wwPDB EM Validation Summary Report (i)

Apr 23, 2024 – 02:12 pm BST

PDB ID	:	7AJU
EMDB ID	:	EMD-11808
Title	:	Cryo-EM structure of the 90S-exosome super-complex (state Post-A1-exosome)
Authors	:	Cheng, J.; Lau, B.; Flemming, D.; Venuta, G.L.; Berninghausen, O.; Beckmann, R.; Hurt, E.
Deposited on	:	2020-09-29
Resolution	:	3.80 Å(reported)
Based on initial model	:	6ZQD

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

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

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

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

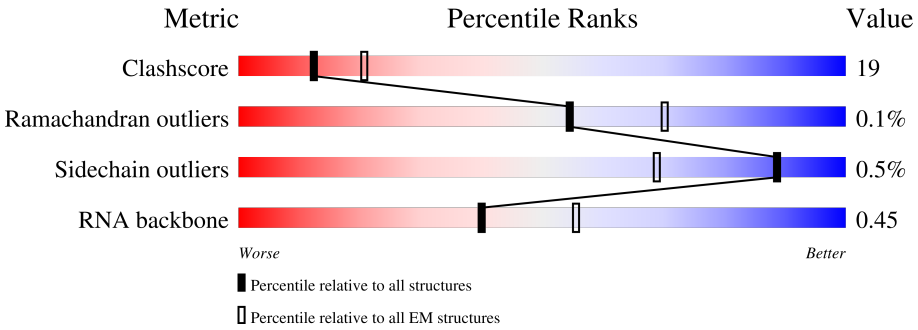
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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)
Clashscore	158937	4297
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	CA	327	42% 32% 26%
1	CB	327	36% 33% 30%
2	DA	255	59% 35% • 6%
3	UA	923	53% 32% 14%
4	UB	810	• 47% 21% 32%
5	UC	610	9% 5% 86%
6	UD	776	44% 41% 15%

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Mol	Chain	Length	Quality of chain
7	UE	643	40% 33% 26%
8	UF	440	42% 24% 33%
9	UG	554	54% 30% 15%
10	UH	713	52% 14% 34%
11	UI	575	8% 7% 85%
12	UJ	1769	36% 27% 37%
13	UK	250	49% 39% 12%
14	UL	943	43% 39% 17%
15	UM	817	43% 50% 7%
16	UN	899	15% 8% 77%
17	UO	513	40% 56%
18	UP	214	13% 14% 72%
19	UQ	896	49% 43% 8%
20	UR	594	47% 34% 19%
21	US	552	58% 30% 12%
22	UT	2493	51% 41% 7%
23	UU	939	56% 38% 6%
24	UV	1237	45% 42% 12%
25	UX	189	50% 37% 12%
26	CD	504	52% 23% 25%
27	CE	511	49% 36% 15%
28	CF	126	56% 33% 8%
28	CG	126	55% 34% 7%
29	CH	573	55% 26% 18%
30	CI	183	52% 43%

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Mol	Chain	Length	Quality of chain
31	CJ	290	50% 39% 12%
32	CK	593	24% 13% 63%
33	CL	1183	42% 26% 32%
34	CM	367	61% 37%
35	CN	297	44% 33% 23%
36	JD	1267	31% 32% 36%
37	JF	252	48% 37% 14%
37	JG	252	52% 38% 9%
38	JH	483	53% 46%
39	JI	1729	15% 85%
40	JL	318	58% 31% 11%
41	JM	217	31% 30% 38%
42	JP	489	59% 33% 6%
43	Db	82	98%
44	JJ	274	46% 26% 27%
45	DE	261	67% 27% 6%
46	DF	225	66% 29% 5%
47	DG	236	61% 31% 8%
48	DH	190	53% 37% 11%
49	DI	200	54% 34% 12%
50	DJ	197	63% 30% 6%
51	DL	156	66% 23% 10%
52	DN	151	79% 21%
53	DO	137	57% 36% 7%
54	DQ	143	57% 30% 13%

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Mol	Chain	Length	Quality of chain
55	DS	146	5% 40% 32% 28%
56	DT	144	6% 62% 37%
57	DW	130	75% 24%
58	DX	145	62% 36%
59	DY	135	76% 24%
60	Dc	67	94% 6%
61	D2	81	36% 47% 17%
62	D3	1802	30% 35% 12% 22%
63	D4	333	19% 38% 10% 33%
64	EA	22	41% 32% 55% 14%
65	EB	305	63% 90% 8%
66	EC	246	46% 94%
67	ED	394	16% 74% 6% 20%
68	EE	223	15% 93% 7%
69	EF	265	15% 95% 5%
70	EG	250	15% 82% 14%
71	EH	240	81% 93% 6%
72	EI	359	36% 77% 18%
73	EJ	292	63% 68% 8% 24%
74	EK	1001	63% 92% 5%
75	EN	1073	67% 80% 10% 10%

2 Entry composition (i)

There are 78 unique types of molecules in this entry. The entry contains 242031 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CA	242	Total	C	N	O	S	0	0
			1881	1193	338	340	10		
1	CB	228	Total	C	N	O	S	0	0
			1782	1131	320	321	10		

- Molecule 2 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	DA	240	Total	C	N	O	S	0	0
			1912	1209	354	345	4		

- Molecule 3 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	UA	792	Total	C	N	O	S	0	0
			6322	4040	1083	1181	18		

- Molecule 4 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	UB	553	Total	C	N	O	S	0	0
			4105	2602	736	756	11		

- Molecule 5 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	UC	86	Total	C	N	O	0	0
			694	430	139	125		

- Molecule 6 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	UD	663	Total	C	N	O	S	0	0
			5269	3339	915	994	21		

- Molecule 7 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UE	475	Total	C	N	O	S	0	0
			3772	2400	649	710	13		

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	UF	293	Total	C	N	O	S	0	0
			2487	1605	435	434	13		

- Molecule 9 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	UG	470	Total	C	N	O	S	0	0
			3718	2345	664	698	11		

- Molecule 10 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	UH	474	Total	C	N	O	S	0	0
			2771	1706	513	549	3		

- Molecule 11 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UI	88	Total	C	N	O	S	0	0
			723	462	131	128	2		

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	UJ	1116	Total	C	N	O	S	0	0
			8961	5802	1468	1666	25		

- Molecule 13 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	UK	219	Total	C	N	O	S	0	0
			1845	1150	356	332	7		

- Molecule 14 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	UL	779	Total	C	N	O	S	0	0
			6199	3974	1034	1164	27		

- Molecule 15 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UM	762	Total	C	N	O	S	0	0
			5970	3787	1007	1148	28		

- Molecule 16 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	UN	203	Total	C	N	O	S	0	0
			1667	1038	313	314	2		

- Molecule 17 is a protein called U3 small nucleolar RNA-associated protein 15.

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

- Molecule 18 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	UP	60	Total	C	N	O	0	0
			495	310	101	84		

- Molecule 19 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	UQ	820	Total	C	N	O	S	0	0
			6557	4171	1107	1260	19		

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	UR	481	Total	C	N	O	S	0	0
			3791	2399	668	714	10		

- Molecule 21 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	US	487	Total	C	N	O	S	0	0
			3587	2305	610	660	12		

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	UT	2313	Total	C	N	O	S	0	0
			18789	12100	3144	3479	66		

- Molecule 23 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	UU	878	Total	C	N	O	S	0	0
			6922	4386	1198	1316	22		

- Molecule 24 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	UV	1083	Total	C	N	O	S	0	0
			8753	5692	1442	1595	24		

- Molecule 25 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	UX	167	Total	C	N	O	S	0	0
			1330	854	241	225	10		

- Molecule 26 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CD	380	Total	C	N	O	S	0	0
			2994	1898	513	574	9		

- Molecule 27 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CE	436	Total	C	N	O	S	0	0
			3326	2093	571	654	8		

- Molecule 28 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CF	121	Total	C	N	O	S	0	0
			916	583	158	171	4		
28	CG	121	Total	C	N	O	S	0	0
			916	583	158	171	4		

- Molecule 29 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CH	467	Total	C	N	O	S	0	0
			3736	2371	655	700	10		

- Molecule 30 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CI	175	Total	C	N	O	S	0	0
			1468	929	276	256	7		

- Molecule 31 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CJ	256	Total	C	N	O	S	0	0
			2081	1306	394	374	7		

- Molecule 32 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CK	222	Total	C	N	O	S	0	0
			1789	1111	311	363	4		

- Molecule 33 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	CL	808	Total	C	N	O	S	0	0
			6551	4187	1171	1165	28		

- Molecule 34 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 35 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	CN	229	Total	C	N	O	S	0	0
			1868	1197	317	347	7		

- Molecule 36 is a protein called Probable ATP-dependent RNA helicase DHR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	JD	811	Total	C	N	O	S	0	0
			6509	4163	1151	1160	35		

- Molecule 37 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	JF	216	Total	C	N	O	S	0	0
			1701	1079	296	315	11		
37	JG	230	Total	C	N	O	S	0	0
			1799	1142	313	333	11		

- Molecule 38 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	JH	261	Total	C	N	O	0	0
			1295	773	261	261		

- Molecule 39 is a protein called rRNA biogenesis protein RRP5.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	JI	265	Total	C	N	O	0	0
			1314	784	265	265		

- Molecule 40 is a protein called Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	JL	283	Total	C	N	O	S	0	0
			2262	1439	401	408	14		

- Molecule 41 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	JM	134	Total	C	N	O	S	0	0
			1131	715	206	207	3		

- Molecule 42 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	JP	461	Total	C	N	O	S	0	0
			3765	2354	686	709	16		

- Molecule 43 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Db	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 44 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	JJ	199	Total	C	N	O	S	0	0
			1573	1001	285	283	4		

- Molecule 45 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	DE	246	Total	C	N	O	S	0	0
			1950	1248	361	338	3		

- Molecule 46 is a protein called 40S ribosomal protein S5.

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

- Molecule 47 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	DG	218	Total	C	N	O	S	0	0
			1755	1102	337	313	3		

- Molecule 48 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	DH	170	Total 1361	C 880	N 235	O 246	0	0

- Molecule 49 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	DI	177	Total 1399	C 869	N 279	O 249	S 2	0	0

- Molecule 50 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	DJ	185	Total 1494	C 943	N 289	O 261	S 1	0	0

- Molecule 51 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	DL	140	Total 1129	C 724	N 215	O 187	S 3	0	0

- Molecule 52 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	DN	150	Total 1192	C 759	N 224	O 207	S 2	0	0

- Molecule 53 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	DO	127	Total 922	C 567	N 185	O 167	S 3	0	0

- Molecule 54 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	DQ	125	Total 969	C 623	N 174	O 172	0	0

- Molecule 55 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	DS	105	Total	C	N	O	S	0	0
			861	545	160	154	2		

- Molecule 56 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	DT	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 57 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	DW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 58 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	DX	143	Total	C	N	O	S	0	0
			1115	705	219	189	2		

- Molecule 59 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	DY	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 60 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 61 is a RNA chain called 5'ETS RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	D2	81	Total	C	N	O	P	0	0
			1741	777	319	564	81		

- Molecule 62 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	D3	1409	Total	C	N	O	P	0	0
			30042	13429	5342	9862	1409		

- Molecule 63 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	D4	223	Total	C	N	O	P	0	0
			4720	2113	816	1568	223		

- Molecule 64 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	EA	22	Total	C	N	O	P	0	0
			366	161	43	140	22		

- Molecule 65 is a protein called Exosome complex component RRP45.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	EB	299	Total	C	N	O	0	0
			1475	877	299	299		

- Molecule 66 is a protein called Exosome complex component SKI6.

Mol	Chain	Residues	Atoms				AltConf	Trace
66	EC	243	Total	C	N	O	0	0
			1199	713	243	243		

- Molecule 67 is a protein called Exosome complex component RRP43.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	ED	317	Total	C	N	O	1	0
			1571	937	317	317		

- Molecule 68 is a protein called Exosome complex component RRP46.

Mol	Chain	Residues	Atoms				AltConf	Trace
68	EE	223	Total	C	N	O	1	0
			1107	661	223	223		

- Molecule 69 is a protein called Exosome complex component RRP42.

Mol	Chain	Residues	Atoms				AltConf	Trace
69	EF	265	Total 1317	C 787	N 265	O 265	1	0

- Molecule 70 is a protein called Exosome complex component MTR3.

Mol	Chain	Residues	Atoms				AltConf	Trace
70	EG	215	Total 1058	C 628	N 215	O 215	0	0

- Molecule 71 is a protein called Exosome complex component RRP40.

Mol	Chain	Residues	Atoms				AltConf	Trace
71	EH	237	Total 1170	C 696	N 237	O 237	0	0

- Molecule 72 is a protein called Exosome complex component RRP4.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	EI	293	Total 1440	C 854	N 293	O 293	0	0

- Molecule 73 is a protein called Exosome complex component CSL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	EJ	222	Total 1091	C 647	N 222	O 222	0	0

- Molecule 74 is a protein called Exosome complex exonuclease DIS3.

Mol	Chain	Residues	Atoms				AltConf	Trace
74	EK	970	Total 4818	C 2878	N 970	O 970	1	0

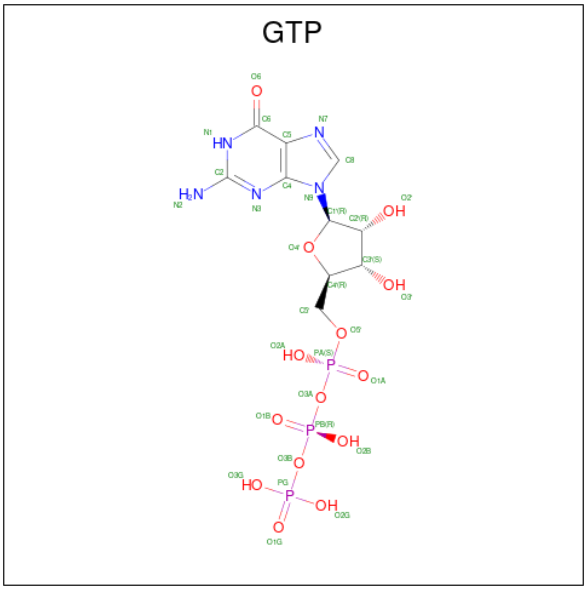
- Molecule 75 is a protein called ATP-dependent RNA helicase DOB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
75	EN	963	Total 4762	C 2839	N 963	O 960	0	0

- Molecule 76 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
76	UX	1	Total Zn 1 1	0
76	Db	1	Total Zn 1 1	0
76	EK	1	Total Zn 1 1	0

- Molecule 77 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 78 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

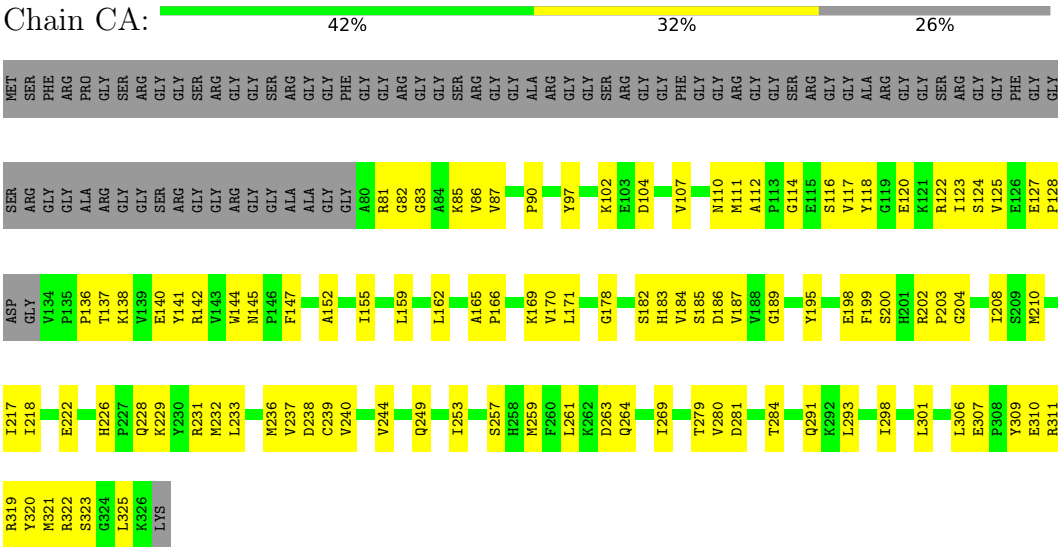
Mol	Chain	Residues	Atoms	AltConf
78	CL	1	Total Mg 1 1	0
78	EK	1	Total Mg 1 1	0

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.

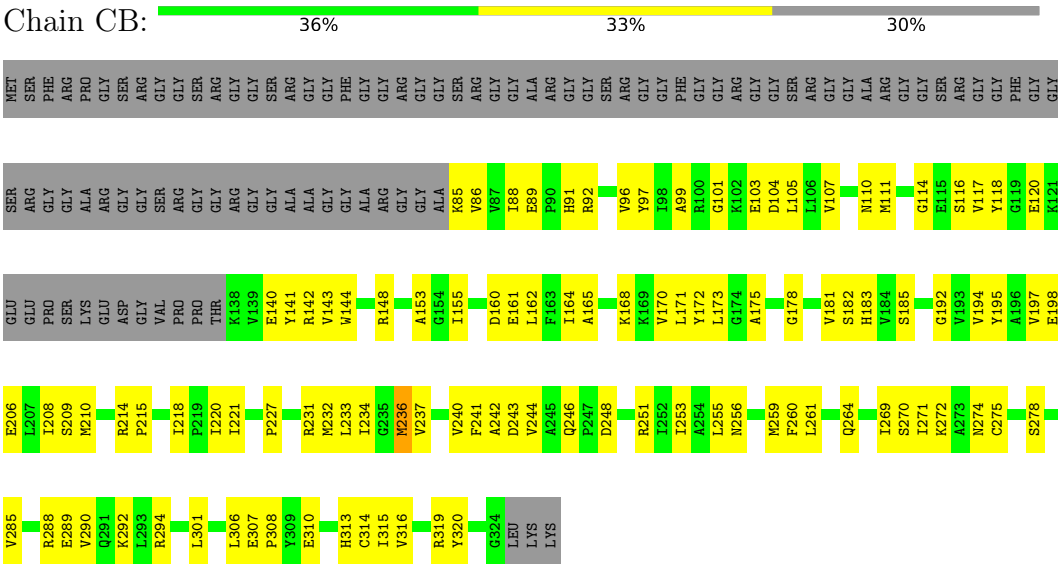
• Molecule 1: rRNA 2'-O-methyltransferase fibrillarin

Chain CA:



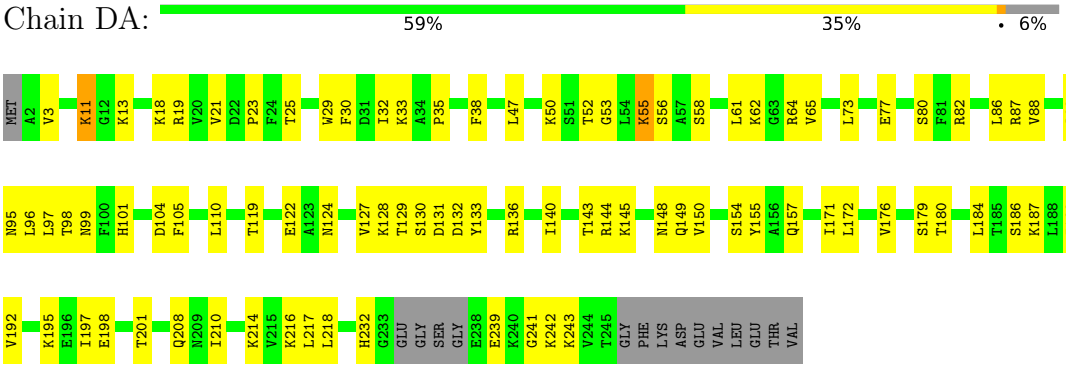
• Molecule 1: rRNA 2'-O-methyltransferase fibrillarin

Chain CB:



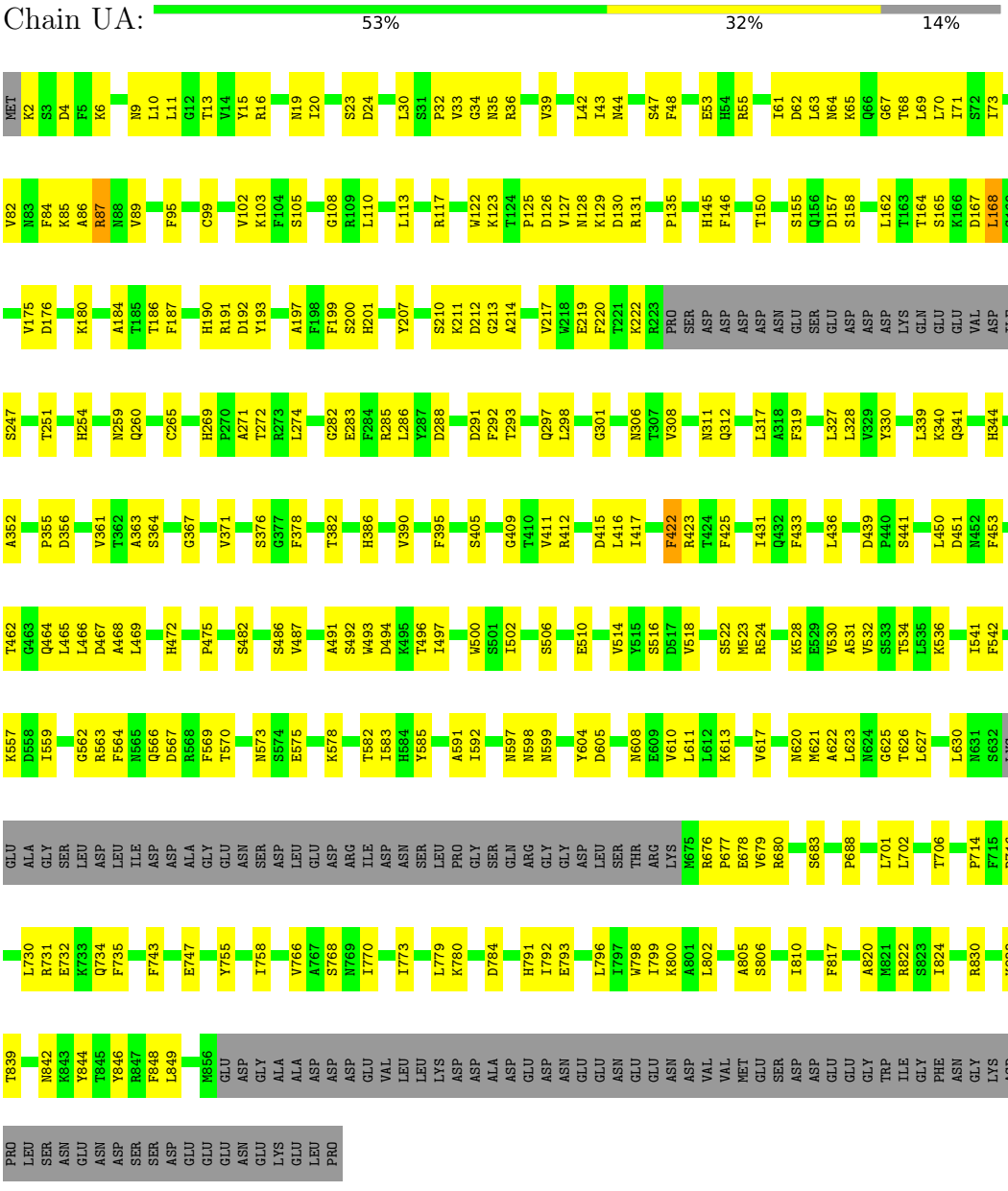
• Molecule 2: 40S ribosomal protein S1-A

Chain DA:



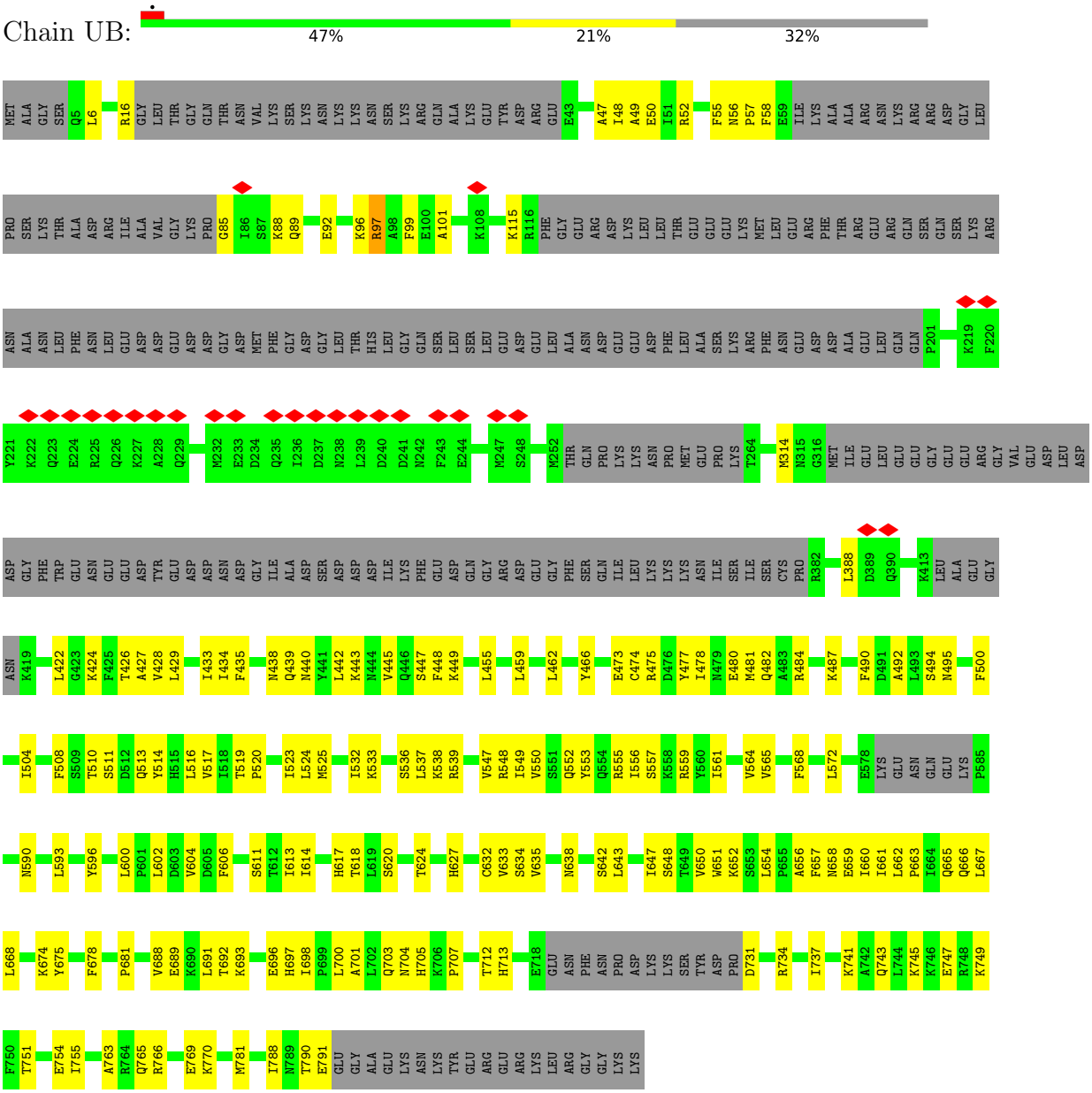
• Molecule 3: Periodic tryptophan protein 2

Chain UA:



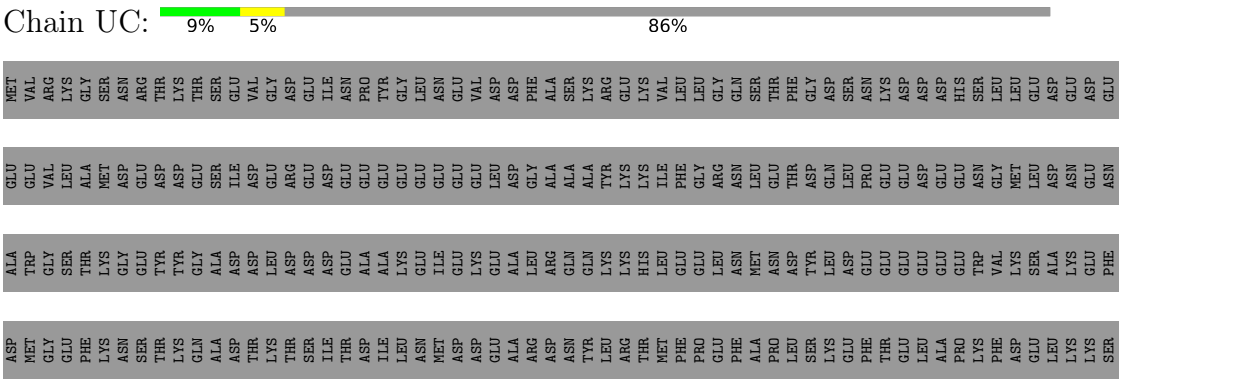
• Molecule 4: Nucleolar complex protein 14

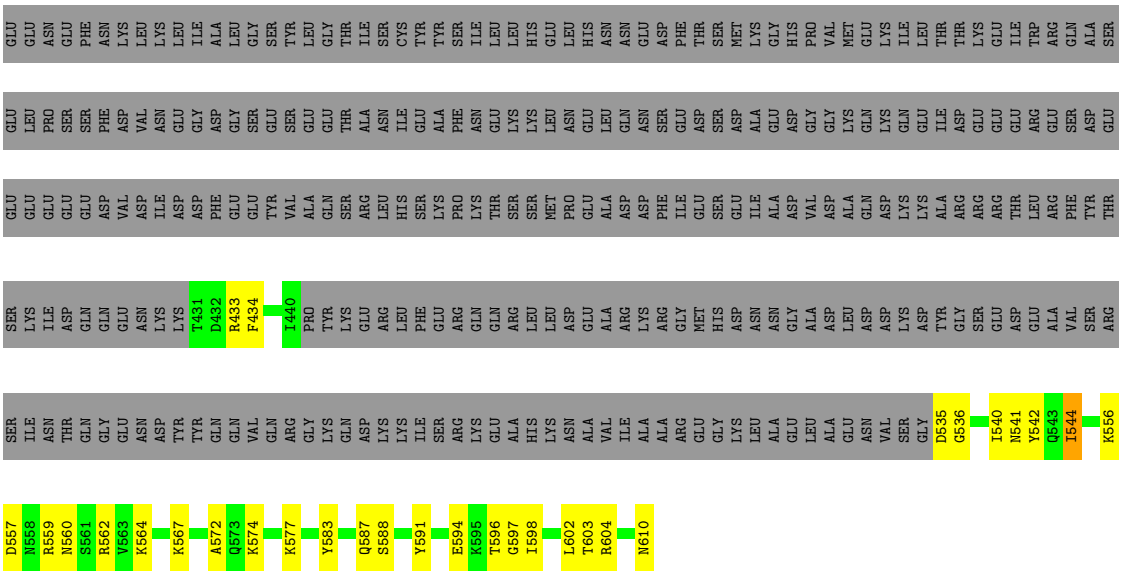
Chain UB:



• Molecule 5: Something about silencing protein 10

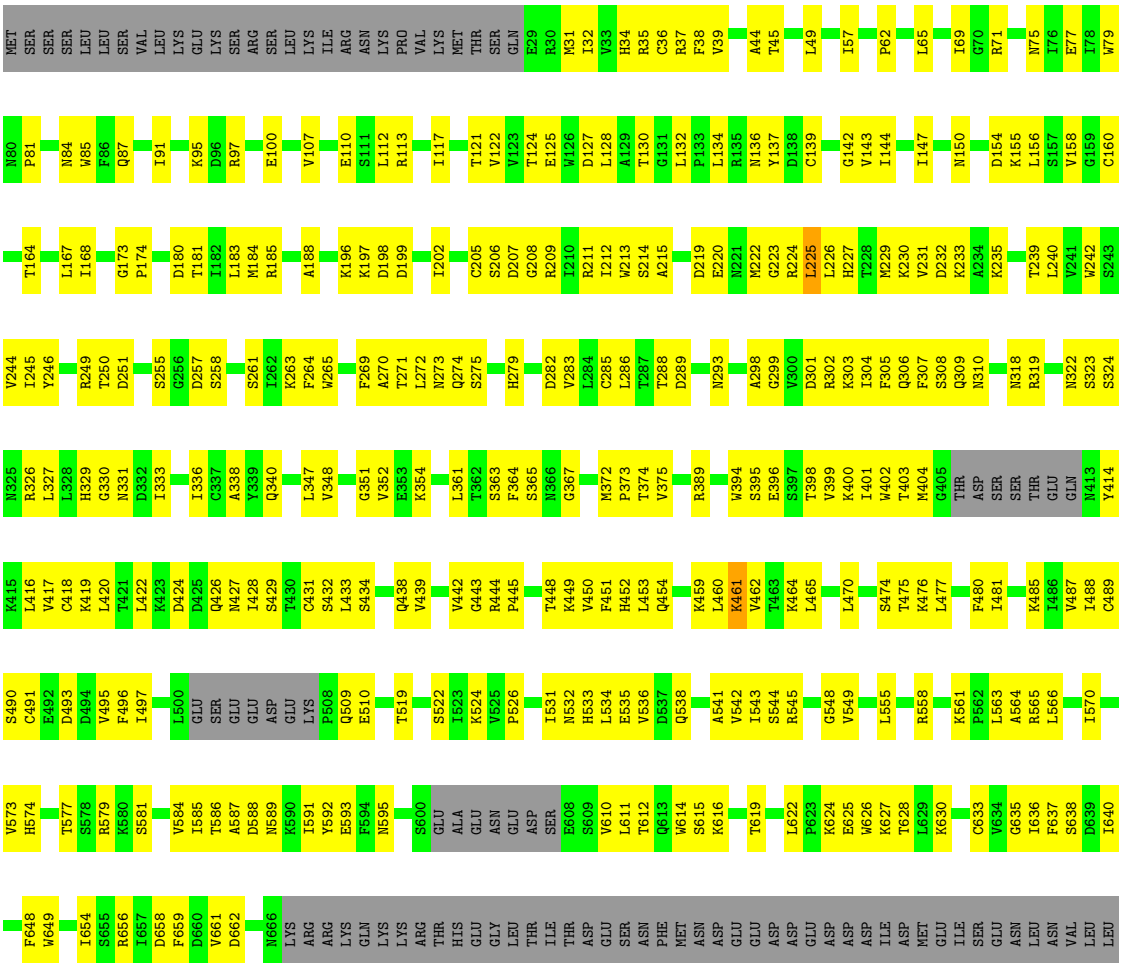
Chain UC:

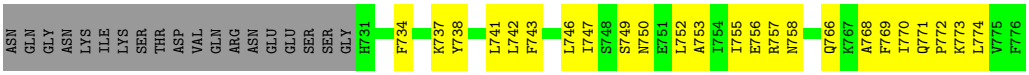




• Molecule 6: U3 small nucleolar RNA-associated protein 4

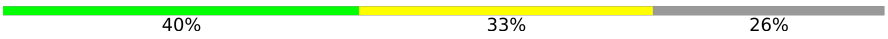
Chain UD:

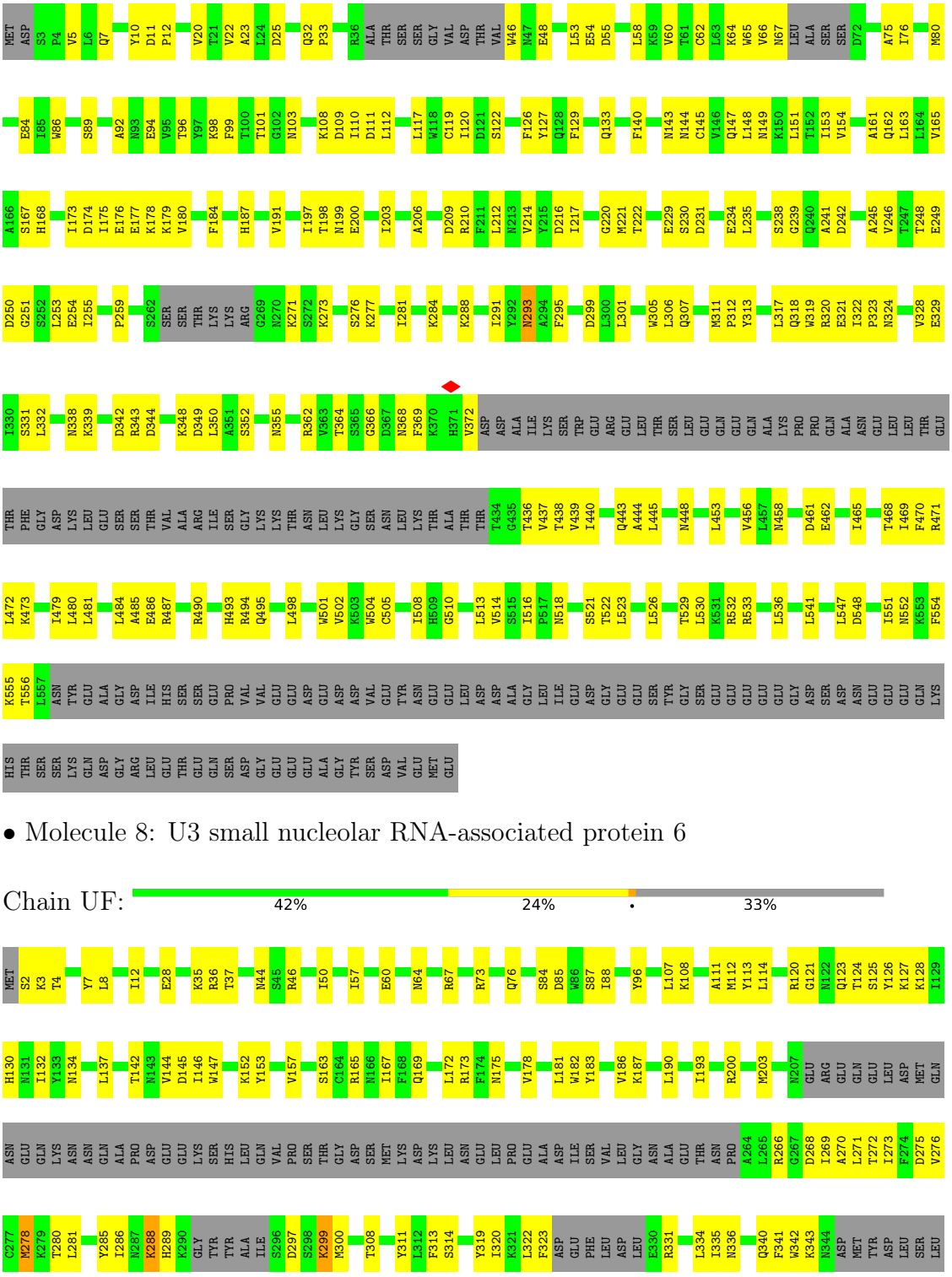




• Molecule 7: U3 small nucleolar RNA-associated protein 5

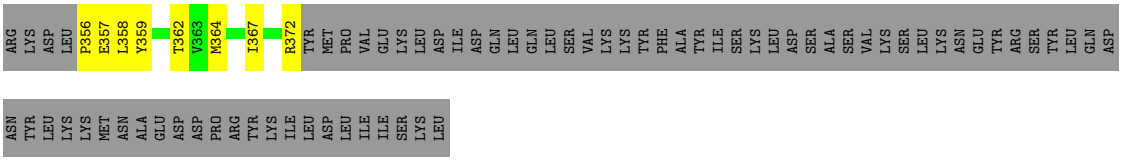
Chain UE:





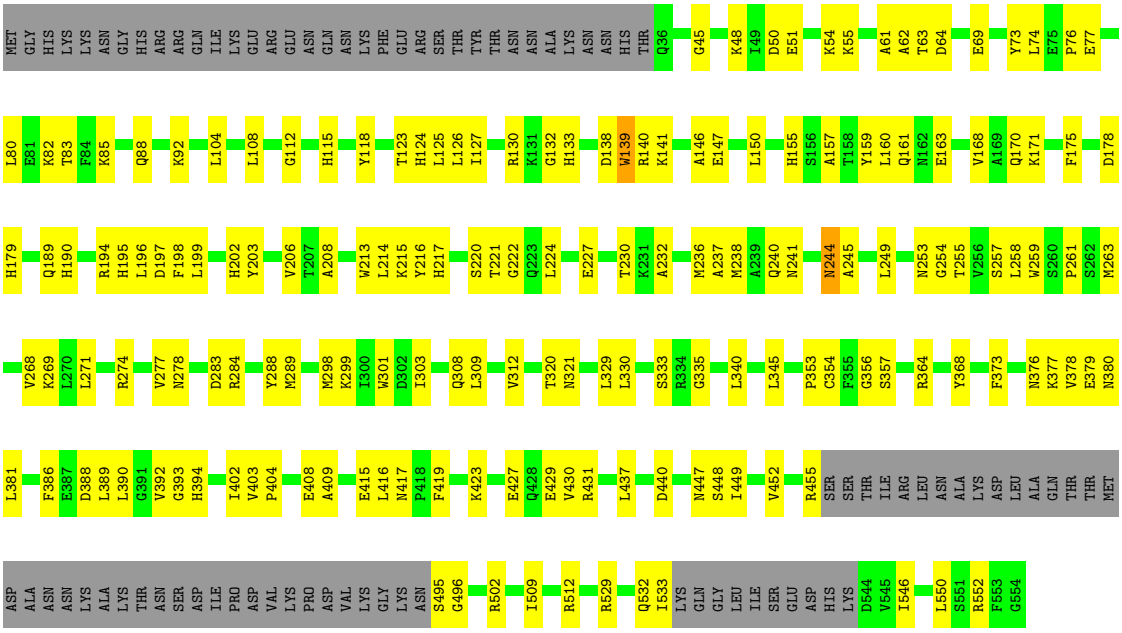
• Molecule 8: U3 small nucleolar RNA-associated protein 6

Chain UF:



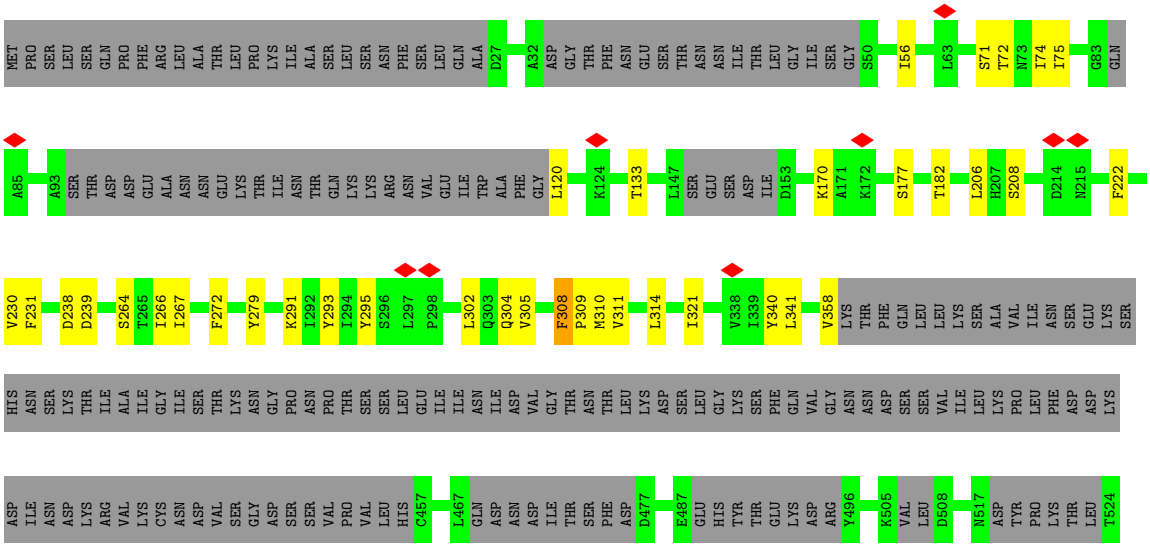
• Molecule 9: U3 small nucleolar RNA-associated protein 7

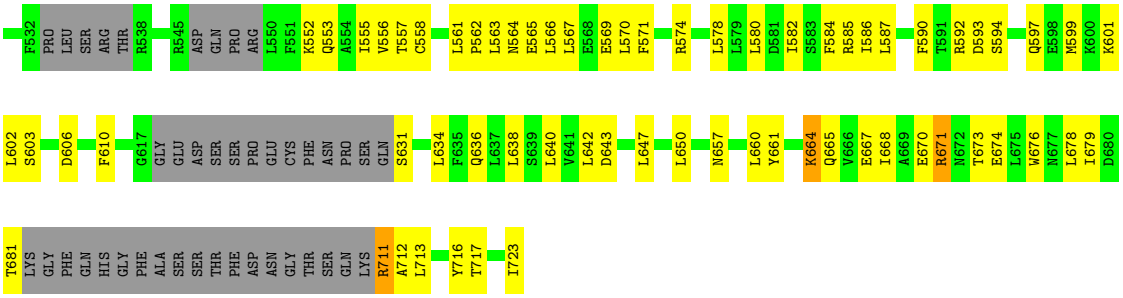
Chain UG:



• Molecule 10: U3 small nucleolar RNA-associated protein 8

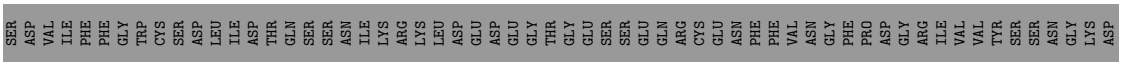
Chain UH:

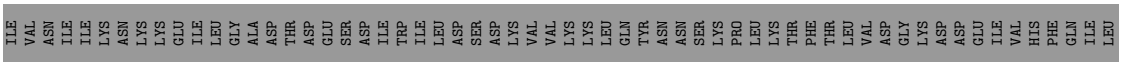


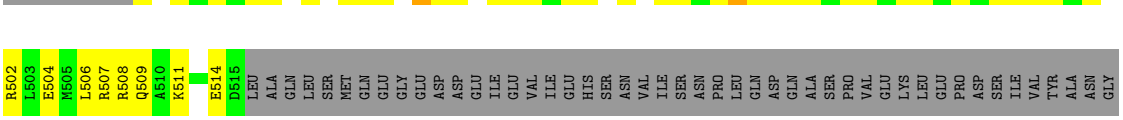


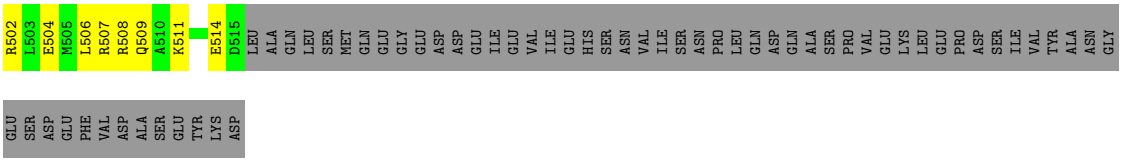
• Molecule 11: U3 small nucleolar RNA-associated protein 9

Chain UI:



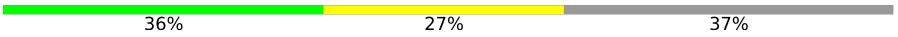


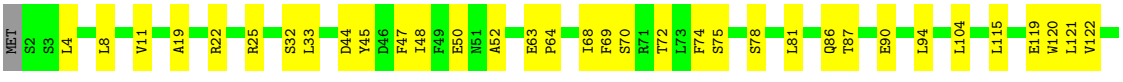


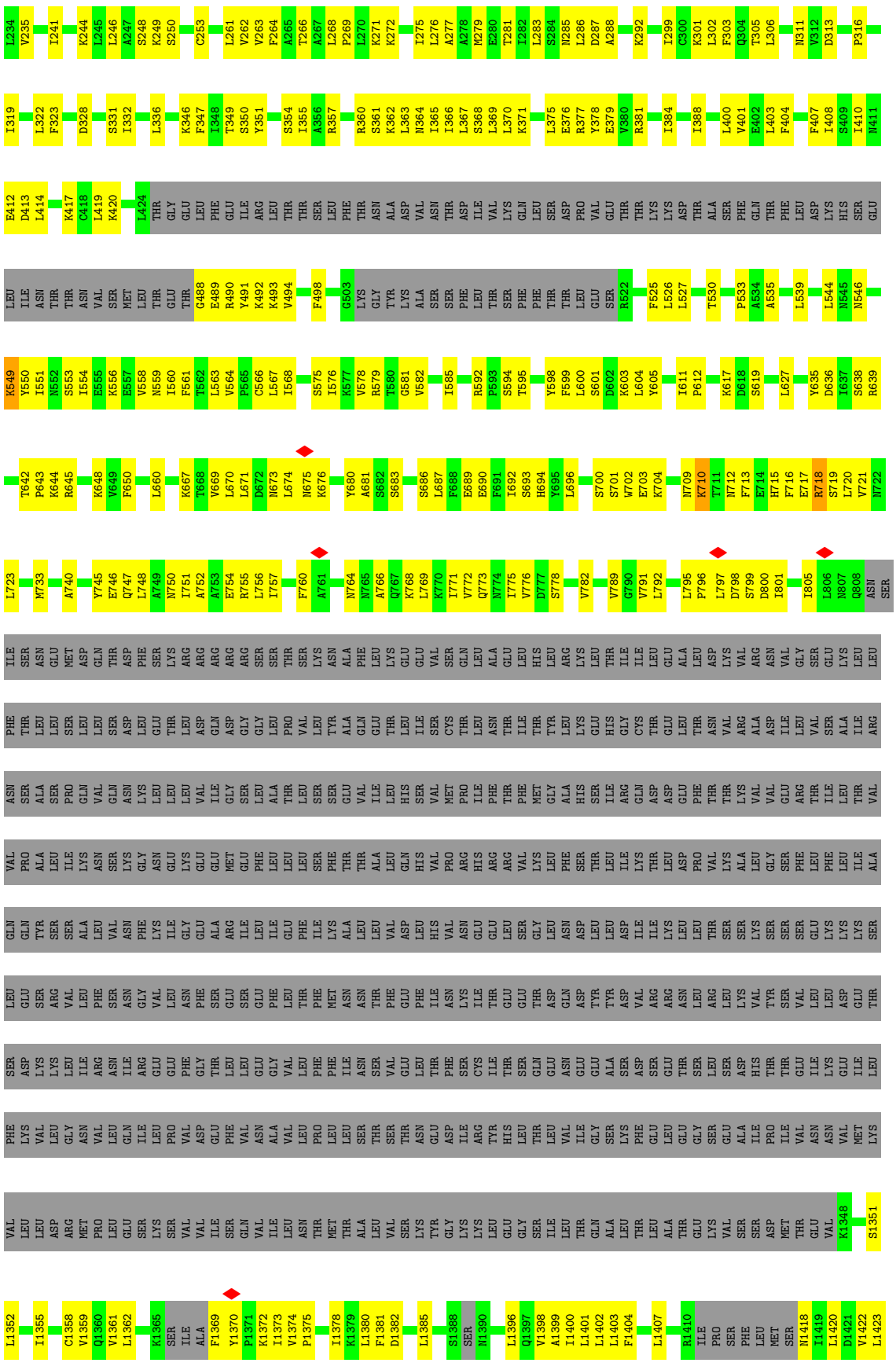


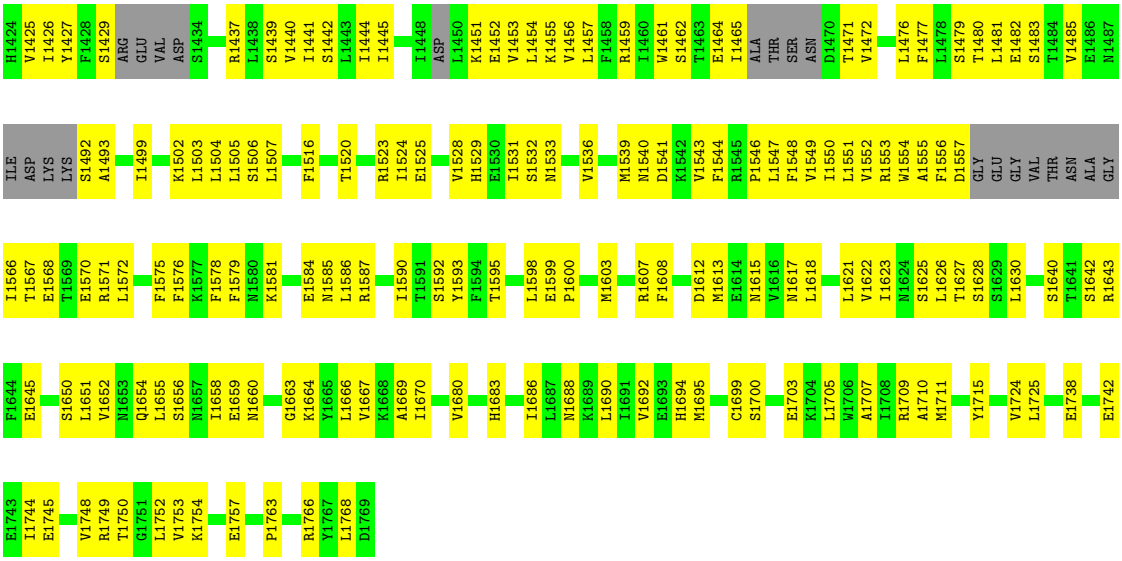
• Molecule 12: U3 small nucleolar RNA-associated protein 10

Chain UJ:



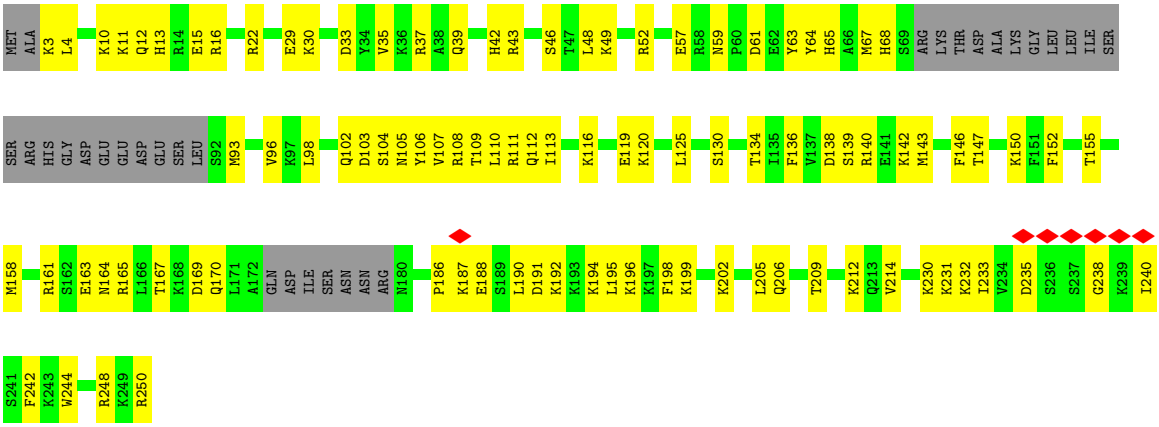






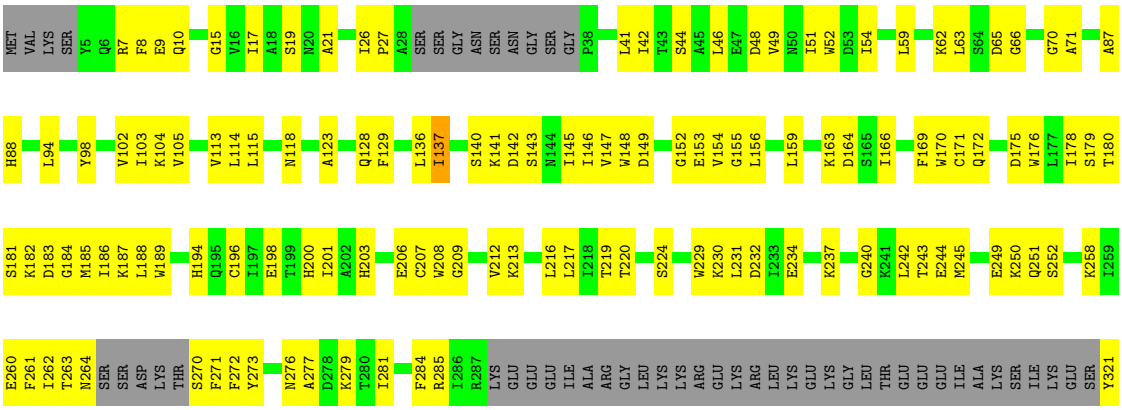
• Molecule 13: U3 small nucleolar RNA-associated protein 11

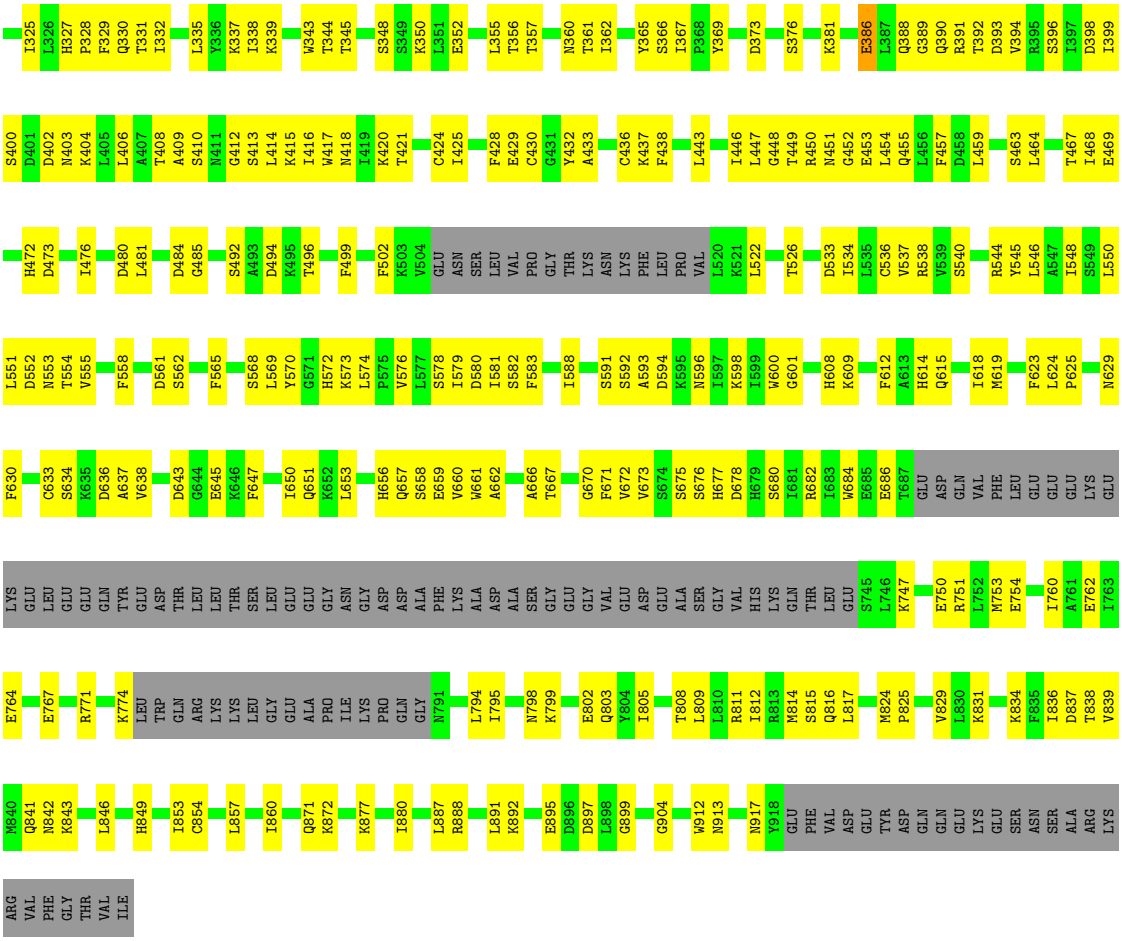
Chain UK:



• Molecule 14: U3 small nucleolar RNA-associated protein 12

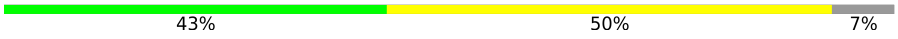
Chain UL:

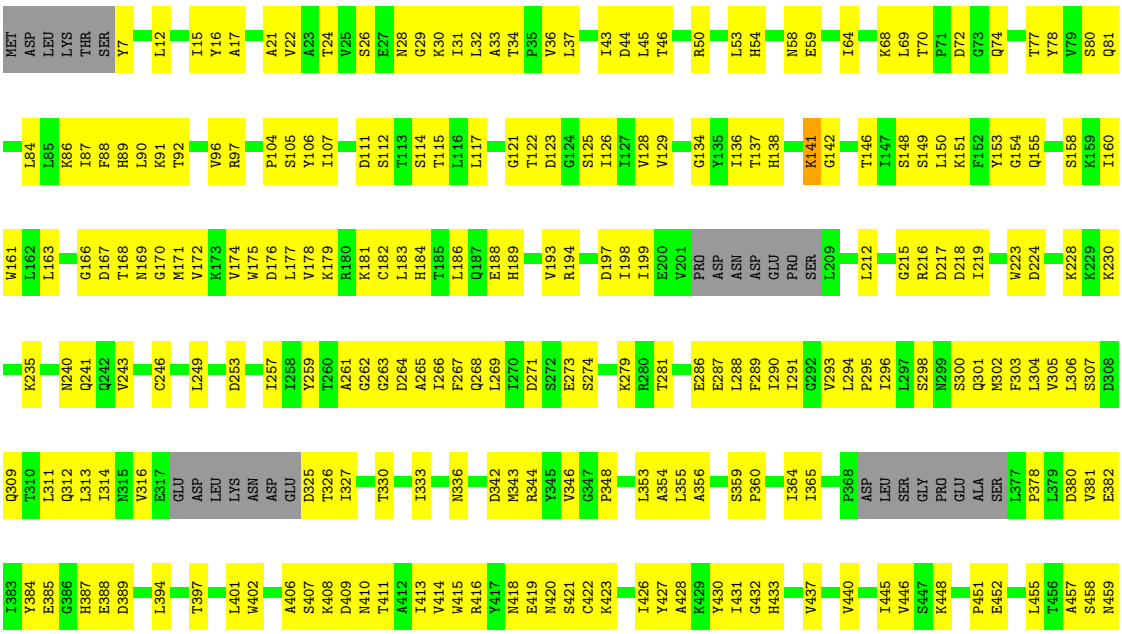


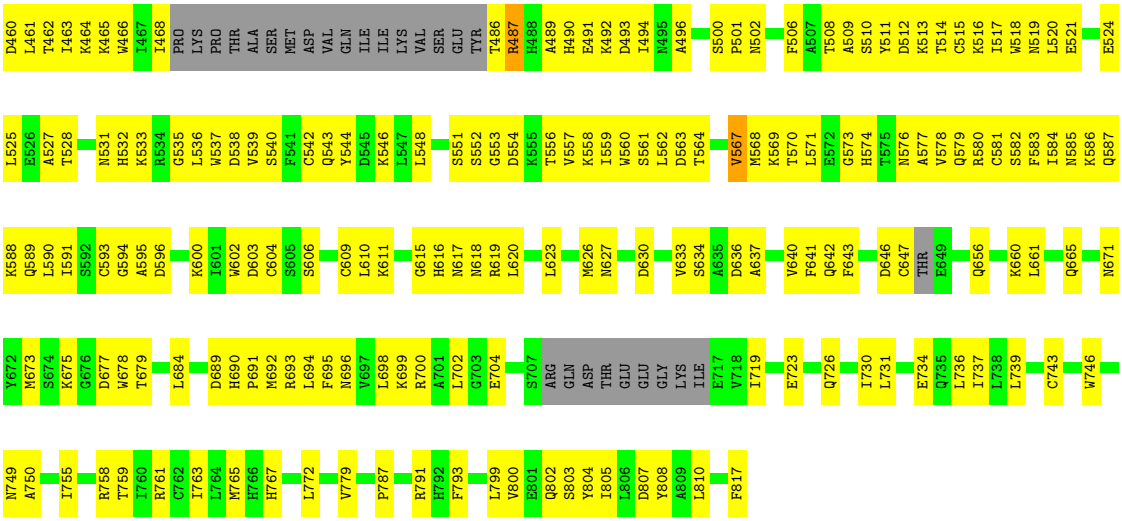


• Molecule 15: U3 small nucleolar RNA-associated protein 13

Chain UM:

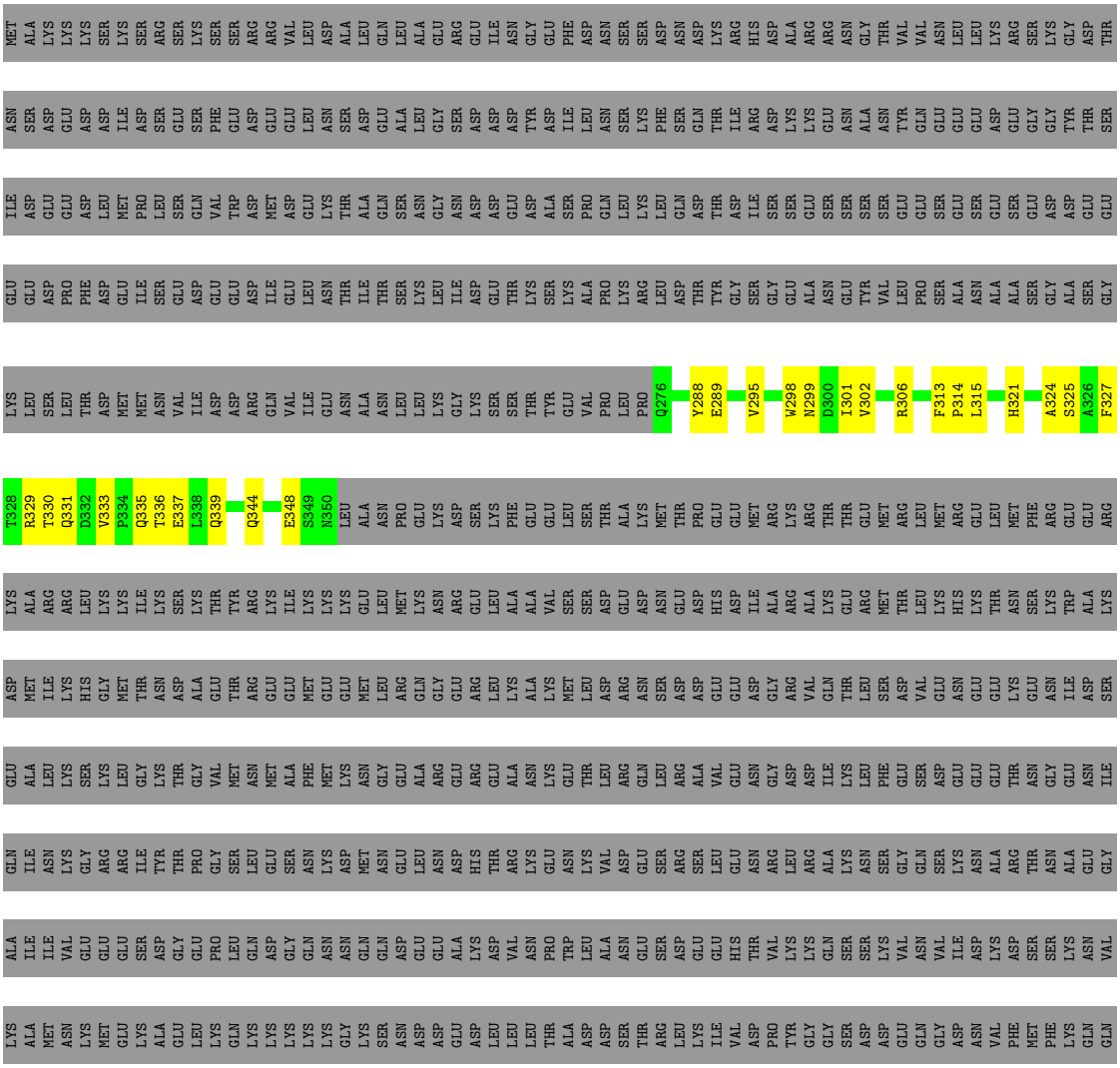


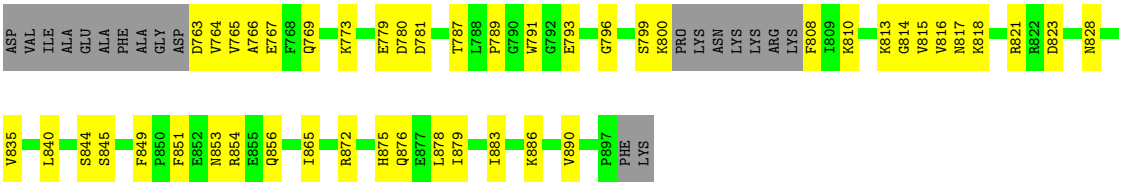




• Molecule 16: U3 small nucleolar RNA-associated protein 14

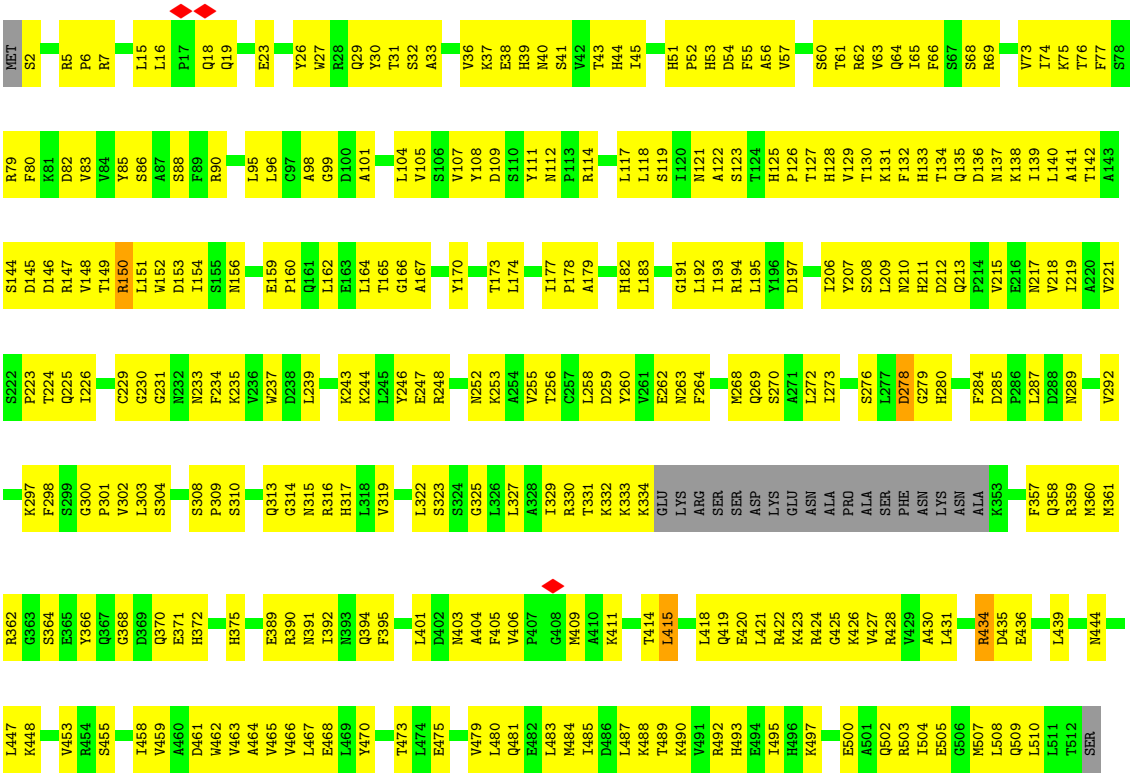
Chain UN: 15% 8% 77%





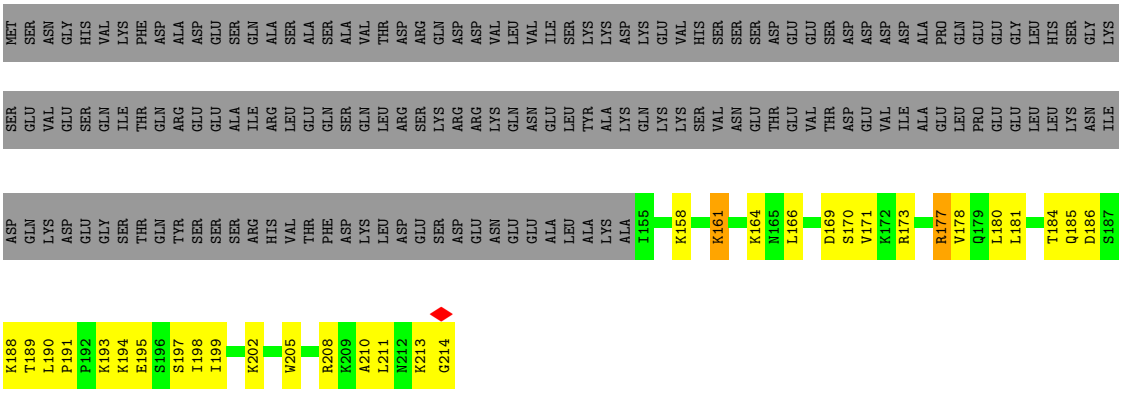
• Molecule 17: U3 small nucleolar RNA-associated protein 15

Chain UO:



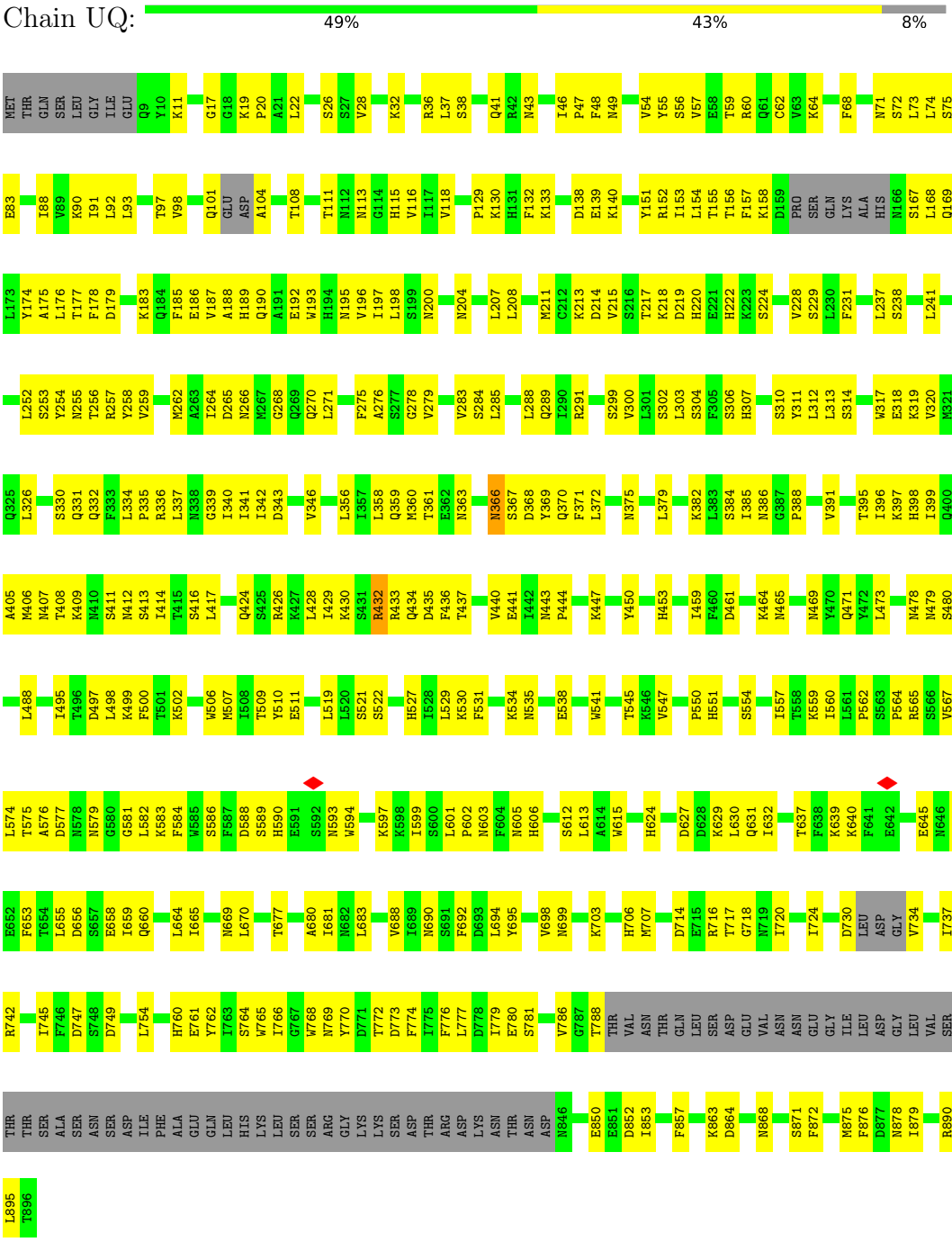
• Molecule 18: Bud site selection protein 21

Chain UP:



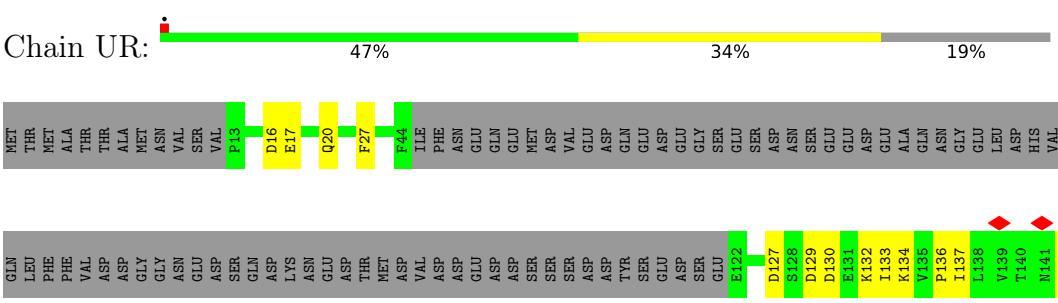
• Molecule 19: NET1-associated nuclear protein 1

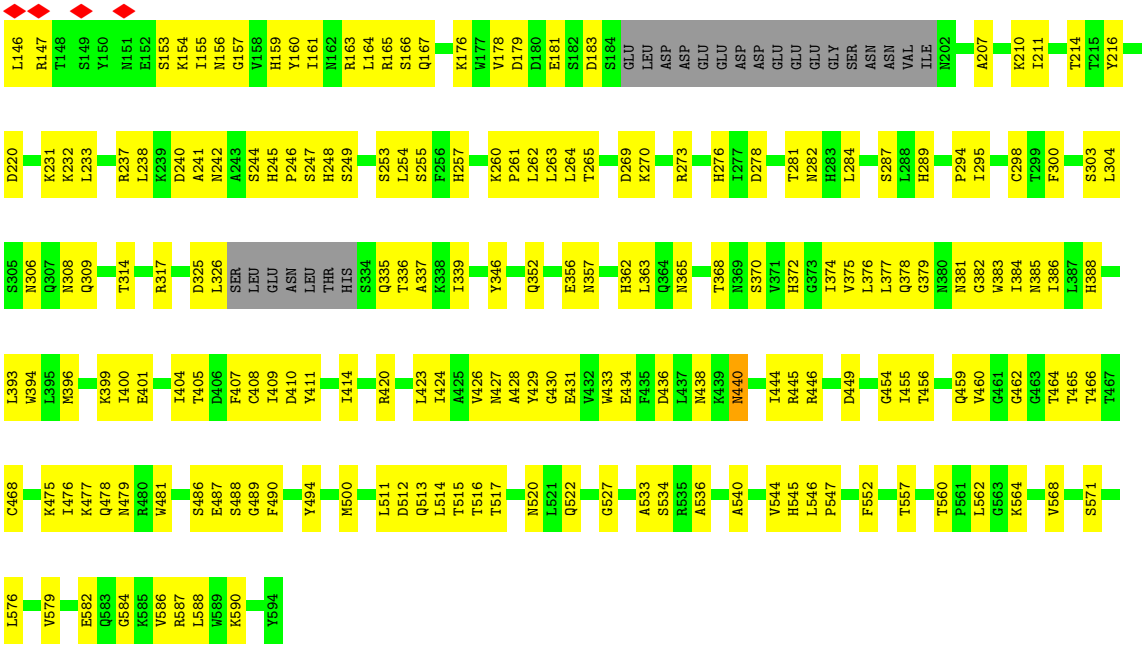
Chain UQ:



• Molecule 20: U3 small nucleolar RNA-associated protein 18

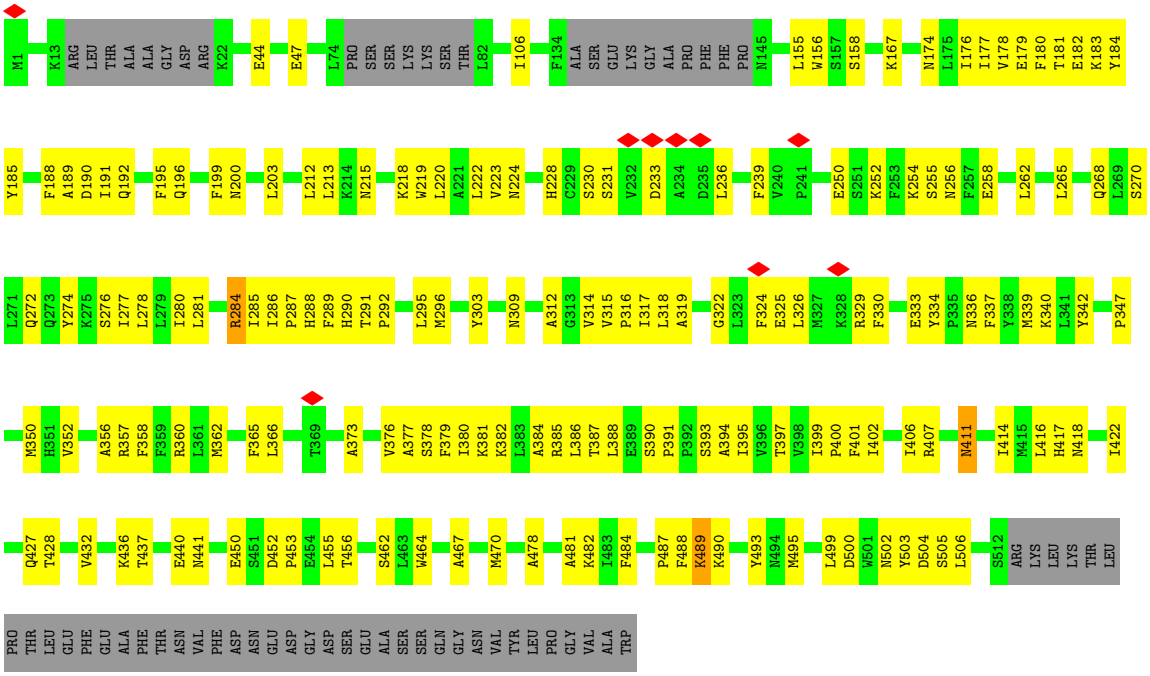
Chain UR:





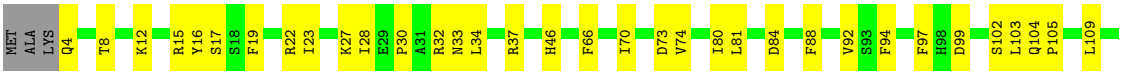
• Molecule 21: Nucleolar complex protein 4

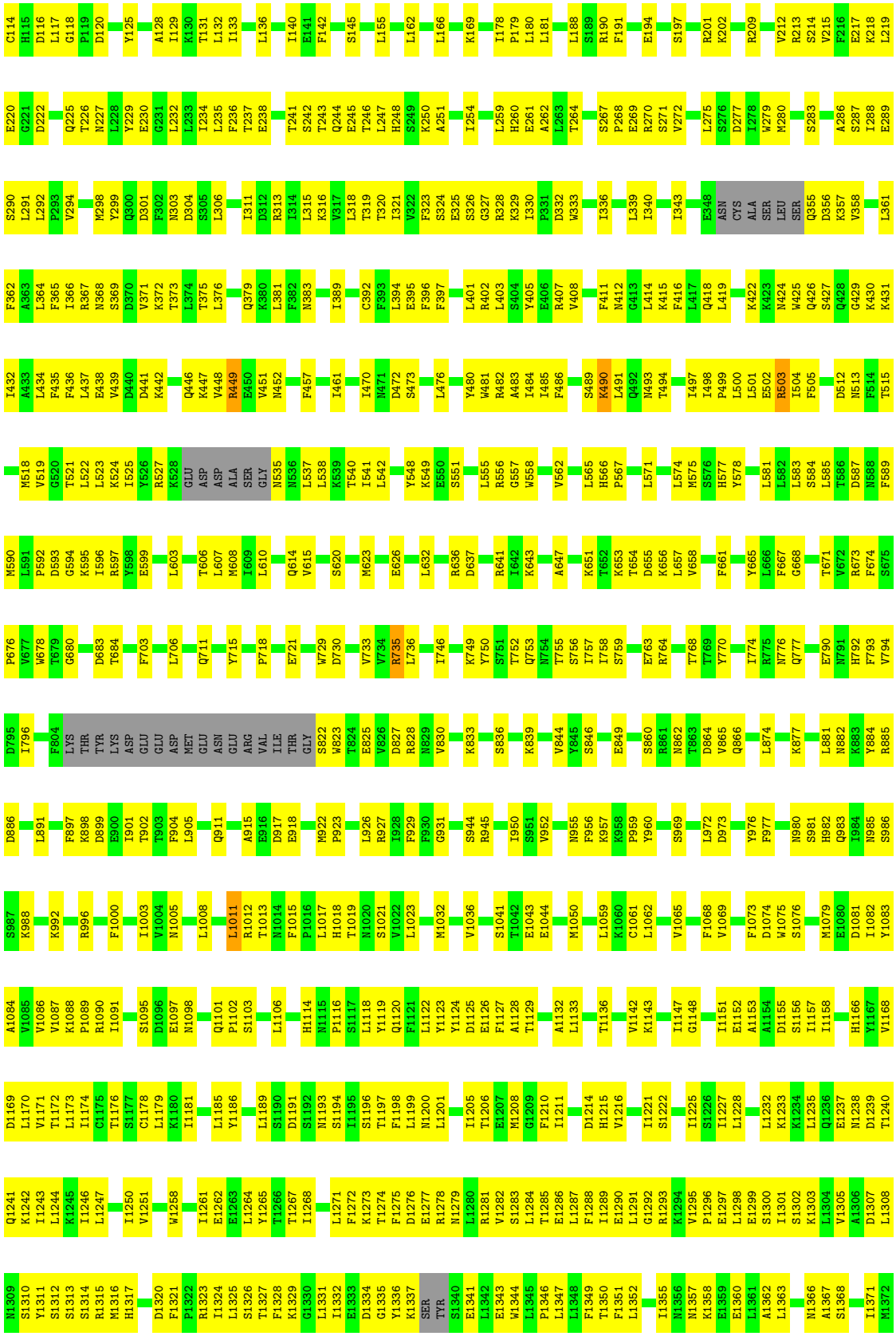
Chain US:

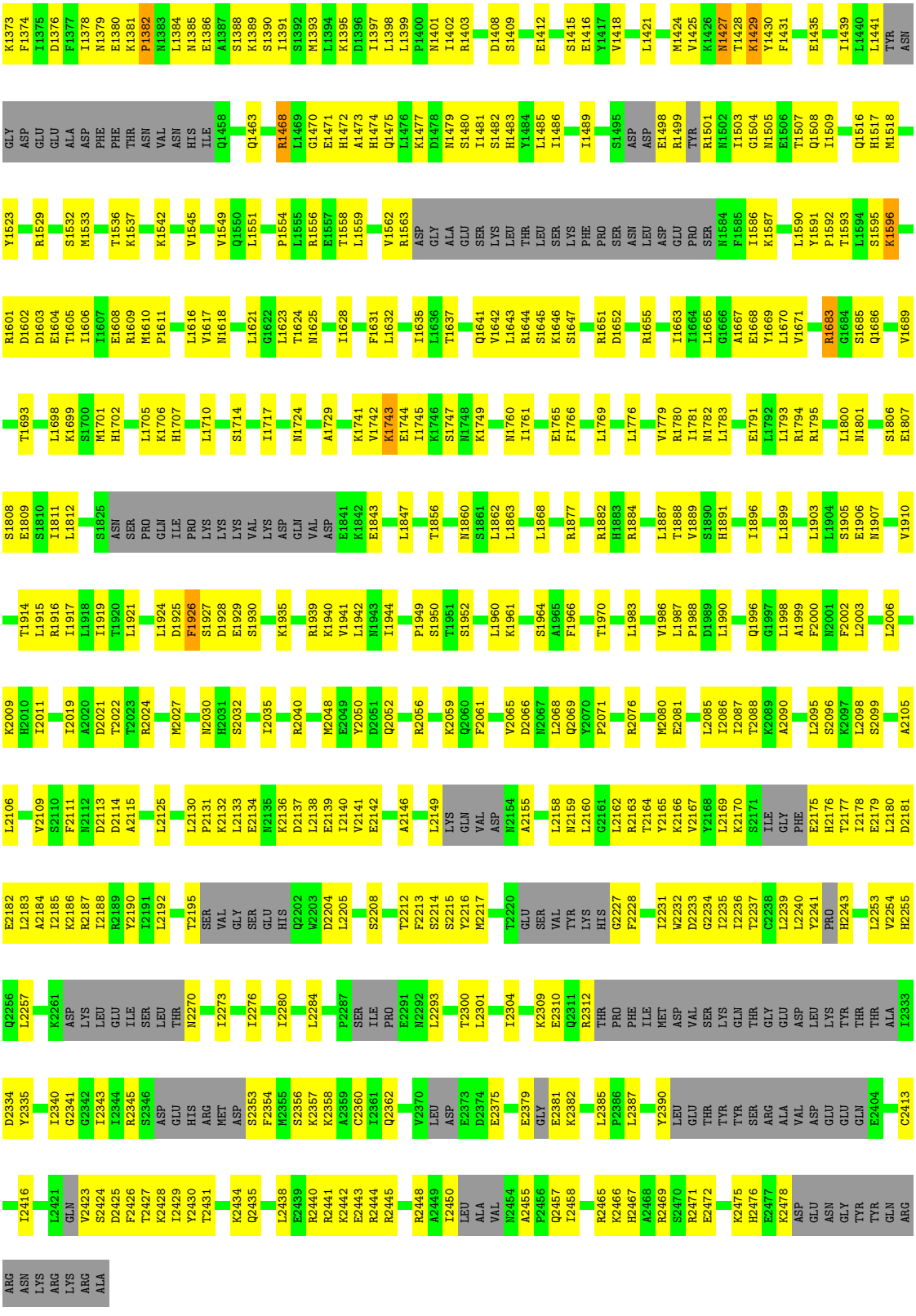


• Molecule 22: U3 small nucleolar RNA-associated protein 20

Chain UT:

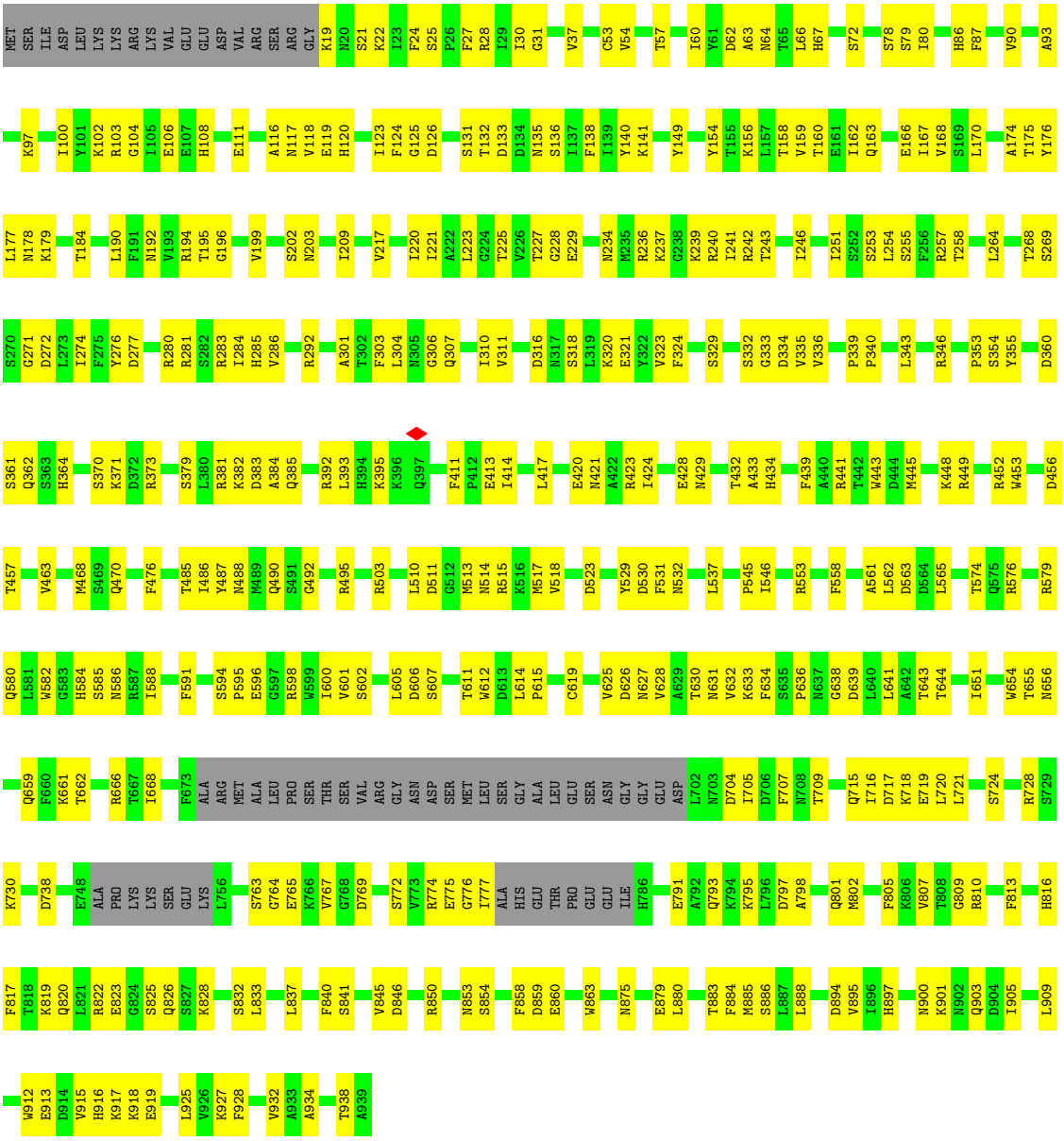






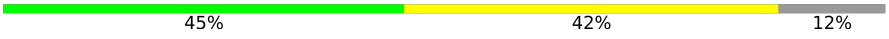
• Molecule 23: U3 small nucleolar RNA-associated protein 21

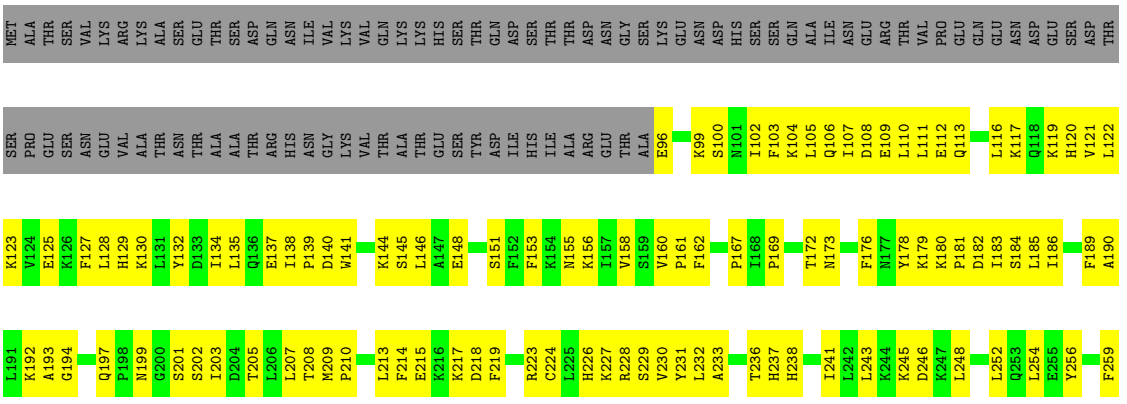
Chain UU:

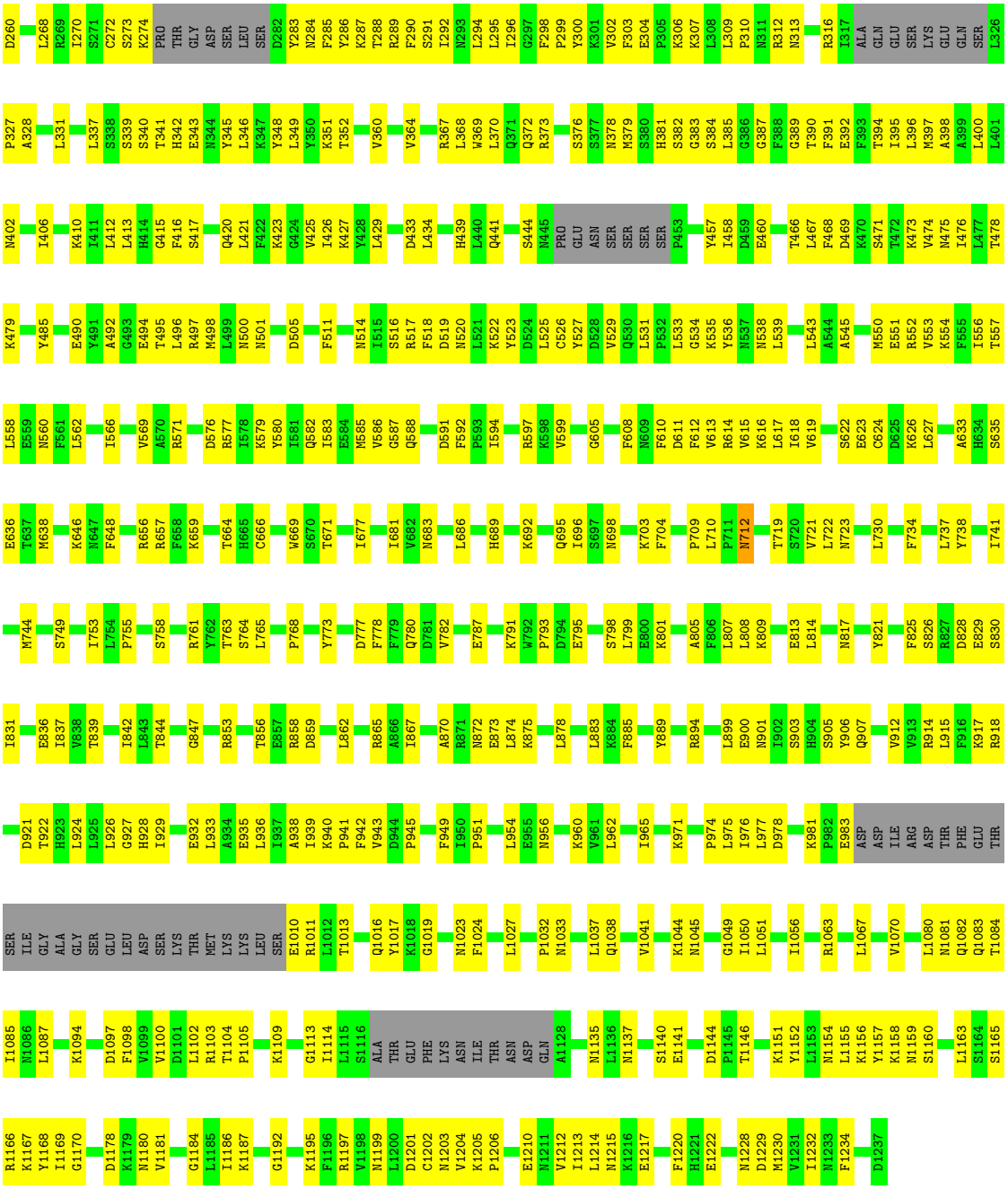


• Molecule 24: U3 small nucleolar RNA-associated protein 22

Chain UV:

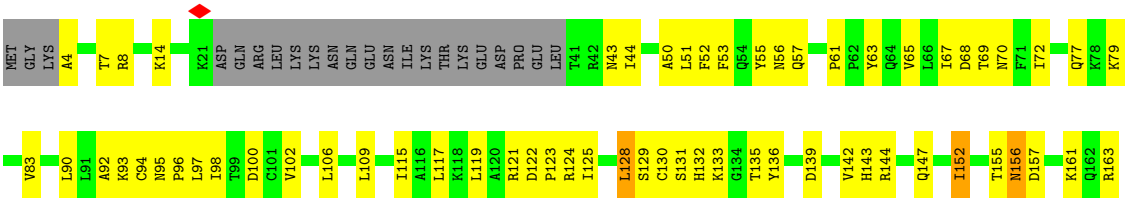


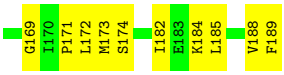




• Molecule 25: rRNA-processing protein FCF1

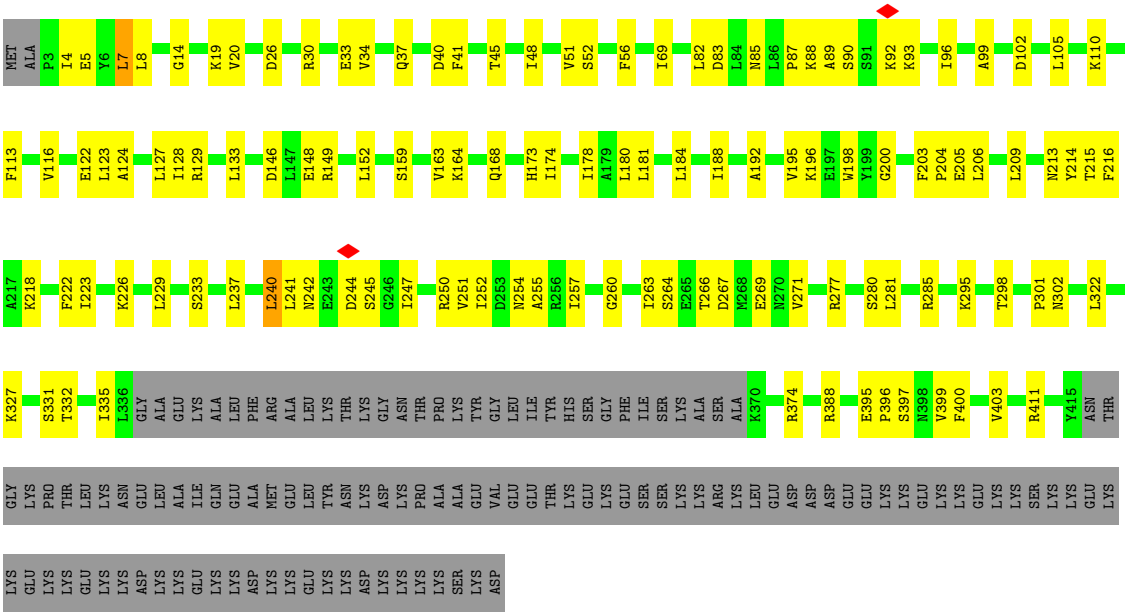
Chain UX:





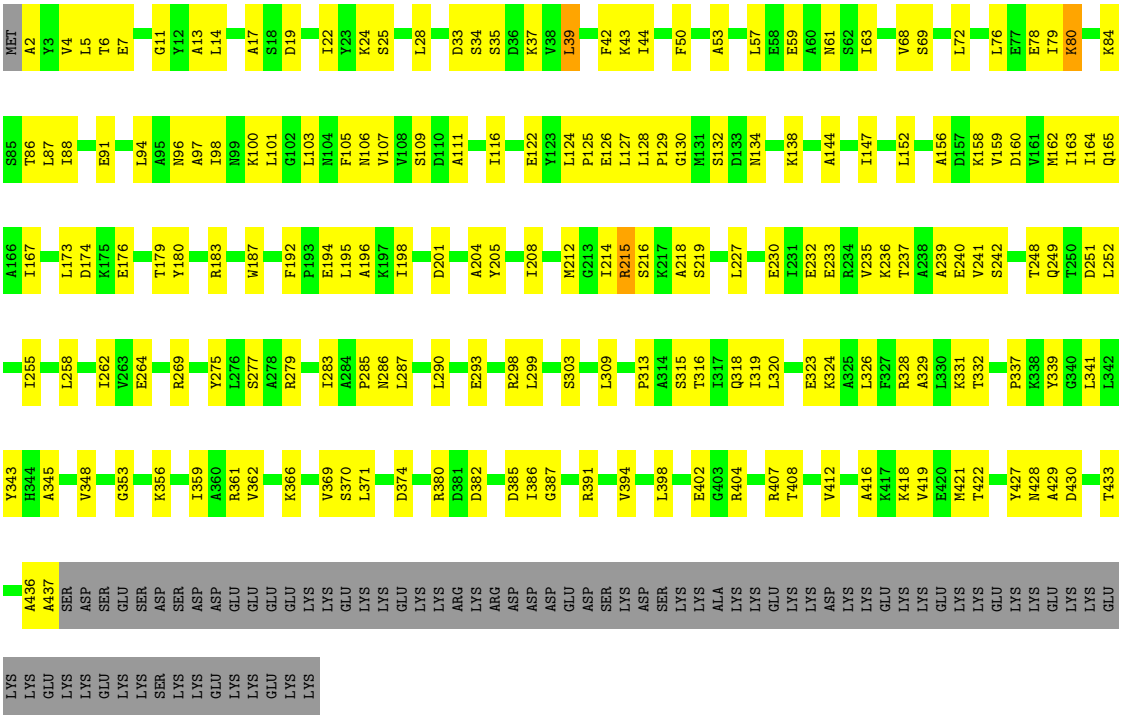
• Molecule 26: Nucleolar protein 56

Chain CD:



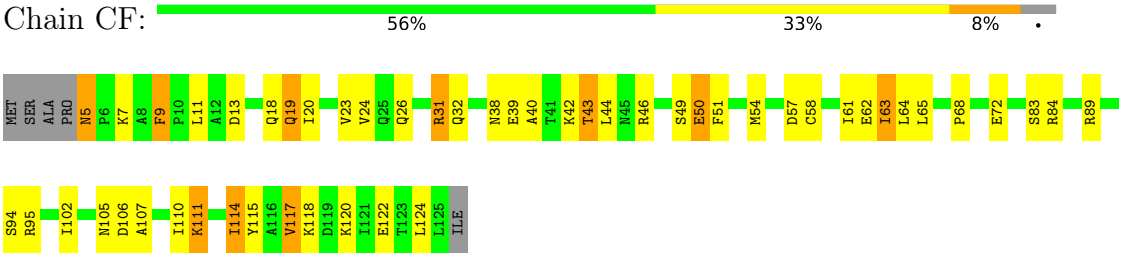
• Molecule 27: Nucleolar protein 58

Chain CE:



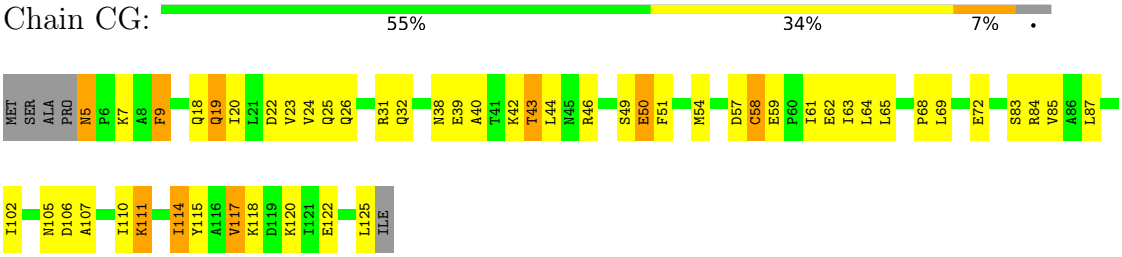
• Molecule 28: 13 kDa ribonucleoprotein-associated protein

Chain CF:



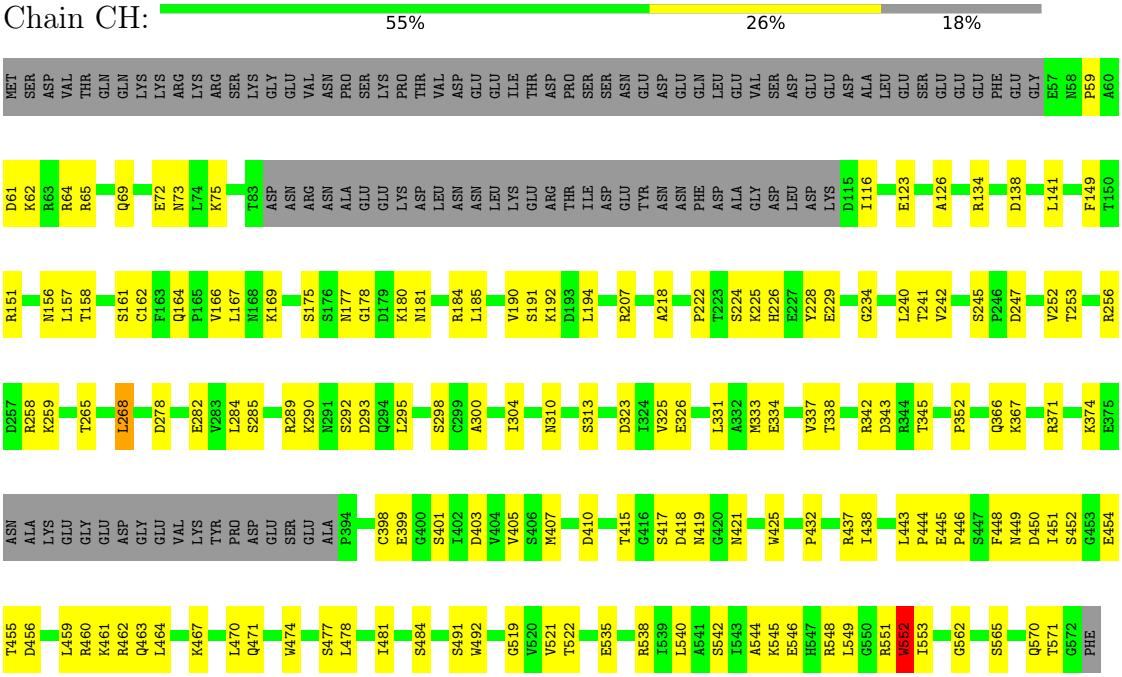
• Molecule 28: 13 kDa ribonucleoprotein-associated protein

Chain CG:



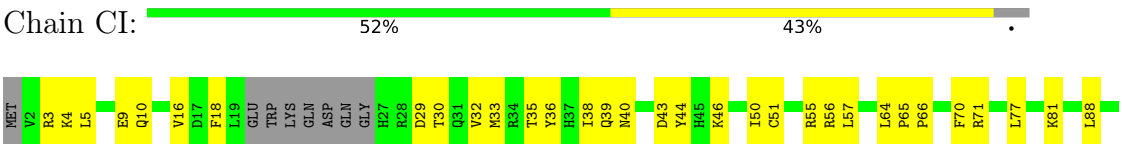
• Molecule 29: Ribosomal RNA-processing protein 9

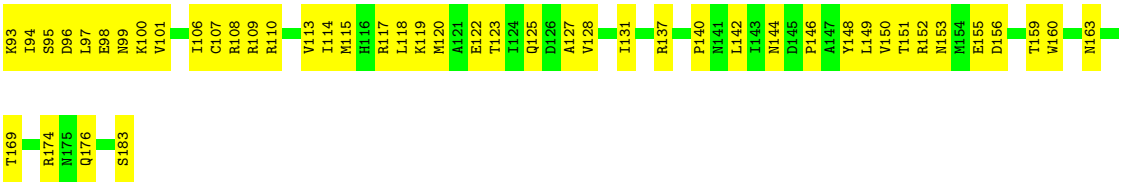
Chain CH:



• Molecule 30: U3 small nucleolar ribonucleoprotein protein IMP3

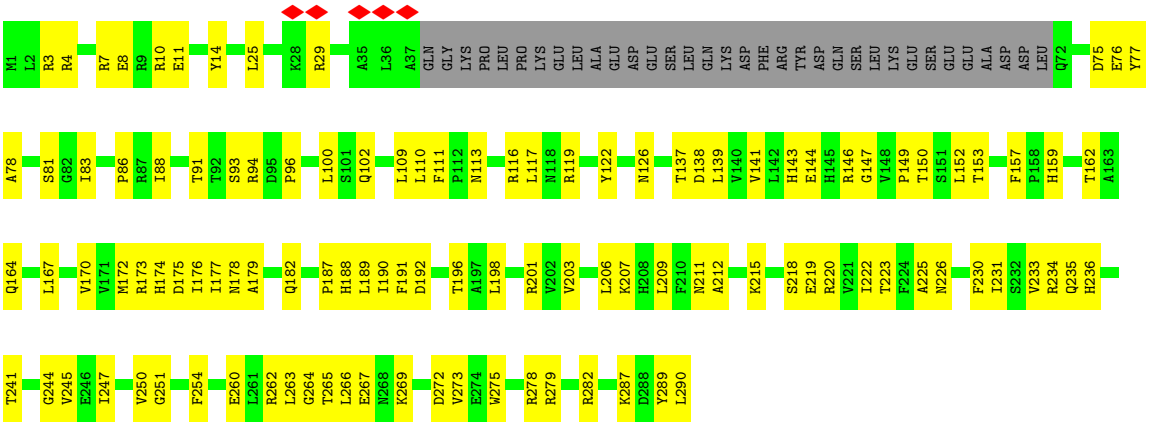
Chain CI:





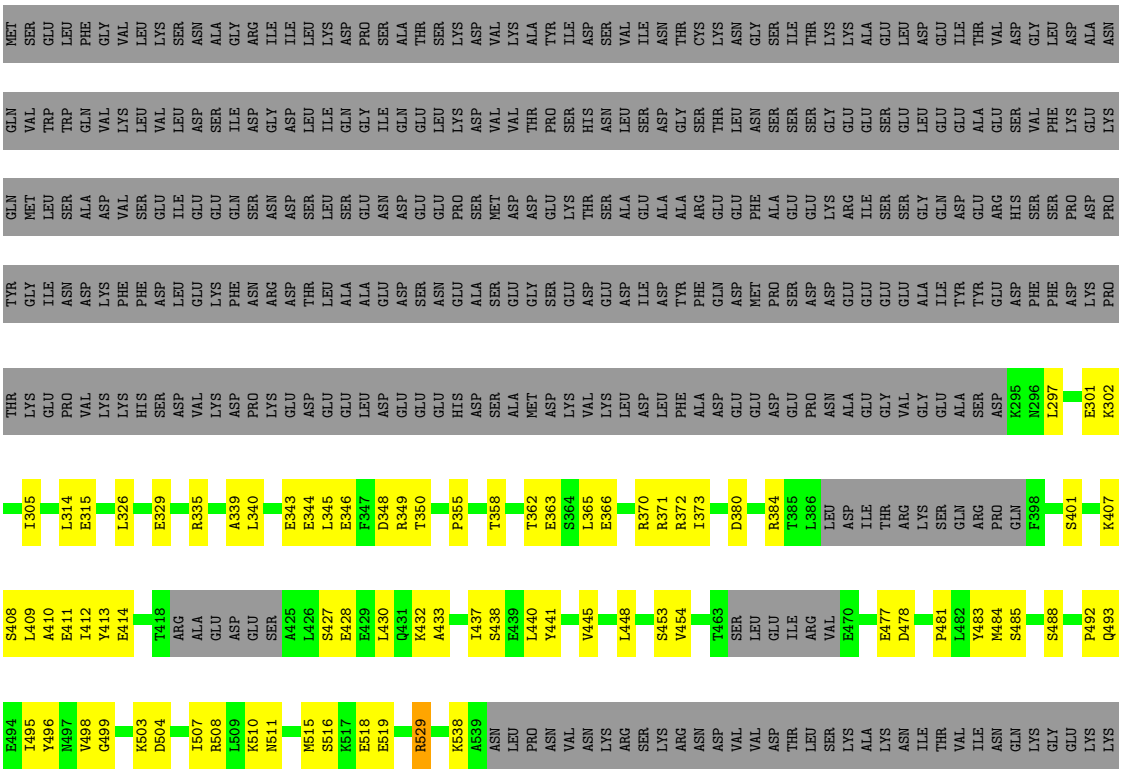
• Molecule 31: U3 small nucleolar ribonucleoprotein protein IMP4

Chain CJ:



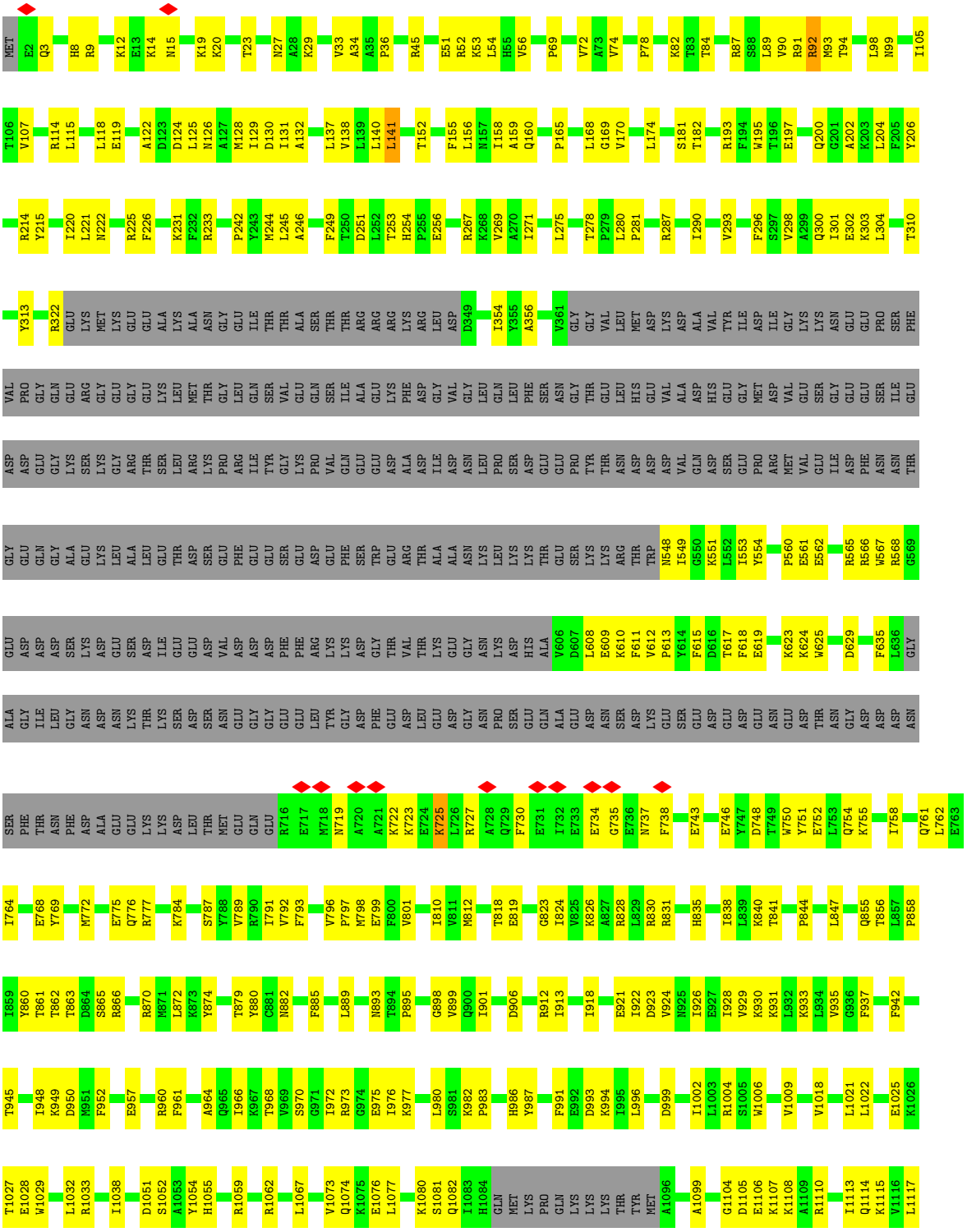
• Molecule 32: U3 small nucleolar RNA-associated protein MPP10

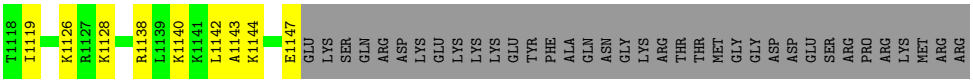
Chain CK:



• Molecule 33: Ribosome biogenesis protein BMS1

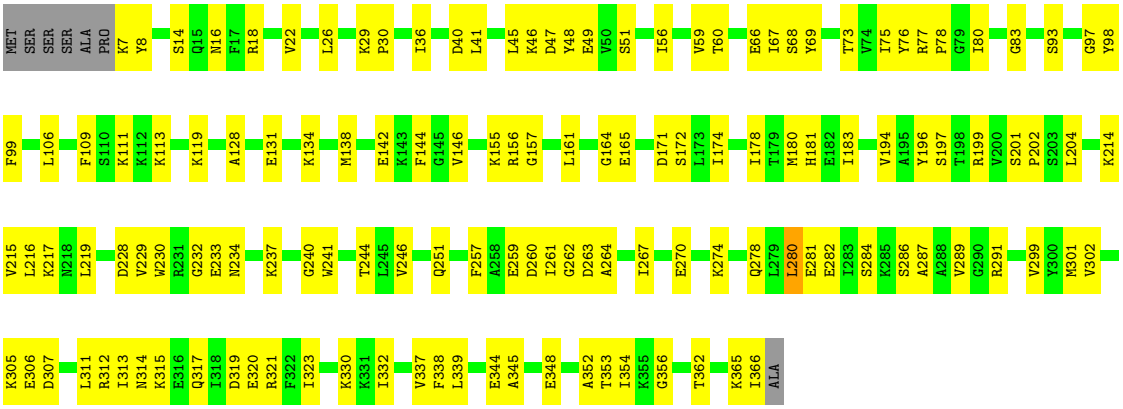
Chain CL:





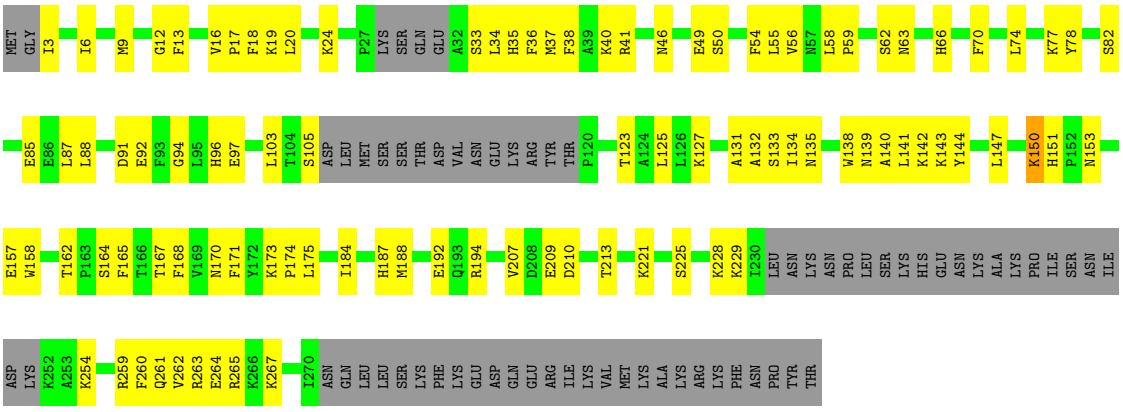
• Molecule 34: RNA 3'-terminal phosphate cyclase-like protein

Chain CM:



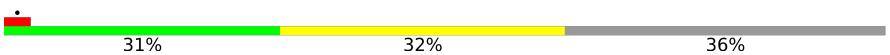
• Molecule 35: Ribosomal RNA-processing protein 7

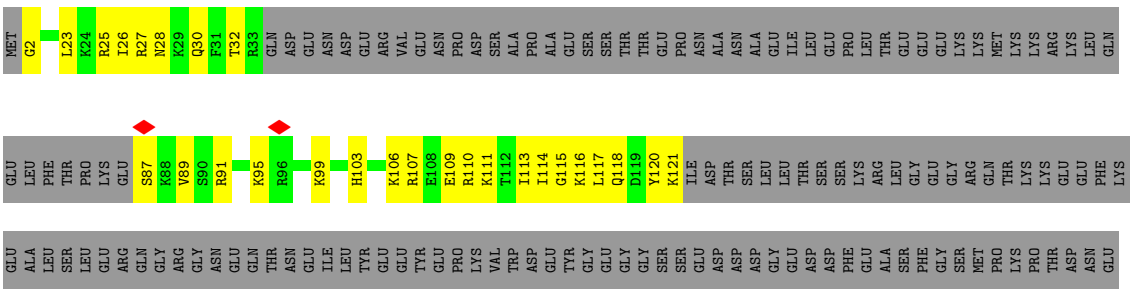
Chain CN:

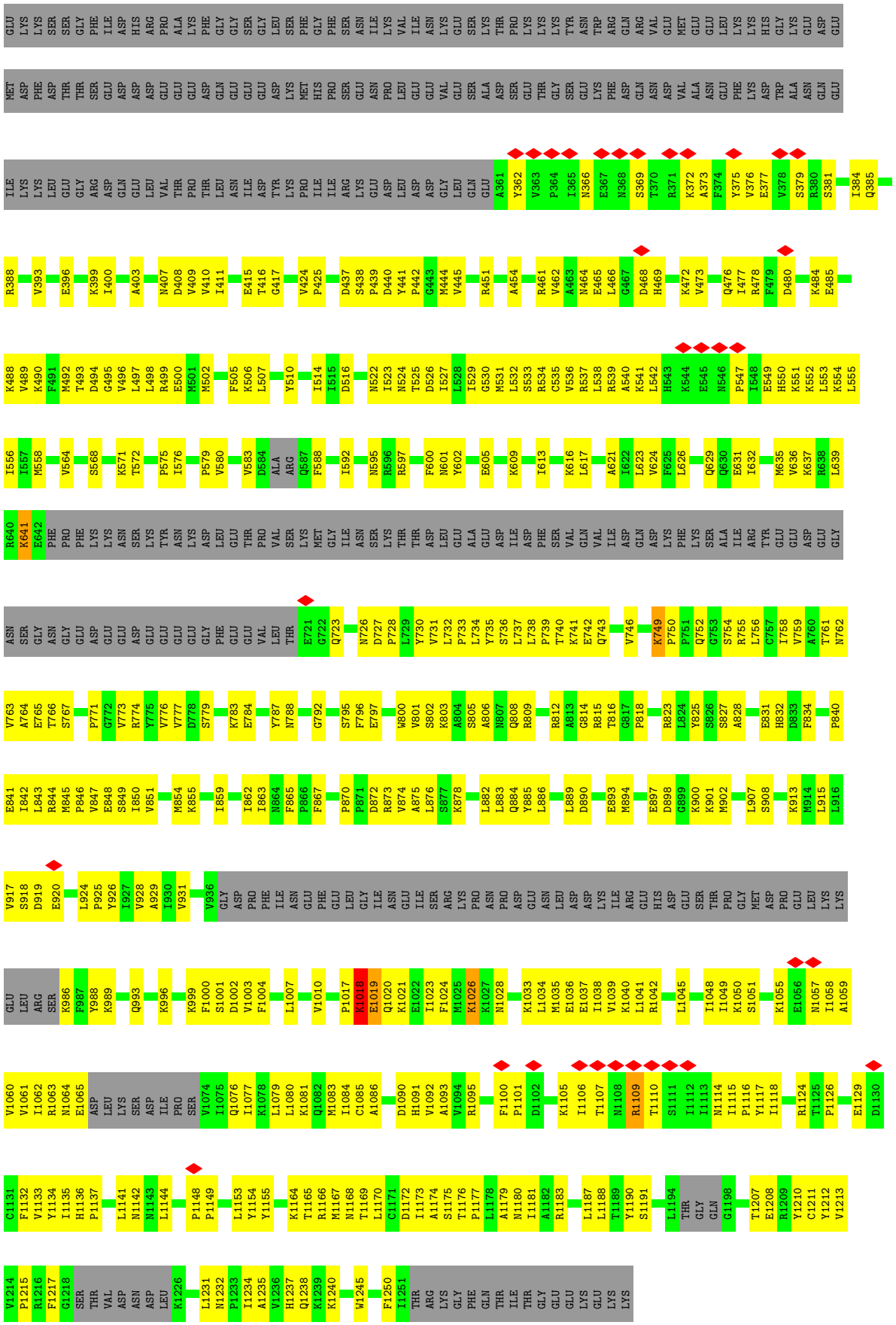


• Molecule 36: Probable ATP-dependent RNA helicase DHR1

Chain JD:

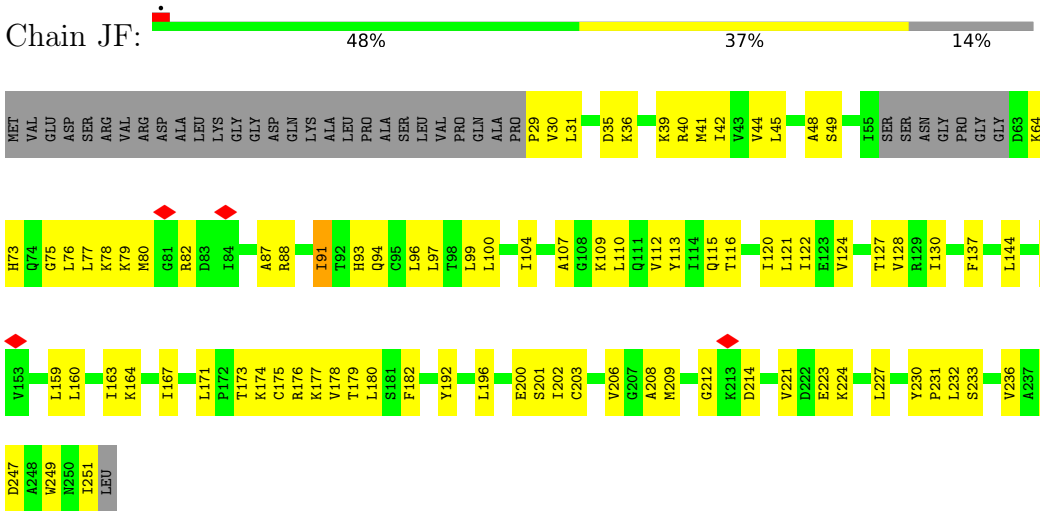





GLU LYS LYS SER SER GLY PHE ILE ASP HIS ARG PRO ALA LYS PHE GLY GLY SER GLY LYS GLU GLU
MET ASP PHE ASP THR THR SER GLU ASP ASP GLU GLU GLU ASP GLN GLU GLU GLU ASP LYS MET HIS PRO SER GLU ASN PRO LEU GLU GLU VAL GLU SER LYS ASP ASP SER GLU THR GLY SER GLU LYS PHE ASP GLN ASN ASP VAL ALA ASN GLU PHE LYS ASP TRP ALA ASN GLN GLU
ILE LYS LYS LEU GLU GLY ARG ASP GLN GLU LEU VAL THR PRO THR LEU ASN ILE ASP TYR LYS PRO ILE ILE ARG LYS GLU ASP GLY LEU GLN GLU A361 Y362 V363 P364 I365 N366 E367 N368 S369 T370 R371 K372 A373 F374 Y375 V376 E377 V378 S379 R380 S381 I384 Q385
R388 V393 E396 K399 I400 A403 N407 D408 V409 V410 I411 E415 T416 G417 V424 P425 D437 S438 P439 D440 Y441 P442 G443 M444 V445 R451 A454 R461 V462 A463 N464 E465 L466 G467 D468 H469 K472 V473 Q476 I477 R478 F479 D480 K484 E485
K488 V489 K490 F491 M492 T493 D494 G495 V496 L497 L498 R499 E500 M501 M502 F505 K506 L507 Y510 I514 I515 D516 N522 I523 N524 T525 D526 I527 L528 I529 G530 M531 L532 S533 R534 C535 V536 R537 L538 R539 A540 K541 L542 H543 K544 E545 N546 P547 I548 E549 H550 K551 K552 L553 K554 L555
I556 I557 M558 V564 S568 K571 T572 P575 I576 P579 V580 V583 D584 A585 R587 F588 I592 N595 R596 R597 F600 N601 Y602 E605 K609 I613 K616 L617 A621 I622 L623 V624 F625 L626 Q629 Q630 E631 I632 M635 V636 K637 R638 L639
R640 K641 E642 PHE PRO PHE LYS LYS ASN SER LYS TYR ASN LYS ASP LEU GLU THR PRO VAL LEU SER LYS MET GLY ILE ASN SER LYS THR THR ASP LEU GLU ALA GLU ASP ILE ASP PHE SER VAL GLN VAL ILE ASP GLN ASP LYS PHE LYS SER ALA ILE ARG TYR GLU GLU ASP GLU GLY
ASN SER GLY ASN GLY GLU ASP GLU GLU ASP GLU GLU GLU GLY PHE GLU GLU VAL LEU THR E721 Q722 Q723 N726 D727 P728 L729 Y730 V731 L732 P733 L734 Y735 S736 L737 L738 P739 T740 K741 E742 Q743 V746 K749 P750 P751 Q752 G753 S754 R755 L756 C757 I758 V759 A760 T761 N762
V763 A764 E765 T766 S767 P771 G772 V773 R774 Y775 V776 V777 D778 S779 K783 E784 Y787 N788 G792 S795 F796 E797 W800 V801 S802 K803 A804 S805 A806 N807 Q808 R809 R812 A813 G814 R815 T816 G817 P818 R823 L824 Y825 S826 S827 A828 E831 H832 D833 F834 P840
E841 I842 L843 R844 M845 P846 V847 E848 S849 I850 V851 M854 K855 I859 I862 I863 N864 F865 P866 F867 P870 P871 D872 R873 V874 A875 L876 S877 K878 L882 L883 Q884 Y885 L886 L889 D890 E893 M894 E897 D898 G899 K900 K901 M902 L907 S908 K913 M914 L915 L916
V917 S918 D919 E920 L924 P925 Y926 I927 V928 A929 I930 V931 V936 GLY ASP PRO PHE ILE ASN GLU PHE GLU LEU GLY ILE ASN GLU ILE SER ARG LYS PRO ASN PRO ASP GLU ASN LEU ASP LYS ILE ARG GLU HIS ASP GLY MET ASP PRO GLU LEU LYS LYS
GLU LEU ARG SER K986 F987 Y988 K989 Q993 K996 K999 F1000 S1001 D1002 V1003 F1004 L1007 V1010 P1017 K1018 E1019 Q1020 K1021 E1022 I1023 F1024 M1025 K1026 K1027 N1028 K1033 L1034 M1035 E1036 E1037 I1038 V1039 K1040 L1041 R1042 L1045 I1048 I1049 K1050 S1051 K1055 E1056 N1057 I1058 A1059
V1060 V1061 I1062 R1063 N1064 E1065 ASP LEU LYS SER ASP ILE PRO SER V1074 I1075 Q1076 I1077 K1078 L1079 L1080 K1081 Q1082 M1083 I1084 C1085 A1086 D1090 H1091 V1092 A1093 V1094 R1095 F1100 P1101 D1102 K1105 I1106 T1107 N1108 R1109 T1110 S1111 I1112 I1113 N1114 I1115 P1116 Y1117 I1118 R1124 T1125 P1126 E1129 D1130
C1131 F1132 V1133 Y1134 I1135 H1136 P1137 L1141 N1142 N1143 L1144 P1148 P1149 L1153 Y1154 Y1155 K1164 T1165 R1166 M1167 N1168 T1169 L1170 C1171 D1172 I1173 A1174 S1175 T1176 P1177 L1178 A1179 N1180 I1181 A1182 R1183 L1187 L1188 T1189 Y1190 S1191 L1194 THR GLY GLN G1198 T1207 E1208 R1209 Y1210 C1211 Y1212 V1213
V1214 P1215 R1216 F1217 G1218 SER THR VAL ASP ASN ASP LEU K1226 L1231 N1232 P1233 I1234 A1235 V1236 H1237 Q1238 K1239 K1240 W1245 F1250 I1251 THR ARG LYS GLY PHE GLN THR ILE THR GLY GLU GLU LYS GLU LYS LYS

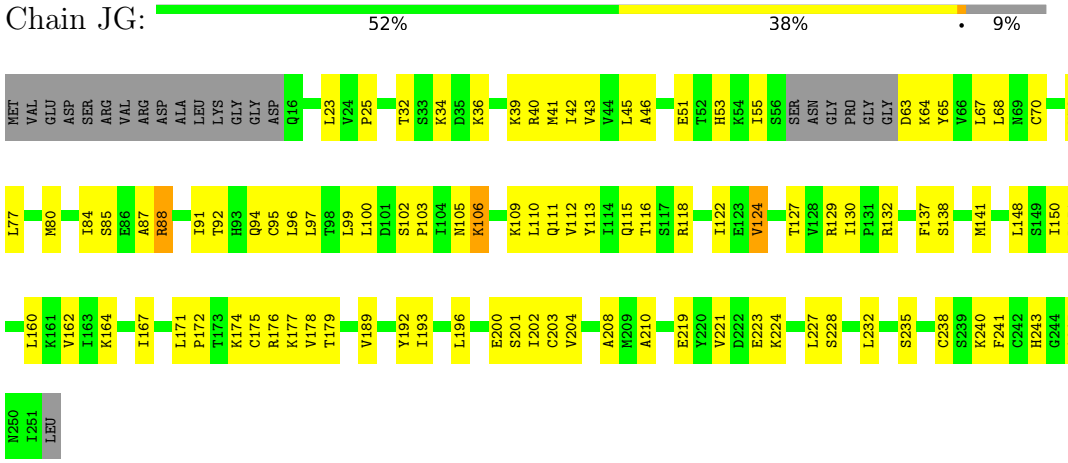
• Molecule 37: Ribosomal RNA small subunit methyltransferase NEP1

Chain JF:



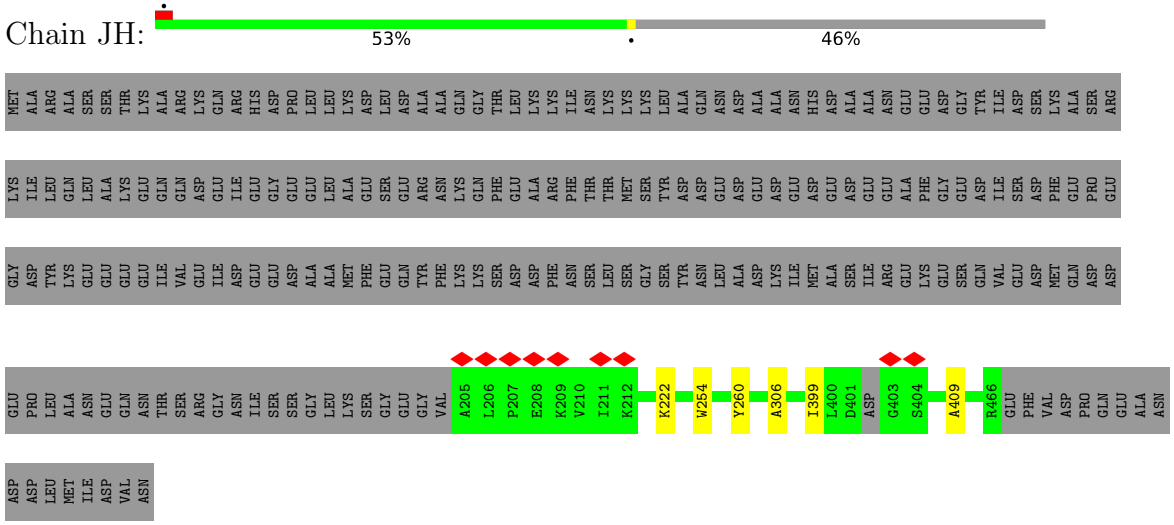
• Molecule 37: Ribosomal RNA small subunit methyltransferase NEP1

Chain JG:



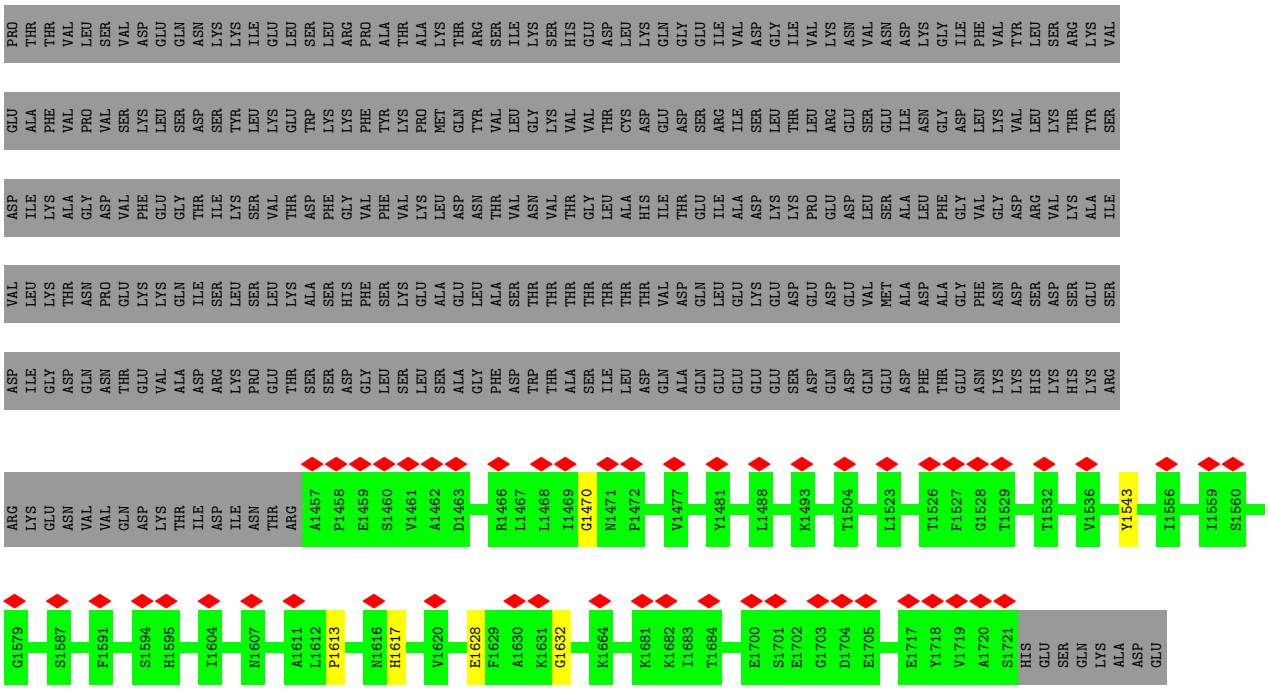
• Molecule 38: Essential nuclear protein 1

Chain JH:



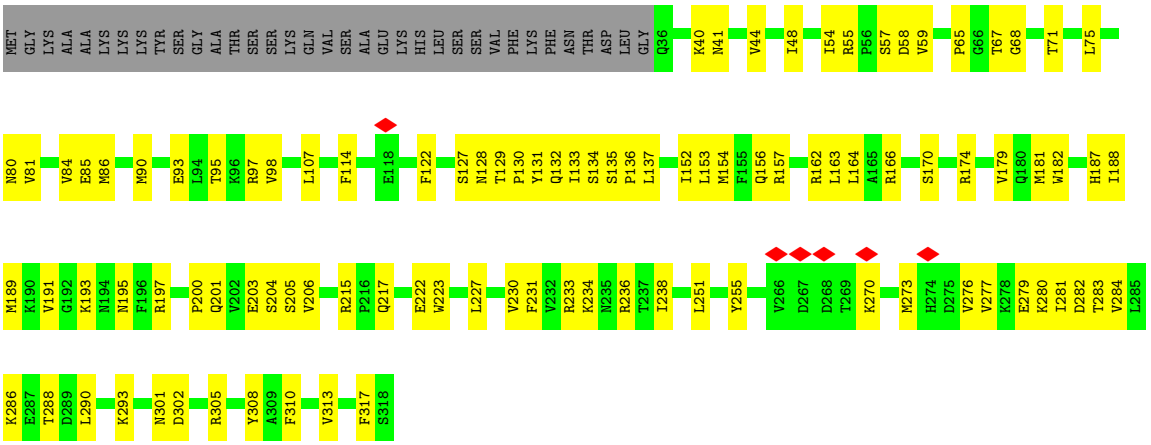
• Molecule 39: rRNA biogenesis protein RRP5

Chain JI:



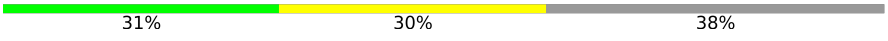
• Molecule 40: Dimethyladenosine transferase

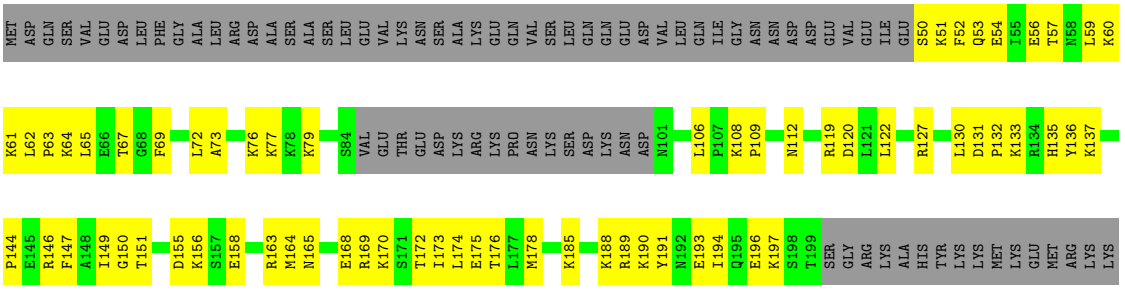
Chain JL:



• Molecule 41: rRNA-processing protein FCF2

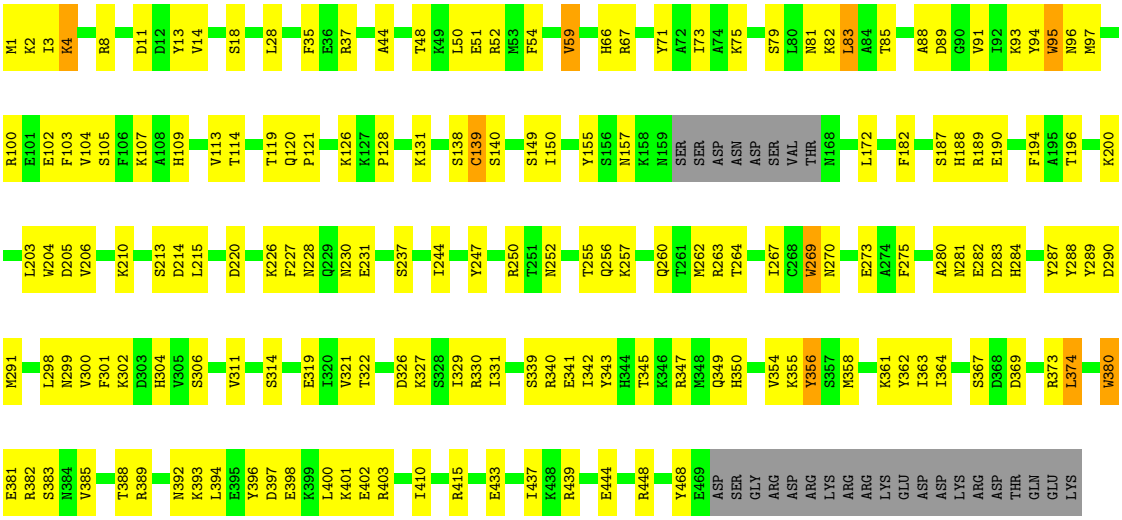
Chain JM:





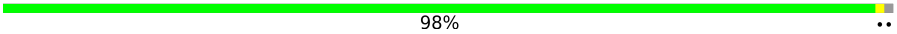
• Molecule 42: Protein SOF1

Chain JP:



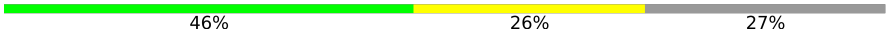
• Molecule 43: 40S ribosomal protein S27-A

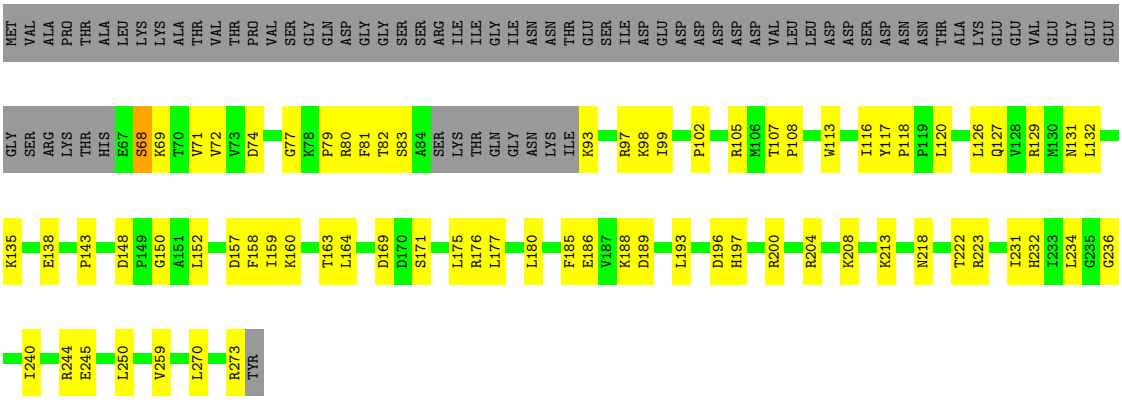
Chain Db:



• Molecule 44: Pre-rRNA-processing protein PNO1

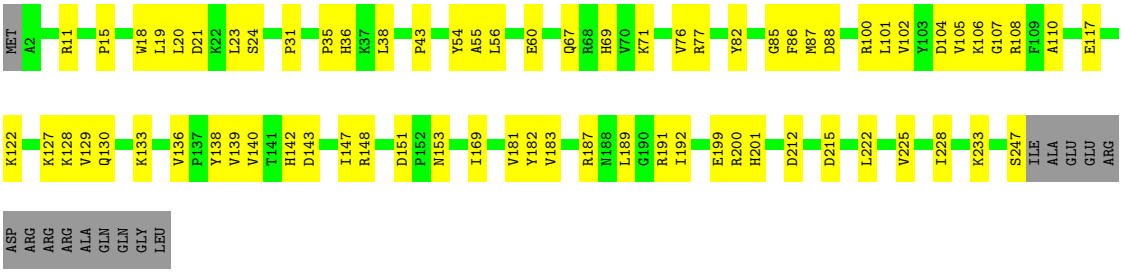
Chain JJ:





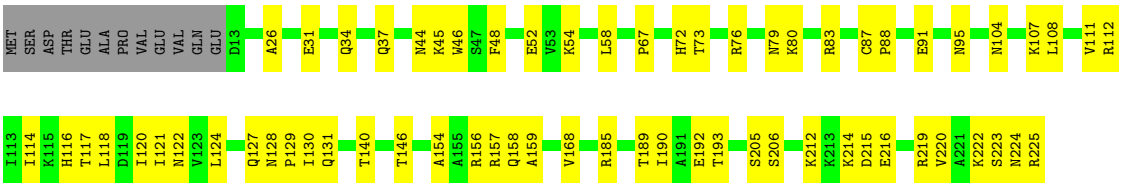
• Molecule 45: 40S ribosomal protein S4-A

Chain DE:



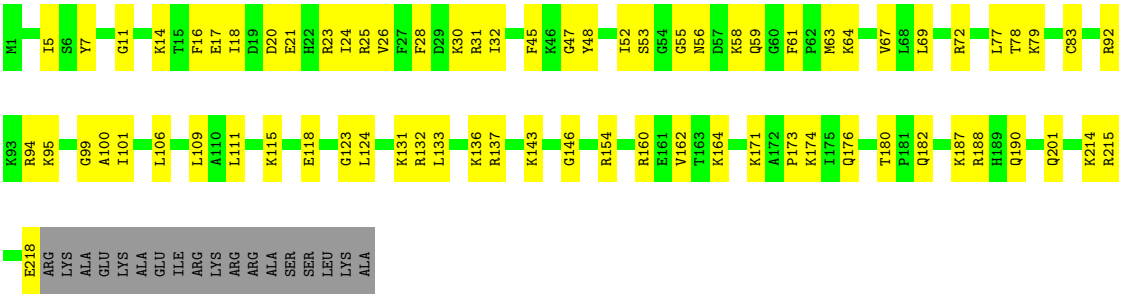
• Molecule 46: 40S ribosomal protein S5

Chain DF:



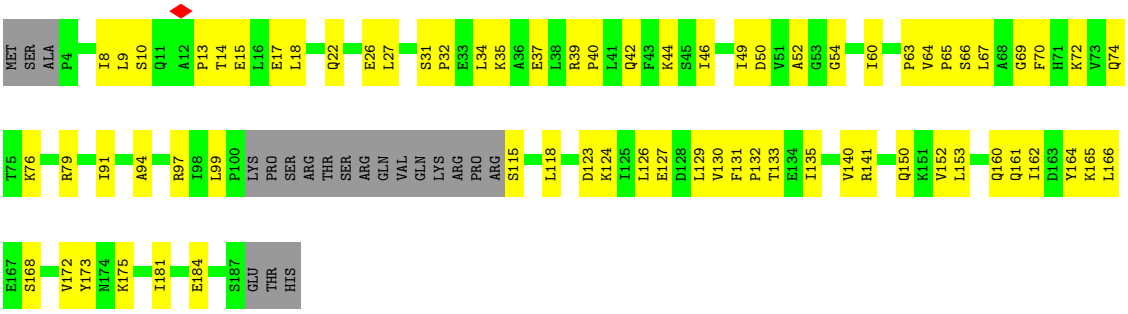
• Molecule 47: 40S ribosomal protein S6-A

Chain DG:



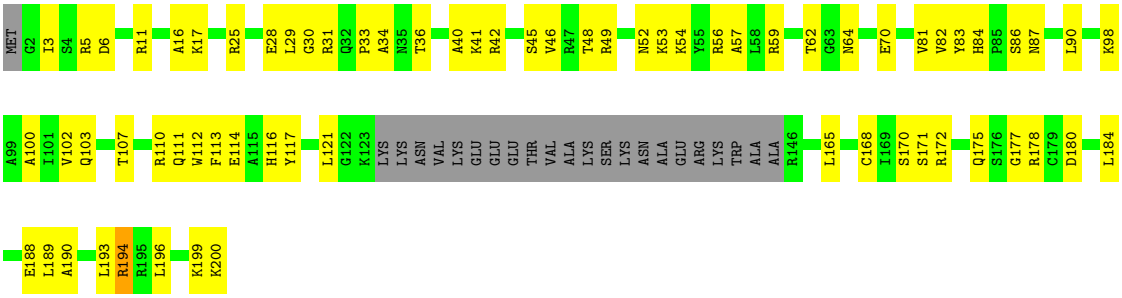
• Molecule 48: 40S ribosomal protein S7-A

Chain DH:



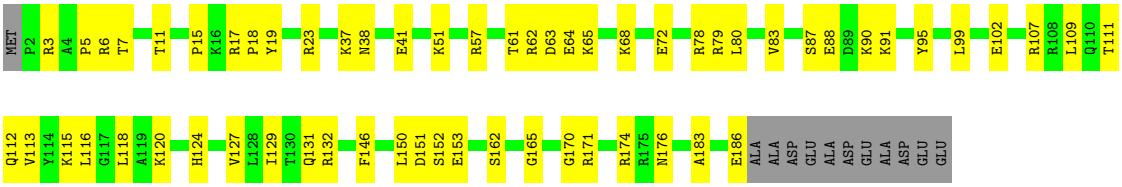
• Molecule 49: 40S ribosomal protein S8-A

Chain DI:



• Molecule 50: 40S ribosomal protein S9-A

Chain DJ:

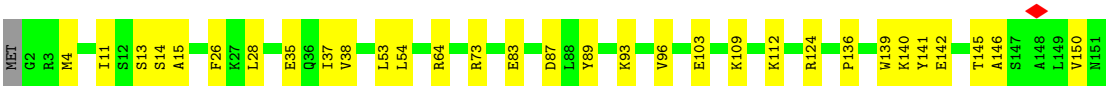


• Molecule 51: 40S ribosomal protein S11-A

Chain DL:

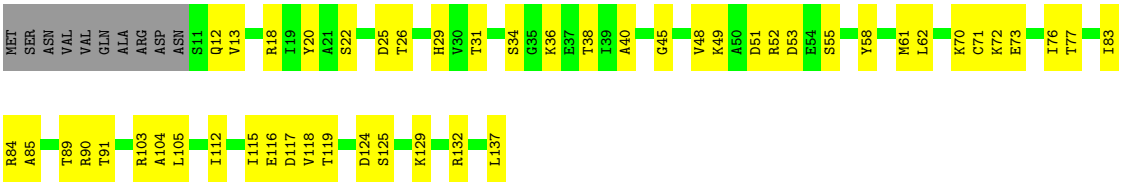
• Molecule 52: 40S ribosomal protein S13

Chain DN:



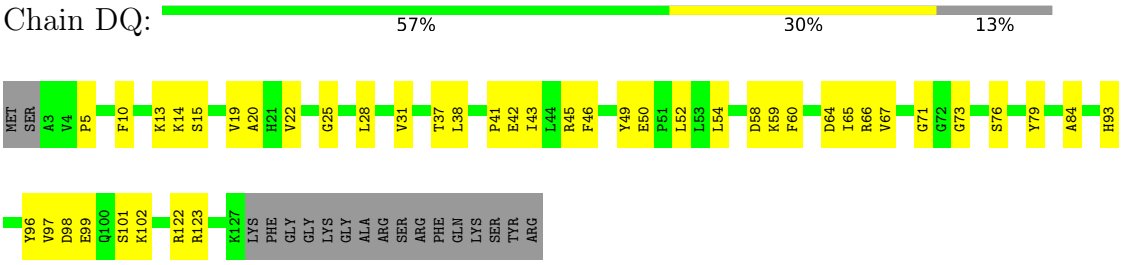
• Molecule 53: 40S ribosomal protein S14-A

Chain DO:



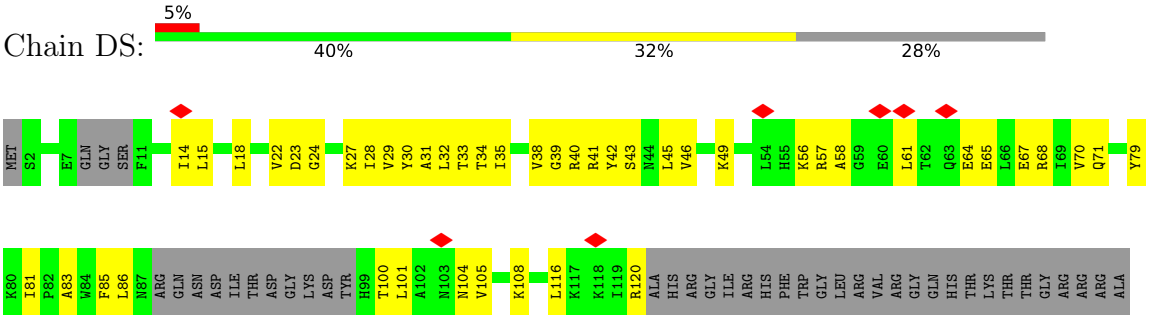
• Molecule 54: 40S ribosomal protein S16-A

Chain DQ:



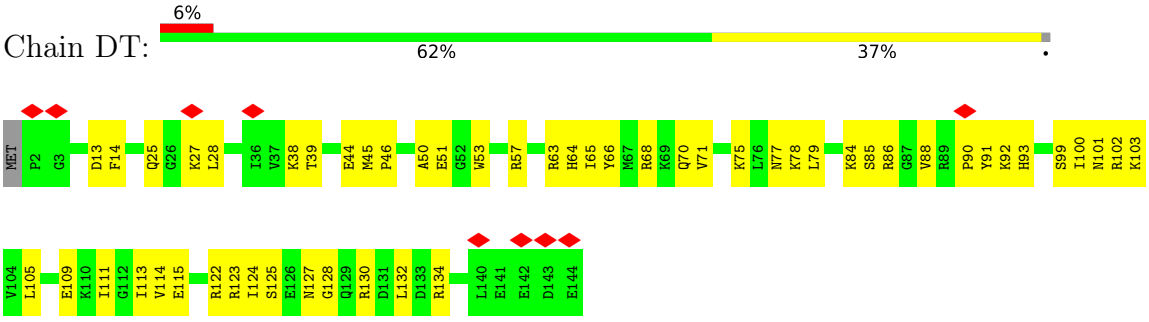
• Molecule 55: 40S ribosomal protein S18-A

Chain DS:



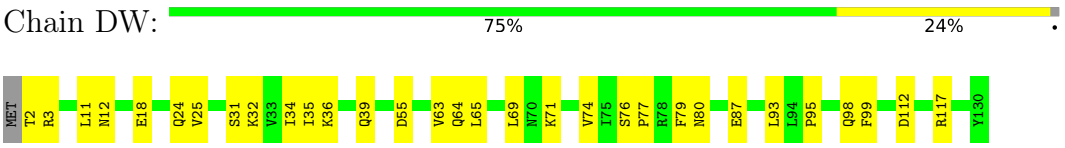
• Molecule 56: 40S ribosomal protein S19-A

Chain DT:



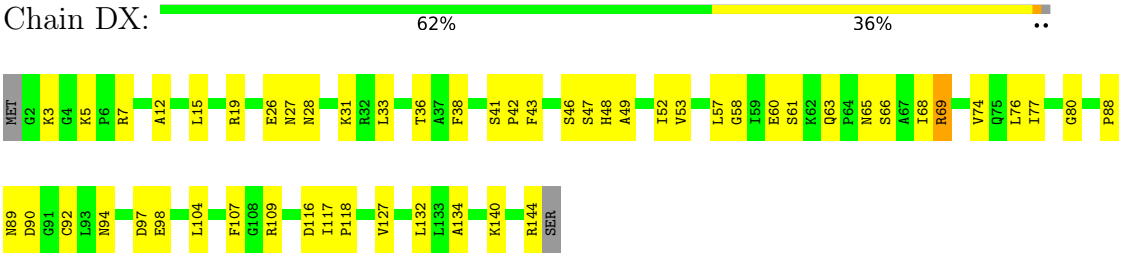
• Molecule 57: 40S ribosomal protein S22-A

Chain DW:



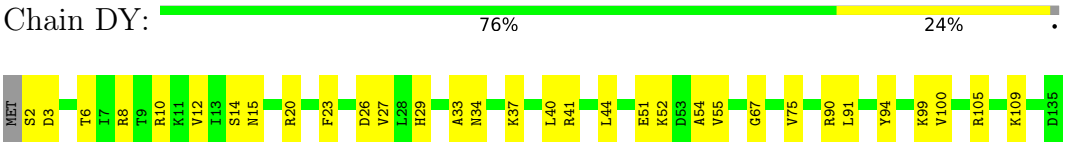
• Molecule 58: 40S ribosomal protein S23-A

Chain DX:



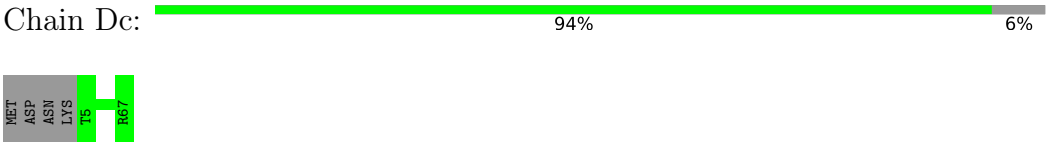
• Molecule 59: 40S ribosomal protein S24-A

Chain DY:



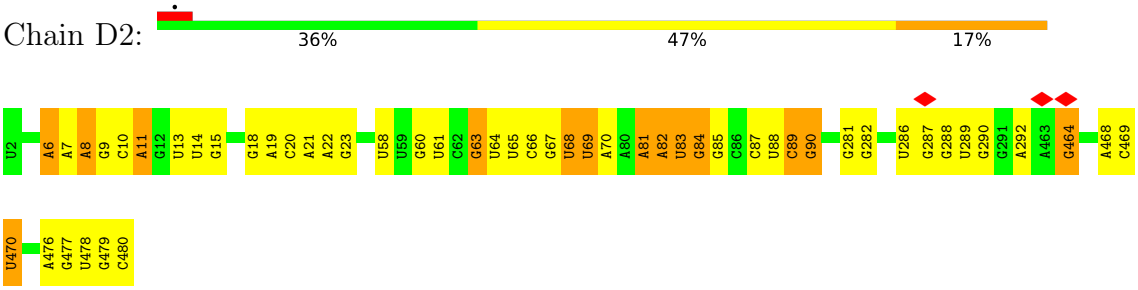
• Molecule 60: 40S ribosomal protein S28-A

Chain Dc:



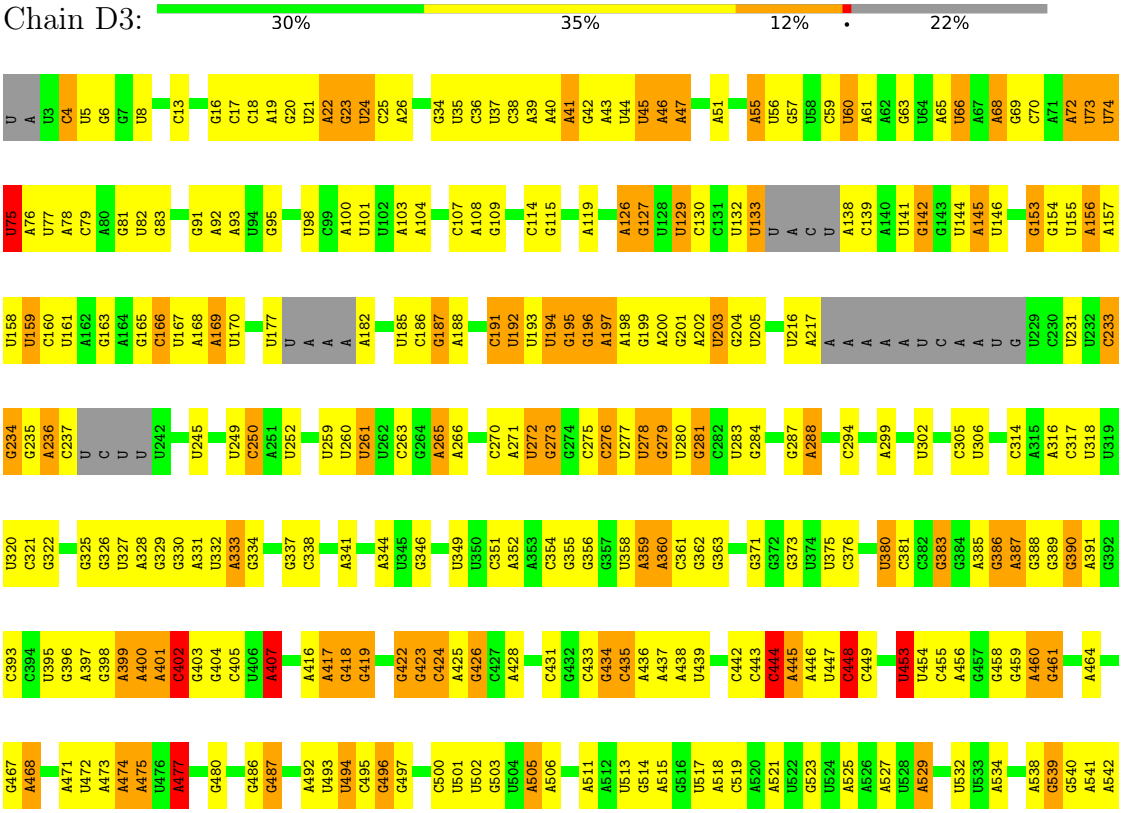
• Molecule 61: 5'ETS RNA

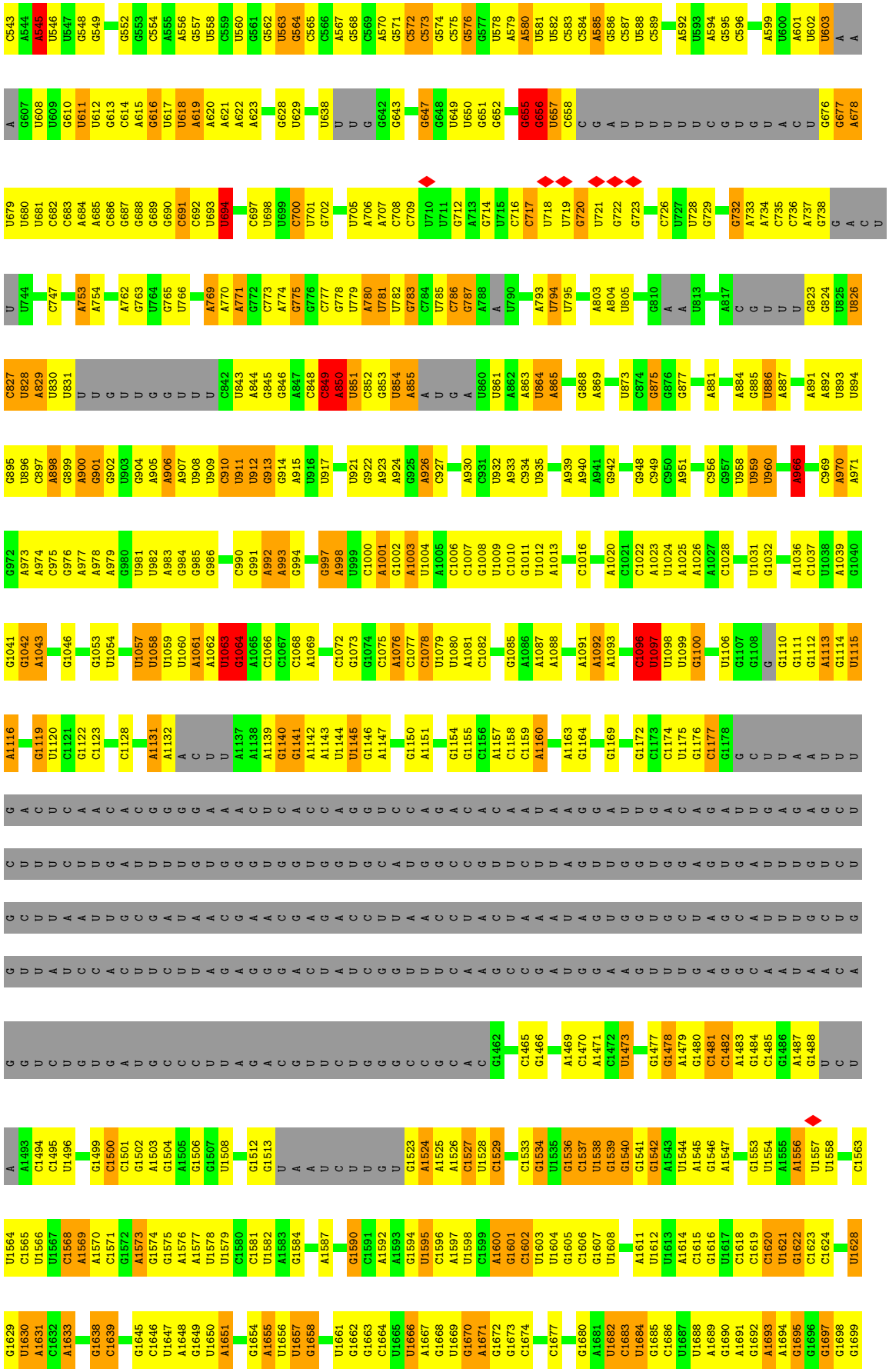
Chain D2:

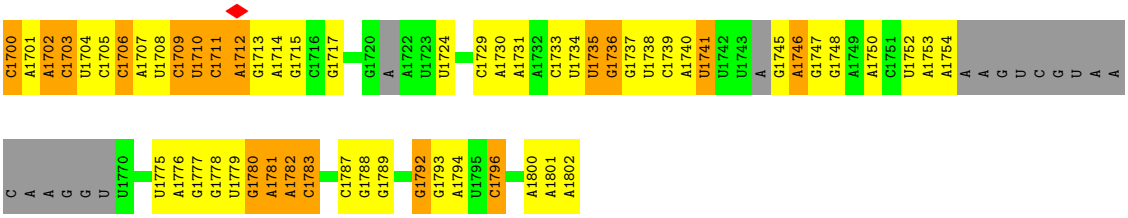


• Molecule 62: 18S rRNA

Chain D3:

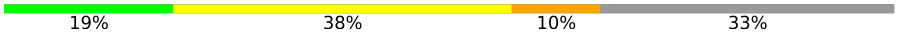


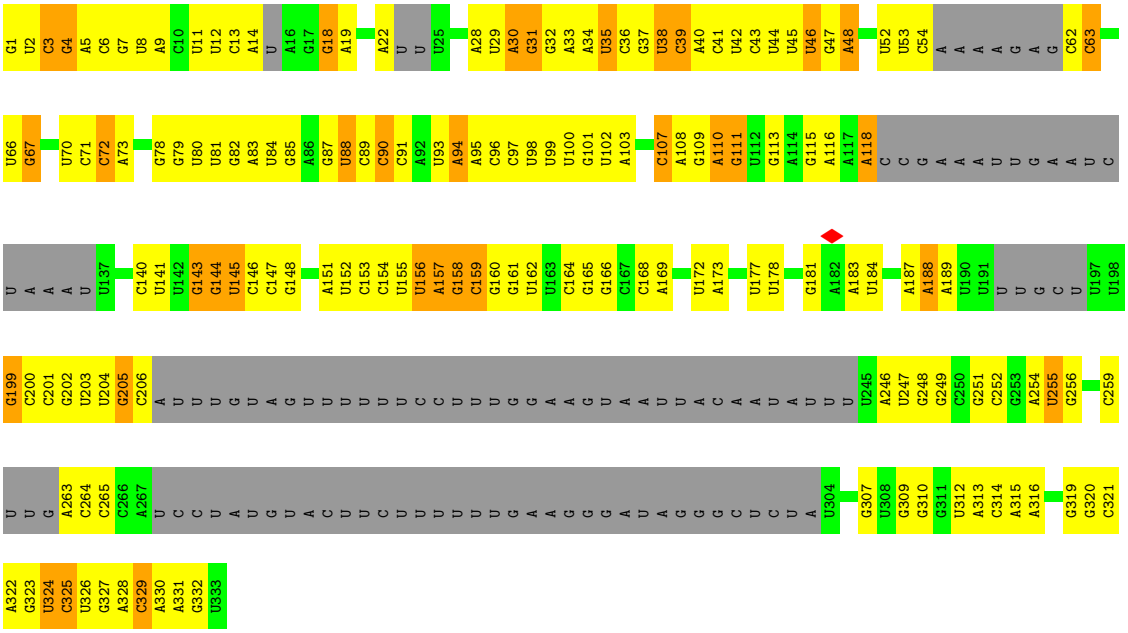




• Molecule 63: U3 snoRNA

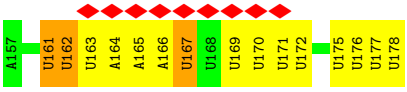
Chain D4:





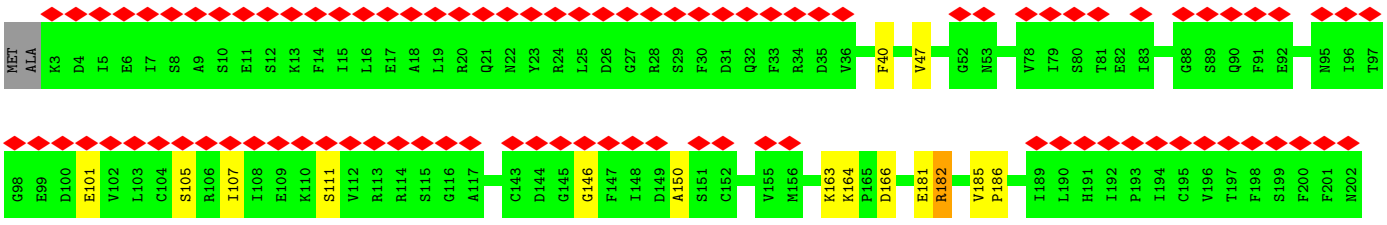
• Molecule 64: RNA

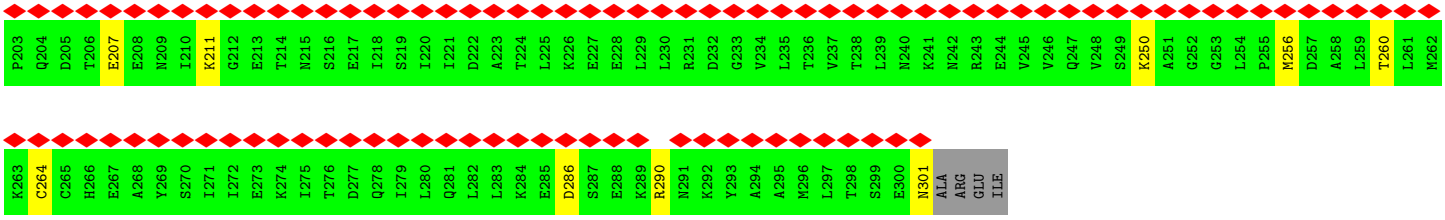
Chain EA:



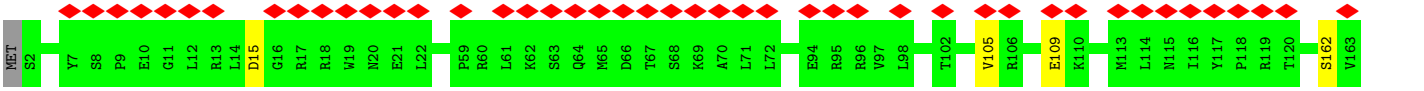
• Molecule 65: Exosome complex component RRP45

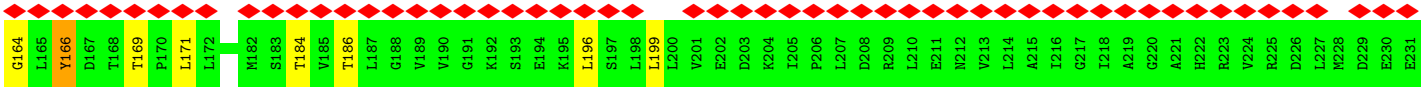
Chain EB:

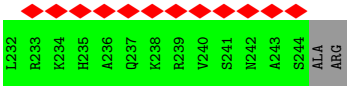




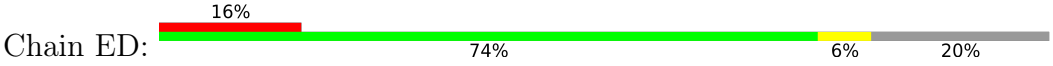
• Molecule 66: Exosome complex component SKI6

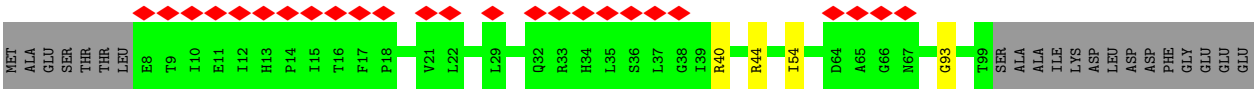


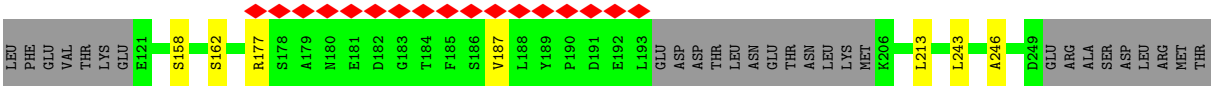


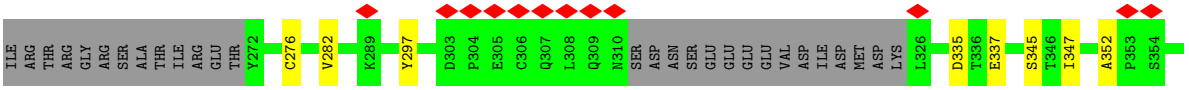


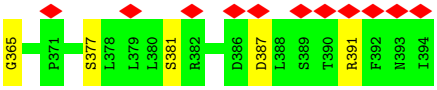
• Molecule 67: Exosome complex component RRP43



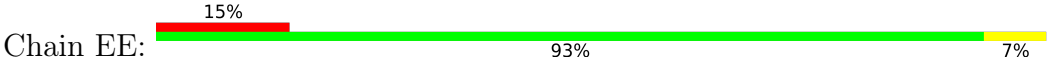


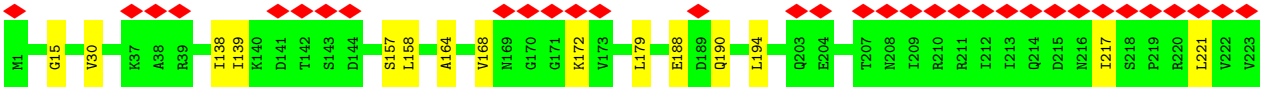






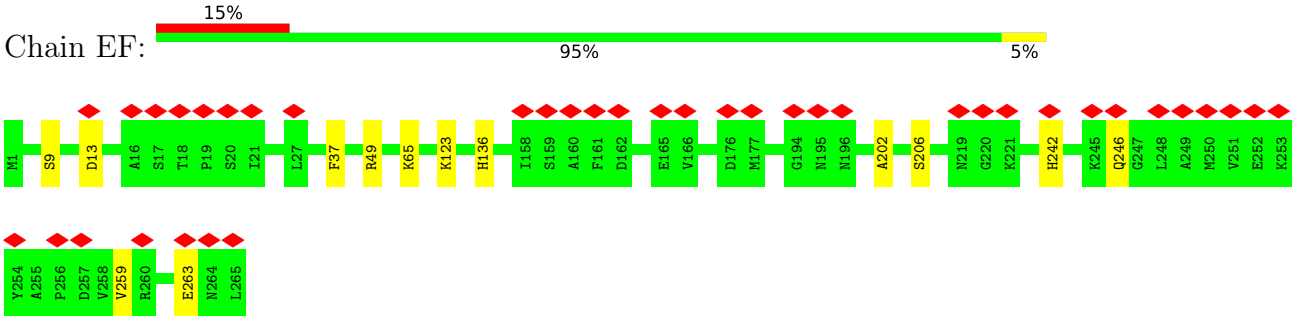
• Molecule 68: Exosome complex component RRP46





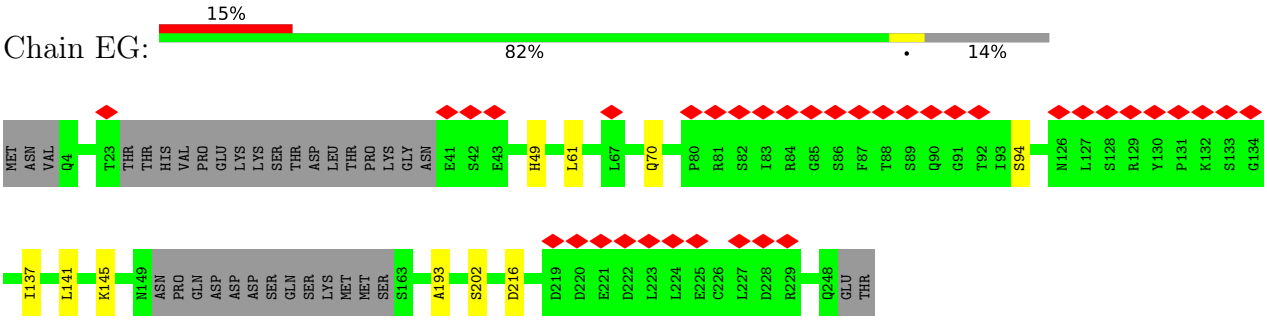
• Molecule 69: Exosome complex component RRP42

Chain EF:



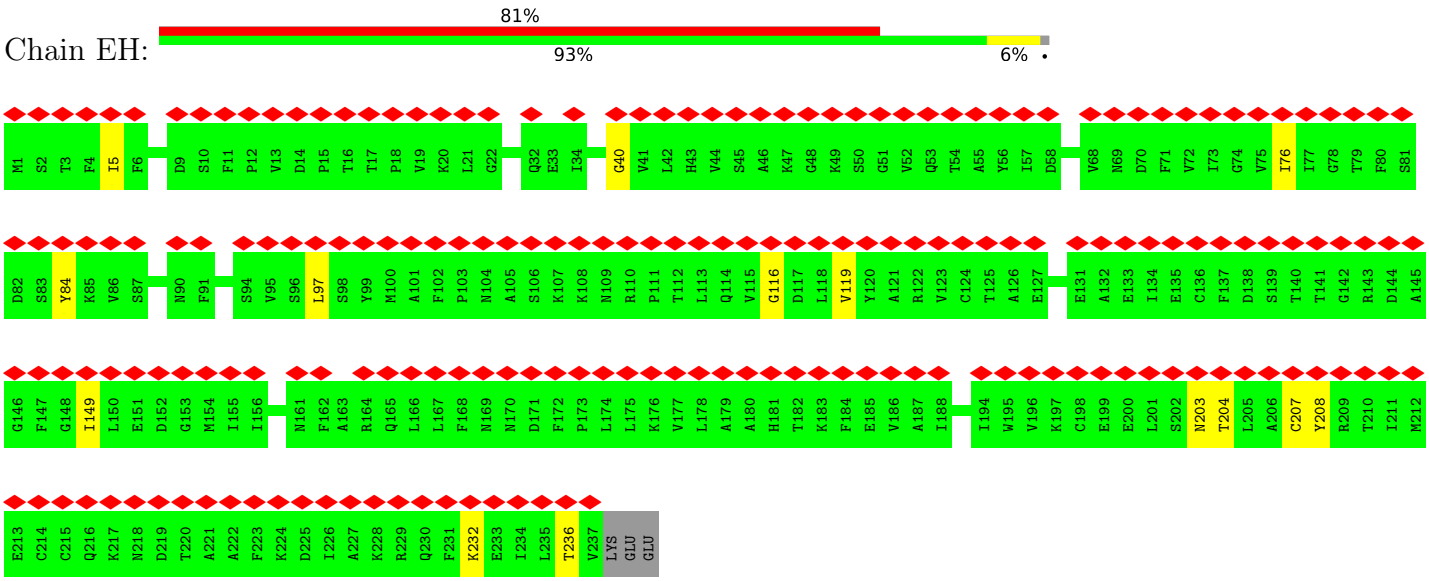
• Molecule 70: Exosome complex component MTR3

Chain EG:



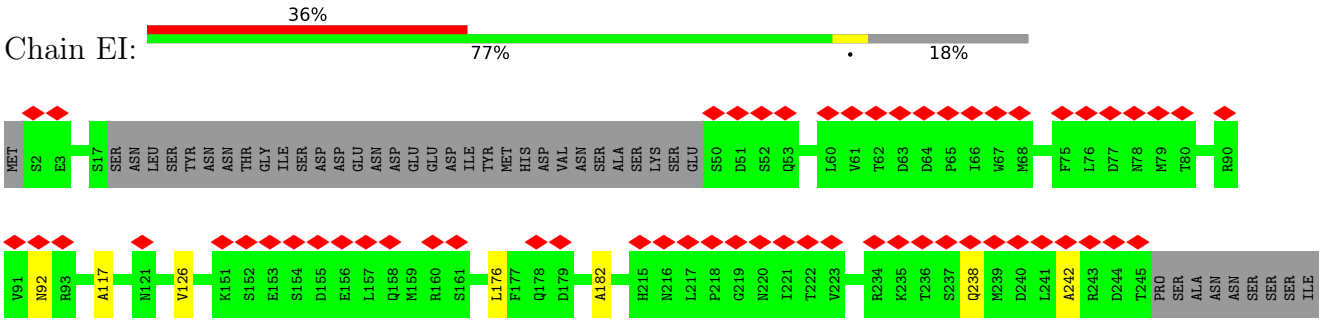
• Molecule 71: Exosome complex component RRP40

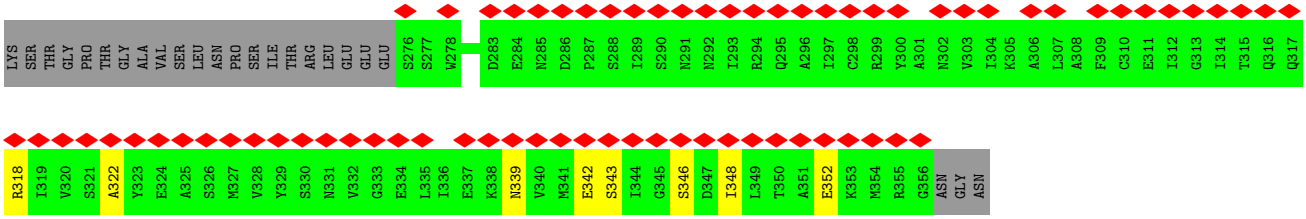
Chain EH:



• Molecule 72: Exosome complex component RRP4

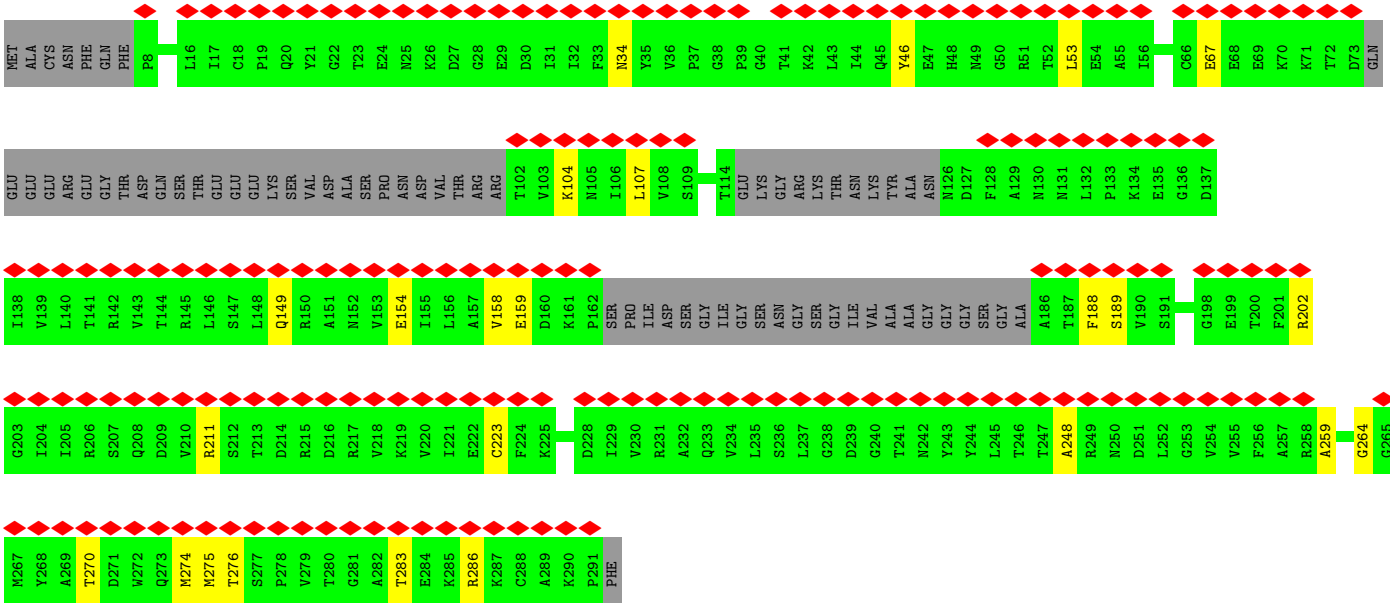
Chain EI:





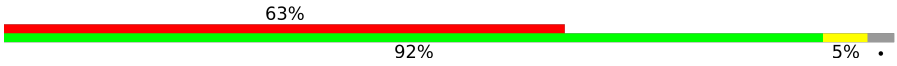
• Molecule 73: Exosome complex component CSL4

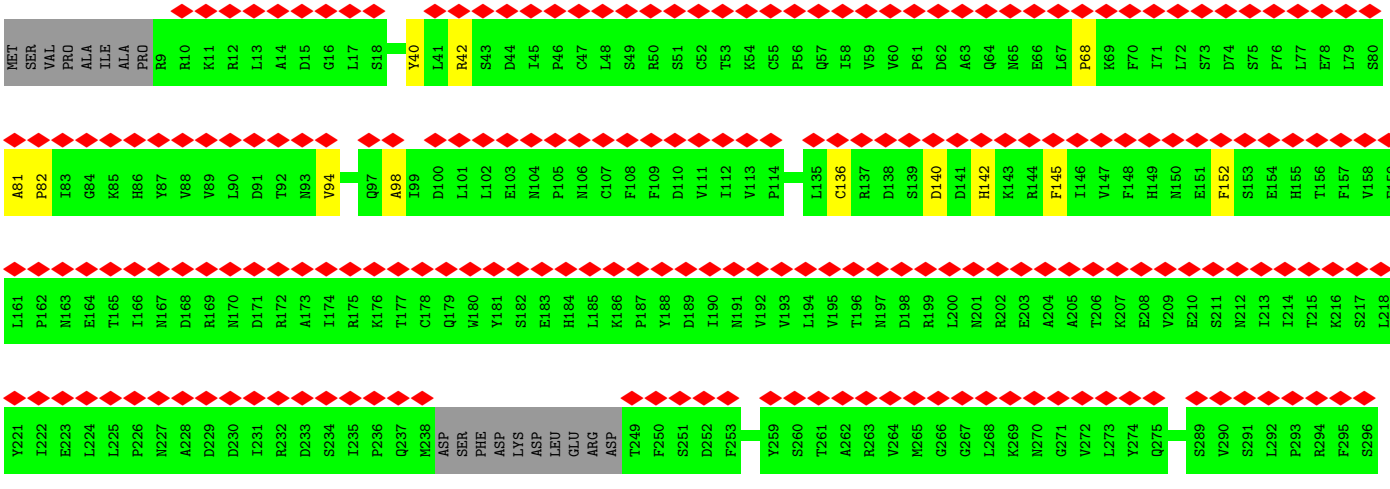
Chain EJ:

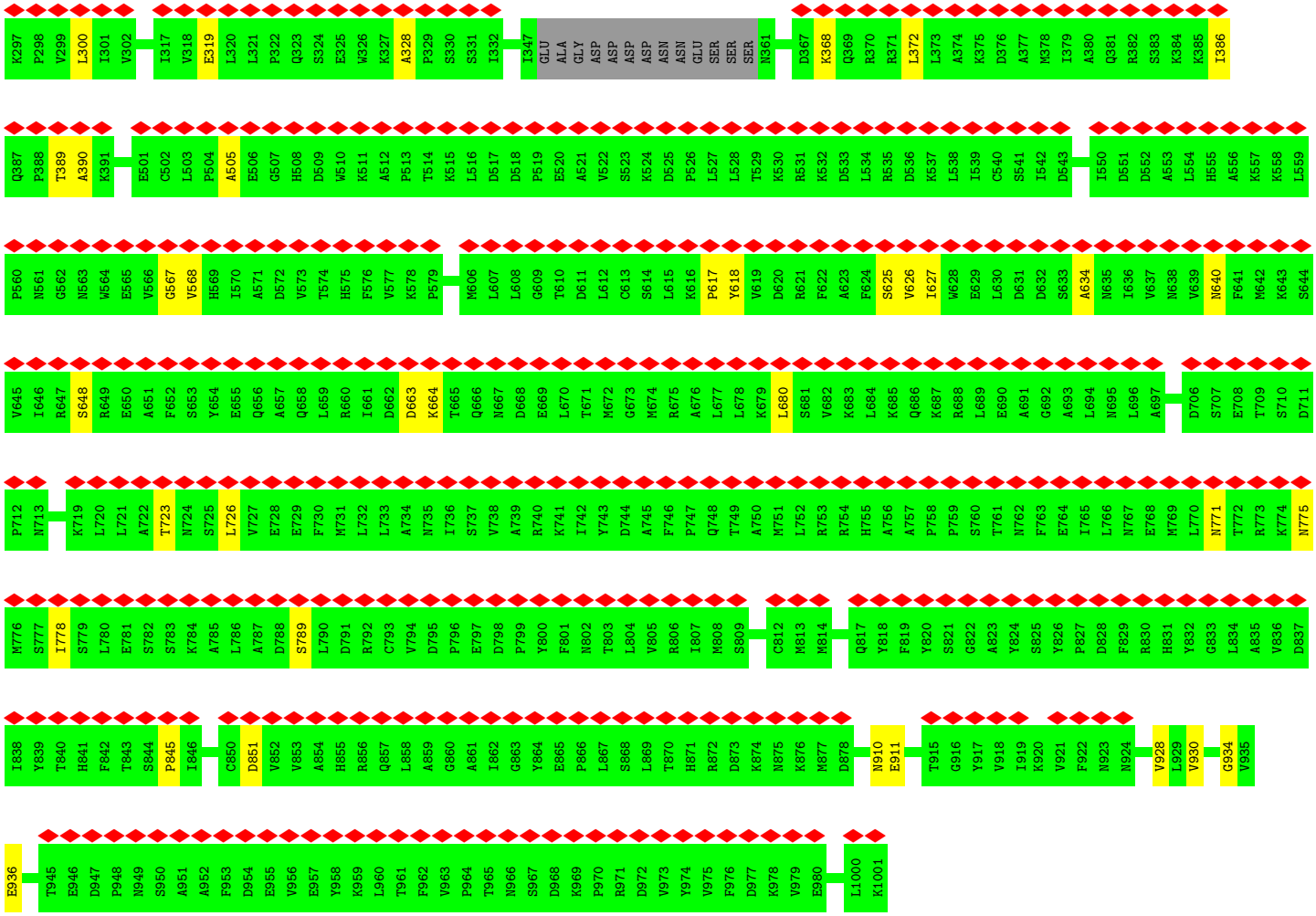


• Molecule 74: Exosome complex exonuclease DIS3

Chain EK:

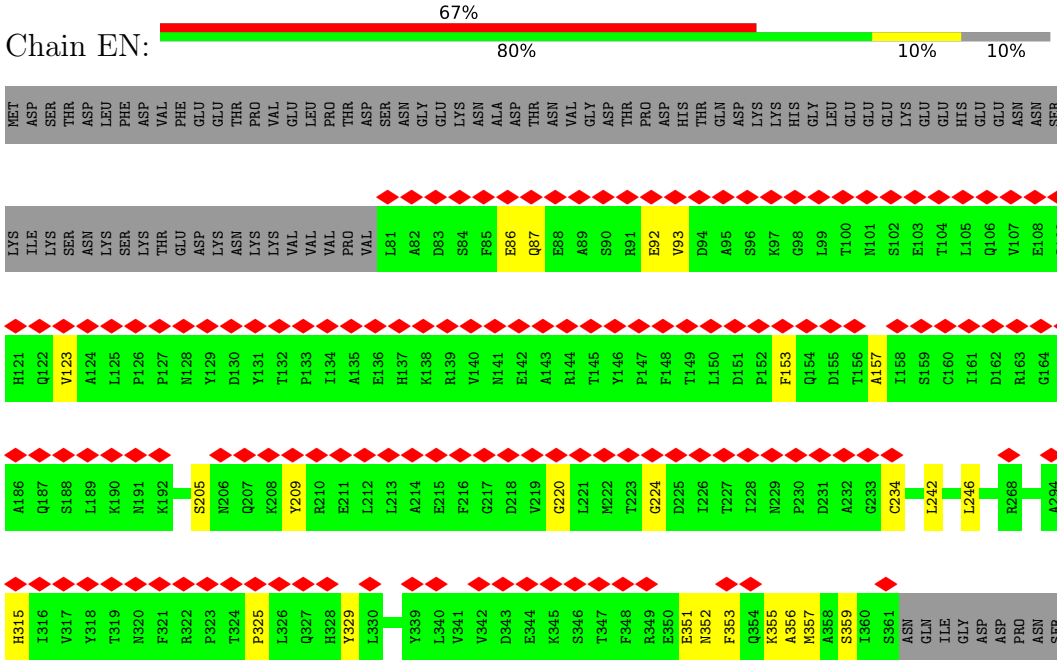


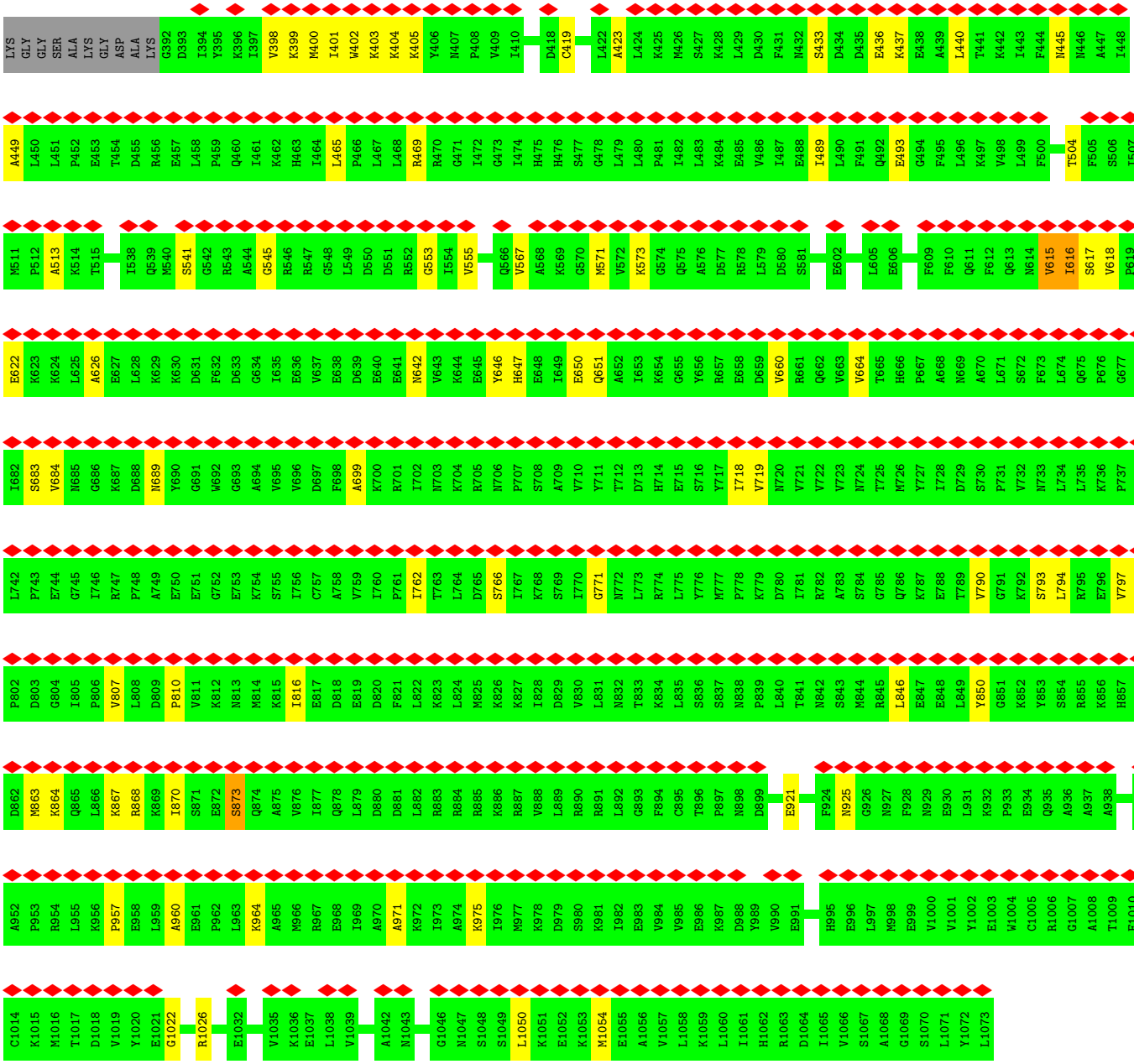




• Molecule 75: ATP-dependent RNA helicase DOB1

Chain EN:




LYS GLY GLY SER ALA LYS GLY ASP ALA LYS
G392 D393 I394 Y395 K396 I397 V398 K399 M400 I401 W402 K403 K404 K405 Y406 N407 P408 V409 I410 D418 C419 L422 A423 L424 K425 M426 S427 K428 L429 D430 F431 N432 S433 D434 D435 E436 K437 E438 A439 L440 T441 K442 I443 F444 N445 N446 A447 I448
A449 L450 L451 P452 E453 T454 D455 R456 E457 L458 P459 Q460 I461 K462 H463 I464 L465 P466 L467 L468 R469 R470 G471 I472 G473 I474 H475 H476 S477 G478 L479 L480 P481 I482 L483 K484 E485 V486 I487 E488 I489 L490 F491 Q492 E493 G494 F495 L496 K497 V498 L499 F500 T504 F505 S506 I507 G508 L509 N510
M511 P512 A513 K514 T515 I538 Q539 M540 S541 G542 R543 A544 G545 R546 R547 G548 L549 D550 D551 R552 G553 I554 V555 Q566 V567 A568 K569 G570 M571 V572 K573 G574 Q575 A576 D577 R578 L579 D580 S581 E602 L605 E606 F609 F610 Q611 F612 Q613 N614 V615 I616 S617 V618 P619 V620 M621
E622 K623 K624 L625 A626 E627 L628 K629 K630 D631 F632 D633 G634 I635 E636 V637 E638 D639 E640 E641 N642 V643 K644 E645 Y646 H647 E648 I649 E650 Q651 A652 I653 K654 G655 Y656 R657 E658 D659 V660 R661 Q662 V663 V664 T665 H666 P667 A668 N669 A670 L671 S672 F673 L674 Q675 P676 G677 R678 L679 V680 E681
I682 S683 V684 N685 G686 K687 D688 N689 Y690 G691 W692 G693 A694 V695 V696 D697 F698 A699 K700 R701 I702 N703 K704 R705 N706 P707 S708 A709 V710 Y711 T712 D713 H714 E715 S716 Y717 I718 V719 N720 V721 V722 V723 N724 T725 M726 Y727 I728 D729 S730 P731 V732 N733 L734 L735 K736 P737 F738 N739 P740 T741
L742 P743 E744 G745 I746 R747 P748 A749 E750 E751 G752 E753 K754 S755 I756 C757 A758 V759 I760 P761 I762 T763 L764 D765 S766 I767 K768 S769 I770 G771 N772 L773 R774 L775 Y776 M777 P778 K779 D780 I781 R782 A783 S784 G785 Q786 K787 E788 T789 V790 G791 K792 S793 L794 R795 E796 V797 N798 R799 R800 F801
P802 D803 G804 I805 P806 V807 L808 D809 P810 V811 K812 N813 M814 K815 I816 E817 D818 E819 D820 F821 L822 K823 L824 M825 K826 K827 I828 D829 V830 L831 N832 T833 K834 L835 S836 S837 N838 P839 L840 T841 N842 S843 M844 R845 L846 E847 E848 L849 Y850 G851 K852 Y853 S854 R855 K856 H857 D858 L859 H860 E861
D862 M863 K864 Q865 L866 K867 R868 K869 I870 S871 E872 S873 Q874 A875 V876 I877 Q878 L879 D880 D881 L882 R883 R884 R885 K886 R887 V888 L889 R890 R891 L892 G893 F894 C895 T896 P897 N898 D899 E921 P924 N925 G926 N927 F928 N929 E930 L931 K932 P933 E934 Q935 A936 A937 A938 C949 K950 E951
A952 P953 R954 L955 K956 P957 E958 L959 A960 E961 P962 L963 K964 A965 M966 R967 E968 I969 A970 A971 K972 I973 A974 K975 I976 M977 K978 D979 S980 K981 I982 E983 V984 V985 E986 K987 D988 Y989 V990 E991 H995 E996 L997 M998 E999 V1000 V1001 Y1002 E1003 W1004 C1005 R1006 G1007 A1008 T1009 F1010 T1011 Q1012 I1013
C1014 K1015 M1016 T1017 D1018 V1019 Y1020 E1021 G1022 R1026 E1032 V1035 K1036 E1037 L1038 V1039 A1042 N1043 G1046 N1047 S1048 S1049 L1050 K1051 E1052 K1053 M1054 E1055 A1056 V1057 L1058 K1059 L1060 I1061 H1062 R1063 D1064 I1065 V1066 S1067 A1068 G1069 S1070 L1071 Y1072 L1073

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35320	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.473	Depositor
Minimum map value	-0.263	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	571.86, 571.86, 571.86	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	CA	0.76	0/1917	0.66	0/2588
1	CB	0.38	0/1815	0.54	1/2448 (0.0%)
2	DA	0.62	0/1937	0.62	0/2593
3	UA	0.65	1/6465 (0.0%)	0.63	2/8752 (0.0%)
4	UB	0.30	0/4158	0.45	0/5607
5	UC	0.69	0/699	0.63	1/919 (0.1%)
6	UD	0.31	0/5369	0.52	1/7272 (0.0%)
7	UE	0.39	0/3840	0.52	0/5208
8	UF	0.52	0/2538	0.56	1/3405 (0.0%)
9	UG	0.64	1/3796 (0.0%)	0.65	1/5126 (0.0%)
10	UH	0.24	0/2773	0.49	0/3798
11	UI	0.24	0/735	0.50	0/987
12	UJ	0.39	0/9111	0.53	1/12323 (0.0%)
13	UK	0.36	0/1869	0.52	0/2472
14	UL	0.43	0/6324	0.57	2/8546 (0.0%)
15	UM	0.43	0/6071	0.59	1/8218 (0.0%)
16	UN	0.58	0/1697	0.58	0/2284
17	UO	0.31	0/3993	0.55	1/5413 (0.0%)
18	UP	0.31	0/499	0.57	0/659
19	UQ	0.30	0/6688	0.50	0/9062
20	UR	0.44	0/3875	0.56	0/5254
21	US	0.26	0/3667	0.45	0/5001
22	UT	0.49	0/19132	0.61	1/25831 (0.0%)
23	UU	0.53	0/7059	0.56	0/9536
24	UV	0.39	0/8962	0.51	0/12120
25	UX	0.78	0/1353	0.72	2/1819 (0.1%)
26	CD	0.55	0/3041	0.57	1/4098 (0.0%)
27	CE	0.38	0/3364	0.55	1/4539 (0.0%)
28	CF	0.63	0/928	0.79	3/1262 (0.2%)
28	CG	0.63	0/928	0.79	3/1262 (0.2%)
29	CH	0.61	1/3809 (0.0%)	0.59	1/5128 (0.0%)
30	CI	0.45	0/1494	0.60	0/2008

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	CJ	0.53	0/2118	0.62	0/2855
32	CK	0.48	0/1808	0.62	3/2424 (0.1%)
33	CL	0.58	0/6691	0.61	1/9000 (0.0%)
34	CM	0.50	0/2832	0.58	1/3825 (0.0%)
35	CN	0.38	0/1909	0.51	0/2571
36	JD	0.33	0/6634	0.53	0/8927
37	JF	0.26	0/1727	0.51	1/2329 (0.0%)
37	JG	0.29	0/1828	0.51	1/2470 (0.0%)
38	JH	0.23	0/1293	0.36	0/1801
39	JI	0.23	0/1313	0.36	0/1830
40	JL	0.32	0/2305	0.51	0/3116
41	JM	0.40	0/1151	0.56	0/1535
42	JP	0.87	5/3844 (0.1%)	0.72	6/5174 (0.1%)
43	Db	0.63	0/620	0.62	0/838
44	JJ	0.55	0/1600	0.62	0/2154
45	DE	0.89	0/1991	0.69	0/2683
46	DF	0.49	0/1690	0.56	0/2285
47	DG	0.53	0/1779	0.60	0/2379
48	DH	0.56	0/1383	0.64	0/1863
49	DI	0.67	0/1422	0.63	0/1899
50	DJ	0.82	0/1519	0.70	1/2035 (0.0%)
51	DL	0.83	0/1155	0.63	1/1557 (0.1%)
52	DN	0.65	0/1215	0.61	0/1638
53	DO	0.61	0/933	0.65	0/1256
54	DQ	0.56	0/986	0.58	0/1330
55	DS	0.28	0/871	0.58	0/1171
56	DT	0.35	0/1130	0.57	0/1517
57	DW	0.92	0/1038	0.74	0/1395
58	DX	0.65	0/1133	0.68	1/1510 (0.1%)
59	DY	0.77	0/1087	0.60	0/1449
60	Dc	0.55	0/499	0.62	0/670
61	D2	0.33	0/1946	0.79	0/3024
62	D3	1.26	54/33586 (0.2%)	1.01	49/52290 (0.1%)
63	D4	0.67	0/5263	0.86	2/8171 (0.0%)
64	EA	0.77	0/405	1.53	6/625 (1.0%)
65	EB	0.47	0/1474	0.57	0/2050
66	EC	0.47	0/1198	0.58	0/1666
67	ED	0.43	0/1569	0.62	0/2179
68	EE	0.46	0/1109	0.61	0/1545
69	EF	0.42	0/1319	0.60	0/1839
70	EG	0.45	0/1055	0.59	0/1462
71	EH	0.45	0/1169	0.64	0/1626
72	EI	0.44	0/1437	0.62	0/1992

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
73	EJ	0.40	0/1087	0.62	0/1504
74	EK	0.39	0/4818	0.57	0/6720
75	EN	0.40	0/4760	0.58	0/6629
All	All	0.65	62/249605 (0.0%)	0.67	97/346346 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	DA	0	1
9	UG	0	2
10	UH	0	3
14	UL	0	1
15	UM	0	1
17	UO	0	1
22	UT	0	2
25	UX	0	1
26	CD	0	1
36	JD	0	1
42	JP	0	2
44	JJ	0	1
51	DL	0	1
59	DY	0	1
66	EC	0	1
67	ED	0	3
68	EE	0	1
69	EF	0	1
70	EG	0	2
72	EI	0	1
73	EJ	0	1
75	EN	0	3
All	All	0	32

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	JP	380	TRP	CB-CG	-6.84	1.38	1.50
3	UA	422	PHE	CB-CG	-6.75	1.39	1.51
62	D3	385	A	N9-C4	-6.50	1.33	1.37
62	D3	407	A	N9-C4	-6.26	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	D3	538	A	N9-C4	-6.21	1.34	1.37

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
64	EA	167	U	N1-C2-O2	13.97	132.58	122.80
64	EA	167	U	N3-C2-O2	-11.26	114.32	122.20
64	EA	167	U	C2-N1-C1'	11.20	131.14	117.70
62	D3	849	C	OP2-P-O3'	-11.15	80.68	105.20
62	D3	850	A	OP1-P-OP2	9.95	134.53	119.60

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	DA	11	LYS	Peptide
9	UG	199	LEU	Peptide
9	UG	452	VAL	Peptide
10	UH	266	ILE	Peptide
10	UH	74	ILE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CA	1881	0	1928	105	0
1	CB	1782	0	1826	100	0
2	DA	1912	0	2023	89	0
3	UA	6322	0	6223	242	0
4	UB	4105	0	3846	152	0
5	UC	694	0	742	31	0
6	UD	5269	0	5281	267	0
7	UE	3772	0	3806	189	0
8	UF	2487	0	2533	99	0
9	UG	3718	0	3721	140	0
10	UH	2771	0	1817	75	0
11	UI	723	0	770	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	UJ	8961	0	9273	378	0
13	UK	1845	0	1926	100	0
14	UL	6199	0	6221	306	0
15	UM	5970	0	6009	358	0
16	UN	1667	0	1658	67	0
17	UO	3911	0	3906	284	0
18	UP	495	0	561	40	0
19	UQ	6557	0	6489	338	0
20	UR	3791	0	3772	200	0
21	US	3587	0	3200	130	0
22	UT	18789	0	19126	887	0
23	UU	6922	0	6886	301	0
24	UV	8753	0	8867	421	0
25	UX	1330	0	1416	59	0
26	CD	2994	0	3018	101	0
27	CE	3326	0	3406	161	0
28	CF	916	0	964	54	0
28	CG	916	0	964	50	0
29	CH	3736	0	3756	124	0
30	CI	1468	0	1519	73	0
31	CJ	2081	0	2112	107	0
32	CK	1789	0	1801	99	0
33	CL	6551	0	6707	284	0
34	CM	2781	0	2878	109	0
35	CN	1868	0	1845	92	0
36	JD	6509	0	6724	354	0
37	JF	1701	0	1767	78	0
37	JG	1799	0	1872	92	0
38	JH	1295	0	570	3	0
39	JI	1314	0	610	5	0
40	JL	2262	0	2330	88	0
41	JM	1131	0	1161	62	0
42	JP	3765	0	3714	145	0
43	Db	610	0	630	0	0
44	JJ	1573	0	1650	70	0
45	DE	1950	0	2035	57	0
46	DF	1669	0	1724	53	0
47	DG	1755	0	1846	70	0
48	DH	1361	0	1437	52	0
49	DI	1399	0	1431	61	0
50	DJ	1494	0	1573	47	0
51	DL	1129	0	1196	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	DN	1192	0	1255	32	0
53	DO	922	0	946	44	0
54	DQ	969	0	1025	37	0
55	DS	861	0	896	38	0
56	DT	1112	0	1124	40	0
57	DW	1021	0	1060	29	0
58	DX	1115	0	1191	53	0
59	DY	1073	0	1132	25	0
60	Dc	497	0	535	0	0
61	D2	1741	0	876	50	0
62	D3	30042	0	15140	753	0
63	D4	4720	0	2397	161	0
64	EA	366	0	184	1	0
65	EB	1475	0	658	14	0
66	EC	1199	0	527	9	0
67	ED	1571	0	699	10	0
68	EE	1107	0	499	7	0
69	EF	1317	0	575	6	0
70	EG	1058	0	478	4	0
71	EH	1170	0	528	7	0
72	EI	1440	0	648	7	0
73	EJ	1091	0	500	12	0
74	EK	4818	0	2108	32	0
75	EN	4762	0	2107	57	0
76	Db	1	0	0	0	0
76	EK	1	0	0	0	0
76	UX	1	0	0	0	0
77	CL	32	0	12	3	0
78	CL	1	0	0	0	0
78	EK	1	0	0	0	0
All	All	242031	0	212166	8401	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 8401 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:UL:671:PHE:HA	14:UL:684:TRP:O	1.25	1.32
3:UA:77:GLY:HA3	3:UA:95:PHE:O	1.27	1.28
9:UG:132:GLY:HA3	9:UG:150:LEU:O	1.33	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:UU:228:GLY:HA3	23:UU:246:ILE:O	1.12	1.22
59:DY:29:HIS:O	59:DY:67:GLY:HA2	1.36	1.21

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CA	238/327 (73%)	211 (89%)	27 (11%)	0	100	100
1	CB	224/327 (68%)	209 (93%)	15 (7%)	0	100	100
2	DA	236/255 (92%)	210 (89%)	26 (11%)	0	100	100
3	UA	786/923 (85%)	699 (89%)	87 (11%)	0	100	100
4	UB	535/810 (66%)	513 (96%)	22 (4%)	0	100	100
5	UC	82/610 (13%)	72 (88%)	10 (12%)	0	100	100
6	UD	653/776 (84%)	589 (90%)	64 (10%)	0	100	100
7	UE	465/643 (72%)	425 (91%)	40 (9%)	0	100	100
8	UF	283/440 (64%)	278 (98%)	5 (2%)	0	100	100
9	UG	464/554 (84%)	410 (88%)	54 (12%)	0	100	100
10	UH	446/713 (63%)	406 (91%)	39 (9%)	1 (0%)	47	79
11	UI	86/575 (15%)	84 (98%)	2 (2%)	0	100	100
12	UJ	1092/1769 (62%)	1030 (94%)	62 (6%)	0	100	100
13	UK	213/250 (85%)	197 (92%)	15 (7%)	1 (0%)	29	66
14	UL	765/943 (81%)	677 (88%)	88 (12%)	0	100	100
15	UM	750/817 (92%)	663 (88%)	87 (12%)	0	100	100
16	UN	197/899 (22%)	180 (91%)	17 (9%)	0	100	100
17	UO	489/513 (95%)	453 (93%)	36 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	UP	58/214 (27%)	55 (95%)	3 (5%)	0	100	100
19	UQ	810/896 (90%)	739 (91%)	71 (9%)	0	100	100
20	UR	473/594 (80%)	435 (92%)	38 (8%)	0	100	100
21	US	479/552 (87%)	456 (95%)	23 (5%)	0	100	100
22	UT	2265/2493 (91%)	2078 (92%)	185 (8%)	2 (0%)	51	83
23	UU	870/939 (93%)	792 (91%)	78 (9%)	0	100	100
24	UV	1071/1237 (87%)	1025 (96%)	46 (4%)	0	100	100
25	UX	163/189 (86%)	148 (91%)	15 (9%)	0	100	100
26	CD	376/504 (75%)	354 (94%)	21 (6%)	1 (0%)	41	74
27	CE	434/511 (85%)	404 (93%)	30 (7%)	0	100	100
28	CF	119/126 (94%)	112 (94%)	7 (6%)	0	100	100
28	CG	119/126 (94%)	112 (94%)	7 (6%)	0	100	100
29	CH	461/573 (80%)	416 (90%)	44 (10%)	1 (0%)	47	79
30	CI	171/183 (93%)	159 (93%)	12 (7%)	0	100	100
31	CJ	252/290 (87%)	220 (87%)	32 (13%)	0	100	100
32	CK	214/593 (36%)	198 (92%)	16 (8%)	0	100	100
33	CL	796/1183 (67%)	723 (91%)	73 (9%)	0	100	100
34	CM	358/367 (98%)	332 (93%)	26 (7%)	0	100	100
35	CN	221/297 (74%)	212 (96%)	9 (4%)	0	100	100
36	JD	793/1267 (63%)	714 (90%)	77 (10%)	2 (0%)	41	74
37	JF	212/252 (84%)	207 (98%)	5 (2%)	0	100	100
37	JG	226/252 (90%)	218 (96%)	8 (4%)	0	100	100
38	JH	257/483 (53%)	250 (97%)	7 (3%)	0	100	100
39	JI	263/1729 (15%)	251 (95%)	12 (5%)	0	100	100
40	JL	281/318 (88%)	269 (96%)	12 (4%)	0	100	100
41	JM	130/217 (60%)	119 (92%)	11 (8%)	0	100	100
42	JP	457/489 (94%)	410 (90%)	47 (10%)	0	100	100
43	Db	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
44	JJ	195/274 (71%)	180 (92%)	15 (8%)	0	100	100
45	DE	244/261 (94%)	231 (95%)	13 (5%)	0	100	100
46	DF	211/225 (94%)	190 (90%)	21 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DG	216/236 (92%)	201 (93%)	15 (7%)	0	100	100
48	DH	166/190 (87%)	150 (90%)	16 (10%)	0	100	100
49	DI	173/200 (86%)	162 (94%)	11 (6%)	0	100	100
50	DJ	183/197 (93%)	168 (92%)	15 (8%)	0	100	100
51	DL	138/156 (88%)	131 (95%)	7 (5%)	0	100	100
52	DN	148/151 (98%)	141 (95%)	7 (5%)	0	100	100
53	DO	125/137 (91%)	110 (88%)	15 (12%)	0	100	100
54	DQ	123/143 (86%)	113 (92%)	10 (8%)	0	100	100
55	DS	99/146 (68%)	91 (92%)	8 (8%)	0	100	100
56	DT	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
57	DW	127/130 (98%)	109 (86%)	18 (14%)	0	100	100
58	DX	141/145 (97%)	125 (89%)	16 (11%)	0	100	100
59	DY	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
60	Dc	61/67 (91%)	56 (92%)	5 (8%)	0	100	100
65	EB	297/305 (97%)	274 (92%)	21 (7%)	2 (1%)	22	60
66	EC	241/246 (98%)	224 (93%)	17 (7%)	0	100	100
67	ED	308/394 (78%)	283 (92%)	24 (8%)	1 (0%)	41	74
68	EE	222/223 (100%)	209 (94%)	13 (6%)	0	100	100
69	EF	264/265 (100%)	250 (95%)	14 (5%)	0	100	100
70	EG	209/250 (84%)	192 (92%)	17 (8%)	0	100	100
71	EH	235/240 (98%)	217 (92%)	18 (8%)	0	100	100
72	EI	287/359 (80%)	262 (91%)	25 (9%)	0	100	100
73	EJ	214/292 (73%)	198 (92%)	16 (8%)	0	100	100
74	EK	965/1001 (96%)	939 (97%)	25 (3%)	1 (0%)	51	83
75	EN	959/1073 (89%)	891 (93%)	64 (7%)	4 (0%)	34	70
All	All	27236/36685 (74%)	25138 (92%)	2082 (8%)	16 (0%)	54	83

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	JD	1019	GLU
75	EN	615	VAL
75	EN	617	SER

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Mol	Chain	Res	Type
10	UH	309	PRO
29	CH	552	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CA	202/240 (84%)	202 (100%)	0	100	100
1	CB	192/240 (80%)	192 (100%)	0	100	100
2	DA	212/224 (95%)	211 (100%)	1 (0%)	88	94
3	UA	695/812 (86%)	693 (100%)	2 (0%)	92	96
4	UB	382/732 (52%)	381 (100%)	1 (0%)	92	96
5	UC	74/538 (14%)	74 (100%)	0	100	100
6	UD	604/713 (85%)	603 (100%)	1 (0%)	93	97
7	UE	428/574 (75%)	426 (100%)	2 (0%)	88	94
8	UF	277/414 (67%)	273 (99%)	4 (1%)	67	81
9	UG	405/480 (84%)	402 (99%)	3 (1%)	84	91
10	UH	125/657 (19%)	122 (98%)	3 (2%)	49	71
11	UI	83/533 (16%)	81 (98%)	2 (2%)	49	71
12	UJ	1031/1633 (63%)	1027 (100%)	4 (0%)	91	95
13	UK	207/234 (88%)	207 (100%)	0	100	100
14	UL	690/832 (83%)	689 (100%)	1 (0%)	93	97
15	UM	668/719 (93%)	666 (100%)	2 (0%)	92	96
16	UN	183/808 (23%)	183 (100%)	0	100	100
17	UO	437/454 (96%)	435 (100%)	2 (0%)	88	94
18	UP	57/196 (29%)	55 (96%)	2 (4%)	36	64
19	UQ	756/826 (92%)	753 (100%)	3 (0%)	91	95
20	UR	424/529 (80%)	423 (100%)	1 (0%)	93	97
21	US	332/506 (66%)	328 (99%)	4 (1%)	71	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	UT	2134/2307 (92%)	2125 (100%)	9 (0%)	91 95
23	UU	768/819 (94%)	766 (100%)	2 (0%)	92 96
24	UV	988/1125 (88%)	984 (100%)	4 (0%)	91 95
25	UX	148/169 (88%)	146 (99%)	2 (1%)	67 81
26	CD	326/435 (75%)	325 (100%)	1 (0%)	92 96
27	CE	352/433 (81%)	350 (99%)	2 (1%)	86 92
28	CF	100/104 (96%)	85 (85%)	15 (15%)	3 18
28	CG	100/104 (96%)	85 (85%)	15 (15%)	3 18
29	CH	407/503 (81%)	407 (100%)	0	100 100
30	CI	165/172 (96%)	165 (100%)	0	100 100
31	CJ	227/258 (88%)	227 (100%)	0	100 100
32	CK	201/535 (38%)	201 (100%)	0	100 100
33	CL	710/1039 (68%)	707 (100%)	3 (0%)	91 95
34	CM	307/312 (98%)	307 (100%)	0	100 100
35	CN	209/274 (76%)	207 (99%)	2 (1%)	76 86
36	JD	724/1140 (64%)	718 (99%)	6 (1%)	81 89
37	JF	195/222 (88%)	195 (100%)	0	100 100
37	JG	206/222 (93%)	204 (99%)	2 (1%)	76 86
40	JL	255/283 (90%)	254 (100%)	1 (0%)	91 95
41	JM	125/200 (62%)	124 (99%)	1 (1%)	81 89
42	JP	416/443 (94%)	416 (100%)	0	100 100
43	Db	70/71 (99%)	69 (99%)	1 (1%)	67 81
44	JJ	174/238 (73%)	174 (100%)	0	100 100
45	DE	210/222 (95%)	210 (100%)	0	100 100
46	DF	180/191 (94%)	180 (100%)	0	100 100
47	DG	187/201 (93%)	187 (100%)	0	100 100
48	DH	151/170 (89%)	151 (100%)	0	100 100
49	DI	142/161 (88%)	141 (99%)	1 (1%)	84 91
50	DJ	158/166 (95%)	158 (100%)	0	100 100
51	DL	125/137 (91%)	125 (100%)	0	100 100
52	DN	127/128 (99%)	127 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
53	DO	90/105 (86%)	90 (100%)	0	100 100
54	DQ	104/119 (87%)	104 (100%)	0	100 100
55	DS	96/129 (74%)	96 (100%)	0	100 100
56	DT	115/116 (99%)	114 (99%)	1 (1%)	78 88
57	DW	110/111 (99%)	110 (100%)	0	100 100
58	DX	118/120 (98%)	118 (100%)	0	100 100
59	DY	112/113 (99%)	112 (100%)	0	100 100
60	Dc	56/60 (93%)	56 (100%)	0	100 100
All	All	19852/26551 (75%)	19746 (100%)	106 (0%)	89 94

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	CE	215	ARG
28	CF	114	ILE
37	JG	88	ARG
28	CF	9	PHE
28	CF	50	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
22	UT	1366	ASN
24	UV	1199	ASN
46	DF	224	ASN
22	UT	2030	ASN
23	UU	490	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
61	D2	76/81 (93%)	23 (30%)	0
62	D3	1387/1802 (76%)	387 (27%)	25 (1%)
63	D4	214/333 (64%)	58 (27%)	4 (1%)
64	EA	21/22 (95%)	15 (71%)	0
All	All	1698/2238 (75%)	483 (28%)	29 (1%)

5 of 483 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
61	D2	6	A
61	D2	8	A
61	D2	11	A
61	D2	14	U
61	D2	15	G

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
62	D3	1058	U
63	D4	156	U
62	D3	1115	U
62	D3	1670	G
62	D3	1096	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
77	GTP	CL	2001	78	26,34,34	1.43	3 (11%)	32,54,54	1.97	7 (21%)

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
77	GTP	CL	2001	78	-	7/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	CL	2001	GTP	C5-C6	-4.96	1.37	1.47
77	CL	2001	GTP	C5-C4	-2.21	1.37	1.43
77	CL	2001	GTP	O4'-C4'	-2.09	1.40	1.45

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
77	CL	2001	GTP	PA-O3A-PB	-5.41	114.25	132.83
77	CL	2001	GTP	PB-O3B-PG	-4.86	116.17	132.83
77	CL	2001	GTP	C5-C6-N1	3.47	120.08	113.95
77	CL	2001	GTP	C2-N1-C6	-3.38	118.87	125.10
77	CL	2001	GTP	C3'-C2'-C1'	3.25	105.87	100.98

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
77	CL	2001	GTP	C5'-O5'-PA-O1A
77	CL	2001	GTP	C5'-O5'-PA-O2A
77	CL	2001	GTP	C3'-C4'-C5'-O5'
77	CL	2001	GTP	O4'-C4'-C5'-O5'
77	CL	2001	GTP	PB-O3A-PA-O1A

There are no ring outliers.

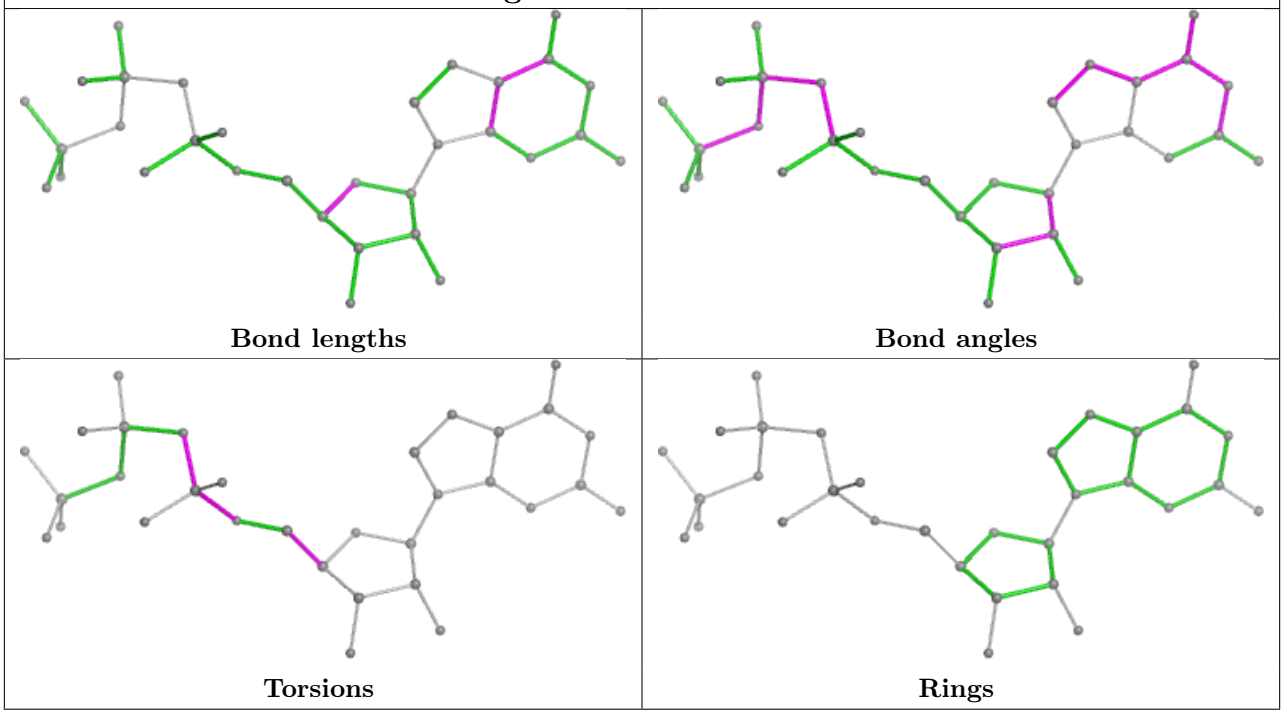
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
77	CL	2001	GTP	3	0

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 CL 2001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
61	D2	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D2	92:C	O3'	281:G	P	62.30

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D2	292:A	O3'	463:A	P	45.10
1	D2	70:A	O3'	80:A	P	19.53
1	D2	24:U	O3'	56:G	P	14.66

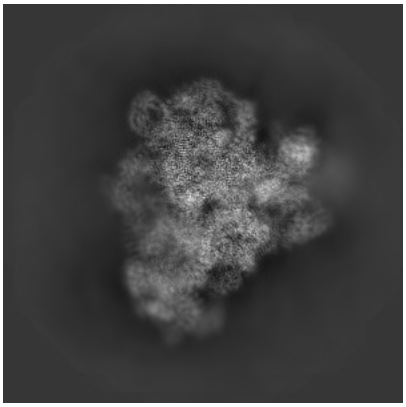
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11808. These allow visual inspection of the internal detail of the map and identification of artifacts.

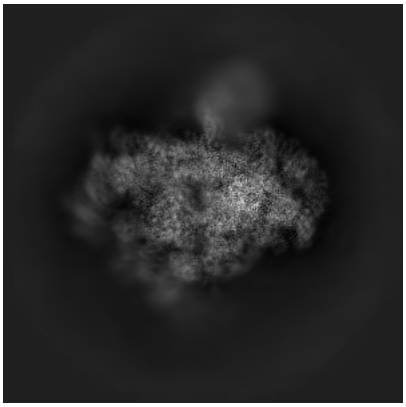
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

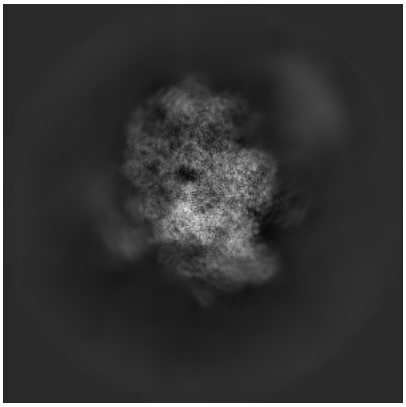
6.1.1 Primary map



X



Y

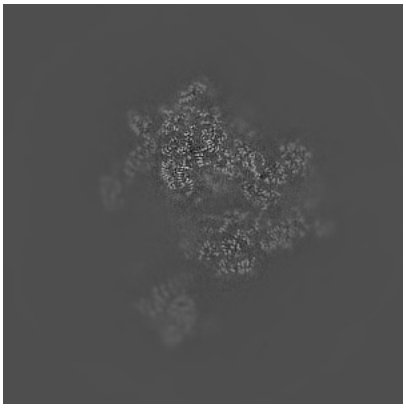


Z

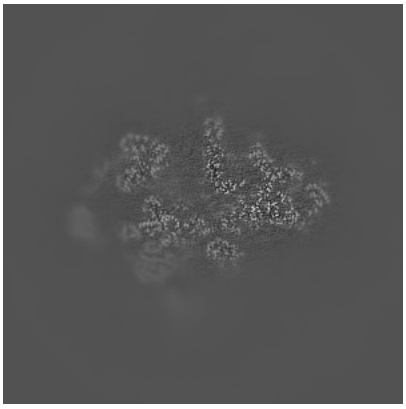
The images above show the map projected in three orthogonal directions.

6.2 Central slices

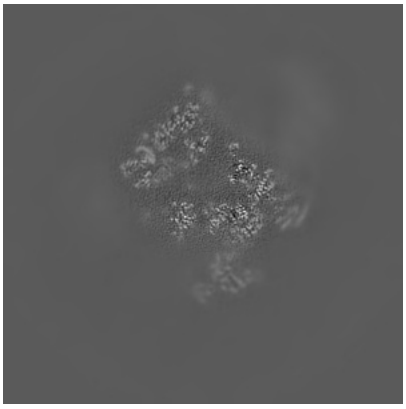
6.2.1 Primary map



X Index: 270



Y Index: 270

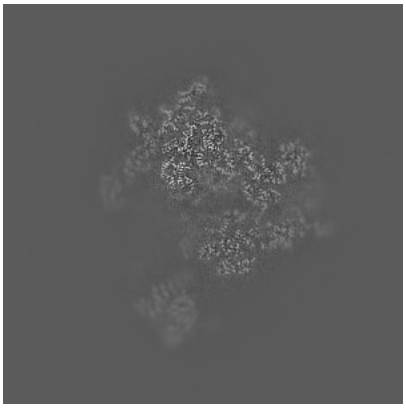


Z Index: 270

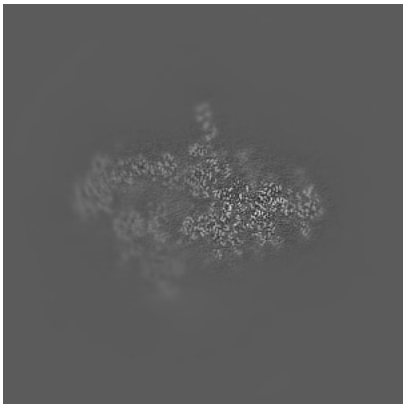
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

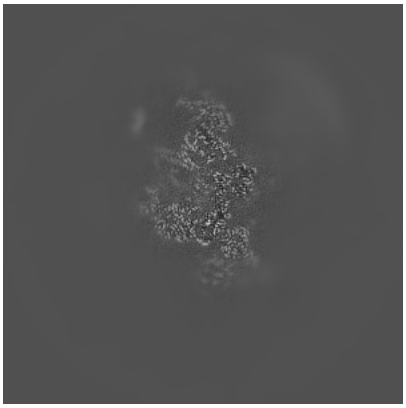
6.3.1 Primary map



X Index: 271



Y Index: 249

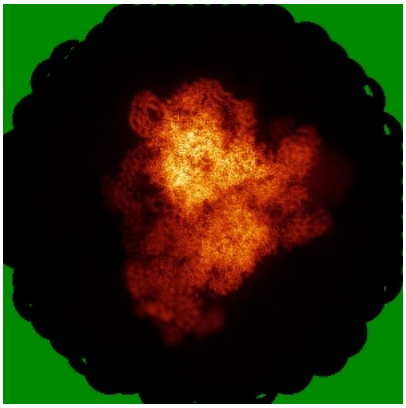


Z Index: 314

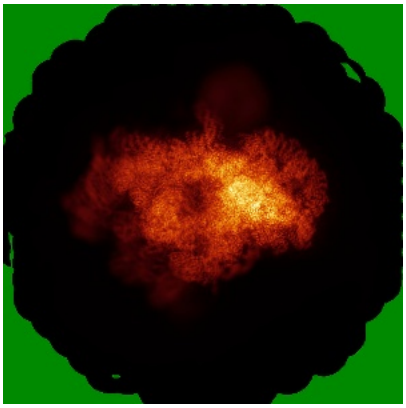
The images above show the largest variance slices of the map in three orthogonal directions.

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

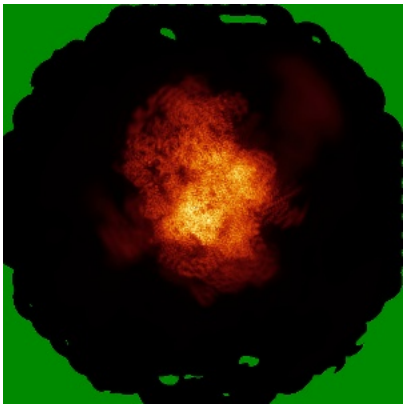
6.4.1 Primary map



X



Y

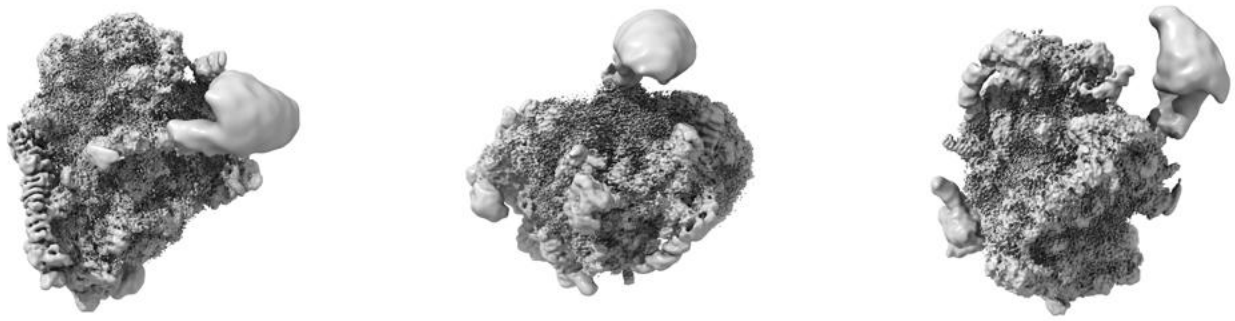


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

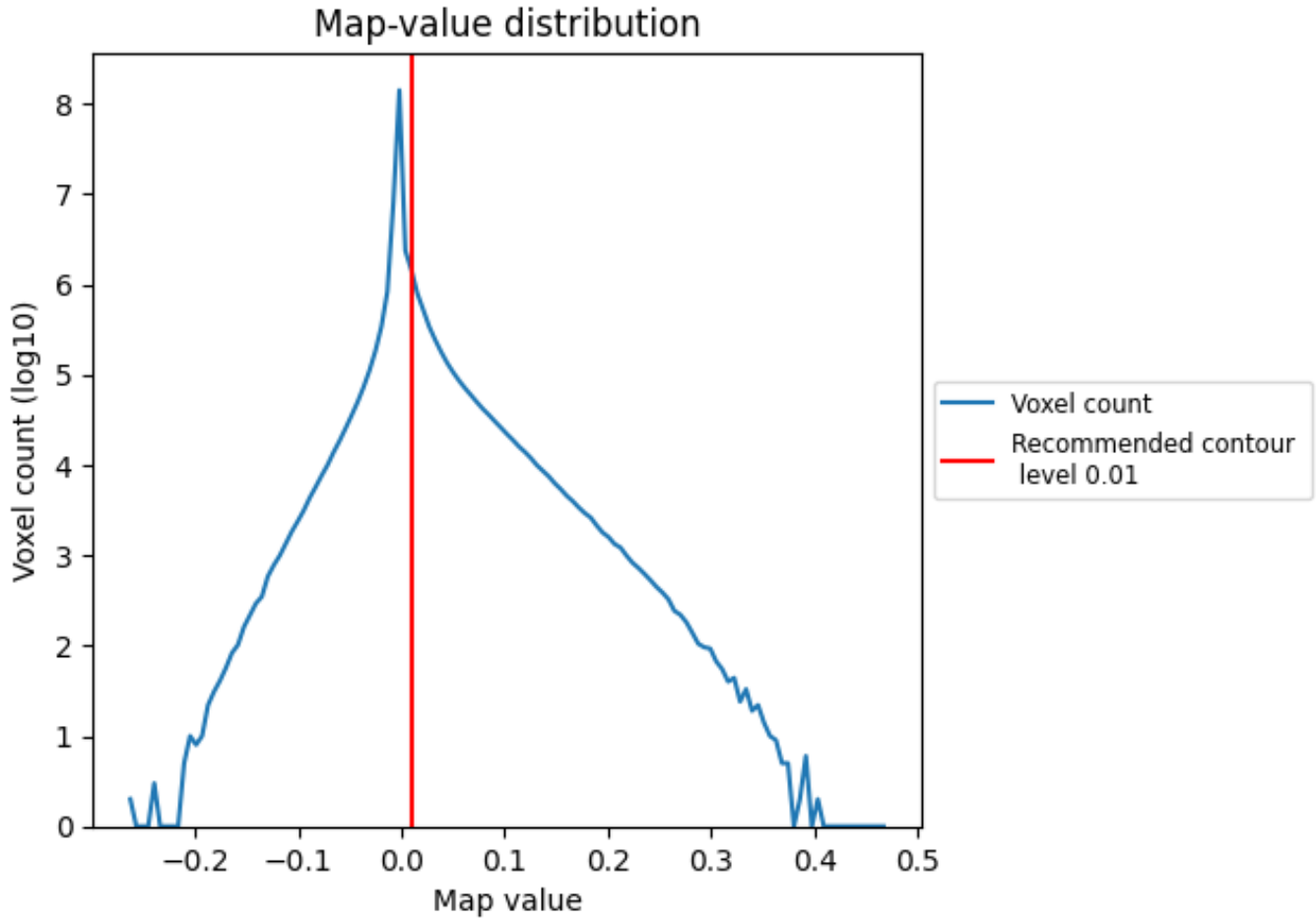
6.6 Mask visualisation (i)

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

7 Map analysis

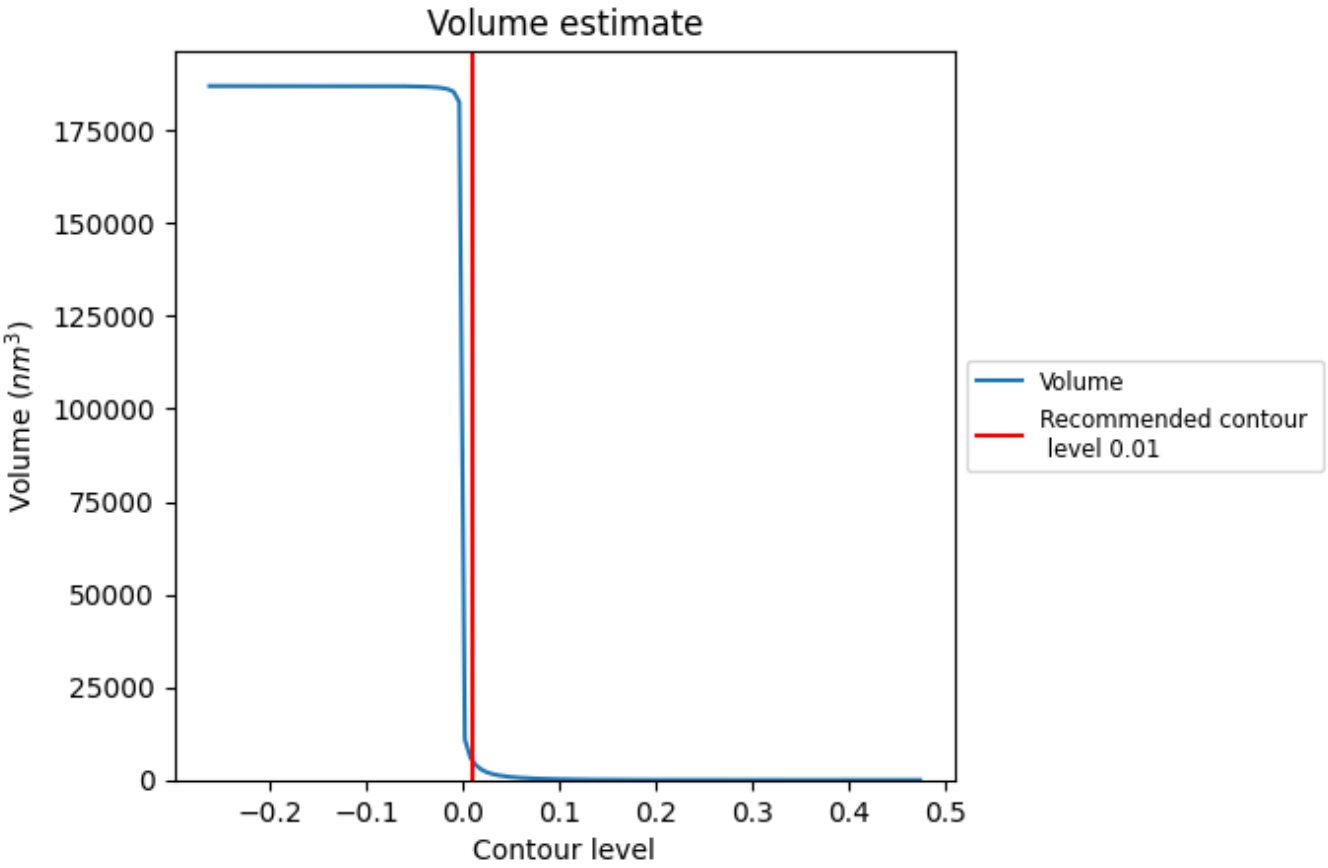
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

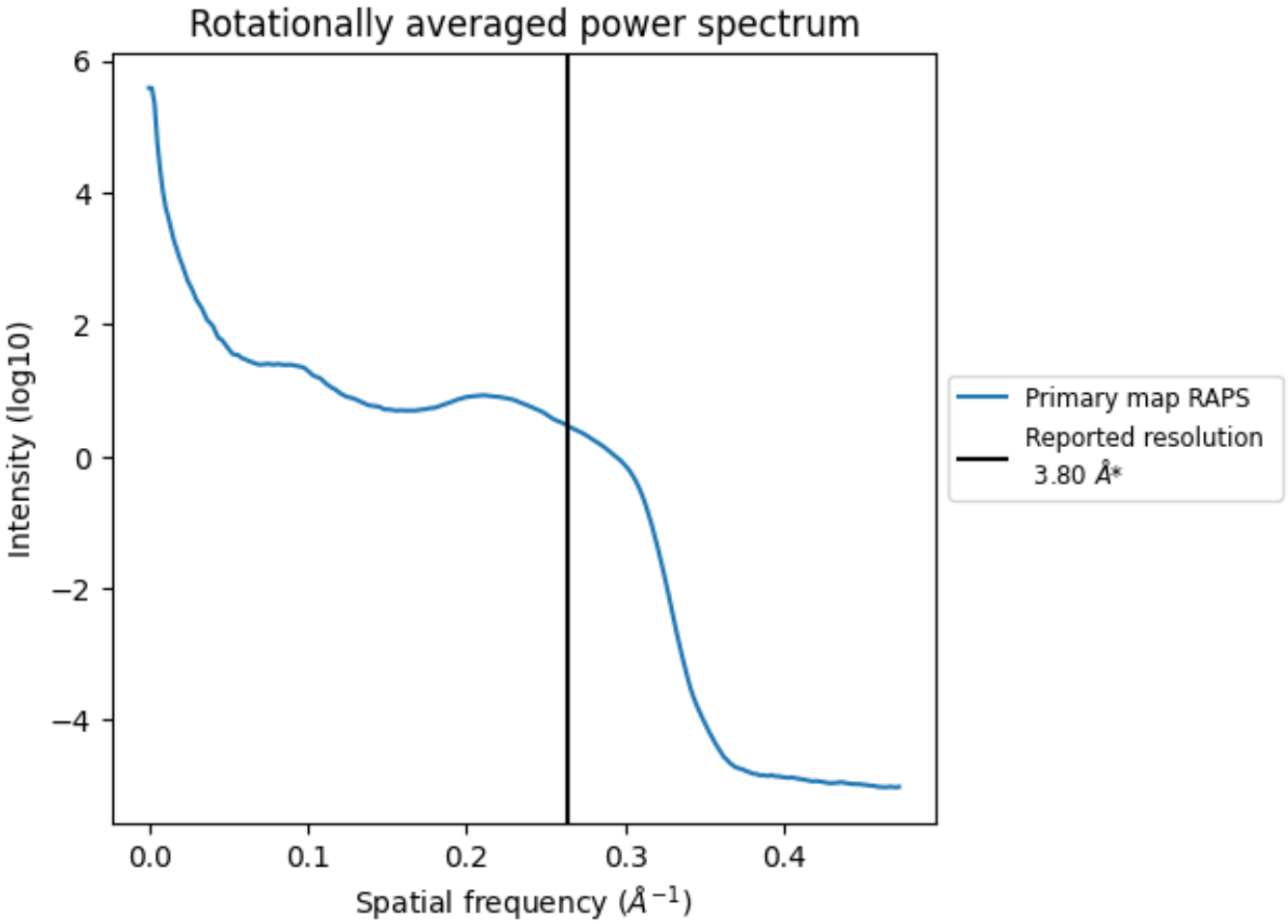
7.2 Volume estimate (i)



The volume at the recommended contour level is 5032 nm^3; this corresponds to an approximate mass of 4545 kDa.

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

7.3 Rotationally averaged power spectrum (i)

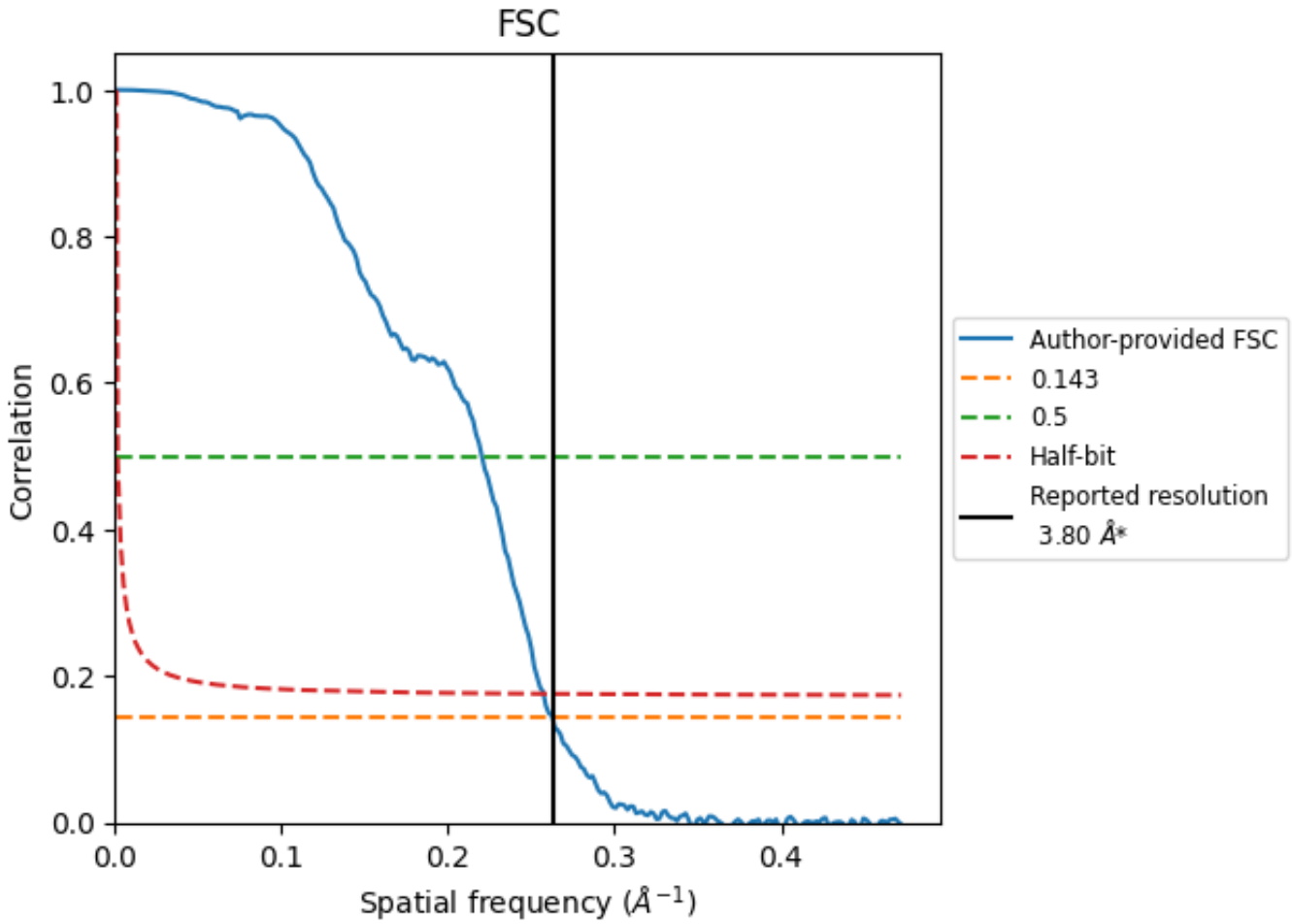


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

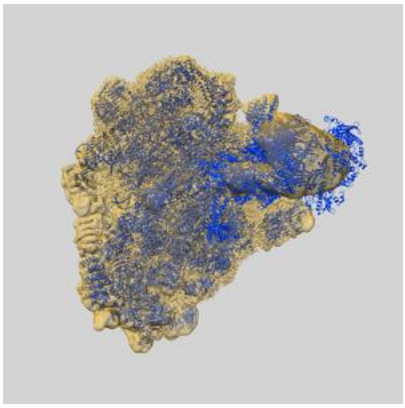
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	4.54	3.89
Unmasked-calculated*	-	-	-

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

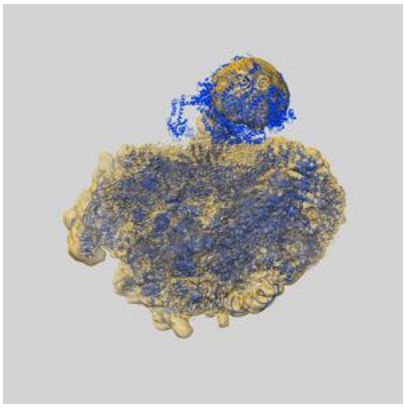
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11808 and PDB model 7AJU. Per-residue inclusion information can be found in section 3 on page 18.

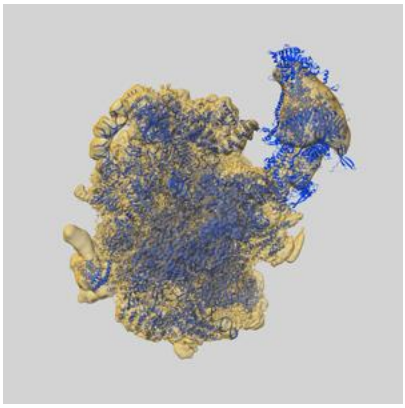
9.1 Map-model overlay



X



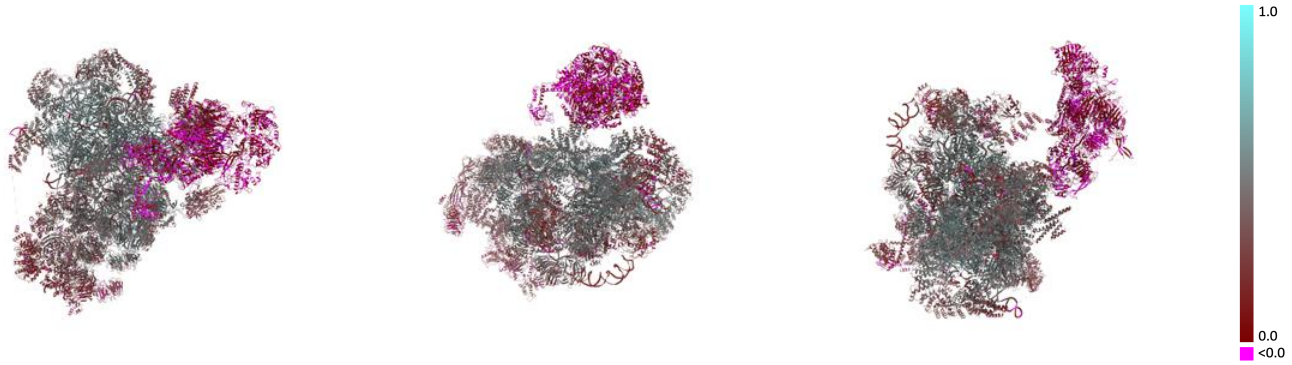
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

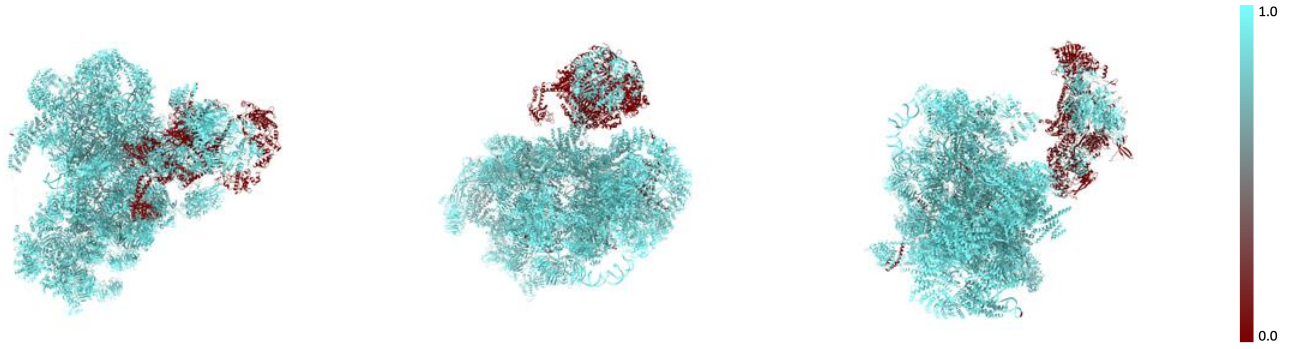
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

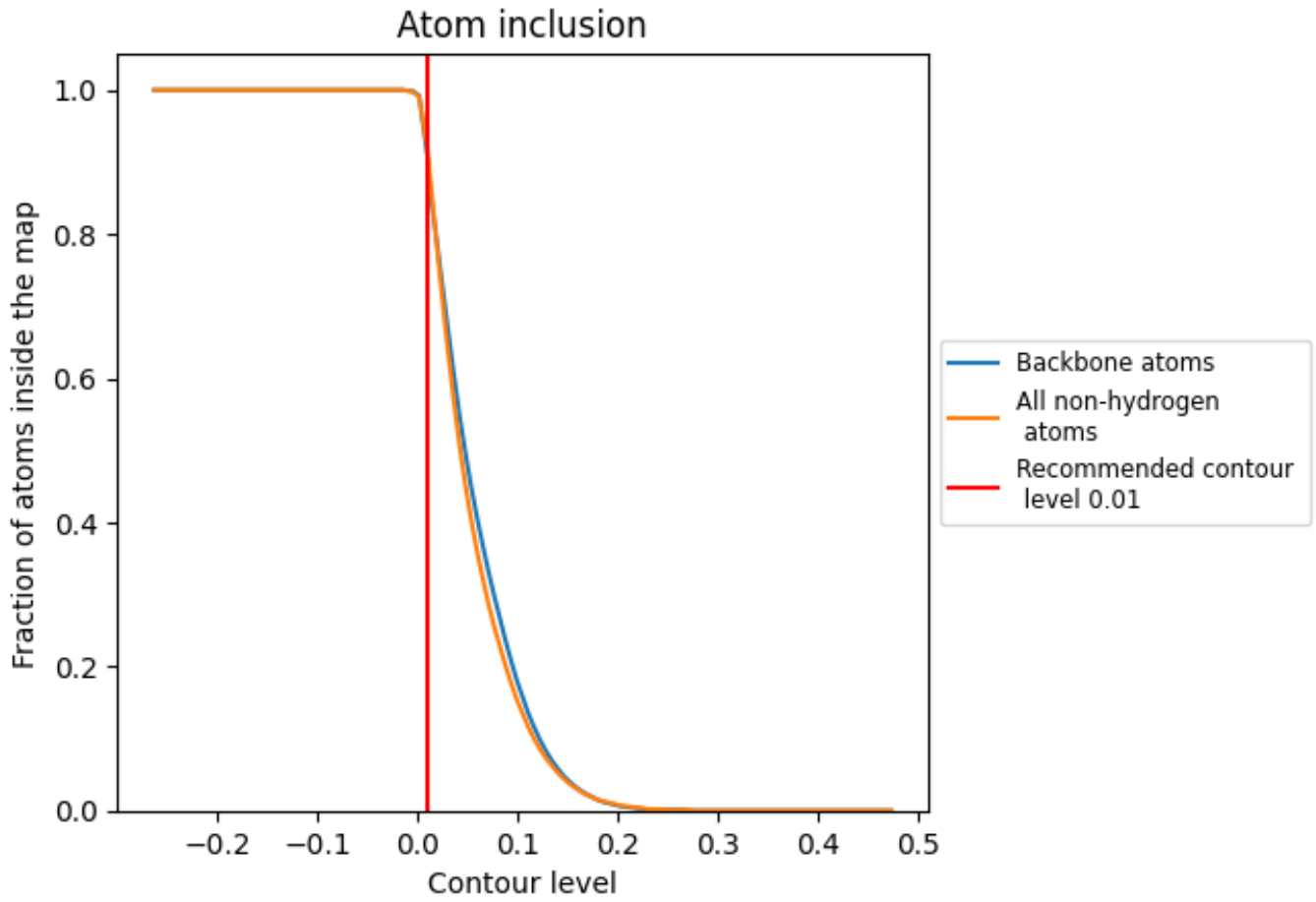
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 92% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9180	0.3660
CA	0.9820	0.5320
CB	0.9630	0.3860
CD	0.9740	0.4510
CE	0.9670	0.3810
CF	0.9510	0.4100
CG	0.9710	0.5040
CH	0.9900	0.5070
CI	0.9530	0.4040
CJ	0.9470	0.4640
CK	0.9780	0.4530
CL	0.9620	0.4670
CM	0.9870	0.4770
CN	0.9760	0.3130
D2	0.9290	0.2450
D3	0.9780	0.4550
D4	0.9470	0.3430
DA	0.9760	0.5000
DE	0.9900	0.5770
DF	0.9820	0.4750
DG	0.9930	0.4920
DH	0.9720	0.4760
DI	0.9870	0.5300
DJ	0.9830	0.5540
DL	0.9920	0.5440
DN	0.9760	0.5150
DO	0.9870	0.5100
DQ	0.9800	0.4990
DS	0.7790	0.2510
DT	0.7880	0.3220
DW	0.9780	0.5690
DX	0.9720	0.5200
DY	0.9820	0.5460
Db	0.9820	0.5430
Dc	0.9940	0.4990

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Chain	Atom inclusion	Q-score
EA	0.5550	-0.0160
EB	0.3590	0.0030
EC	0.5350	0.0130
ED	0.7980	0.0450
EE	0.8410	0.0480
EF	0.8530	0.0380
EG	0.8260	0.0300
EH	0.1750	0.0420
EI	0.5400	0.0270
EJ	0.1710	0.0100
EK	0.3440	0.0230
EN	0.2480	0.0260
JD	0.9160	0.2530
JF	0.9440	0.1520
JG	0.9410	0.2340
JH	0.9590	0.1490
JI	0.7860	0.1720
JJ	0.9760	0.4860
JL	0.9250	0.3520
JM	0.9550	0.4290
JP	0.9860	0.5510
UA	0.9790	0.5040
UB	0.9330	0.1870
UC	0.9690	0.4960
UD	0.9730	0.3120
UE	0.9530	0.3570
UF	0.9840	0.4230
UG	0.9810	0.5010
UH	0.9720	0.1410
UI	0.9690	0.1760
UJ	0.9340	0.3300
UK	0.9130	0.3730
UL	0.9840	0.4080
UM	0.9720	0.4070
UN	0.9770	0.4800
UO	0.9410	0.2560
UP	0.9330	0.3080
UQ	0.9640	0.2520
UR	0.9620	0.4270
US	0.9320	0.1770
UT	0.9780	0.4140
UU	0.9820	0.4700

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Chain	Atom inclusion	Q-score
UV	0.9740	0.3420
UX	0.9580	0.5330