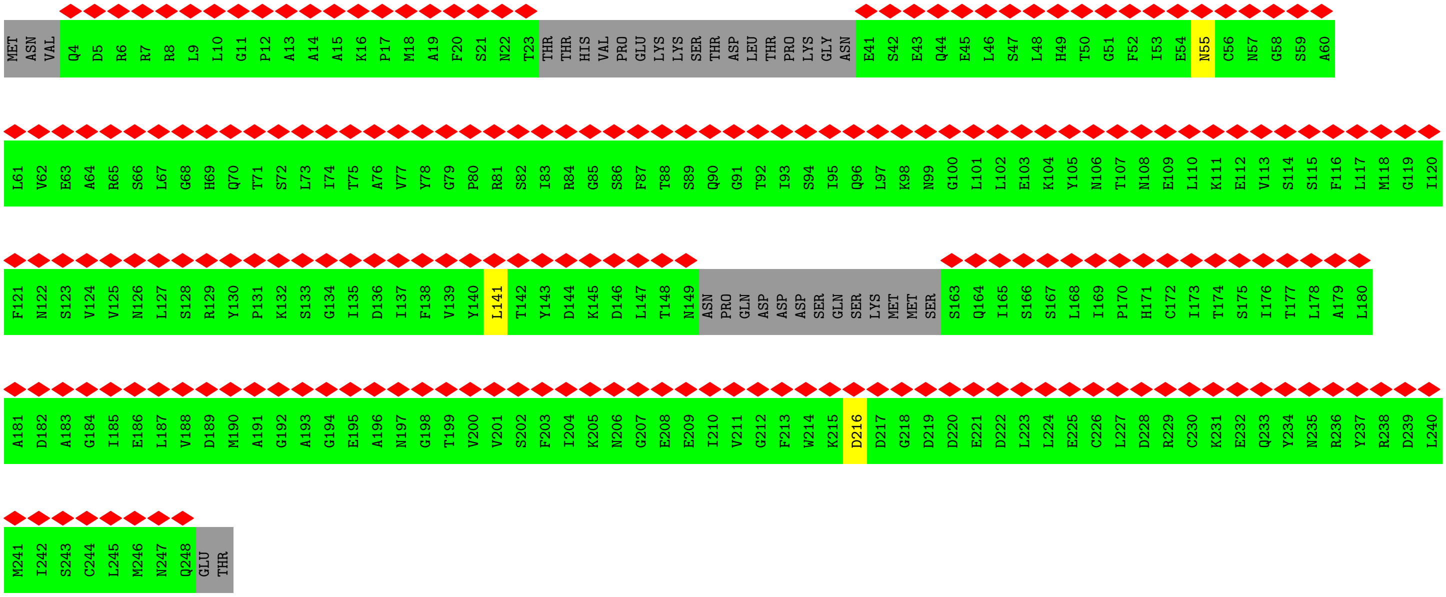
- Molecule 70: Exosome complex component RRP42

Chain R2:



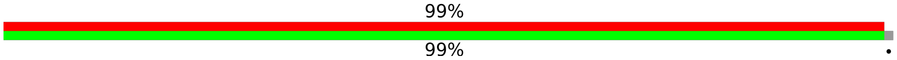
- Molecule 71: Exosome complex component MTR3

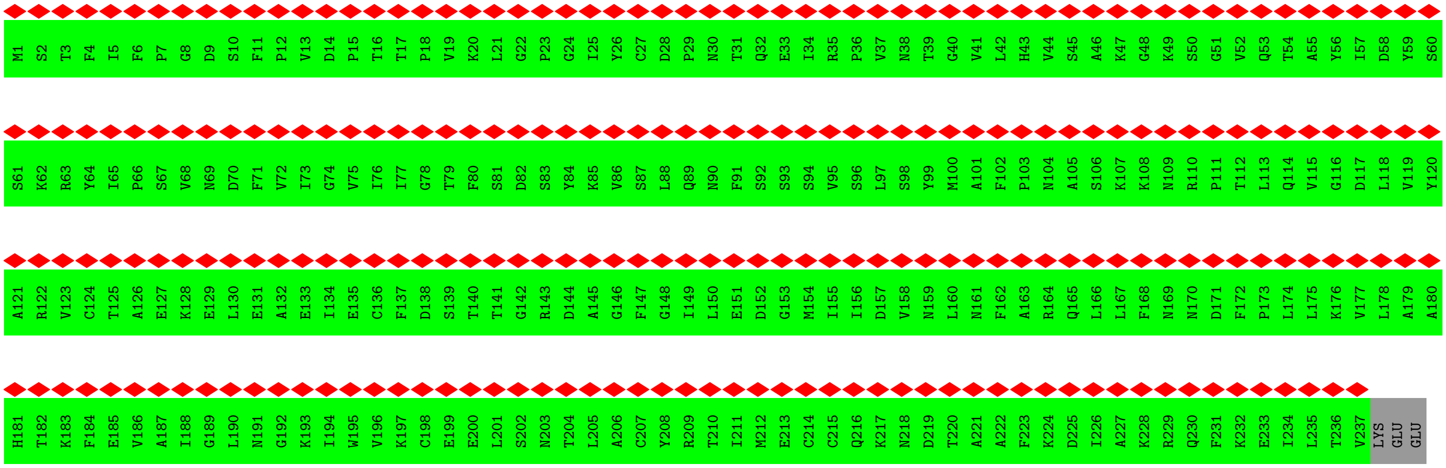
Chain M3:



- Molecule 72: Exosome complex component RRP40

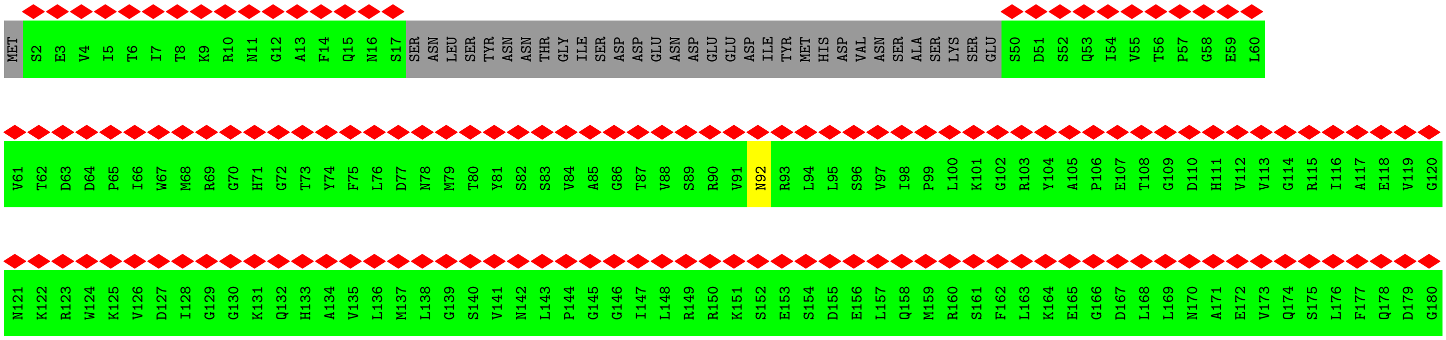
Chain R0:

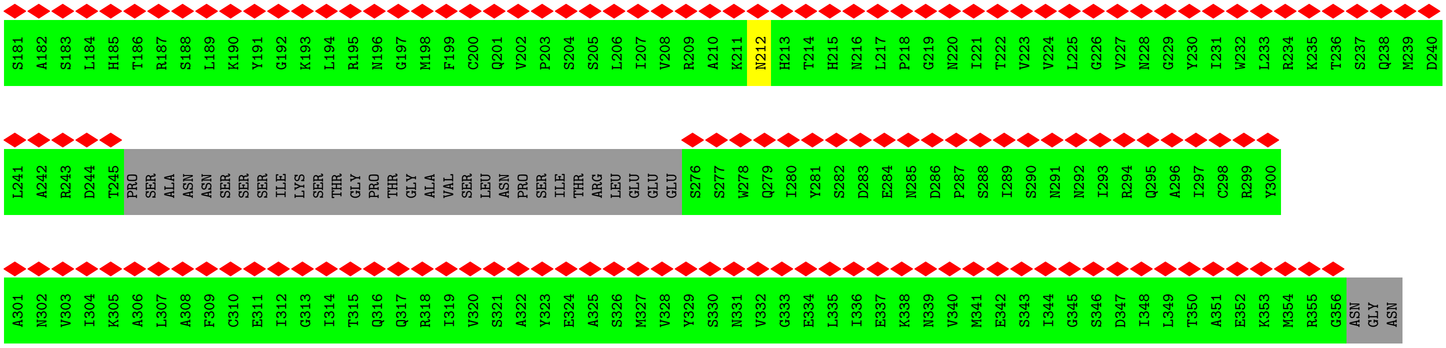




- Molecule 73: Exosome complex component RRP4

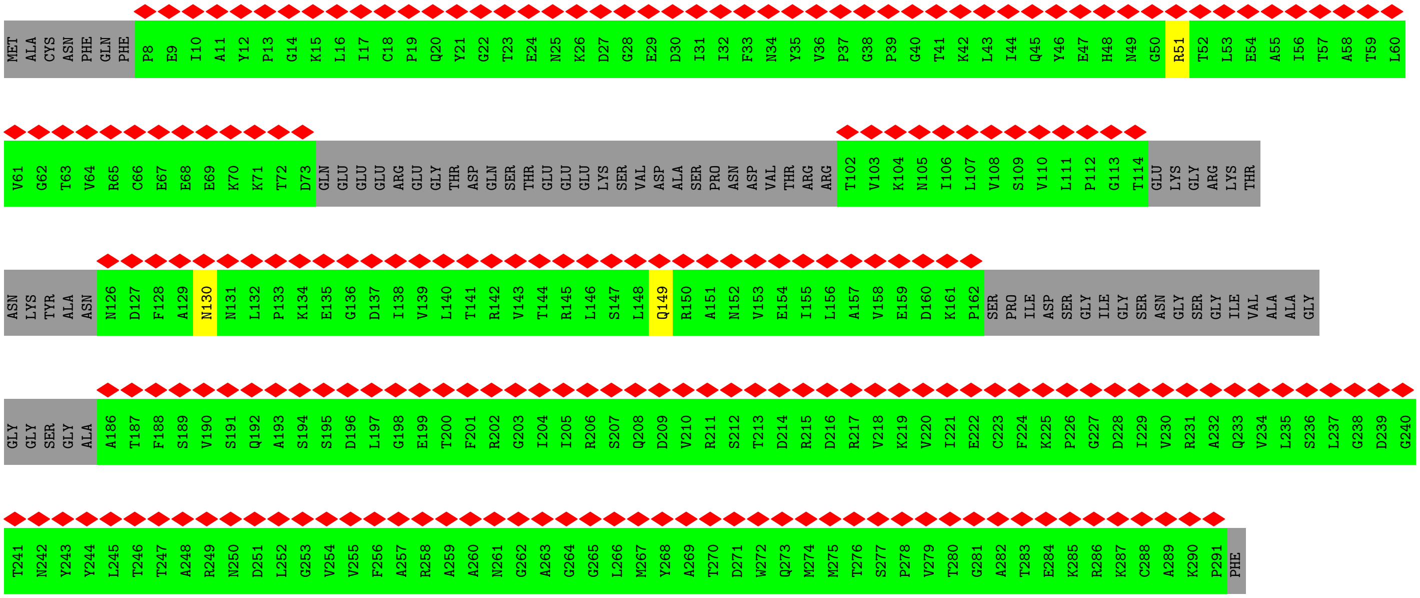
Chain r4:





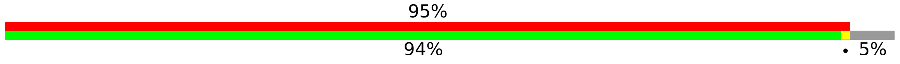
- Molecule 74: Exosome complex component CSL4

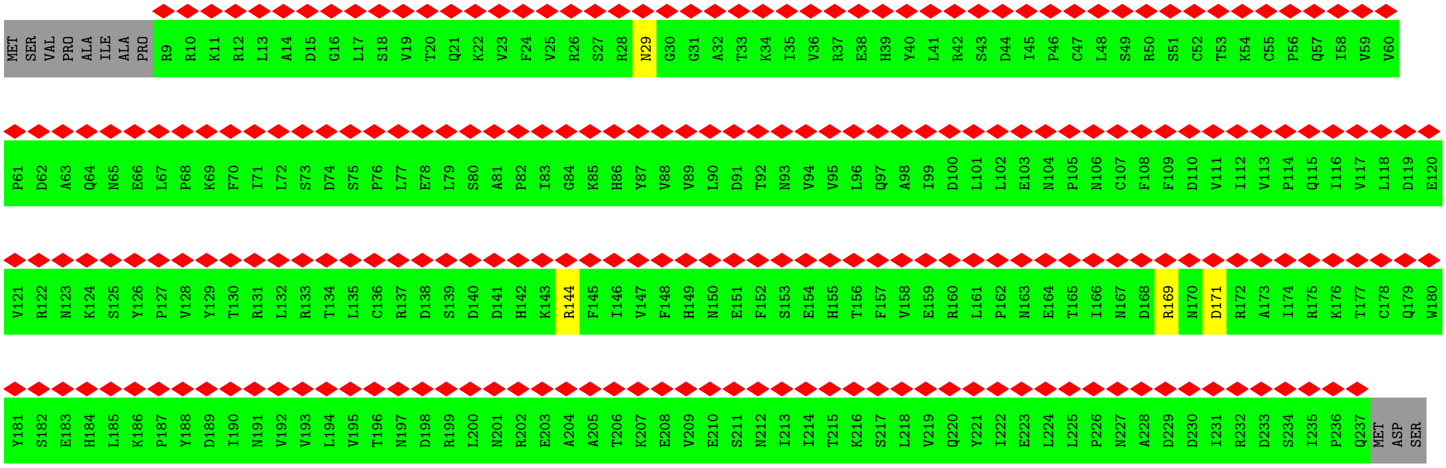
Chain C4:

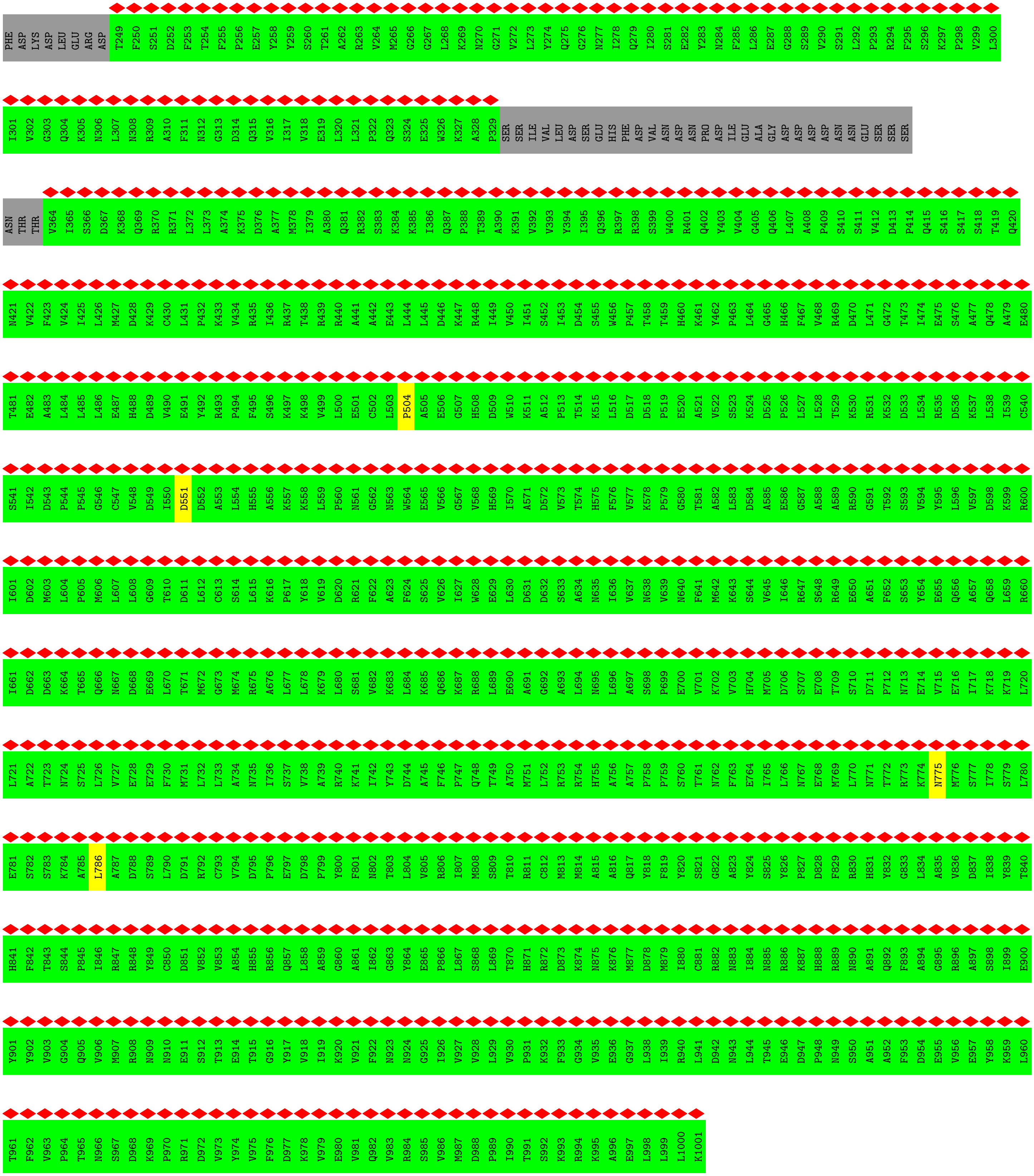


- Molecule 75: Exosome complex exonuclease DIS3

Chain R4:

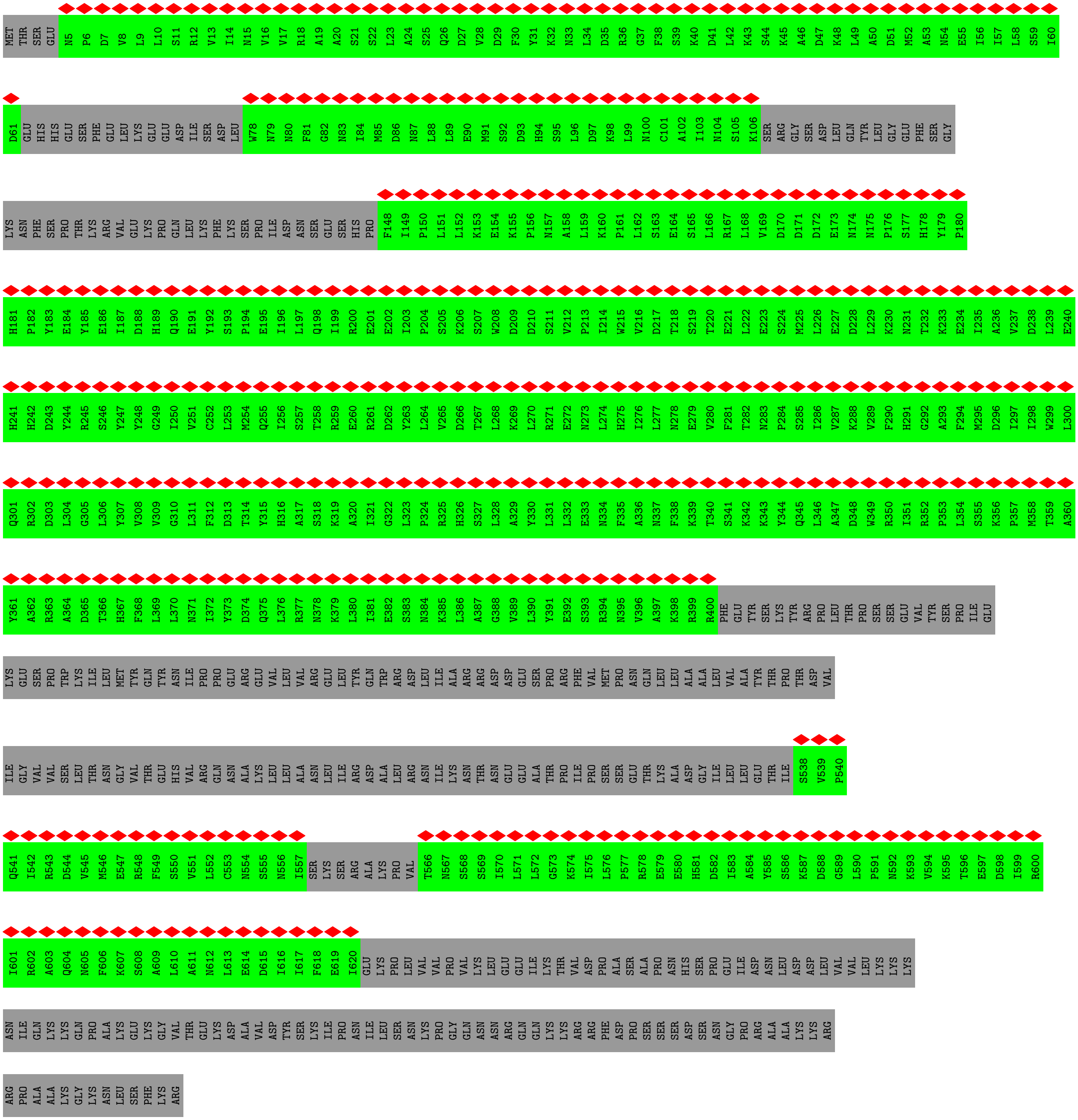






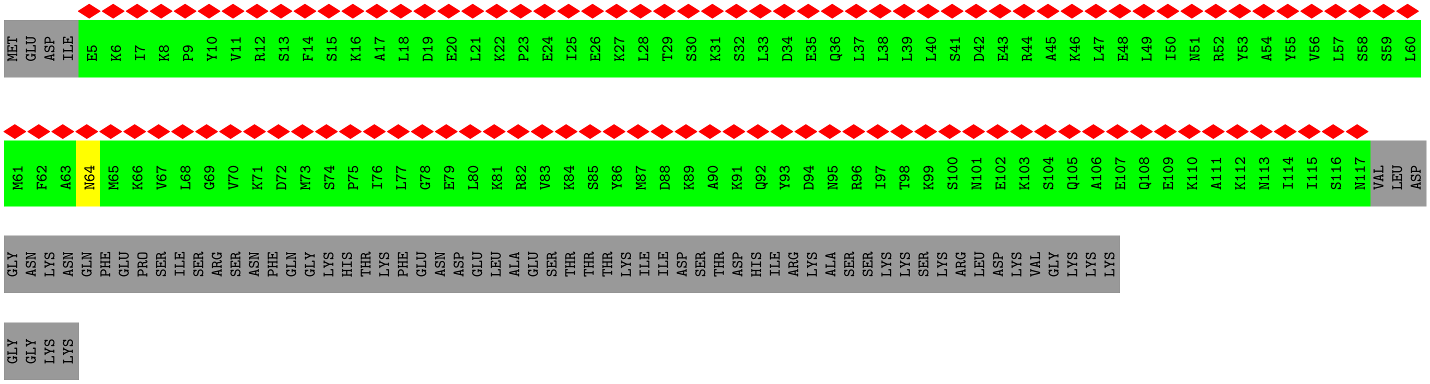
- Molecule 76: Exosome complex exonuclease RRP6

Chain r6:



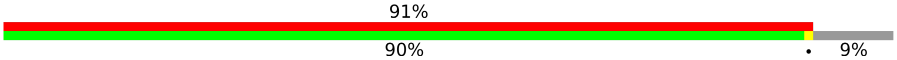
- Molecule 77: Exosome complex protein LRP1

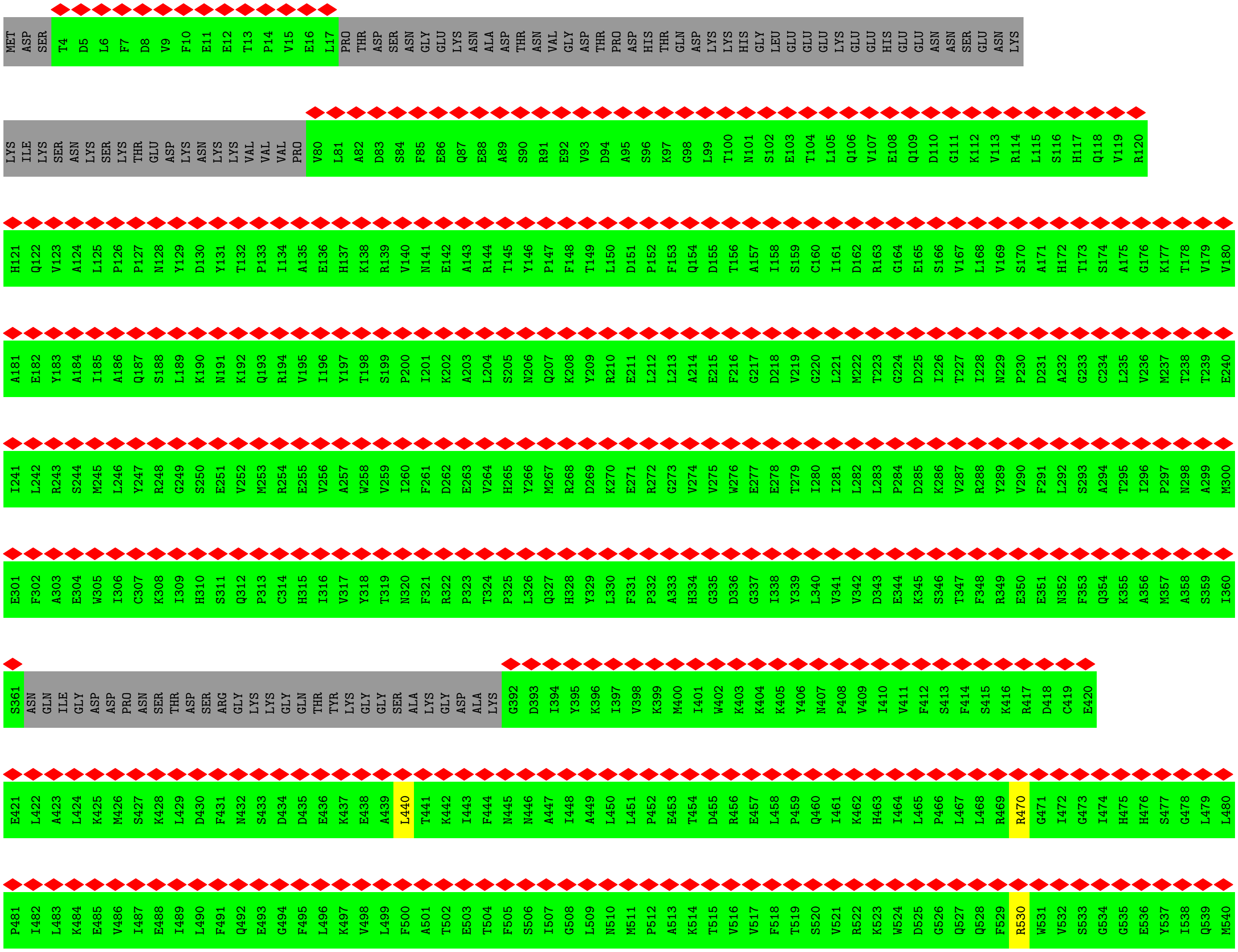
Chain R7:

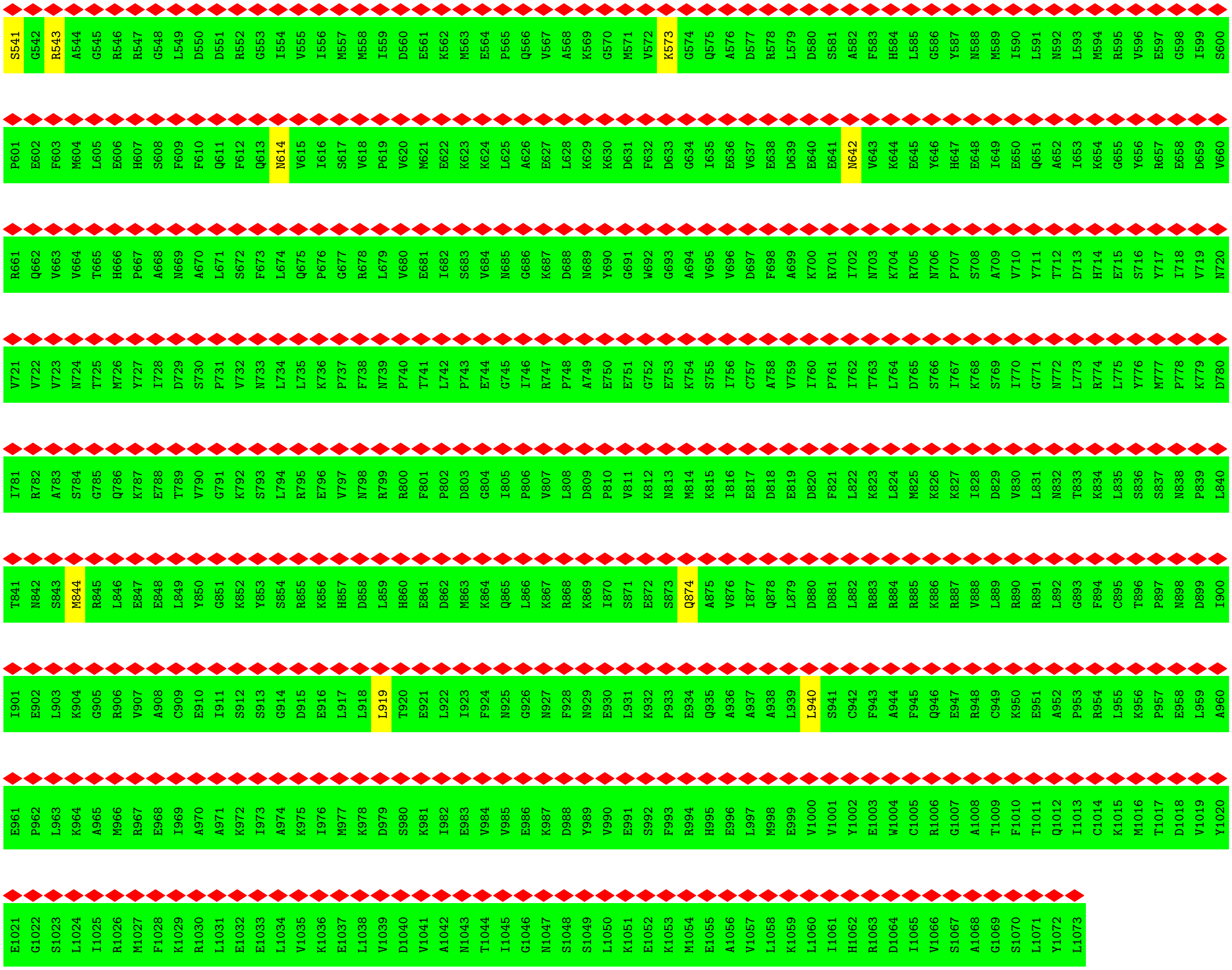


- Molecule 78: ATP-dependent RNA helicase DOB1

Chain M4:

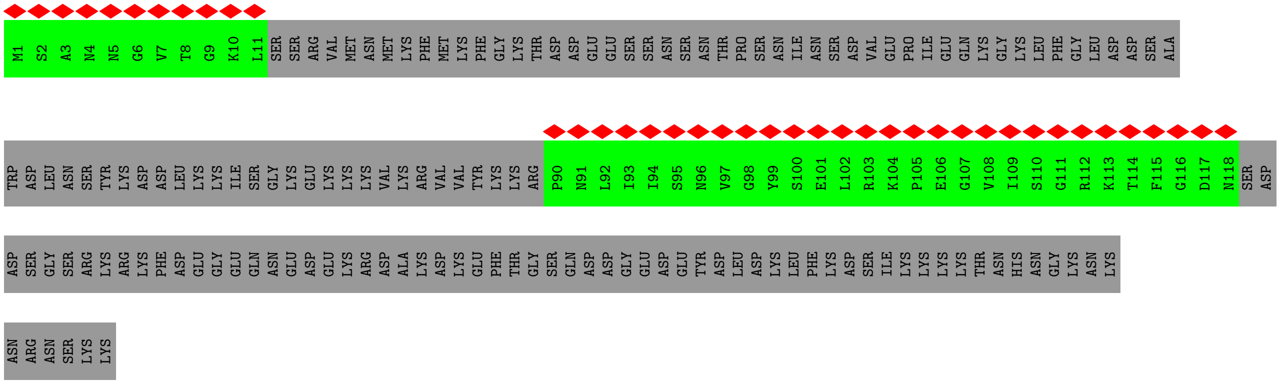






- Molecule 79: M-phase phosphoprotein 6 homolog

Chain M6:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219545	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	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.120	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	531.19995, 531.19995, 531.19995	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3279998, 1.3279998, 1.3279998	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, ADP

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	0.61	0/5088	1.20	47/7888 (0.6%)
2	5A	0.44	0/2833	1.13	12/4401 (0.3%)
3	SA	0.56	0/31829	1.17	228/49545 (0.5%)
4	SC	0.39	0/1949	0.66	2/2609 (0.1%)
5	SF	0.37	0/1954	0.65	1/2640 (0.0%)
6	SG	0.38	0/1690	0.61	0/2285
7	SH	0.29	0/1476	0.56	1/1975 (0.1%)
8	SI	0.36	0/1341	0.76	3/1806 (0.2%)
9	SJ	0.30	0/1202	0.58	0/1610
10	SK	0.41	0/1432	0.65	2/1917 (0.1%)
11	SM	0.29	0/1139	0.52	0/1535
12	SO	0.37	0/1109	0.57	0/1495
13	SP	0.37	0/859	0.63	0/1161
14	SR	0.46	0/990	0.63	0/1335
15	ST	0.30	0/914	0.59	0/1229
16	SU	0.34	0/1092	0.55	0/1466
17	SX	0.39	0/1020	0.64	0/1371
18	SY	0.40	0/804	0.57	0/1074
19	SZ	0.44	0/1000	0.66	0/1334
20	Sc	0.38	0/613	0.62	0/828
21	Sd	0.41	0/499	0.60	0/670
22	3B	0.50	0/1914	0.66	1/2582 (0.0%)
22	3C	0.41	0/1787	0.66	2/2413 (0.1%)
23	3D	0.41	0/3020	0.60	2/4066 (0.0%)
24	3E	0.37	0/3088	0.61	1/4193 (0.0%)
25	3F	0.45	0/3569	0.62	0/4806
26	3G	0.42	0/928	0.74	2/1262 (0.2%)
26	3H	0.46	0/928	0.74	2/1262 (0.2%)
27	A4	0.41	0/5282	0.65	2/7154 (0.0%)
28	A5	0.37	0/4021	0.65	4/5462 (0.1%)
29	A8	0.27	0/3328	0.59	2/4565 (0.0%)
30	A9	0.28	0/951	0.65	2/1287 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	AE	0.33	0/10367	0.57	18/14163 (0.1%)
32	AF	0.33	0/3941	0.59	1/5344 (0.0%)
33	AG	0.36	0/6694	0.62	4/9070 (0.0%)
34	B1	0.43	0/6459	0.63	0/8744
35	B2	0.38	0/6624	0.65	3/8950 (0.0%)
36	B3	0.37	0/6001	0.66	3/8120 (0.0%)
37	B8	0.44	0/3730	0.63	3/5058 (0.1%)
38	BE	0.42	0/7012	0.63	5/9493 (0.1%)
39	B6	0.40	0/3138	0.60	2/4226 (0.0%)
40	5B	0.32	0/486	0.71	1/643 (0.2%)
41	5C	0.40	0/3902	0.61	3/5265 (0.1%)
42	5D	0.34	0/1801	0.57	0/2379
43	5E	0.34	0/1745	0.62	1/2335 (0.0%)
44	5F	0.37	0/1559	0.60	0/2097
45	5G	0.42	0/1993	0.65	2/2689 (0.1%)
46	5H	0.40	0/704	0.59	1/931 (0.1%)
47	5I	0.49	0/3844	0.61	0/5174
48	5J	0.37	0/1147	0.56	0/1531
49	5K	0.44	0/1213	0.63	1/1638 (0.1%)
50	RD	0.30	0/2454	0.56	3/3310 (0.1%)
51	RE	0.34	0/9015	0.58	4/12195 (0.0%)
52	RF	0.32	0/2004	0.62	0/2697
53	RG	0.27	0/1727	0.62	2/2329 (0.1%)
53	RH	0.32	0/1828	0.61	1/2470 (0.0%)
54	RJ	0.41	0/6126	0.59	1/8247 (0.0%)
55	RK	0.38	0/2832	0.61	0/3825
56	RN	0.30	0/4521	0.58	5/6083 (0.1%)
57	RO	0.29	0/3824	0.59	6/5226 (0.1%)
58	RP	0.31	0/12292	0.58	48/16822 (0.3%)
59	RQ	0.35	0/2443	0.62	4/3317 (0.1%)
60	RS	0.30	0/2104	0.58	0/2854
61	RT	0.34	0/1679	0.63	1/2261 (0.0%)
62	RW	0.30	0/760	0.46	1/1059 (0.1%)
63	RZ	0.31	0/6730	0.58	1/9088 (0.0%)
66	R5	0.57	0/2340	0.64	1/3161 (0.0%)
67	R1	0.54	0/1910	0.68	0/2579
68	R3	0.50	0/2628	0.69	2/3569 (0.1%)
69	R6	0.54	0/1722	0.70	0/2339
70	R2	0.51	0/2077	0.69	0/2828
71	M3	0.53	0/1661	0.65	0/2243
72	R0	0.55	0/1828	0.68	0/2486
73	r4	0.52	0/2269	0.66	0/3066
74	C4	0.48	0/1676	0.66	0/2277

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	R4	0.42	0/7575	0.61	3/10290 (0.0%)
76	r6	0.35	0/2540	0.51	0/3497
77	R7	0.39	0/903	0.58	0/1210
78	M4	0.49	0/7772	0.66	3/10521 (0.0%)
79	M6	0.43	0/277	0.66	0/371
All	All	0.42	0/259526	0.74	450/359296 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	SC	0	2
5	SF	0	1
7	SH	0	2
8	SI	0	2
14	SR	0	1
17	SX	0	1
19	SZ	0	1
20	Sc	0	1
25	3F	0	3
26	3G	0	2
26	3H	0	1
27	A4	0	1
28	A5	0	2
29	A8	0	2
33	AG	0	4
34	B1	0	2
35	B2	0	2
36	B3	0	7
38	BE	0	3
39	B6	0	2
40	5B	0	1
46	5H	0	1
47	5I	0	2
49	5K	0	1
51	RE	0	2
52	RF	0	1
54	RJ	0	1
56	RN	0	1
57	RO	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
58	RP	0	9
59	RQ	0	1
62	RW	0	1
63	RZ	0	2
67	R1	0	1
68	R3	0	3
69	R6	0	1
70	R2	0	1
71	M3	0	2
73	r4	0	1
74	C4	0	1
75	R4	0	1
78	M4	0	3
All	All	0	81

There are no bond length outliers.

All (450) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5A	494	C	C2-N1-C1'	14.08	134.28	118.80
3	SA	185	U	C2-N1-C1'	10.48	130.27	117.70
1	3A	269	C	C2-N1-C1'	10.38	130.22	118.80
3	SA	185	U	N1-C2-O2	10.12	129.88	122.80
3	SA	1473	U	C2-N1-C1'	10.10	129.82	117.70
3	SA	1473	U	N1-C2-O2	9.84	129.69	122.80
2	5A	494	C	C6-N1-C1'	-9.80	109.04	120.80
1	3A	269	C	N1-C2-O2	9.66	124.70	118.90
3	SA	75	U	N1-C2-O2	9.60	129.52	122.80
3	SA	185	U	N3-C2-O2	-9.60	115.48	122.20
3	SA	75	U	C2-N1-C1'	9.53	129.14	117.70
2	5A	494	C	C6-N1-C2	-9.33	116.57	120.30
3	SA	75	U	N3-C2-O2	-9.25	115.72	122.20
3	SA	767	U	N3-C2-O2	-9.15	115.80	122.20
3	SA	1784	C	N3-C2-O2	-9.14	115.50	121.90
3	SA	658	C	N1-C2-O2	9.09	124.35	118.90
3	SA	1473	U	N3-C2-O2	-8.89	115.97	122.20
26	3H	21	LEU	CA-CB-CG	8.80	135.54	115.30
3	SA	658	C	C2-N1-C1'	8.66	128.33	118.80
3	SA	827	C	C2-N1-C1'	8.63	128.29	118.80
22	3C	306	LEU	CA-CB-CG	8.46	134.76	115.30
4	SC	54	LEU	CA-CB-CG	8.43	134.68	115.30
3	SA	190	C	N3-C2-O2	-8.28	116.10	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	827	C	N1-C2-O2	8.23	123.84	118.90
3	SA	767	U	C2-N1-C1'	8.19	127.52	117.70
1	3A	269	C	C6-N1-C2	-8.12	117.05	120.30
3	SA	767	U	N1-C2-O2	8.10	128.47	122.80
3	SA	827	C	N3-C2-O2	-8.02	116.28	121.90
2	5A	494	C	C5-C6-N1	8.02	125.01	121.00
3	SA	1472	C	C2-N1-C1'	7.99	127.59	118.80
28	A5	25	ASP	CB-CG-OD1	7.98	125.48	118.30
33	AG	383	LEU	CA-CB-CG	7.85	133.36	115.30
3	SA	1533	C	P-O3'-C3'	7.84	129.11	119.70
3	SA	230	C	C5-C6-N1	7.83	124.91	121.00
1	3A	105	C	C2-N1-C1'	7.80	127.39	118.80
3	SA	820	U	C2-N1-C1'	7.73	126.98	117.70
3	SA	287	G	O4'-C1'-N9	7.72	114.38	108.20
22	3B	306	LEU	CA-CB-CG	7.71	133.03	115.30
26	3G	65	LEU	CA-CB-CG	7.68	132.97	115.30
2	5A	494	C	N1-C2-O2	7.59	123.45	118.90
57	RO	519	PRO	N-CA-CB	7.56	112.37	103.30
1	3A	269	C	C5-C6-N1	7.54	124.77	121.00
3	SA	1664	C	C2-N1-C1'	7.53	127.08	118.80
3	SA	648	G	C4-N9-C1'	7.52	136.28	126.50
3	SA	648	G	N3-C4-N9	7.47	130.48	126.00
45	5G	129	ASP	CB-CG-OD1	7.38	124.95	118.30
3	SA	532	U	N3-C2-O2	-7.32	117.08	122.20
40	5B	190	LEU	CA-CB-CG	7.30	132.08	115.30
3	SA	864	U	N1-C2-O2	7.29	127.91	122.80
3	SA	820	U	N1-C2-O2	7.28	127.89	122.80
26	3G	67	LEU	CA-CB-CG	7.23	131.92	115.30
3	SA	185	U	C6-N1-C1'	-7.22	111.10	121.20
3	SA	864	U	C2-N1-C1'	7.19	126.33	117.70
3	SA	139	C	P-O3'-C3'	7.16	128.29	119.70
3	SA	302	U	C2-N1-C1'	7.15	126.28	117.70
3	SA	1472	C	N1-C2-O2	7.11	123.16	118.90
3	SA	136	C	N1-C2-O2	7.10	123.16	118.90
56	RN	522	LEU	CA-CB-CG	7.06	131.55	115.30
3	SA	864	U	N3-C2-O2	-7.04	117.27	122.20
3	SA	1267	G	N3-C4-C5	-7.02	125.09	128.60
1	3A	102	U	N3-C2-O2	-7.01	117.29	122.20
30	A9	452	LEU	CA-CB-CG	7.01	131.43	115.30
3	SA	536	C	N1-C2-O2	6.98	123.09	118.90
3	SA	1451	C	N3-C2-O2	-6.94	117.04	121.90
3	SA	1657	U	C2-N1-C1'	6.93	126.02	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	648	G	C8-N9-C1’	-6.89	118.04	127.00
3	SA	1566	U	N3-C2-O2	-6.88	117.38	122.20
3	SA	1053	G	O5’-P-OP1	-6.88	99.51	105.70
1	3A	314	C	C2-N1-C1’	6.86	126.35	118.80
3	SA	569	C	C6-N1-C2	-6.84	117.56	120.30
28	A5	569	PRO	N-CA-CB	6.82	111.49	103.30
8	SI	118	LEU	CA-CB-CG	6.82	130.98	115.30
3	SA	1784	C	C6-N1-C2	-6.80	117.58	120.30
3	SA	1675	C	N1-C2-O2	6.78	122.97	118.90
1	3A	46	U	N3-C2-O2	-6.78	117.45	122.20
3	SA	773	C	O4’-C1’-N1	6.77	113.62	108.20
1	3A	104	C	C2-N1-C1’	6.77	126.25	118.80
1	3A	269	C	C6-N1-C1’	-6.77	112.68	120.80
2	5A	10	C	N3-C2-O2	-6.74	117.18	121.90
3	SA	784	C	N3-C2-O2	-6.73	117.19	121.90
3	SA	1476	C	C2-N1-C1’	6.73	126.21	118.80
3	SA	747	C	N1-C2-O2	6.73	122.94	118.90
3	SA	1803	G	P-O3’-C3’	6.71	127.75	119.70
3	SA	507	U	C2-N1-C1’	6.70	125.75	117.70
3	SA	1476	C	C6-N1-C2	-6.69	117.62	120.30
3	SA	532	U	N1-C2-O2	6.69	127.48	122.80
3	SA	487	G	C2-N3-C4	6.68	115.24	111.90
1	3A	27	U	N1-C2-O2	6.67	127.47	122.80
3	SA	1267	G	N3-C4-N9	6.66	129.99	126.00
57	RO	141	PRO	N-CA-CB	6.66	111.29	103.30
58	RP	923	PRO	N-CA-CB	6.65	111.28	103.30
3	SA	1267	G	C4-N9-C1’	6.65	135.14	126.50
3	SA	815	G	N3-C4-C5	-6.64	125.28	128.60
1	3A	269	C	N3-C2-O2	-6.63	117.26	121.90
3	SA	1066	C	N3-C2-O2	-6.61	117.27	121.90
3	SA	815	G	C4-N9-C1’	6.61	135.09	126.50
3	SA	258	C	C6-N1-C2	-6.59	117.66	120.30
1	3A	104	C	C6-N1-C2	-6.59	117.66	120.30
3	SA	189	C	C2-N1-C1’	6.58	126.04	118.80
3	SA	658	C	C6-N1-C2	-6.58	117.67	120.30
50	RD	1223	PRO	N-CA-CB	6.57	111.19	103.30
57	RO	110	PRO	N-CA-CB	6.57	111.18	103.30
3	SA	532	U	C2-N1-C1’	6.56	125.57	117.70
2	5A	10	C	N1-C2-O2	6.55	122.83	118.90
24	3E	253	ASP	CB-CG-OD1	6.53	124.18	118.30
3	SA	658	C	N3-C2-O2	-6.52	117.33	121.90
3	SA	1451	C	N1-C2-O2	6.52	122.81	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	1473	U	C6-N1-C1’	-6.52	112.07	121.20
3	SA	1657	U	N1-C2-O2	6.51	127.36	122.80
35	B2	443	LEU	CA-CB-CG	6.51	130.27	115.30
3	SA	136	C	C2-N1-C1’	6.50	125.96	118.80
3	SA	747	C	C2-N1-C1’	6.50	125.95	118.80
26	3H	22	ASP	CB-CG-OD1	6.50	124.15	118.30
3	SA	1216	C	N3-C2-O2	-6.49	117.36	121.90
3	SA	1440	C	C2-N1-C1’	6.47	125.92	118.80
3	SA	1441	C	N3-C2-O2	-6.45	117.38	121.90
2	5A	57	C	C5-C6-N1	6.45	124.22	121.00
3	SA	1784	C	N1-C2-O2	6.44	122.76	118.90
3	SA	189	C	N1-C2-O2	6.42	122.75	118.90
3	SA	453	U	C2-N1-C1’	6.40	125.38	117.70
3	SA	777	C	C2-N1-C1’	6.38	125.82	118.80
1	3A	46	U	N1-C2-O2	6.36	127.25	122.80
3	SA	1664	C	N1-C2-O2	6.36	122.71	118.90
58	RP	707	PRO	N-CA-CB	6.34	110.91	103.30
3	SA	1440	C	C6-N1-C2	-6.33	117.77	120.30
1	3A	27	U	C2-N1-C1’	6.31	125.27	117.70
3	SA	339	C	C2-N1-C1’	6.30	125.73	118.80
32	AF	277	LEU	CA-CB-CG	6.29	129.76	115.30
1	3A	102	U	N1-C2-O2	6.26	127.18	122.80
3	SA	827	C	C6-N1-C2	-6.26	117.80	120.30
3	SA	1441	C	C6-N1-C2	-6.26	117.80	120.30
41	5C	74	LEU	CA-CB-CG	6.25	129.67	115.30
3	SA	230	C	C2-N1-C1’	6.24	125.66	118.80
3	SA	1476	C	C5-C6-N1	6.24	124.12	121.00
3	SA	190	C	C6-N1-C2	-6.24	117.81	120.30
3	SA	1657	U	N3-C2-O2	-6.22	117.84	122.20
3	SA	1472	C	N3-C2-O2	-6.20	117.56	121.90
58	RP	2116	PRO	N-CA-CB	6.20	110.74	103.30
1	3A	105	C	C6-N1-C2	-6.20	117.82	120.30
3	SA	229	U	C2-N1-C1’	6.19	125.13	117.70
3	SA	507	U	N1-C2-O2	6.19	127.13	122.80
1	3A	42	U	C5-C6-N1	6.19	125.79	122.70
3	SA	50	C	C2-N1-C1’	6.18	125.60	118.80
3	SA	176	C	C6-N1-C2	-6.18	117.83	120.30
3	SA	1527	C	C2-N1-C1’	6.16	125.58	118.80
1	3A	248	G	P-O3’-C3’	6.16	127.09	119.70
3	SA	230	C	N1-C2-O2	6.13	122.58	118.90
3	SA	1053	G	C8-N9-C4	-6.13	103.95	106.40
3	SA	815	G	N3-C4-N9	6.12	129.68	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SA	35	U	N3-C2-O2	-6.11	117.92	122.20
3	SA	1473	U	C5-C6-N1	6.11	125.76	122.70
3	SA	75	U	C6-N1-C1'	-6.09	112.67	121.20
3	SA	1448	G	N1-C6-O6	-6.08	116.25	119.90
3	SA	777	C	C6-N1-C2	-6.07	117.87	120.30
58	RP	2092	PRO	N-CA-CB	6.05	110.56	103.30
78	M4	940	LEU	CA-CB-CG	-6.05	101.38	115.30
31	AE	1412	PRO	N-CA-CB	6.05	110.56	103.30
3	SA	262	U	N1-C2-O2	6.04	127.03	122.80
59	RQ	644	PRO	N-CA-CB	6.03	110.54	103.30
1	3A	27	U	N3-C2-O2	-6.03	117.98	122.20
3	SA	487	G	C8-N9-C4	-6.02	103.99	106.40
3	SA	1566	U	N1-C2-O2	6.02	127.02	122.80
41	5C	389	LEU	CA-CB-CG	6.02	129.15	115.30
1	3A	260	U	C2-N1-C1'	6.01	124.92	117.70
58	RP	616	PRO	N-CA-CB	6.01	110.51	103.30
10	SK	118	LEU	CA-CB-CG	6.00	129.11	115.30
3	SA	1448	G	C5-C6-O6	6.00	132.20	128.60
38	BE	756	LEU	CA-CB-CG	6.00	129.10	115.30
38	BE	782	PRO	N-CA-CB	6.00	110.50	103.30
3	SA	1440	C	N1-C2-O2	6.00	122.50	118.90
3	SA	1441	C	N1-C2-O2	5.99	122.50	118.90
58	RP	567	PRO	N-CA-CB	5.98	110.47	103.30
58	RP	629	PRO	N-CA-CB	5.98	110.47	103.30
1	3A	105	C	N1-C2-O2	5.98	122.49	118.90
38	BE	750	PRO	N-CA-CB	5.98	110.47	103.30
31	AE	992	PRO	N-CA-CB	5.97	110.47	103.30
3	SA	873	U	C2-N1-C1'	5.96	124.86	117.70
3	SA	1216	C	C6-N1-C2	-5.96	117.91	120.30
3	SA	820	U	N3-C2-O2	-5.95	118.03	122.20
3	SA	332	U	N1-C2-O2	5.94	126.96	122.80
3	SA	302	U	N1-C2-O2	5.94	126.96	122.80
3	SA	873	U	N1-C2-O2	5.94	126.96	122.80
3	SA	1269	U	N3-C2-O2	-5.93	118.05	122.20
58	RP	718	PRO	N-CA-CB	5.93	110.42	103.30
3	SA	962	C	N3-C2-O2	-5.93	117.75	121.90
1	3A	260	U	N1-C2-O2	5.92	126.94	122.80
58	RP	1089	PRO	N-CA-CB	5.92	110.40	103.30
56	RN	201	PRO	N-CA-CB	5.91	110.39	103.30
3	SA	484	C	P-O3'-C3'	5.91	126.79	119.70
35	B2	785	PRO	N-CA-CB	5.90	110.38	103.30
58	RP	293	PRO	N-CA-CB	5.90	110.38	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	280	U	P-O3'-C3'	5.90	126.78	119.70
3	SA	648	G	N3-C4-C5	-5.89	125.65	128.60
58	RP	1633	PRO	N-CA-CB	5.89	110.37	103.30
3	SA	230	C	C6-N1-C2	-5.89	117.94	120.30
7	SH	171	LYS	C-N-CA	5.89	136.43	121.70
3	SA	773	C	P-O3'-C3'	5.89	126.77	119.70
3	SA	1594	G	P-O3'-C3'	5.89	126.76	119.70
3	SA	1709	C	N3-C2-O2	-5.89	117.78	121.90
63	RZ	658	PRO	N-CA-CB	5.88	110.36	103.30
56	RN	412	PRO	N-CA-CB	5.87	110.35	103.30
50	RD	1205	PRO	N-CA-CB	5.87	110.34	103.30
58	RP	2290	PRO	N-CA-CB	5.87	110.34	103.30
58	RP	1183	PRO	N-CA-CB	5.87	110.34	103.30
58	RP	798	PRO	N-CA-CB	5.85	110.32	103.30
3	SA	302	U	N3-C2-O2	-5.85	118.11	122.20
58	RP	1382	PRO	N-CA-CB	5.84	110.31	103.30
58	RP	268	PRO	N-CA-CB	5.84	110.30	103.30
3	SA	1269	U	C2-N1-C1'	5.83	124.69	117.70
3	SA	1709	C	N1-C2-O2	5.82	122.39	118.90
3	SA	658	C	C6-N1-C1'	-5.82	113.82	120.80
58	RP	676	PRO	N-CA-CB	5.82	110.28	103.30
57	RO	75	PRO	N-CA-CB	5.81	110.28	103.30
58	RP	786	PRO	N-CA-CB	5.81	110.28	103.30
3	SA	1527	C	C6-N1-C2	-5.80	117.98	120.30
39	B6	334	LEU	CA-CB-CG	5.79	128.62	115.30
58	RP	1149	PRO	N-CA-CB	5.79	110.25	103.30
1	3A	248	G	O4'-C1'-N9	5.79	112.83	108.20
3	SA	542	A	P-O3'-C3'	5.79	126.65	119.70
58	RP	1487	PRO	N-CA-CB	5.79	110.24	103.30
3	SA	332	U	N3-C2-O2	-5.78	118.15	122.20
58	RP	954	PRO	N-CA-CB	5.78	110.24	103.30
1	3A	204	U	N3-C2-O2	-5.78	118.15	122.20
3	SA	332	U	C2-N1-C1'	5.78	124.64	117.70
58	RP	936	PRO	N-CA-CB	5.78	110.23	103.30
1	3A	105	C	C5-C6-N1	5.78	123.89	121.00
3	SA	0	U	P-O3'-C3'	5.78	126.63	119.70
31	AE	1252	PRO	N-CA-CB	5.77	110.23	103.30
3	SA	773	C	C2-N1-C1'	-5.77	112.46	118.80
56	RN	400	PRO	N-CA-CB	5.76	110.22	103.30
3	SA	781	U	P-O3'-C3'	5.76	126.61	119.70
58	RP	1322	PRO	N-CA-CB	5.76	110.21	103.30
58	RP	443	PRO	N-CA-CB	5.75	110.21	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	RP	592	PRO	N-CA-CB	5.75	110.20	103.30
3	SA	1472	C	C6-N1-C1’	-5.75	113.90	120.80
58	RP	686	PRO	N-CA-CB	5.75	110.20	103.30
59	RQ	801	PRO	N-CA-CB	5.74	110.19	103.30
3	SA	827	C	C6-N1-C1’	-5.74	113.92	120.80
3	SA	1510	U	N1-C2-O2	5.74	126.82	122.80
2	5A	494	C	N3-C2-O2	-5.74	117.89	121.90
31	AE	890	PRO	N-CA-CB	5.73	110.18	103.30
30	A9	414	PRO	N-CA-CB	5.73	110.18	103.30
57	RO	144	PRO	N-CA-CB	5.73	110.18	103.30
58	RP	511	PRO	N-CA-CB	5.73	110.18	103.30
31	AE	962	PRO	N-CA-CB	5.73	110.18	103.30
58	RP	1116	PRO	N-CA-CB	5.73	110.18	103.30
31	AE	1021	PRO	N-CA-CB	5.73	110.17	103.30
31	AE	1498	PRO	N-CA-CB	5.73	110.17	103.30
58	RP	454	PRO	N-CA-CB	5.73	110.17	103.30
3	SA	487	G	N3-C4-C5	-5.72	125.74	128.60
3	SA	448	C	C6-N1-C2	-5.72	118.01	120.30
28	A5	481	LEU	CA-CB-CG	5.72	128.45	115.30
31	AE	1375	PRO	N-CA-CB	5.72	110.16	103.30
49	5K	146	LEU	CA-CB-CG	5.72	128.45	115.30
3	SA	278	U	P-O3’-C3’	5.71	126.56	119.70
31	AE	1297	PRO	N-CA-CB	5.71	110.15	103.30
1	3A	247	U	C2-N1-C1’	5.71	124.55	117.70
3	SA	1664	C	C6-N1-C1’	-5.70	113.96	120.80
37	B8	521	LEU	CA-CB-CG	5.70	128.40	115.30
58	RP	2287	PRO	N-CA-CB	5.69	110.13	103.30
33	AG	601	LEU	CA-CB-CG	5.69	128.38	115.30
58	RP	1576	PRO	N-CA-CB	5.69	110.13	103.30
57	RO	37	PRO	N-CA-CB	5.69	110.12	103.30
59	RQ	662	PRO	N-CA-CB	5.68	110.11	103.30
31	AE	1283	PRO	N-CA-CB	5.67	110.11	103.30
58	RP	331	PRO	N-CA-CB	5.67	110.11	103.30
58	RP	1016	PRO	N-CA-CB	5.67	110.10	103.30
59	RQ	354	PRO	N-CA-CB	5.67	110.10	103.30
58	RP	1025	PRO	N-CA-CB	5.66	110.09	103.30
58	RP	1102	PRO	N-CA-CB	5.66	110.09	103.30
3	SA	784	C	N1-C2-O2	5.66	122.29	118.90
3	SA	1717	G	C4-N9-C1’	5.66	133.85	126.50
62	RW	26	PRO	N-CA-CB	5.65	110.08	103.30
38	BE	614	LEU	CA-CB-CG	5.64	128.28	115.30
38	BE	909	LEU	CA-CB-CG	5.64	128.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	1733	C	N1-C2-O2	5.64	122.28	118.90
29	A8	637	LEU	CA-CB-CG	5.63	128.26	115.30
3	SA	197	A	O4'-C1'-N9	5.63	112.70	108.20
58	RP	879	PRO	N-CA-CB	5.63	110.06	103.30
3	SA	149	C	C2-N1-C1'	5.63	124.99	118.80
3	SA	908	U	N1-C2-O2	5.63	126.74	122.80
3	SA	281	G	N1-C6-O6	-5.62	116.53	119.90
56	RN	507	LEU	CA-CB-CG	5.62	128.22	115.30
3	SA	262	U	N3-C2-O2	-5.61	118.27	122.20
3	SA	536	C	N3-C2-O2	-5.61	117.97	121.90
31	AE	1600	PRO	N-CA-CB	5.61	110.03	103.30
1	3A	46	U	C2-N1-C1'	5.60	124.42	117.70
36	B3	698	LEU	CA-CB-CG	5.60	128.18	115.30
1	3A	147	C	C5-C6-N1	5.60	123.80	121.00
3	SA	1661	U	N3-C2-O2	-5.60	118.28	122.20
36	B3	525	LEU	CA-CB-CG	5.59	128.15	115.30
53	RH	148	LEU	CA-CB-CG	5.59	128.15	115.30
3	SA	883	C	C6-N1-C2	-5.58	118.07	120.30
50	RD	1514	LEU	CA-CB-CG	5.58	128.13	115.30
58	RP	2242	PRO	N-CA-CB	5.58	109.99	103.30
58	RP	1400	PRO	N-CA-CB	5.58	109.99	103.30
58	RP	1582	PRO	N-CA-CB	5.58	109.99	103.30
3	SA	107	C	C2-N1-C1'	5.57	124.92	118.80
3	SA	686	C	N1-C2-O2	5.57	122.24	118.90
3	SA	536	C	C2-N1-C1'	5.56	124.92	118.80
3	SA	747	C	N3-C2-O2	-5.56	118.01	121.90
3	SA	1440	C	C5-C6-N1	5.56	123.78	121.00
31	AE	1546	PRO	N-CA-CB	5.56	109.97	103.30
58	RP	1346	PRO	N-CA-CB	5.56	109.97	103.30
3	SA	658	C	C5-C6-N1	5.56	123.78	121.00
1	3A	204	U	N1-C2-O2	5.55	126.69	122.80
58	RP	937	PRO	N-CA-CB	5.54	109.95	103.30
31	AE	1371	PRO	N-CA-CB	5.54	109.95	103.30
31	AE	935	PRO	N-CA-CB	5.54	109.94	103.30
53	RG	96	LEU	CA-CB-CG	5.54	128.03	115.30
3	SA	1568	C	P-O3'-C3'	5.53	126.34	119.70
58	RP	771	PRO	N-CA-CB	5.53	109.93	103.30
3	SA	196	G	N1-C6-O6	-5.53	116.58	119.90
31	AE	1376	PRO	N-CA-CB	5.52	109.93	103.30
58	RP	959	PRO	N-CA-CB	5.52	109.93	103.30
58	RP	1592	PRO	N-CA-CB	5.51	109.92	103.30
3	SA	176	C	C6-N1-C1'	5.51	127.41	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	267	U	N3-C2-O2	-5.50	118.35	122.20
37	B8	530	LEU	CA-CB-CG	5.50	127.95	115.30
23	3D	219	LEU	CA-CB-CG	5.50	127.95	115.30
10	SK	128	LEU	CA-CB-CG	5.49	127.92	115.30
33	AG	449	LEU	CA-CB-CG	5.48	127.91	115.30
46	5H	441	PRO	N-CA-CB	5.48	109.88	103.30
3	SA	908	U	N3-C2-O2	-5.48	118.36	122.20
37	B8	449	ASP	CB-CG-OD1	5.48	123.23	118.30
43	5E	314	LEU	CA-CB-CG	5.47	127.89	115.30
3	SA	1510	U	N3-C2-O2	-5.47	118.37	122.20
58	RP	2131	PRO	N-CA-CB	5.47	109.86	103.30
68	R3	360	LEU	CB-CG-CD2	-5.46	101.72	111.00
3	SA	686	C	C2-N1-C1'	5.46	124.80	118.80
27	A4	563	LEU	CA-CB-CG	5.46	127.85	115.30
53	RG	50	LEU	CA-CB-CG	5.44	127.80	115.30
3	SA	1216	C	N1-C2-O2	5.43	122.16	118.90
3	SA	1490	C	N1-C2-O2	5.43	122.16	118.90
1	3A	314	C	C6-N1-C2	-5.42	118.13	120.30
3	SA	211	U	C2-N1-C1'	5.42	124.21	117.70
3	SA	1267	G	C8-N9-C1'	-5.42	119.95	127.00
3	SA	1161	C	C5-C6-N1	5.42	123.71	121.00
1	3A	41	C	C6-N1-C2	-5.41	118.14	120.30
3	SA	75	U	C5-C6-N1	5.40	125.40	122.70
1	3A	147	C	C6-N1-C2	-5.40	118.14	120.30
51	RE	531	LEU	CA-CB-CG	5.39	127.71	115.30
1	3A	311	G	C4-N9-C1'	5.39	133.51	126.50
3	SA	88	U	N3-C2-O2	-5.38	118.44	122.20
41	5C	270	LEU	CA-CB-CG	5.38	127.67	115.30
3	SA	650	U	C5-C6-N1	5.37	125.39	122.70
4	SC	172	LEU	CA-CB-CG	5.37	127.64	115.30
2	5A	479	G	N1-C6-O6	-5.37	116.68	119.90
3	SA	185	U	C5-C6-N1	5.36	125.38	122.70
3	SA	192	U	C2-N1-C1'	5.36	124.14	117.70
58	RP	579	PRO	N-CA-CB	5.36	109.74	103.30
3	SA	901	G	C4-N9-C1'	5.36	133.47	126.50
3	SA	1254	U	N1-C2-O2	5.36	126.55	122.80
3	SA	916	U	N1-C2-O2	5.35	126.55	122.80
3	SA	815	G	C8-N9-C1'	-5.34	120.05	127.00
8	SI	77	LEU	CA-CB-CG	5.34	127.59	115.30
1	3A	104	C	C5-C6-N1	5.32	123.66	121.00
3	SA	777	C	N1-C2-O2	5.31	122.09	118.90
3	SA	1067	C	C6-N1-C2	-5.31	118.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	335	U	P-O3'-C3'	5.30	126.06	119.70
3	SA	482	U	N3-C2-O2	-5.30	118.49	122.20
3	SA	767	U	C6-N1-C1'	-5.30	113.79	121.20
28	A5	51	LEU	CA-CB-CG	5.30	127.48	115.30
3	SA	648	G	C6-C5-N7	-5.28	127.23	130.40
35	B2	551	LEU	CA-CB-CG	5.28	127.44	115.30
3	SA	136	C	N3-C2-O2	-5.28	118.20	121.90
1	3A	308	U	N1-C2-O2	5.28	126.49	122.80
1	3A	44	U	N3-C2-O2	-5.26	118.52	122.20
3	SA	633	U	N3-C2-O2	-5.26	118.52	122.20
31	AE	1391	PRO	N-CA-CB	5.25	109.60	103.30
58	RP	1538	PRO	N-CA-CB	5.25	109.60	103.30
51	RE	1087	LEU	CA-CB-CG	5.25	127.37	115.30
3	SA	1161	C	C6-N1-C2	-5.24	118.21	120.30
3	SA	870	C	C6-N1-C2	-5.23	118.21	120.30
75	R4	171	ASP	CB-CG-OD2	5.23	123.01	118.30
5	SF	193	GLY	N-CA-C	5.23	126.18	113.10
3	SA	453	U	N3-C2-O2	-5.22	118.54	122.20
3	SA	302	U	C5-C6-N1	5.22	125.31	122.70
54	RJ	1021	LEU	CA-CB-CG	5.22	127.31	115.30
3	SA	35	U	N1-C2-O2	5.22	126.45	122.80
3	SA	820	U	C6-N1-C1'	-5.22	113.90	121.20
3	SA	1052	U	O4'-C1'-N1	5.21	112.37	108.20
66	R5	229	LEU	CA-CB-CG	-5.21	103.31	115.30
39	B6	327	LEU	CB-CG-CD1	5.21	119.86	111.00
1	3A	260	U	N3-C2-O2	-5.20	118.56	122.20
51	RE	655	LEU	CA-CB-CG	5.20	127.25	115.30
3	SA	1554	U	N1-C2-O2	5.19	126.43	122.80
3	SA	1646	C	N1-C2-O2	5.19	122.01	118.90
3	SA	916	U	N3-C2-O2	-5.19	118.57	122.20
3	SA	921	U	C2-N1-C1'	5.19	123.92	117.70
3	SA	448	C	C2-N1-C1'	5.18	124.50	118.80
3	SA	1609	U	N3-C2-O2	-5.17	118.58	122.20
75	R4	551	ASP	CB-CG-OD2	5.17	122.95	118.30
3	SA	1783	C	C6-N1-C2	-5.17	118.23	120.30
33	AG	520	LEU	CA-CB-CG	5.17	127.19	115.30
3	SA	196	G	C5-C6-O6	5.17	131.70	128.60
3	SA	309	C	N1-C2-O2	5.17	122.00	118.90
1	3A	107	C	P-O3'-C3'	5.16	125.89	119.70
2	5A	550	C	N1-C2-O2	5.16	122.00	118.90
3	SA	448	C	C5-C6-N1	5.15	123.58	121.00
2	5A	57	C	C6-N1-C2	-5.15	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SA	1267	G	C2-N3-C4	5.15	114.47	111.90
23	3D	40	ASP	CB-CG-OD1	5.14	122.92	118.30
3	SA	873	U	N3-C2-O2	-5.13	118.61	122.20
3	SA	1540	G	N3-C4-C5	-5.13	126.03	128.60
45	5G	209	LEU	CA-CB-CG	5.13	127.10	115.30
1	3A	268	U	N3-C2-O2	-5.12	118.62	122.20
3	SA	331	A	C8-N9-C4	-5.12	103.75	105.80
3	SA	453	U	C5-C6-N1	5.12	125.26	122.70
1	3A	107	C	OP1-P-O3'	5.11	116.44	105.20
1	3A	32	G	C2-N3-C4	5.11	114.45	111.90
3	SA	1440	C	N3-C2-O2	-5.10	118.33	121.90
3	SA	262	U	C2-N1-C1'	5.09	123.81	117.70
1	3A	314	C	C5-C6-N1	5.08	123.54	121.00
61	RT	226	LEU	CA-CB-CG	5.08	126.99	115.30
22	3C	233	LEU	CA-CB-CG	5.08	126.99	115.30
78	M4	440	LEU	CA-CB-CG	5.08	126.98	115.30
3	SA	1510	U	C2-N1-C1'	5.08	123.79	117.70
3	SA	1064	G	C4-N9-C1'	5.07	133.09	126.50
78	M4	919	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	3A	46	U	C5-C6-N1	5.07	125.23	122.70
75	R4	786	LEU	CA-CB-CG	5.07	126.95	115.30
3	SA	1191	U	C2-N1-C1'	5.06	123.77	117.70
31	AE	403	LEU	CA-CB-CG	5.06	126.94	115.30
1	3A	105	C	C6-N1-C1'	-5.06	114.73	120.80
3	SA	280	U	OP2-P-O3'	5.06	116.33	105.20
3	SA	1703	C	N1-C2-O2	5.05	121.93	118.90
31	AE	571	LEU	CA-CB-CG	-5.05	103.69	115.30
51	RE	429	LEU	CA-CB-CG	5.05	126.91	115.30
8	SI	64	VAL	CA-CB-CG1	5.04	118.47	110.90
3	SA	507	U	C6-N1-C1'	-5.04	114.14	121.20
3	SA	575	C	N1-C2-O2	5.03	121.92	118.90
29	A8	637	LEU	CB-CG-CD2	-5.03	102.44	111.00
68	R3	303	ASP	CB-CG-OD1	5.03	122.83	118.30
36	B3	379	LEU	CA-CB-CG	5.03	126.87	115.30
3	SA	1439	C	C6-N1-C2	-5.03	118.29	120.30
58	RP	202	LYS	C-N-CA	5.03	134.27	121.70
3	SA	1594	G	OP2-P-O3'	5.02	116.25	105.20
3	SA	1269	U	N1-C2-O2	5.02	126.32	122.80
3	SA	14	C	N3-C2-O2	-5.02	118.39	121.90
3	SA	1686	C	C6-N1-C2	-5.02	118.29	120.30
3	SA	965	U	C2-N1-C1'	5.01	123.72	117.70
3	SA	1623	C	C6-N1-C2	-5.01	118.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3A	269	C	C2-N3-C4	5.01	122.41	119.90
1	3A	75	C	C6-N1-C2	-5.01	118.30	120.30
3	SA	-5	G	C4-N9-C1'	5.01	133.01	126.50
3	SA	453	U	N1-C2-O2	5.01	126.30	122.80
27	A4	134	LEU	CA-CB-CG	5.00	126.81	115.30
3	SA	1633	A	C4-N9-C1'	5.00	135.30	126.30
3	SA	1706	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (81) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	3F	141	LEU	Peptide
25	3F	173	GLU	Peptide
25	3F	237	ASP	Peptide
26	3G	59	GLU	Peptide
26	3G	9	PHE	Peptide
26	3H	59	GLU	Peptide
40	5B	192	PRO	Peptide
46	5H	576	LEU	Peptide
47	5I	185	ILE	Peptide
47	5I	87	SER	Peptide
49	5K	68	ASP	Peptide
27	A4	353	GLU	Peptide
28	A5	436	THR	Peptide
28	A5	50	PHE	Peptide
29	A8	256	SER	Peptide
29	A8	529	HIS	Peptide
33	AG	119	LEU	Peptide
33	AG	140	LYS	Peptide
33	AG	557	ILE	Peptide
33	AG	780	GLU	Peptide
34	B1	519	LEU	Peptide
34	B1	709	THR	Peptide
35	B2	160	ARG	Peptide
35	B2	552	ASP	Peptide
36	B3	220	ILE	Peptide
36	B3	236	THR	Peptide
36	B3	410	ASN	Peptide
36	B3	437	VAL	Peptide
36	B3	50	ARG	Peptide
36	B3	567	VAL	Peptide

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Mol	Chain	Res	Type	Group
36	B3	594	GLY	Peptide
39	B6	322	LEU	Peptide
39	B6	326	PHE	Peptide
38	BE	591	PHE	Peptide
38	BE	811	LEU	Peptide
38	BE	94	TYR	Peptide
74	C4	149	GLN	Peptide
71	M3	141	LEU	Peptide
71	M3	216	ASP	Peptide
78	M4	541	SER	Peptide
78	M4	573	LYS	Peptide
78	M4	874	GLN	Peptide
67	R1	166	TYR	Peptide
70	R2	136	HIS	Peptide
68	R3	335	ASP	Peptide
68	R3	352	ALA	Peptide
68	R3	54	ILE	Peptide
75	R4	504	PRO	Peptide
69	R6	188	GLU	Peptide
51	RE	1028	ARG	Peptide
51	RE	1094	LYS	Peptide
52	RF	171	PHE	Peptide
54	RJ	948	ILE	Peptide
56	RN	327	GLY	Peptide
57	RO	493	TYR	Peptide
57	RO	53	ARG	Peptide
58	RP	1739	HIS	Peptide
58	RP	1745	ILE	Peptide
58	RP	1907	ASN	Peptide
58	RP	1995	ARG	Peptide
58	RP	2009	LYS	Peptide
58	RP	203	CYS	Peptide
58	RP	2113	ASP	Peptide
58	RP	2114	ASP	Peptide
58	RP	33	ASN	Peptide
59	RQ	728	ARG	Peptide
62	RW	171	GLU	Peptide
63	RZ	1001	SER	Peptide
63	RZ	1069	SER	Peptide
4	SC	16	GLN	Peptide
4	SC	18	LYS	Peptide
5	SF	207	LEU	Peptide

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Mol	Chain	Res	Type	Group
7	SH	147	LEU	Peptide
7	SH	152	ASP	Peptide
8	SI	134	GLU	Peptide
8	SI	64	VAL	Peptide
14	SR	123	ARG	Peptide
17	SX	108	ALA	Peptide
19	SZ	34	ASN	Peptide
20	Sc	49	HIS	Peptide
73	r4	92	ASN	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	240/255 (94%)	210 (88%)	30 (12%)	0	100	100
5	SF	245/261 (94%)	198 (81%)	47 (19%)	0	100	100
6	SG	211/225 (94%)	194 (92%)	17 (8%)	0	100	100
7	SH	178/236 (75%)	159 (89%)	15 (8%)	4 (2%)	6	37
8	SI	161/190 (85%)	137 (85%)	24 (15%)	0	100	100
9	SJ	144/200 (72%)	126 (88%)	18 (12%)	0	100	100
10	SK	172/197 (87%)	154 (90%)	17 (10%)	1 (1%)	25	63
11	SM	135/156 (86%)	117 (87%)	18 (13%)	0	100	100
12	SO	132/151 (87%)	123 (93%)	9 (7%)	0	100	100
13	SP	114/137 (83%)	96 (84%)	18 (16%)	0	100	100
14	SR	123/143 (86%)	110 (89%)	13 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	ST	107/146 (73%)	91 (85%)	16 (15%)	0	100	100
16	SU	136/144 (94%)	123 (90%)	13 (10%)	0	100	100
17	SX	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
18	SY	102/145 (70%)	88 (86%)	14 (14%)	0	100	100
19	SZ	121/135 (90%)	106 (88%)	15 (12%)	0	100	100
20	Sc	78/82 (95%)	66 (85%)	12 (15%)	0	100	100
21	Sd	61/67 (91%)	56 (92%)	5 (8%)	0	100	100
22	3B	238/327 (73%)	215 (90%)	23 (10%)	0	100	100
22	3C	220/327 (67%)	200 (91%)	20 (9%)	0	100	100
23	3D	372/504 (74%)	342 (92%)	30 (8%)	0	100	100
24	3E	433/511 (85%)	392 (90%)	40 (9%)	1 (0%)	47	79
25	3F	431/573 (75%)	394 (91%)	37 (9%)	0	100	100
26	3G	119/126 (94%)	114 (96%)	5 (4%)	0	100	100
26	3H	119/126 (94%)	110 (92%)	9 (8%)	0	100	100
27	A4	643/776 (83%)	568 (88%)	75 (12%)	0	100	100
28	A5	501/643 (78%)	447 (89%)	52 (10%)	2 (0%)	34	71
29	A8	534/713 (75%)	407 (76%)	127 (24%)	0	100	100
30	A9	126/575 (22%)	111 (88%)	15 (12%)	0	100	100
31	AE	1516/1769 (86%)	1374 (91%)	138 (9%)	4 (0%)	41	75
32	AF	483/513 (94%)	440 (91%)	43 (9%)	0	100	100
33	AG	811/896 (90%)	726 (90%)	84 (10%)	1 (0%)	51	84
34	B1	785/900 (87%)	709 (90%)	75 (10%)	1 (0%)	51	84
35	B2	814/943 (86%)	716 (88%)	98 (12%)	0	100	100
36	B3	733/817 (90%)	585 (80%)	147 (20%)	1 (0%)	51	84
37	B8	453/594 (76%)	397 (88%)	56 (12%)	0	100	100
38	BE	886/939 (94%)	804 (91%)	81 (9%)	1 (0%)	51	84
39	B6	369/440 (84%)	341 (92%)	26 (7%)	2 (0%)	29	67
40	5B	56/214 (26%)	51 (91%)	5 (9%)	0	100	100
41	5C	474/554 (86%)	424 (90%)	50 (10%)	0	100	100
42	5D	201/250 (80%)	175 (87%)	26 (13%)	0	100	100
43	5E	205/593 (35%)	187 (91%)	18 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	5F	180/183 (98%)	169 (94%)	11 (6%)	0	100	100
45	5G	237/290 (82%)	215 (91%)	22 (9%)	0	100	100
46	5H	91/610 (15%)	81 (89%)	9 (10%)	1 (1%)	14	51
47	5I	457/489 (94%)	413 (90%)	44 (10%)	0	100	100
48	5J	130/217 (60%)	117 (90%)	13 (10%)	0	100	100
49	5K	148/189 (78%)	134 (90%)	14 (10%)	0	100	100
50	RD	310/1729 (18%)	281 (91%)	25 (8%)	4 (1%)	12	48
51	RE	1080/1237 (87%)	998 (92%)	81 (8%)	1 (0%)	51	84
52	RF	233/297 (78%)	205 (88%)	26 (11%)	2 (1%)	17	55
53	RG	212/252 (84%)	191 (90%)	21 (10%)	0	100	100
53	RH	226/252 (90%)	207 (92%)	19 (8%)	0	100	100
54	RJ	726/1183 (61%)	670 (92%)	56 (8%)	0	100	100
55	RK	358/367 (98%)	332 (93%)	26 (7%)	0	100	100
56	RN	568/810 (70%)	513 (90%)	55 (10%)	0	100	100
57	RO	518/552 (94%)	462 (89%)	50 (10%)	6 (1%)	13	49
58	RP	1948/2493 (78%)	1778 (91%)	156 (8%)	14 (1%)	22	61
59	RQ	333/899 (37%)	287 (86%)	42 (13%)	4 (1%)	13	49
60	RS	247/480 (52%)	224 (91%)	23 (9%)	0	100	100
61	RT	207/326 (64%)	188 (91%)	19 (9%)	0	100	100
62	RW	149/206 (72%)	135 (91%)	13 (9%)	1 (1%)	22	61
63	RZ	831/1267 (66%)	737 (89%)	91 (11%)	3 (0%)	34	71
66	R5	297/305 (97%)	275 (93%)	22 (7%)	0	100	100
67	R1	242/246 (98%)	224 (93%)	18 (7%)	0	100	100
68	R3	332/394 (84%)	304 (92%)	27 (8%)	1 (0%)	41	75
69	R6	222/223 (100%)	209 (94%)	13 (6%)	0	100	100
70	R2	264/265 (100%)	250 (95%)	14 (5%)	0	100	100
71	M3	209/250 (84%)	192 (92%)	17 (8%)	0	100	100
72	R0	235/240 (98%)	216 (92%)	19 (8%)	0	100	100
73	r4	287/359 (80%)	263 (92%)	24 (8%)	0	100	100
74	C4	214/292 (73%)	198 (92%)	16 (8%)	0	100	100
75	R4	942/1001 (94%)	875 (93%)	67 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	r6	404/733 (55%)	367 (91%)	37 (9%)	0	100	100
77	R7	111/184 (60%)	108 (97%)	3 (3%)	0	100	100
78	M4	972/1073 (91%)	908 (93%)	64 (7%)	0	100	100
79	M6	36/186 (19%)	32 (89%)	4 (11%)	0	100	100
All	All	28063/37702 (74%)	25255 (90%)	2753 (10%)	55 (0%)	50	79

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	A5	569	PRO
50	RD	1223	PRO
57	RO	141	PRO
57	RO	519	PRO
58	RP	707	PRO
58	RP	718	PRO
58	RP	922	MET
58	RP	923	PRO
58	RP	925	VAL
58	RP	2115	ALA
59	RQ	257	ILE
59	RQ	353	ASN
63	RZ	583	VAL
63	RZ	676	ILE
63	RZ	682	VAL
33	AG	558	THR
34	B1	710	ILE
52	RF	122	ASN
52	RF	172	TYR
57	RO	110	PRO
58	RP	727	VAL
58	RP	1149	PRO
7	SH	154	ARG
7	SH	173	PRO
31	AE	1370	TYR
58	RP	616	PRO
7	SH	149	LYS
31	AE	1390	ASN
31	AE	1568	GLU
36	B3	71	PRO
39	B6	327	LEU
50	RD	1204	VAL

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Mol	Chain	Res	Type
58	RP	76	THR
58	RP	685	LEU
10	SK	118	LEU
39	B6	328	ASP
46	5H	440	ILE
50	RD	1222	LYS
57	RO	143	PHE
58	RP	1088	LYS
59	RQ	643	GLU
68	R3	337	GLU
58	RP	615	VAL
58	RP	928	ILE
62	RW	26	PRO
24	3E	68	VAL
38	BE	749	ALA
50	RD	1180	VAL
51	RE	1032	PRO
57	RO	28	ILE
28	A5	568	GLU
7	SH	153	VAL
57	RO	140	ALA
31	AE	1448	ILE
59	RQ	354	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	SC	213/224 (95%)	210 (99%)	3 (1%)	67	81
5	SF	199/222 (90%)	197 (99%)	2 (1%)	76	86
6	SG	180/191 (94%)	178 (99%)	2 (1%)	73	85
7	SH	153/201 (76%)	151 (99%)	2 (1%)	69	82
8	SI	146/170 (86%)	144 (99%)	2 (1%)	67	81
9	SJ	122/161 (76%)	118 (97%)	4 (3%)	38	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	SK	150/166 (90%)	149 (99%)	1 (1%)	84	90
11	SM	124/137 (90%)	124 (100%)	0	100	100
12	SO	117/128 (91%)	117 (100%)	0	100	100
13	SP	88/105 (84%)	86 (98%)	2 (2%)	50	70
14	SR	105/119 (88%)	105 (100%)	0	100	100
15	ST	99/129 (77%)	99 (100%)	0	100	100
16	SU	111/116 (96%)	111 (100%)	0	100	100
17	SX	108/111 (97%)	107 (99%)	1 (1%)	78	88
18	SY	86/120 (72%)	86 (100%)	0	100	100
19	SZ	103/113 (91%)	103 (100%)	0	100	100
20	Sc	69/71 (97%)	69 (100%)	0	100	100
21	Sd	56/60 (93%)	55 (98%)	1 (2%)	59	77
22	3B	201/240 (84%)	199 (99%)	2 (1%)	76	86
22	3C	189/240 (79%)	188 (100%)	1 (0%)	88	93
23	3D	322/435 (74%)	320 (99%)	2 (1%)	86	92
24	3E	265/433 (61%)	264 (100%)	1 (0%)	91	94
25	3F	382/503 (76%)	379 (99%)	3 (1%)	81	89
26	3G	100/104 (96%)	99 (99%)	1 (1%)	76	86
26	3H	100/104 (96%)	100 (100%)	0	100	100
27	A4	587/713 (82%)	581 (99%)	6 (1%)	76	86
28	A5	431/574 (75%)	428 (99%)	3 (1%)	84	90
29	A8	174/657 (26%)	173 (99%)	1 (1%)	86	92
30	A9	89/533 (17%)	86 (97%)	3 (3%)	37	61
31	AE	770/1633 (47%)	761 (99%)	9 (1%)	71	84
32	AF	431/454 (95%)	426 (99%)	5 (1%)	71	84
33	AG	750/826 (91%)	748 (100%)	2 (0%)	92	95
34	B1	694/789 (88%)	691 (100%)	3 (0%)	91	94
35	B2	712/832 (86%)	705 (99%)	7 (1%)	76	86
36	B3	659/719 (92%)	655 (99%)	4 (1%)	86	92
37	B8	407/529 (77%)	403 (99%)	4 (1%)	76	86
38	BE	741/819 (90%)	737 (100%)	4 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	B6	323/414 (78%)	319 (99%)	4 (1%)	71	84
40	5B	56/196 (29%)	55 (98%)	1 (2%)	59	77
41	5C	418/480 (87%)	416 (100%)	2 (0%)	88	93
42	5D	198/234 (85%)	197 (100%)	1 (0%)	88	93
43	5E	193/535 (36%)	192 (100%)	1 (0%)	88	93
44	5F	171/172 (99%)	168 (98%)	3 (2%)	59	77
45	5G	214/258 (83%)	213 (100%)	1 (0%)	88	93
46	5H	63/538 (12%)	63 (100%)	0	100	100
47	5I	416/443 (94%)	413 (99%)	3 (1%)	84	90
48	5J	124/200 (62%)	123 (99%)	1 (1%)	81	89
49	5K	133/169 (79%)	133 (100%)	0	100	100
50	RD	226/1544 (15%)	222 (98%)	4 (2%)	59	77
51	RE	994/1125 (88%)	987 (99%)	7 (1%)	84	90
52	RF	221/274 (81%)	220 (100%)	1 (0%)	88	93
53	RG	195/222 (88%)	192 (98%)	3 (2%)	65	80
53	RH	206/222 (93%)	204 (99%)	2 (1%)	76	86
54	RJ	654/1039 (63%)	642 (98%)	12 (2%)	59	77
55	RK	307/312 (98%)	304 (99%)	3 (1%)	76	86
56	RN	435/732 (59%)	431 (99%)	4 (1%)	78	88
57	RO	329/506 (65%)	327 (99%)	2 (1%)	86	92
58	RP	556/2307 (24%)	550 (99%)	6 (1%)	73	85
59	RQ	206/808 (26%)	204 (99%)	2 (1%)	76	86
60	RS	225/421 (53%)	225 (100%)	0	100	100
61	RT	178/282 (63%)	178 (100%)	0	100	100
63	RZ	717/1140 (63%)	712 (99%)	5 (1%)	84	90
66	R5	255/266 (96%)	255 (100%)	0	100	100
67	R1	210/218 (96%)	207 (99%)	3 (1%)	67	81
68	R3	282/349 (81%)	281 (100%)	1 (0%)	91	94
69	R6	196/197 (100%)	196 (100%)	0	100	100
70	R2	237/240 (99%)	237 (100%)	0	100	100
71	M3	181/219 (83%)	180 (99%)	1 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	R0	194/209 (93%)	194 (100%)	0	100	100
73	r4	243/311 (78%)	242 (100%)	1 (0%)	91	94
74	C4	174/240 (72%)	172 (99%)	2 (1%)	73	85
75	R4	812/901 (90%)	808 (100%)	4 (0%)	88	93
76	r6	150/671 (22%)	150 (100%)	0	100	100
77	R7	99/168 (59%)	98 (99%)	1 (1%)	76	86
78	M4	810/953 (85%)	804 (99%)	6 (1%)	84	90
79	M6	25/168 (15%)	25 (100%)	0	100	100
All	All	21859/33364 (66%)	21691 (99%)	168 (1%)	82	89

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	SC	22	ASP
4	SC	59	ASP
4	SC	162	ARG
5	SF	52	LEU
5	SF	81	THR
6	SG	54	LYS
6	SG	125	THR
7	SH	46	LYS
7	SH	214	LYS
8	SI	34	LEU
8	SI	83	LYS
9	SJ	25	ARG
9	SJ	49	ARG
9	SJ	62	THR
9	SJ	200	LYS
10	SK	17	ARG
13	SP	89	THR
13	SP	124	ASP
17	SX	79	PHE
21	Sd	38	ARG
22	3B	233	LEU
22	3B	305	THR
22	3C	297	ARG
23	3D	218	LYS
23	3D	267	ASP
24	3E	370	SER

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Mol	Chain	Res	Type
25	3F	169	LYS
25	3F	225	LYS
25	3F	405	VAL
26	3G	30	LEU
27	A4	45	THR
27	A4	67	LEU
27	A4	231	VAL
27	A4	313	LYS
27	A4	519	THR
27	A4	550	VAL
28	A5	28	ARG
28	A5	194	LEU
28	A5	339	LYS
29	A8	664	LYS
30	A9	457	LYS
30	A9	476	LYS
30	A9	502	ARG
31	AE	132	THR
31	AE	156	LYS
31	AE	197	ASP
31	AE	321	LYS
31	AE	374	ARG
31	AE	404	PHE
31	AE	723	LEU
31	AE	732	PHE
31	AE	1713	LEU
32	AF	95	LEU
32	AF	165	THR
32	AF	199	ARG
32	AF	257	CYS
32	AF	432	TYR
33	AG	336	ARG
33	AG	565	ARG
34	B1	163	THR
34	B1	192	ASP
34	B1	398	ARG
35	B2	75	ARG
35	B2	175	ASP
35	B2	286	ILE
35	B2	333	ARG
35	B2	343	TRP
35	B2	447	LEU

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Mol	Chain	Res	Type
35	B2	576	VAL
36	B3	65	THR
36	B3	466	TRP
36	B3	618	ASN
36	B3	753	HIS
37	B8	282	ASN
37	B8	384	ILE
37	B8	410	ASP
37	B8	542	ARG
38	BE	218	LEU
38	BE	484	ILE
38	BE	510	LEU
38	BE	890	LYS
39	B6	174	PHE
39	B6	299	LYS
39	B6	352	ARG
39	B6	358	LEU
40	5B	188	LYS
41	5C	291	THR
41	5C	442	ILE
42	5D	58	ARG
43	5E	538	LYS
44	5F	5	LEU
44	5F	13	LEU
44	5F	34	ARG
45	5G	116	ARG
47	5I	83	LEU
47	5I	238	THR
47	5I	255	THR
48	5J	119	ARG
50	RD	1466	ARG
50	RD	1503	LYS
50	RD	1565	LYS
50	RD	1685	ARG
51	RE	223	ARG
51	RE	245	LYS
51	RE	288	THR
51	RE	546	THR
51	RE	781	ASP
51	RE	899	LEU
51	RE	1236	THR
52	RF	158	TRP

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Mol	Chain	Res	Type
53	RG	40	ARG
53	RG	95	CYS
53	RG	171	LEU
53	RH	78	LYS
53	RH	118	ARG
54	RJ	92	ARG
54	RJ	113	ARG
54	RJ	114	ARG
54	RJ	214	ARG
54	RJ	230	MET
54	RJ	566	ARG
54	RJ	769	TYR
54	RJ	833	ARG
54	RJ	866	ARG
54	RJ	948	ILE
54	RJ	973	ARG
54	RJ	1033	ARG
55	RK	77	ARG
55	RK	135	TRP
55	RK	171	ASP
56	RN	116	ARG
56	RN	468	ARG
56	RN	486	LYS
56	RN	588	PHE
57	RO	291	THR
57	RO	408	LYS
58	RP	36	LYS
58	RP	114	CYS
58	RP	154	CYS
58	RP	1819	PHE
58	RP	1875	LEU
58	RP	1995	ARG
59	RQ	728	ARG
59	RQ	808	PHE
63	RZ	386	LYS
63	RZ	452	ARG
63	RZ	584	ASP
63	RZ	586	ARG
63	RZ	1109	ARG
67	R1	77	ASN
67	R1	86	ARG
67	R1	225	ARG

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Mol	Chain	Res	Type
68	R3	73	ASN
71	M3	55	ASN
73	r4	212	ASN
74	C4	51	ARG
74	C4	130	ASN
75	R4	29	ASN
75	R4	144	ARG
75	R4	169	ARG
75	R4	775	ASN
77	R7	64	ASN
78	M4	470	ARG
78	M4	530	ARG
78	M4	543	ARG
78	M4	614	ASN
78	M4	642	ASN
78	M4	844	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (291) such sidechains are listed below:

Mol	Chain	Res	Type
4	SC	101	HIS
4	SC	211	HIS
5	SF	142	HIS
6	SG	95	ASN
6	SG	131	GLN
7	SH	176	GLN
7	SH	182	GLN
7	SH	201	GLN
8	SI	174	ASN
8	SI	180	GLN
9	SJ	32	GLN
9	SJ	44	HIS
10	SK	112	GLN
11	SM	8	GLN
11	SM	106	ASN
14	SR	77	GLN
15	ST	71	GLN
17	SX	39	GLN
17	SX	80	ASN
18	SY	99	ASN
19	SZ	29	HIS
19	SZ	107	GLN

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Mol	Chain	Res	Type
20	Sc	9	HIS
20	Sc	19	HIS
22	3B	291	GLN
22	3C	91	HIS
22	3C	216	ASN
22	3C	256	ASN
22	3C	291	GLN
23	3D	24	GLN
23	3D	65	ASN
23	3D	85	ASN
23	3D	172	ASN
23	3D	213	ASN
24	3E	261	GLN
24	3E	286	ASN
25	3F	128	GLN
25	3F	181	ASN
25	3F	226	HIS
25	3F	230	ASN
25	3F	310	ASN
25	3F	321	HIS
25	3F	366	GLN
25	3F	463	GLN
25	3F	471	GLN
25	3F	547	HIS
25	3F	561	ASN
26	3G	32	GLN
26	3G	38	ASN
26	3G	75	ASN
26	3H	5	ASN
26	3H	18	GLN
27	A4	34	HIS
27	A4	108	ASN
27	A4	309	GLN
27	A4	317	ASN
27	A4	359	ASN
27	A4	529	ASN
28	A5	27	GLN
28	A5	168	HIS
28	A5	293	ASN
28	A5	316	ASN
28	A5	333	ASN
28	A5	491	GLN

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Mol	Chain	Res	Type
28	A5	495	GLN
28	A5	499	ASN
29	A8	504	ASN
29	A8	657	ASN
29	A8	677	ASN
30	A9	425	ASN
30	A9	474	HIS
31	AE	14	ASN
31	AE	219	ASN
31	AE	628	ASN
31	AE	634	ASN
31	AE	709	ASN
32	AF	24	GLN
32	AF	44	HIS
32	AF	72	GLN
32	AF	133	HIS
32	AF	217	ASN
32	AF	315	ASN
32	AF	391	ASN
32	AF	403	ASN
32	AF	481	GLN
33	AG	33	ASN
33	AG	50	ASN
33	AG	120	ASN
33	AG	166	ASN
33	AG	169	GLN
33	AG	190	GLN
33	AG	393	ASN
33	AG	439	ASN
33	AG	489	ASN
33	AG	579	ASN
33	AG	606	HIS
34	B1	45	ASN
34	B1	128	ASN
34	B1	421	ASN
34	B1	464	GLN
34	B1	597	ASN
34	B1	707	ASN
34	B1	734	GLN
34	B1	837	ASN
34	B1	842	ASN
35	B2	20	ASN

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Mol	Chain	Res	Type
35	B2	264	ASN
35	B2	327	HIS
35	B2	390	GLN
35	B2	629	ASN
36	B3	210	ASN
36	B3	337	HIS
36	B3	585	ASN
36	B3	616	HIS
36	B3	667	GLN
36	B3	696	ASN
36	B3	757	GLN
36	B3	766	HIS
36	B3	767	HIS
37	B8	159	HIS
37	B8	162	ASN
37	B8	242	ASN
37	B8	282	ASN
37	B8	283	HIS
37	B8	296	GLN
37	B8	310	GLN
37	B8	352	GLN
37	B8	362	HIS
37	B8	381	ASN
37	B8	438	ASN
37	B8	492	ASN
37	B8	593	HIS
38	BE	96	ASN
38	BE	192	ASN
38	BE	421	ASN
38	BE	481	ASN
38	BE	490	GLN
38	BE	532	ASN
38	BE	820	GLN
38	BE	877	ASN
38	BE	903	GLN
39	B6	10	GLN
39	B6	90	GLN
39	B6	287	ASN
39	B6	336	ASN
39	B6	383	GLN
40	5B	207	ASN
40	5B	212	ASN

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Mol	Chain	Res	Type
41	5C	36	GLN
41	5C	101	ASN
41	5C	151	ASN
41	5C	162	ASN
41	5C	251	HIS
41	5C	253	ASN
41	5C	278	ASN
41	5C	394	HIS
41	5C	424	GLN
41	5C	435	ASN
42	5D	102	GLN
42	5D	105	ASN
42	5D	112	GLN
42	5D	206	GLN
43	5E	303	GLN
44	5F	8	HIS
44	5F	59	ASN
44	5F	74	HIS
45	5G	5	GLN
45	5G	181	ASN
46	5H	573	GLN
46	5H	587	GLN
47	5I	20	GLN
47	5I	23	GLN
47	5I	27	ASN
47	5I	46	ASN
47	5I	61	GLN
47	5I	109	HIS
47	5I	134	ASN
47	5I	207	ASN
47	5I	228	ASN
47	5I	242	ASN
47	5I	260	GLN
47	5I	276	ASN
47	5I	293	ASN
47	5I	371	ASN
47	5I	466	HIS
48	5J	118	GLN
48	5J	135	HIS
48	5J	184	ASN
48	5J	195	GLN
49	5K	46	GLN

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Mol	Chain	Res	Type
49	5K	138	ASN
50	RD	1485	GLN
50	RD	1515	ASN
50	RD	1525	ASN
51	RE	261	ASN
51	RE	333	ASN
51	RE	407	ASN
51	RE	414	HIS
51	RE	443	HIS
51	RE	582	GLN
51	RE	588	GLN
51	RE	647	ASN
51	RE	811	GLN
51	RE	1073	ASN
51	RE	1078	HIS
51	RE	1203	ASN
51	RE	1228	ASN
52	RF	57	ASN
52	RF	122	ASN
52	RF	136	ASN
52	RF	148	HIS
52	RF	187	HIS
53	RG	105	ASN
54	RJ	222	ASN
54	RJ	254	HIS
54	RJ	314	GLN
54	RJ	1037	GLN
54	RJ	1074	GLN
55	RK	317	GLN
56	RN	432	HIS
56	RN	467	ASN
56	RN	515	HIS
56	RN	569	GLN
56	RN	631	GLN
56	RN	783	HIS
57	RO	256	ASN
57	RO	260	ASN
57	RO	304	ASN
57	RO	306	GLN
57	RO	331	ASN
57	RO	434	ASN
57	RO	472	HIS

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Mol	Chain	Res	Type
58	RP	33	ASN
58	RP	112	GLN
58	RP	1787	ASN
58	RP	1865	ASN
58	RP	1957	GLN
59	RQ	303	GLN
59	RQ	876	GLN
60	RS	269	ASN
60	RS	290	ASN
60	RS	300	ASN
60	RS	426	GLN
61	RT	127	GLN
61	RT	142	ASN
63	RZ	385	GLN
63	RZ	794	GLN
63	RZ	884	GLN
63	RZ	1114	ASN
63	RZ	1232	ASN
67	R1	30	ASN
67	R1	64	GLN
67	R1	77	ASN
68	R3	73	ASN
68	R3	153	GLN
68	R3	239	GLN
68	R3	287	ASN
69	R6	81	HIS
69	R6	216	ASN
70	R2	150	ASN
70	R2	183	ASN
70	R2	219	ASN
71	M3	55	ASN
71	M3	235	ASN
73	r4	212	ASN
75	R4	29	ASN
75	R4	170	ASN
75	R4	197	ASN
75	R4	555	HIS
75	R4	775	ASN
75	R4	855	HIS
75	R4	857	GLN
76	r6	83	ASN
76	r6	604	GLN

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Mol	Chain	Res	Type
76	r6	612	ASN
77	R7	64	ASN
77	R7	95	ASN
77	R7	113	ASN
78	M4	191	ASN
78	M4	445	ASN
78	M4	475	HIS
78	M4	539	GLN
78	M4	588	ASN
78	M4	614	ASN
78	M4	669	ASN
78	M4	786	GLN
78	M4	832	ASN
78	M4	874	GLN
78	M4	929	ASN
78	M4	946	GLN
78	M4	1043	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3A	202/333 (60%)	78 (38%)	4 (1%)
2	5A	110/700 (15%)	42 (38%)	0
3	SA	1315/1812 (72%)	510 (38%)	20 (1%)
All	All	1627/2845 (57%)	630 (38%)	24 (1%)

All (630) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3A	3	C
1	3A	4	G
1	3A	23	U
1	3A	24	U
1	3A	25	U
1	3A	28	A
1	3A	30	A
1	3A	31	G
1	3A	33	A
1	3A	34	A
1	3A	35	U
1	3A	36	C

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Mol	Chain	Res	Type
1	3A	38	U
1	3A	46	U
1	3A	48	A
1	3A	49	C
1	3A	51	C
1	3A	52	U
1	3A	53	U
1	3A	72	C
1	3A	80	U
1	3A	81	U
1	3A	82	G
1	3A	87	G
1	3A	90	C
1	3A	91	C
1	3A	101	G
1	3A	103	A
1	3A	104	C
1	3A	105	C
1	3A	107	C
1	3A	108	A
1	3A	109	G
1	3A	111	G
1	3A	115	G
1	3A	116	A
1	3A	118	A
1	3A	141	U
1	3A	144	G
1	3A	147	C
1	3A	160	G
1	3A	163	U
1	3A	165	G
1	3A	199	G
1	3A	203	U
1	3A	206	C
1	3A	207	A
1	3A	243	U
1	3A	244	U
1	3A	245	U
1	3A	246	A
1	3A	247	U
1	3A	248	G
1	3A	249	G

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Mol	Chain	Res	Type
1	3A	252	C
1	3A	254	A
1	3A	256	G
1	3A	261	U
1	3A	262	G
1	3A	263	A
1	3A	265	C
1	3A	266	C
1	3A	267	A
1	3A	272	A
1	3A	290	G
1	3A	296	G
1	3A	305	G
1	3A	307	G
1	3A	309	G
1	3A	310	G
1	3A	311	G
1	3A	312	U
1	3A	314	C
1	3A	319	G
1	3A	322	A
1	3A	324	U
1	3A	325	C
1	3A	329	C
2	5A	7	A
2	5A	8	A
2	5A	9	G
2	5A	10	C
2	5A	11	A
2	5A	14	U
2	5A	15	G
2	5A	16	A
2	5A	58	U
2	5A	61	U
2	5A	64	U
2	5A	70	A
2	5A	82	A
2	5A	83	U
2	5A	84	G
2	5A	85	G
2	5A	86	C
2	5A	89	C

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Mol	Chain	Res	Type
2	5A	90	G
2	5A	91	U
2	5A	279	A
2	5A	280	A
2	5A	281	G
2	5A	468	A
2	5A	470	U
2	5A	471	C
2	5A	481	U
2	5A	482	A
2	5A	483	U
2	5A	495	G
2	5A	497	A
2	5A	534	A
2	5A	539	A
2	5A	540	U
2	5A	541	U
2	5A	544	C
2	5A	546	G
2	5A	548	A
2	5A	552	G
2	5A	585	C
2	5A	586	A
2	5A	590	G
3	SA	-5	G
3	SA	-4	A
3	SA	-3	U
3	SA	-1	G
3	SA	0	U
3	SA	1	U
3	SA	5	U
3	SA	6	G
3	SA	17	C
3	SA	18	C
3	SA	20	G
3	SA	21	U
3	SA	22	A
3	SA	23	G
3	SA	25	C
3	SA	26	A
3	SA	34	G
3	SA	40	A

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Mol	Chain	Res	Type
3	SA	42	G
3	SA	43	A
3	SA	44	U
3	SA	45	U
3	SA	46	A
3	SA	47	A
3	SA	57	G
3	SA	60	U
3	SA	66	U
3	SA	68	A
3	SA	69	G
3	SA	72	A
3	SA	73	U
3	SA	74	U
3	SA	76	A
3	SA	81	G
3	SA	104	A
3	SA	107	C
3	SA	108	A
3	SA	109	G
3	SA	114	C
3	SA	115	G
3	SA	116	U
3	SA	117	U
3	SA	125	U
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	132	U
3	SA	133	U
3	SA	134	U
3	SA	135	A
3	SA	136	C
3	SA	137	U
3	SA	138	A
3	SA	140	A
3	SA	145	A
3	SA	146	U
3	SA	153	G

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Mol	Chain	Res	Type
3	SA	155	U
3	SA	156	A
3	SA	162	A
3	SA	169	A
3	SA	170	U
3	SA	176	C
3	SA	177	U
3	SA	178	U
3	SA	179	A
3	SA	180	A
3	SA	181	A
3	SA	182	A
3	SA	184	C
3	SA	185	U
3	SA	186	C
3	SA	187	G
3	SA	189	C
3	SA	191	C
3	SA	192	U
3	SA	194	U
3	SA	195	G
3	SA	196	G
3	SA	200	A
3	SA	202	A
3	SA	203	U
3	SA	204	G
3	SA	211	U
3	SA	215	A
3	SA	231	U
3	SA	232	U
3	SA	233	C
3	SA	234	G
3	SA	235	G
3	SA	238	U
3	SA	239	C
3	SA	240	U
3	SA	241	U
3	SA	242	U
3	SA	248	U
3	SA	249	U
3	SA	250	C
3	SA	256	A

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Mol	Chain	Res	Type
3	SA	259	U
3	SA	260	U
3	SA	261	U
3	SA	262	U
3	SA	265	A
3	SA	267	U
3	SA	271	A
3	SA	272	U
3	SA	276	C
3	SA	278	U
3	SA	279	G
3	SA	280	U
3	SA	281	G
3	SA	288	A
3	SA	302	U
3	SA	306	U
3	SA	313	U
3	SA	314	C
3	SA	316	A
3	SA	320	U
3	SA	321	C
3	SA	322	G
3	SA	323	A
3	SA	331	A
3	SA	332	U
3	SA	333	A
3	SA	336	G
3	SA	337	G
3	SA	351	C
3	SA	352	A
3	SA	354	C
3	SA	426	G
3	SA	430	G
3	SA	433	C
3	SA	435	C
3	SA	437	A
3	SA	438	A
3	SA	439	U
3	SA	440	U
3	SA	444	C
3	SA	445	A
3	SA	448	C

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Mol	Chain	Res	Type
3	SA	452	A
3	SA	453	U
3	SA	454	U
3	SA	468	A
3	SA	471	A
3	SA	475	A
3	SA	477	A
3	SA	484	C
3	SA	485	A
3	SA	487	G
3	SA	488	G
3	SA	492	A
3	SA	493	U
3	SA	494	U
3	SA	495	C
3	SA	496	G
3	SA	499	U
3	SA	500	C
3	SA	501	U
3	SA	504	U
3	SA	505	A
3	SA	507	U
3	SA	508	U
3	SA	510	G
3	SA	513	U
3	SA	514	G
3	SA	515	A
3	SA	516	G
3	SA	519	C
3	SA	525	A
3	SA	532	U
3	SA	534	A
3	SA	539	G
3	SA	540	G
3	SA	541	A
3	SA	542	A
3	SA	543	C
3	SA	544	A
3	SA	545	A
3	SA	548	G
3	SA	551	G
3	SA	552	G

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Mol	Chain	Res	Type
3	SA	563	U
3	SA	564	G
3	SA	565	C
3	SA	570	A
3	SA	572	C
3	SA	573	C
3	SA	574	G
3	SA	575	C
3	SA	579	A
3	SA	580	A
3	SA	582	U
3	SA	583	C
3	SA	584	C
3	SA	585	A
3	SA	587	C
3	SA	594	A
3	SA	595	G
3	SA	601	A
3	SA	602	U
3	SA	603	U
3	SA	623	A
3	SA	624	G
3	SA	635	A
3	SA	638	U
3	SA	648	G
3	SA	649	U
3	SA	658	C
3	SA	667	U
3	SA	670	U
3	SA	674	C
3	SA	686	C
3	SA	687	G
3	SA	690	G
3	SA	694	U
3	SA	695	U
3	SA	696	C
3	SA	697	C
3	SA	698	U
3	SA	699	U
3	SA	700	C
3	SA	702	G
3	SA	744	U

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Mol	Chain	Res	Type
3	SA	746	A
3	SA	747	C
3	SA	748	U
3	SA	749	U
3	SA	750	U
3	SA	751	G
3	SA	752	A
3	SA	754	A
3	SA	755	A
3	SA	756	A
3	SA	757	A
3	SA	758	U
3	SA	759	U
3	SA	760	A
3	SA	763	G
3	SA	765	G
3	SA	766	U
3	SA	771	A
3	SA	772	G
3	SA	773	C
3	SA	774	A
3	SA	775	G
3	SA	778	G
3	SA	779	U
3	SA	780	A
3	SA	781	U
3	SA	782	U
3	SA	783	G
3	SA	784	C
3	SA	785	U
3	SA	787	G
3	SA	789	A
3	SA	790	U
3	SA	791	A
3	SA	792	U
3	SA	794	U
3	SA	795	U
3	SA	796	A
3	SA	797	G
3	SA	798	C
3	SA	802	G
3	SA	803	A

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Mol	Chain	Res	Type
3	SA	804	A
3	SA	811	A
3	SA	812	A
3	SA	813	U
3	SA	815	G
3	SA	816	G
3	SA	820	U
3	SA	821	U
3	SA	822	U
3	SA	827	C
3	SA	828	U
3	SA	842	C
3	SA	850	A
3	SA	858	G
3	SA	859	A
3	SA	860	U
3	SA	862	A
3	SA	863	A
3	SA	864	U
3	SA	865	A
3	SA	873	U
3	SA	875	G
3	SA	876	G
3	SA	881	A
3	SA	898	A
3	SA	906	A
3	SA	912	U
3	SA	913	G
3	SA	914	G
3	SA	921	U
3	SA	928	U
3	SA	929	A
3	SA	931	C
3	SA	933	A
3	SA	935	U
3	SA	944	A
3	SA	951	A
3	SA	960	U
3	SA	966	A
3	SA	969	C
3	SA	1039	A
3	SA	1052	U

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Mol	Chain	Res	Type
3	SA	1053	G
3	SA	1056	U
3	SA	1057	U
3	SA	1058	U
3	SA	1059	U
3	SA	1060	U
3	SA	1063	U
3	SA	1064	G
3	SA	1076	A
3	SA	1114	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	1133	A
3	SA	1134	C
3	SA	1135	U
3	SA	1136	U
3	SA	1140	G
3	SA	1144	U
3	SA	1145	U
3	SA	1146	G
3	SA	1158	C
3	SA	1164	G
3	SA	1176	G
3	SA	1178	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	1204	A
3	SA	1205	C

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Mol	Chain	Res	Type
3	SA	1206	U
3	SA	1210	C
3	SA	1211	A
3	SA	1212	G
3	SA	1213	G
3	SA	1216	C
3	SA	1217	A
3	SA	1218	G
3	SA	1219	A
3	SA	1220	C
3	SA	1223	A
3	SA	1228	G
3	SA	1229	G
3	SA	1233	G
3	SA	1235	C
3	SA	1236	A
3	SA	1252	C
3	SA	1254	U
3	SA	1256	A
3	SA	1257	U
3	SA	1258	U
3	SA	1259	U
3	SA	1260	U
3	SA	1262	U
3	SA	1263	G
3	SA	1264	G
3	SA	1266	U
3	SA	1267	G
3	SA	1268	G
3	SA	1269	U
3	SA	1270	G
3	SA	1272	U
3	SA	1273	G
3	SA	1274	C
3	SA	1435	G
3	SA	1436	A
3	SA	1437	U
3	SA	1441	C
3	SA	1443	U
3	SA	1453	G
3	SA	1454	G
3	SA	1470	C

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Mol	Chain	Res	Type
3	SA	1471	A
3	SA	1472	C
3	SA	1473	U
3	SA	1474	G
3	SA	1476	C
3	SA	1483	A
3	SA	1488	G
3	SA	1489	U
3	SA	1490	C
3	SA	1491	U
3	SA	1492	A
3	SA	1493	A
3	SA	1506	G
3	SA	1525	A
3	SA	1534	G
3	SA	1535	U
3	SA	1537	C
3	SA	1538	U
3	SA	1539	G
3	SA	1540	G
3	SA	1542	G
3	SA	1553	G
3	SA	1554	U
3	SA	1555	A
3	SA	1556	A
3	SA	1557	U
3	SA	1558	U
3	SA	1559	A
3	SA	1560	U
3	SA	1569	A
3	SA	1573	A
3	SA	1574	G
3	SA	1577	A
3	SA	1584	G
3	SA	1590	G
3	SA	1595	U
3	SA	1596	C
3	SA	1600	A
3	SA	1601	G
3	SA	1602	C
3	SA	1607	G
3	SA	1614	A

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Mol	Chain	Res	Type
3	SA	1618	C
3	SA	1619	C
3	SA	1622	G
3	SA	1628	U
3	SA	1630	U
3	SA	1631	A
3	SA	1633	A
3	SA	1639	C
3	SA	1640	C
3	SA	1651	A
3	SA	1654	G
3	SA	1655	A
3	SA	1656	U
3	SA	1657	U
3	SA	1658	G
3	SA	1662	G
3	SA	1663	G
3	SA	1676	U
3	SA	1679	G
3	SA	1680	G
3	SA	1681	A
3	SA	1682	U
3	SA	1683	C
3	SA	1689	A
3	SA	1697	G
3	SA	1698	G
3	SA	1700	C
3	SA	1701	A
3	SA	1703	C
3	SA	1704	U
3	SA	1707	A
3	SA	1708	U
3	SA	1709	C
3	SA	1710	U
3	SA	1711	C
3	SA	1712	A
3	SA	1713	G
3	SA	1717	G
3	SA	1718	G
3	SA	1719	A
3	SA	1724	U
3	SA	1725	U

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Mol	Chain	Res	Type
3	SA	1726	G
3	SA	1727	G
3	SA	1728	A
3	SA	1731	A
3	SA	1734	U
3	SA	1736	G
3	SA	1737	G
3	SA	1738	U
3	SA	1742	U
3	SA	1743	U
3	SA	1744	A
3	SA	1746	A
3	SA	1749	A
3	SA	1753	A
3	SA	1754	A
3	SA	1755	A
3	SA	1778	G
3	SA	1790	A
3	SA	1791	A
3	SA	1792	G
3	SA	1793	G
3	SA	1794	A
3	SA	1795	U
3	SA	1796	C
3	SA	1799	U
3	SA	1800	A
3	SA	1801	A
3	SA	1802	A
3	SA	1803	G
3	SA	1804	A

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3A	24	U
1	3A	102	U
1	3A	107	C
1	3A	248	G
3	SA	0	U
3	SA	68	A
3	SA	136	C
3	SA	139	C

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Mol	Chain	Res	Type
3	SA	278	U
3	SA	280	U
3	SA	335	U
3	SA	484	C
3	SA	503	G
3	SA	542	A
3	SA	773	C
3	SA	781	U
3	SA	1052	U
3	SA	1063	U
3	SA	1490	C
3	SA	1533	C
3	SA	1568	C
3	SA	1594	G
3	SA	1754	A
3	SA	1803	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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
81	GTP	RJ	1201	82	26,34,34	1.20	1 (3%)	32,54,54	1.70	7 (21%)
83	ADP	RZ	1301	-	24,29,29	0.96	1 (4%)	29,45,45	1.37	4 (13%)

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
81	GTP	RJ	1201	82	-	5/18/38/38	0/3/3/3
83	ADP	RZ	1301	-	-	4/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	RJ	1201	GTP	C5-C6	-4.23	1.38	1.47
83	RZ	1301	ADP	C5-C4	2.45	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	RJ	1201	GTP	PA-O3A-PB	-4.49	117.41	132.83
81	RJ	1201	GTP	PB-O3B-PG	-4.12	118.69	132.83
83	RZ	1301	ADP	N3-C2-N1	-3.40	123.36	128.68
81	RJ	1201	GTP	C5-C6-N1	3.36	119.88	113.95
81	RJ	1201	GTP	C8-N7-C5	3.10	108.89	102.99
83	RZ	1301	ADP	C3'-C2'-C1'	3.02	105.52	100.98
81	RJ	1201	GTP	C2-N1-C6	-2.97	119.63	125.10
83	RZ	1301	ADP	C4-C5-N7	-2.93	106.35	109.40
81	RJ	1201	GTP	C3'-C2'-C1'	2.75	105.12	100.98
83	RZ	1301	ADP	PA-O3A-PB	-2.26	125.06	132.83
81	RJ	1201	GTP	O6-C6-C5	-2.00	120.46	124.37

There are no chirality outliers.

All (9) torsion outliers are listed below:

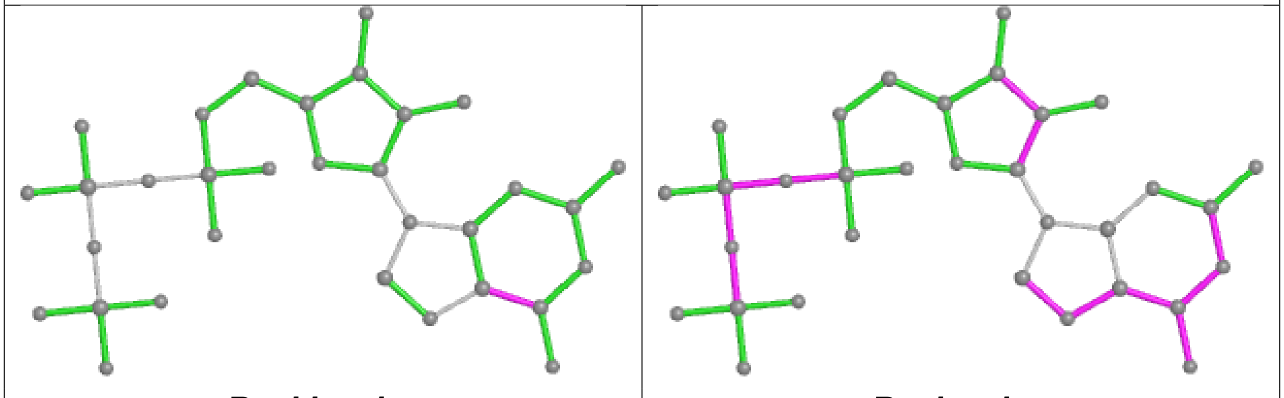
Mol	Chain	Res	Type	Atoms
83	RZ	1301	ADP	C5'-O5'-PA-O2A
83	RZ	1301	ADP	C5'-O5'-PA-O3A
81	RJ	1201	GTP	O4'-C4'-C5'-O5'
81	RJ	1201	GTP	C3'-C4'-C5'-O5'
81	RJ	1201	GTP	PA-O3A-PB-O2B
83	RZ	1301	ADP	O4'-C4'-C5'-O5'
81	RJ	1201	GTP	PG-O3B-PB-O2B
83	RZ	1301	ADP	C3'-C4'-C5'-O5'
81	RJ	1201	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

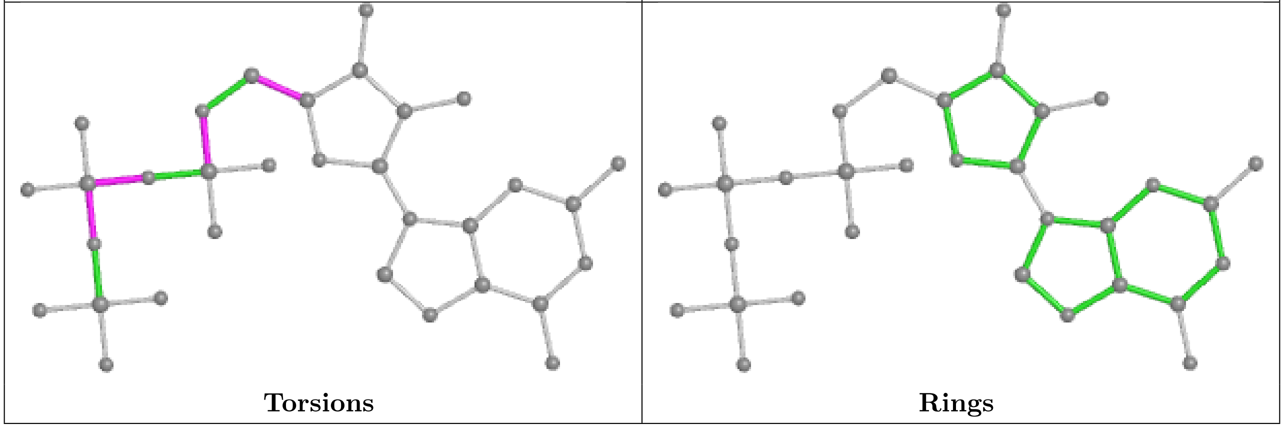
No monomer is involved in short contacts.

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

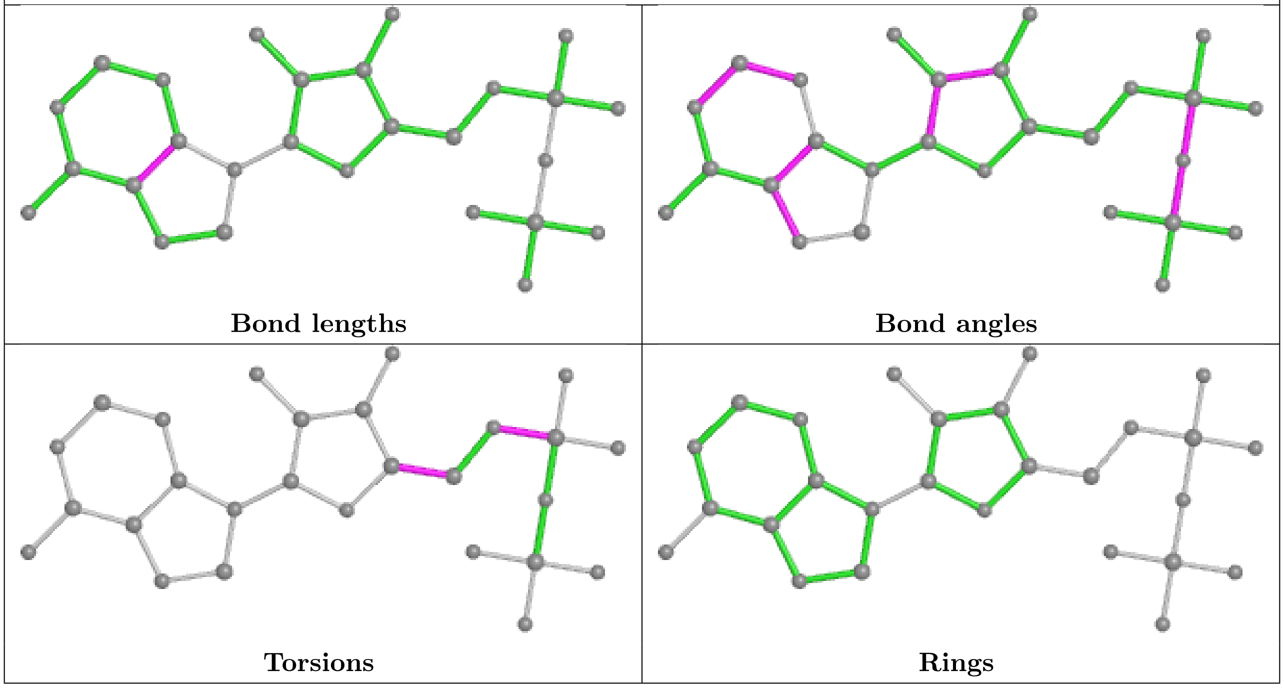


Bond lengths **Bond angles**



Torsions **Rings**

Ligand ADP RZ 1301



Bond lengths

Bond angles

Torsions

Rings

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.

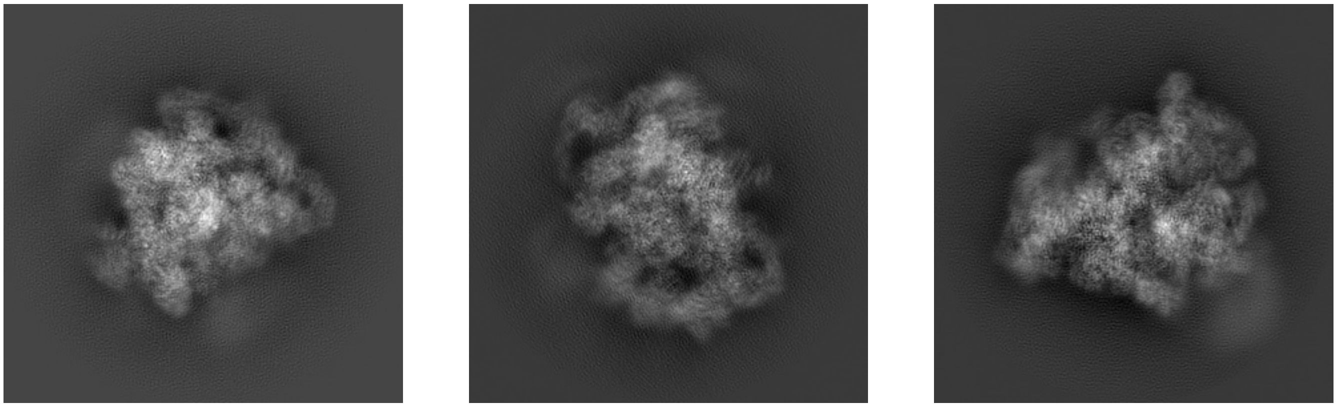
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30574. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

6.1.1 Primary map

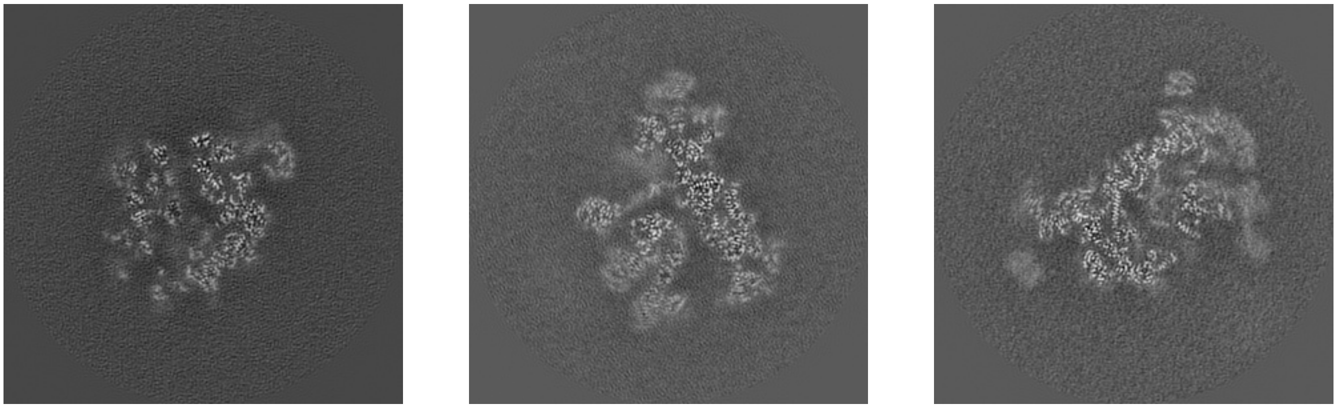


X Y Z

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

6.2 Central slices

6.2.1 Primary map

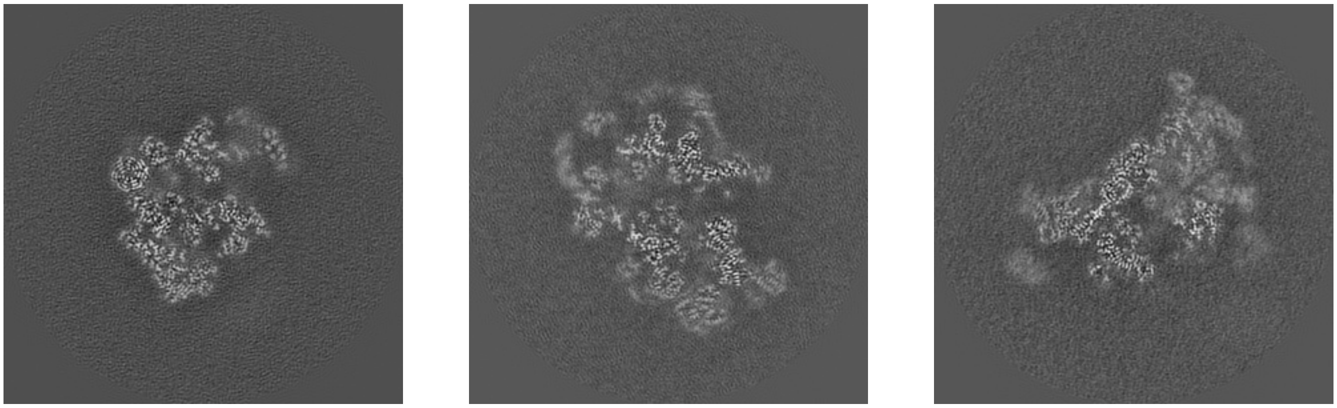


X Index: 200 Y Index: 200 Z Index: 200

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

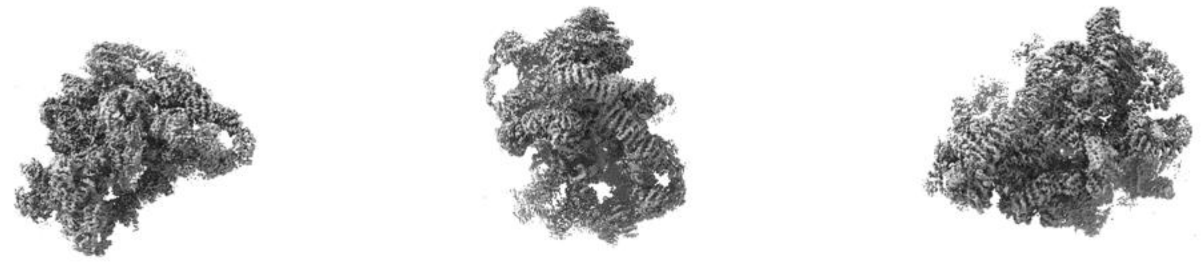


X Index: 186 Y Index: 178 Z Index: 192

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

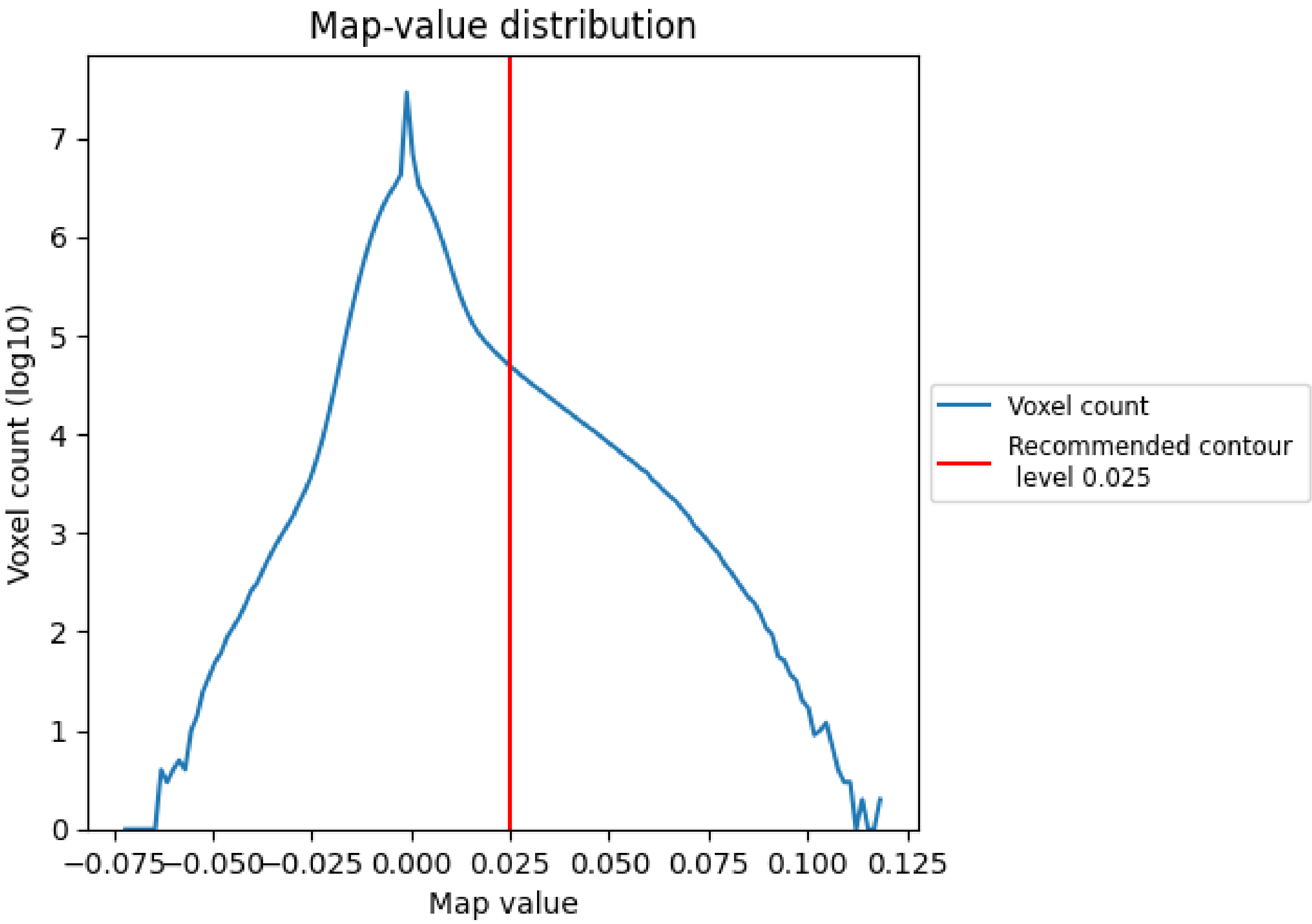
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

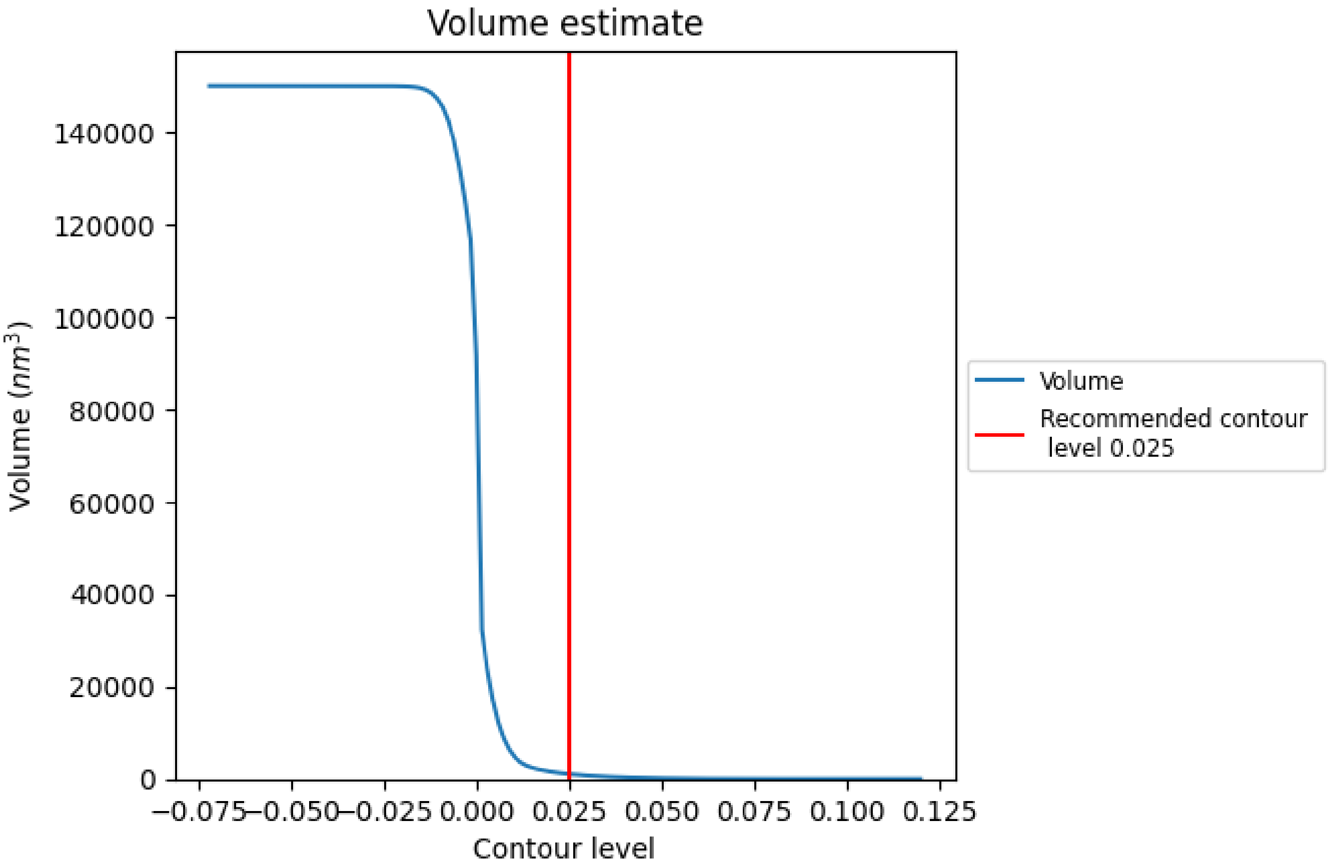
This section contains the results of statistical analysis of the map.

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.

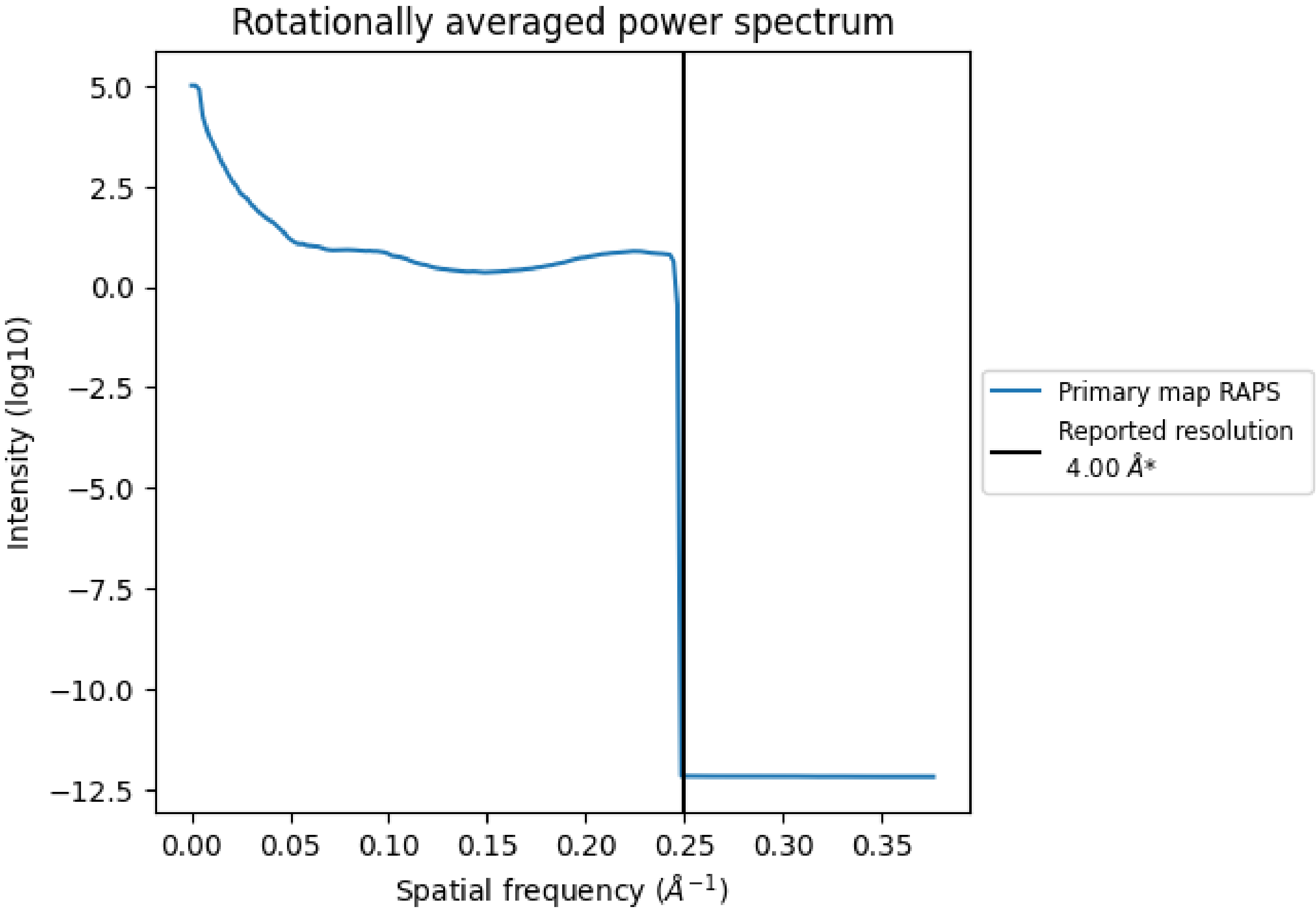
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1074 nm^3; this corresponds to an approximate mass of 970 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 0.250 Å^{-1}

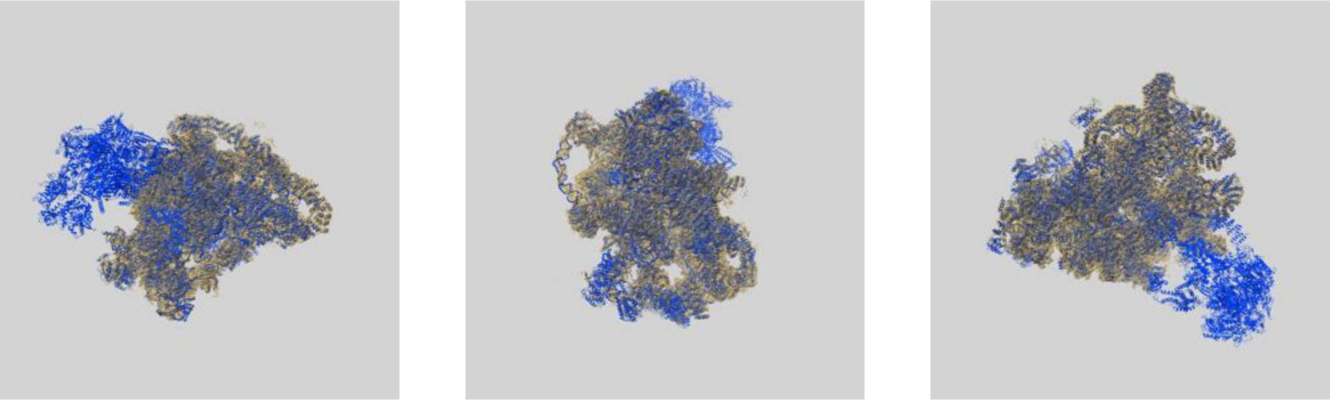
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30574 and PDB model 7D4I. Per-residue inclusion information can be found in section 3 on page 20.

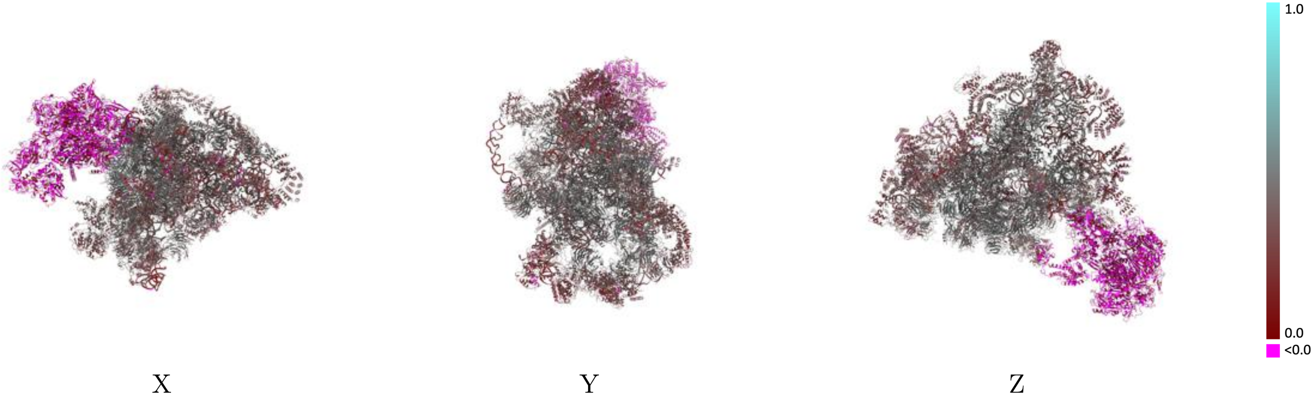
9.1 Map-model overlay (i)



X Y Z

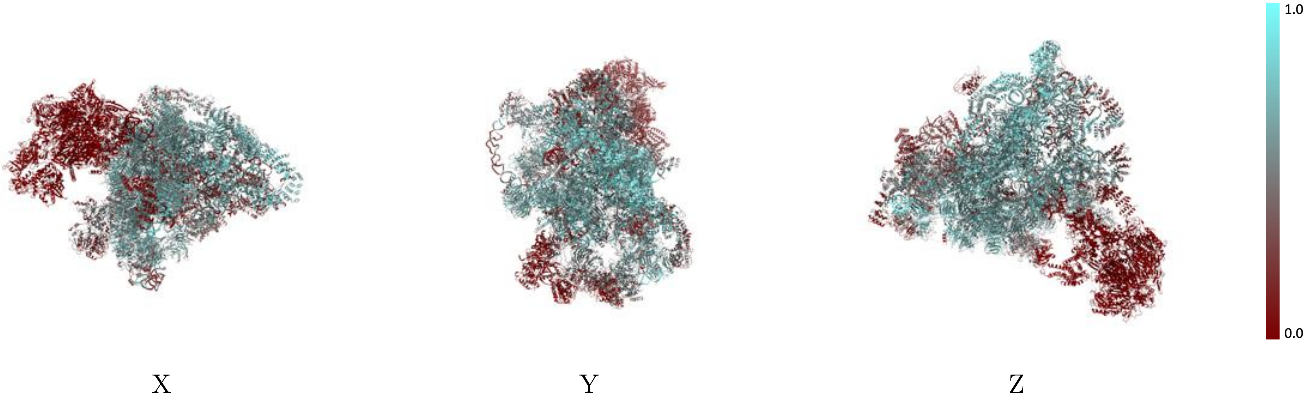
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



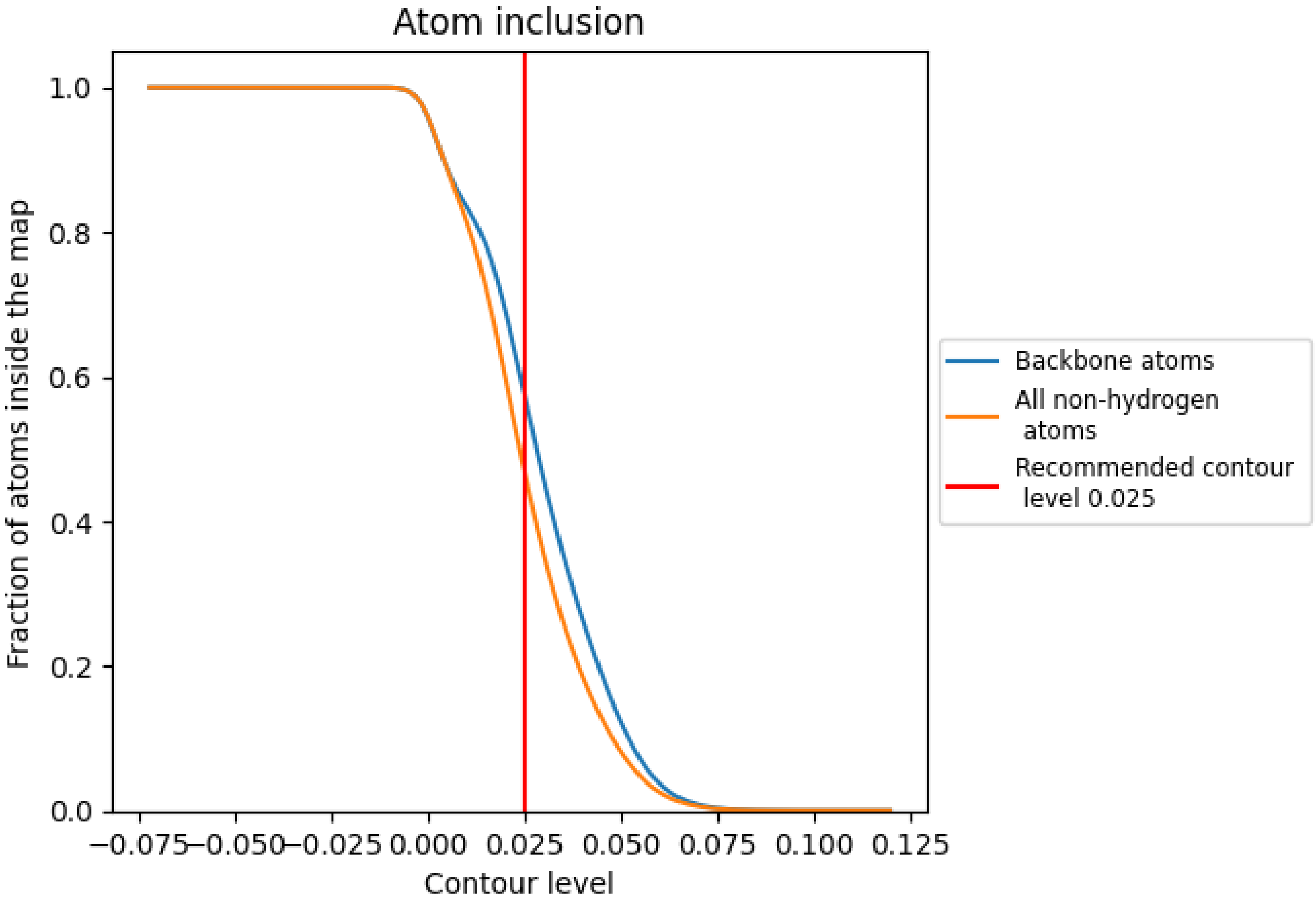
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 58% of all backbone atoms, 47% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4723	0.3390
3A	0.6875	0.3800
3B	0.7032	0.4820
3C	0.6511	0.4460
3D	0.6824	0.4450
3E	0.6469	0.4270
3F	0.6890	0.4600
3G	0.6460	0.4550
3H	0.6858	0.4620
5A	0.4290	0.2980
5B	0.4732	0.4040
5C	0.6099	0.4530
5D	0.5588	0.4350
5E	0.5352	0.4230
5F	0.4976	0.4190
5G	0.6040	0.4550
5H	0.6422	0.4620
5I	0.6999	0.4760
5J	0.5669	0.4540
5K	0.6692	0.4760
A4	0.6528	0.4270
A5	0.5791	0.4240
A8	0.1932	0.3060
A9	0.4449	0.3310
AE	0.5486	0.3640
AF	0.5387	0.4190
AG	0.5808	0.4120
B1	0.6430	0.4640
B2	0.6441	0.4170
B3	0.6321	0.4210
B6	0.6328	0.4130
B8	0.6833	0.4570
BE	0.6634	0.4540
C4	0.0000	0.0140
M3	0.0000	0.0020

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Chain	Atom inclusion	Q-score
M4	0.0000	0.0070
M6	0.0000	-0.0180
R0	0.0000	0.0240
R1	0.0000	-0.0040
R2	0.0000	-0.0020
R3	0.0000	-0.0050
R4	0.0000	-0.0040
R5	0.0000	-0.0020
R6	0.0000	0.0200
R7	0.0000	-0.0180
RD	0.0438	0.2830
RE	0.5242	0.3780
RF	0.4603	0.3590
RG	0.1548	0.3120
RH	0.2784	0.3730
RJ	0.6415	0.4430
RK	0.6323	0.4350
RN	0.1619	0.3150
RO	0.2538	0.3260
RP	0.5767	0.3540
RQ	0.4825	0.4150
RS	0.0673	0.2410
RT	0.5494	0.4390
RW	0.5617	0.3770
RZ	0.3569	0.3490
SA	0.6215	0.3510
SC	0.6416	0.4550
SF	0.5579	0.4330
SG	0.6223	0.4540
SH	0.2821	0.3650
SI	0.4954	0.3850
SJ	0.2726	0.3480
SK	0.6779	0.4600
SM	0.1885	0.3280
SO	0.6663	0.4340
SP	0.6449	0.4560
SR	0.6688	0.4730
ST	0.3580	0.3880
SU	0.4626	0.4250
SX	0.6487	0.4510
SY	0.6184	0.4530
SZ	0.6587	0.4520

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Chain	Atom inclusion	Q-score
Sc	0.6706	0.4620
Sd	0.6625	0.4830
X1	0.4407	0.3940
X2	0.1574	0.3330
r4	0.0000	0.0010
r6	0.0000	0.0010