wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 01:04 am GMT

PDB ID	:	6ZQC
EMDB ID	:	EMD-11359
Title	:	Cryo-EM structure of the 90S pre-ribosome from Saccharomyces cerevisiae, state Pre-A1
Authors	:	Cheng, J.; Lau, B.; Venuta, G.L.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on	:	2020-07-09
Resolution	:	3.80 Å(reported)

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

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

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

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

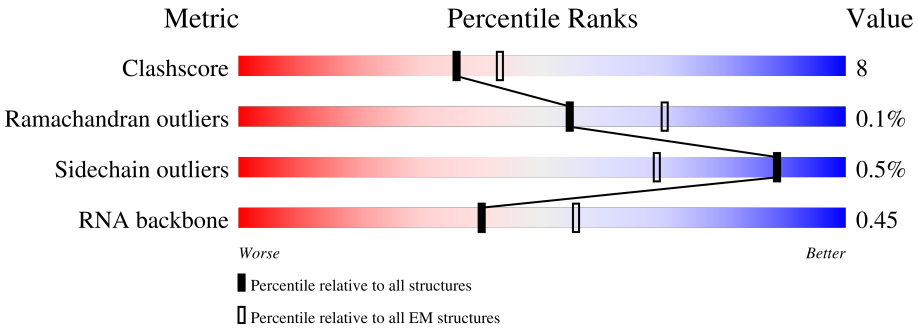
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	62% 12% 26%
1	CB	327	54% 16% 30%
2	DA	255	75% 20% 6%
3	JA	1056	57% 19% 23%
3	JB	1056	10% 77% 21%
4	UA	923	72% 17% 10%
5	UB	810	52% 10% 37%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	UC	610	
7	UD	776	
8	UE	643	
9	UF	440	
10	UG	554	
11	UH	713	
12	UI	575	
13	UJ	1769	
14	UK	250	
15	UL	943	
16	UM	817	
17	UN	899	
18	UO	513	
19	UP	214	
20	UQ	896	
21	UR	594	
22	US	552	
23	UT	2493	
24	UU	939	
25	UV	1237	
26	UX	189	
27	UZ	274	
28	CD	504	
29	CE	511	
30	CF	126	

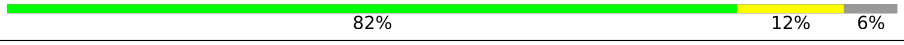
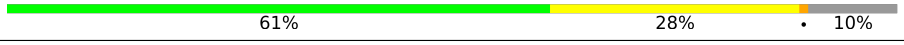
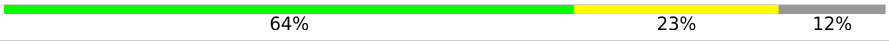
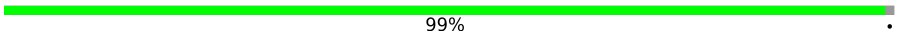
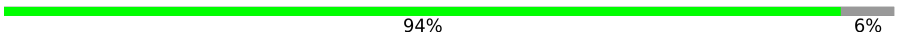
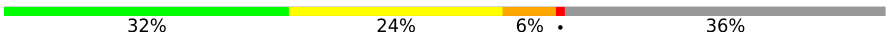
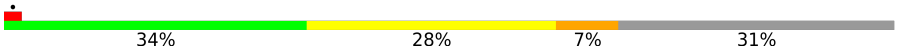
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	CG	126	74% 23%
31	CH	573	67% 14% 19%
32	CI	183	80% 19%
33	CJ	290	73% 23%
34	CK	593	30% 5% 65%
35	CL	1183	52% 13% 34%
36	CM	367	81% 17%
37	CN	297	60% 18% 22%
38	JC	707	33% 17% 50%
39	JF	252	71% 14% 14%
39	JG	252	67% 23% 9%
40	JH	483	7% 53% 46%
41	JI	1729	12% 15% 85%
42	JJ	274	51% 15% 34%
43	JK	534	5% 92%
44	JM	217	47% 15% 38%
45	JN	346	46% 8% 46%
46	JO	316	63% 9% 27%
47	JP	489	75% 19% 6%
48	JQ	206	27% 69%
49	DE	261	69% 25% 6%
50	DF	225	81% 14% 5%
51	DG	236	66% 25% 8%
52	DH	190	71% 26%
53	DI	200	65% 24% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	DJ	197	
55	DL	156	
56	DN	151	
57	DO	137	
58	DQ	143	
59	DS	146	
60	DW	130	
61	DX	145	
62	DY	135	
63	Db	82	
64	Dc	67	
65	D2	700	
66	D3	1808	
67	D4	333	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
70	GTP	CL	2001	-	-	X	-

2 Entry composition (i)

There are 70 unique types of molecules in this entry. The entry contains 234757 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 RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	JA	812	Total	C	N	O	S	0	0
			5916	3745	1044	1102	25		
3	JB	835	Total	C	N	O		0	0
			4132	2462	835	835			

- Molecule 4 is a protein called Periodic tryptophan protein 2.

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

- Molecule 5 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	UB	507	Total	C	N	O	S	0	0
			3734	2367	663	695	9		

- Molecule 6 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	UC	128	Total 1026	C 633	N 204	O 189	0	0

- Molecule 7 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UD	675	Total 5361	C 3395	N 929	O 1015	S 22	0	0

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 5.

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

- Molecule 9 is a protein called U3 small nucleolar RNA-associated protein 6.

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

- Molecule 10 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	UG	533	Total 4218	C 2646	N 758	O 802	S 12	0	0

- Molecule 11 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UH	442	Total 2701	C 1680	N 494	O 524	S 3	0	0

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	UI	104	Total 860	C 556	N 152	O 150	S 2	0	0

- Molecule 13 is a protein called U3 small nucleolar RNA-associated protein 10.

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

- Molecule 14 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	UK	242	Total	C	N	O	S	0	0
			2021	1254	389	371	7		

- Molecule 15 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UL	842	Total	C	N	O	S	0	0
			6726	4303	1129	1267	27		

- Molecule 16 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	UM	762	Total	C	N	O	S	0	0
			5969	3785	1007	1149	28		

- Molecule 17 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	UN	147	Total	C	N	O	S	0	0
			1227	765	233	227	2		

- Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 15.

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

- Molecule 19 is a protein called Bud site selection protein 21.

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

- Molecule 20 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	UQ	832	Total	C	N	O	S	0	0
			6662	4236	1124	1283	19		

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	UR	482	Total	C	N	O	S	0	0
			3799	2405	669	715	10		

- Molecule 22 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	US	494	Total	C	N	O	S	0	0
			3622	2326	617	667	12		

- Molecule 23 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	UT	2255	Total	C	N	O	S	0	0
			17290	11076	2927	3235	52		

- Molecule 24 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	UU	848	Total	C	N	O	S	0	0
			6678	4241	1149	1267	21		

- Molecule 25 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	UV	1081	Total	C	N	O	S	0	0
			8736	5681	1440	1591	24		

- Molecule 26 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	UX	174	Total	C	N	O	S	0	0
			1395	890	255	240	10		

- Molecule 27 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	UZ	247	Total	C	N	O	S	0	0
			2006	1284	356	358	8		

- Molecule 28 is a protein called Nucleolar protein 56.

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

- Molecule 29 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CE	435	Total	C	N	O	S	0	0
			3325	2093	571	653	8		

- Molecule 30 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CF	123	Total	C	N	O	S	0	0
			931	594	160	173	4		
30	CG	123	Total	C	N	O	S	0	0
			928	591	160	173	4		

- Molecule 31 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CH	465	Total	C	N	O	S	0	0
			3725	2365	653	697	10		

- Molecule 32 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CI	182	Total	C	N	O	S	0	0
			1530	967	287	269	7		

- Molecule 33 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	CJ	282	Total	C	N	O	S	0	0
			2296	1441	430	418	7		

- Molecule 34 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	CK	207	Total	C	N	O	S	0	0
			1667	1034	297	332	4		

- Molecule 35 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	CL	781	Total	C	N	O	S	0	0
			6332	4063	1122	1117	30		

- Molecule 36 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 37 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	CN	232	Total	C	N	O	S	0	0
			1893	1213	322	351	7		

- Molecule 38 is a protein called Ribosome biogenesis protein ENP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	JC	354	Total	C	N	O	S	0	0
			2845	1795	489	552	9		

- Molecule 39 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

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

- Molecule 40 is a protein called Essential nuclear protein 1.

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

- Molecule 41 is a protein called rRNA biogenesis protein RRP5.

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

- Molecule 42 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	JJ	182	Total	C	N	O	S	0	0
			1442	923	259	256	4		

- Molecule 43 is a protein called Protein BFR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	JK	42	Total	C	N	O	0	0
			334	213	54	67		

- Molecule 44 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	JM	135	Total	C	N	O	S	0	0
			1137	721	211	201	4		

- Molecule 45 is a protein called Protein FAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	JN	186	Total	C	N	O	S	0	0
			1428	879	287	259	3		

- Molecule 46 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	JO	230	Total	C	N	O	S	0	0
			1876	1203	330	332	11		

- Molecule 47 is a protein called Protein SOF1.

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

- Molecule 48 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	JQ	63	Total 381	C 234	N 69	O 78	0	0

- Molecule 49 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	DE	245	Total 1944	C 1245	N 360	O 336	S 3	0	0

- Molecule 50 is a protein called 40S ribosomal protein S5.

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

- Molecule 51 is a protein called 40S ribosomal protein S6-A.

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

- Molecule 52 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	DH	184	Total 1481	C 951	N 265	O 265	0	0

- Molecule 53 is a protein called 40S ribosomal protein S8-A.

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

- Molecule 54 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 55 is a protein called 40S ribosomal protein S11-A.

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

- Molecule 56 is a protein called 40S ribosomal protein S13.

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

- Molecule 57 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	DO	120	Total	C	N	O	S	0	0
			881	544	167	167	3		

- Molecule 58 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	DQ	125	Total	C	N	O	0	0
			973	625	174	174		

- Molecule 59 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	DS	104	Total	C	N	O	0	0
			516	308	104	104		

- Molecule 60 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 61 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 62 is a protein called 40S ribosomal protein S24-A.

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

- Molecule 63 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 64 is a protein called 40S ribosomal protein S28-A.

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

- Molecule 65 is a RNA chain called 5ETS RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	D2	446	Total	C	N	O	P	0	0
			9508	4250	1682	3130	446		

- Molecule 66 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	D3	1327	Total	C	N	O	P	0	0
			28287	12644	5022	9294	1327		

- Molecule 67 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	D4	230	Total	C	N	O	P	0	0
			4872	2181	844	1617	230		

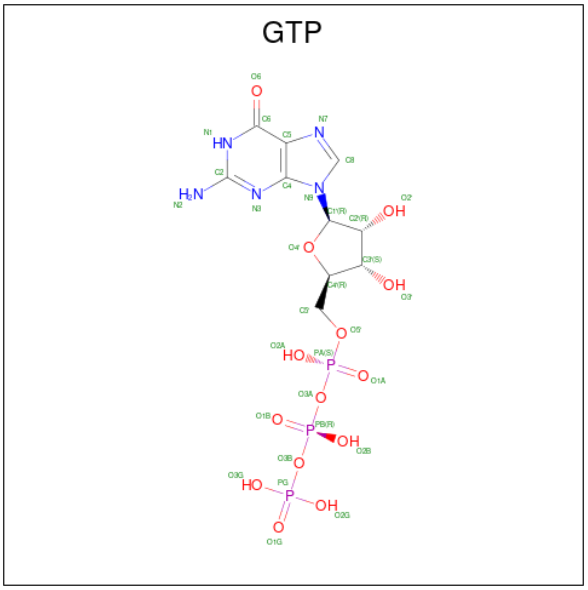
- Molecule 68 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
68	UX	1	Total	Zn	0
			1	1	
68	Db	1	Total	Zn	0
			1	1	

- Molecule 69 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
69	UX	1	Total Mg 1 1	0
69	CL	1	Total Mg 1 1	0

- Molecule 70 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



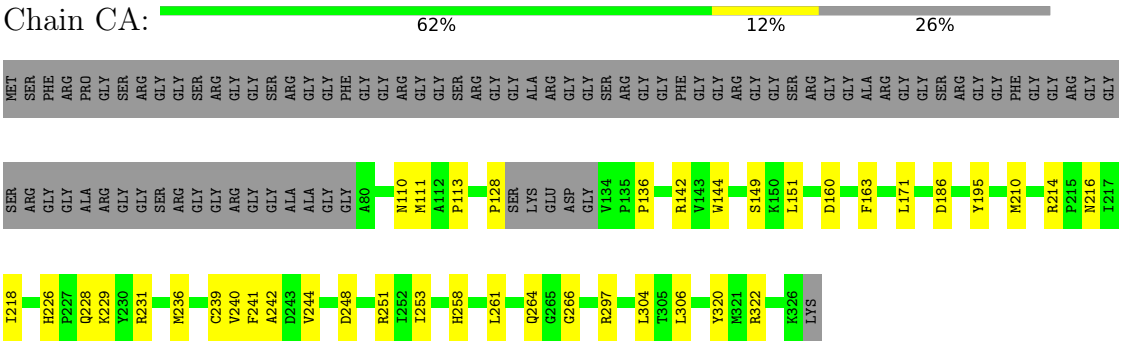
Mol	Chain	Residues	Atoms	AltConf
70	CL	1	Total C N O P 32 10 5 14 3	0

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.

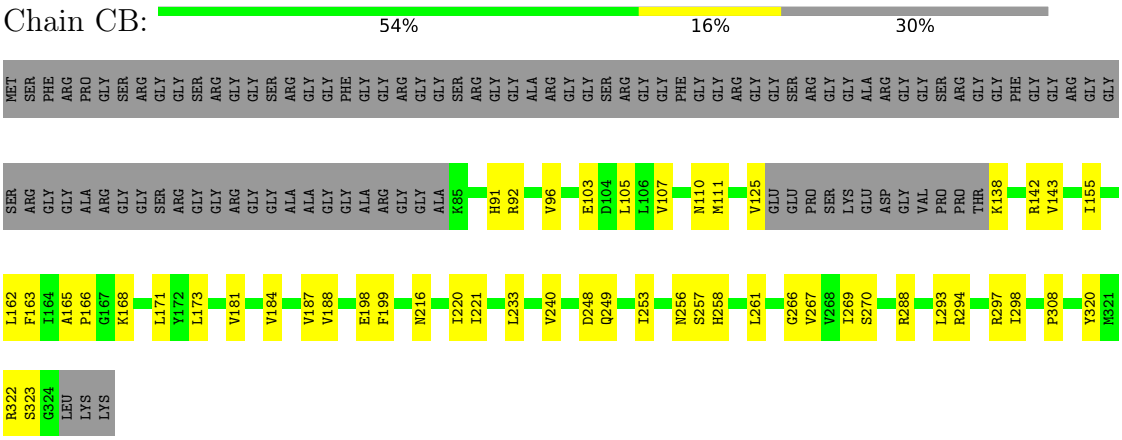
• Molecule 1: rRNA 2'-O-methyltransferase fibrillarin

Chain CA:



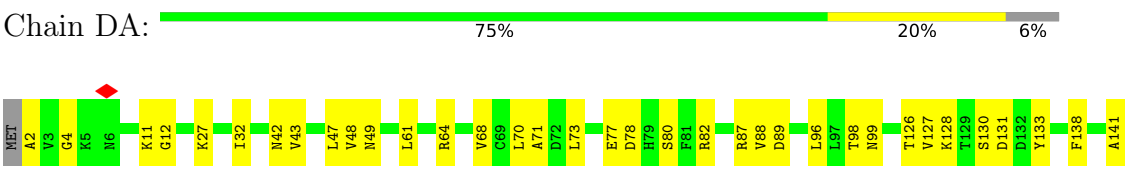
• Molecule 1: rRNA 2'-O-methyltransferase fibrillarin

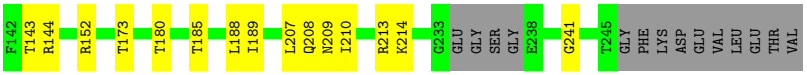
Chain CB:



• Molecule 2: 40S ribosomal protein S1-A

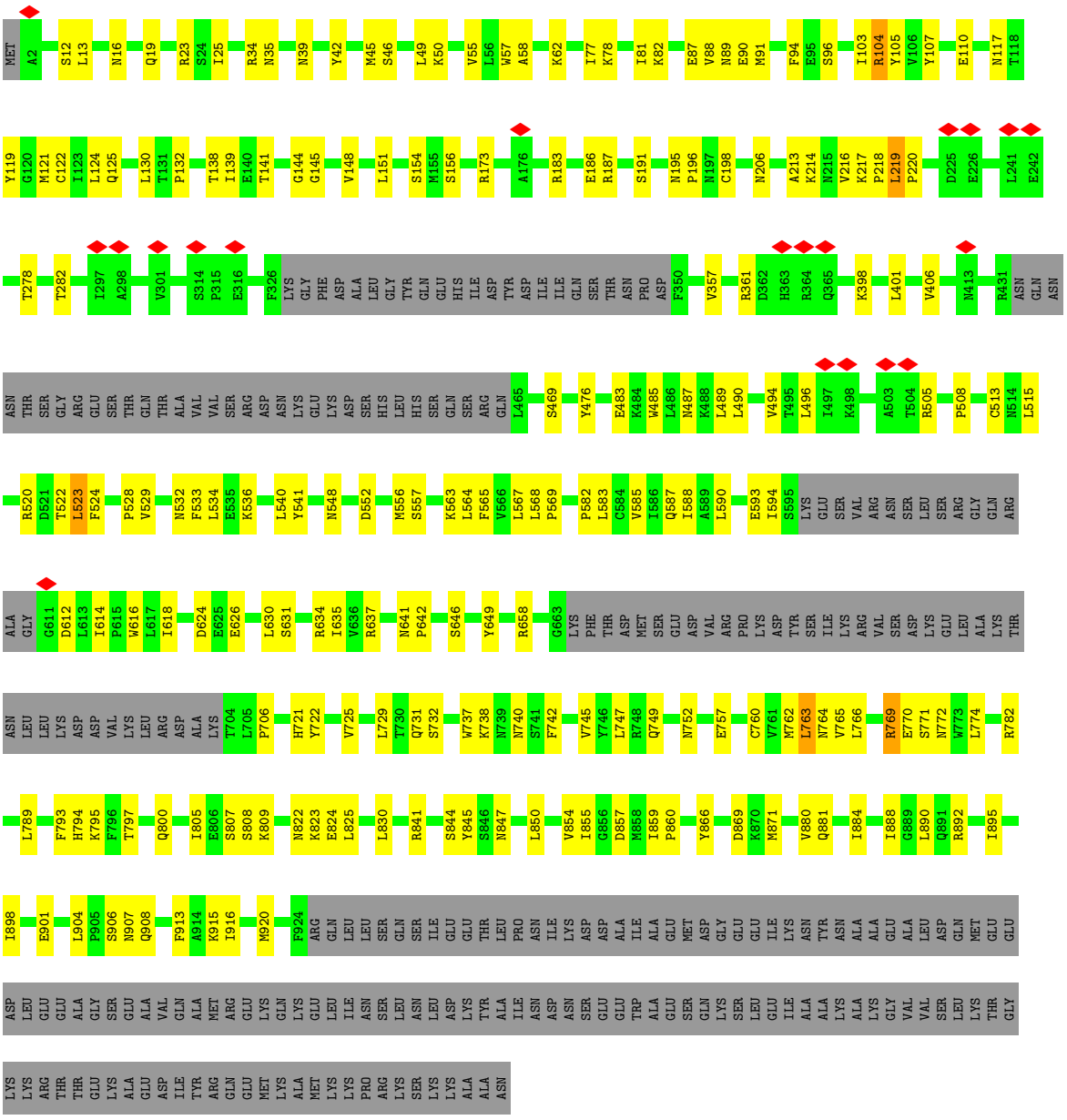
Chain DA:





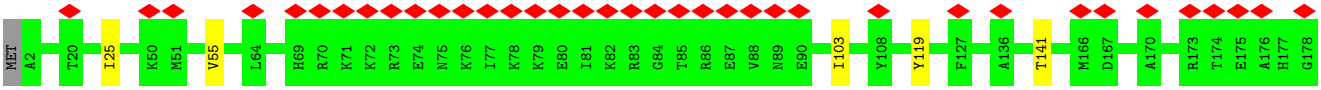
• Molecule 3: RNA cytidine acetyltransferase

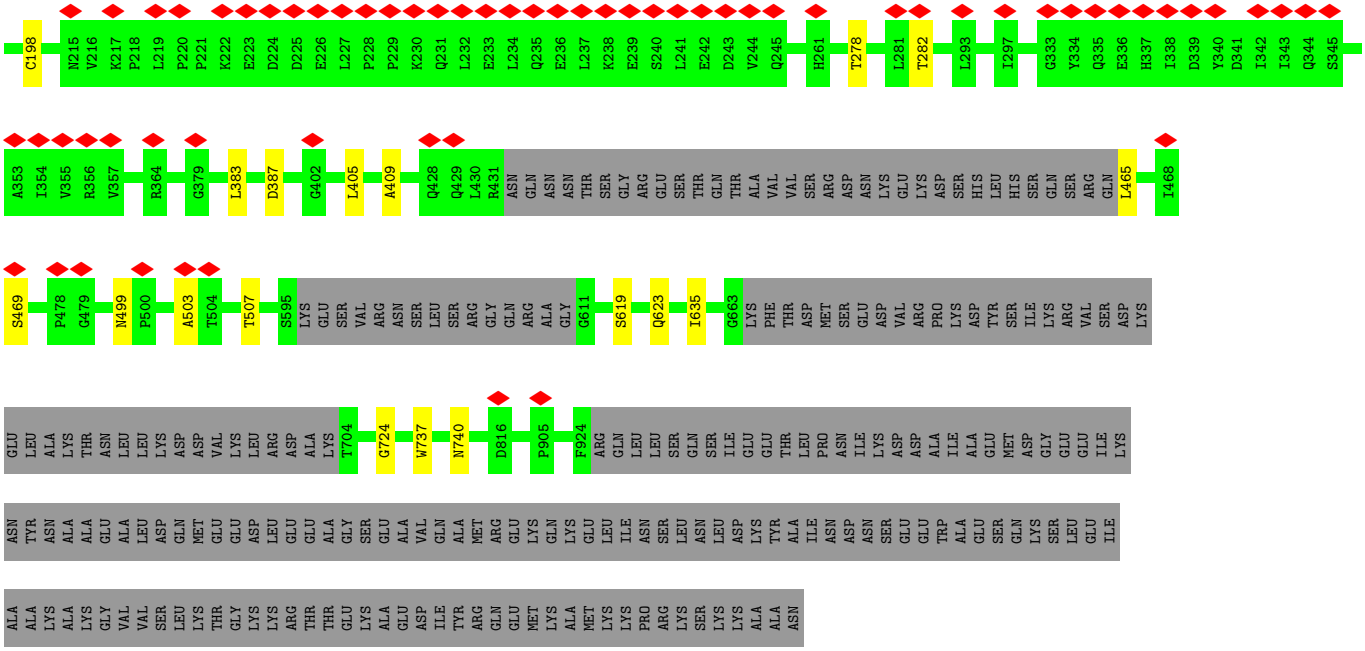
Chain JA:



• Molecule 3: RNA cytidine acetyltransferase

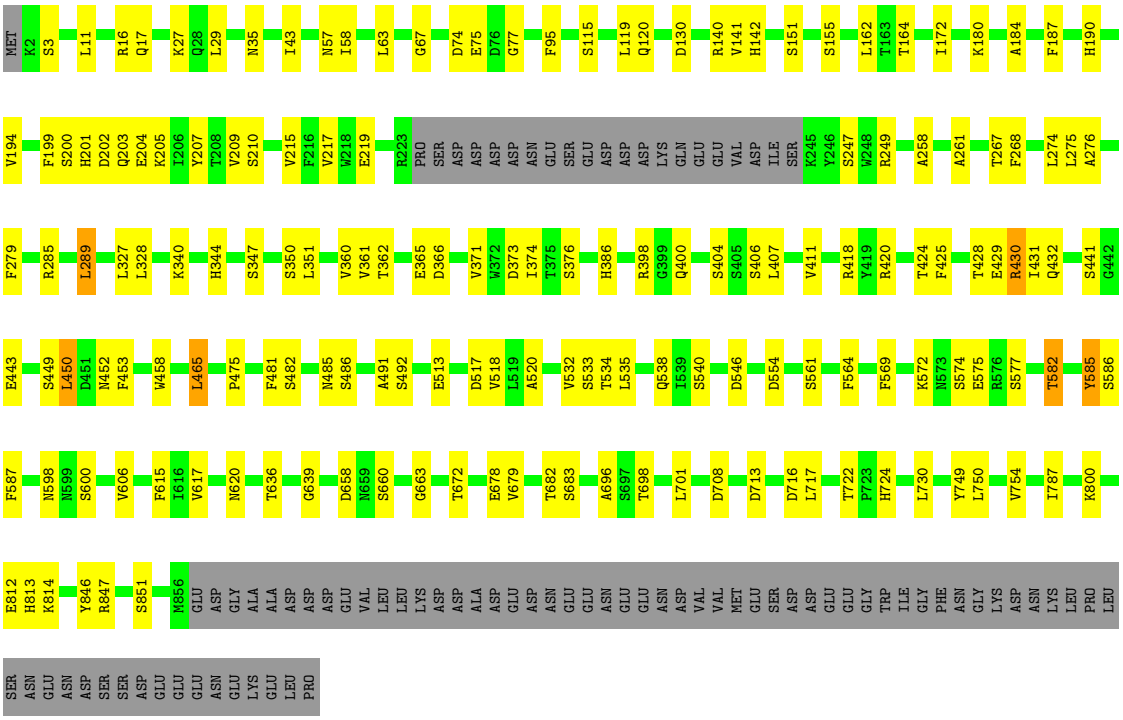
Chain JB:





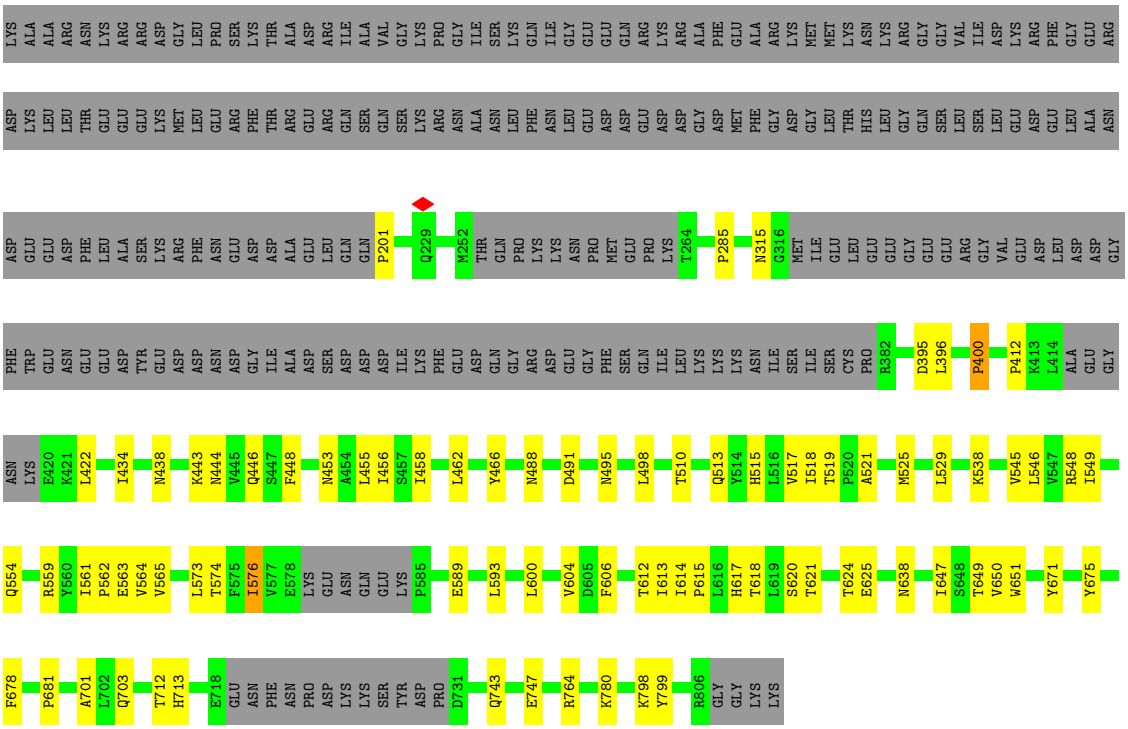
• Molecule 4: Periodic tryptophan protein 2

Chain UA:



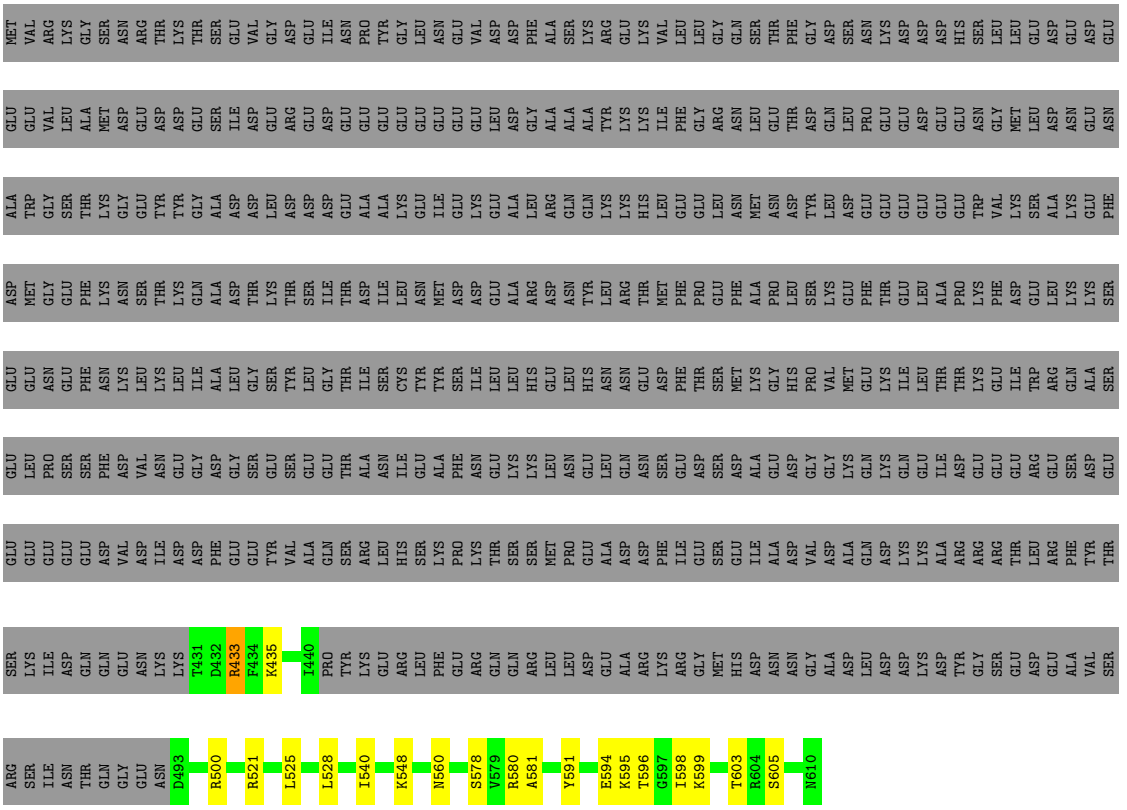
• Molecule 5: Nucleolar complex protein 14

Chain UB:



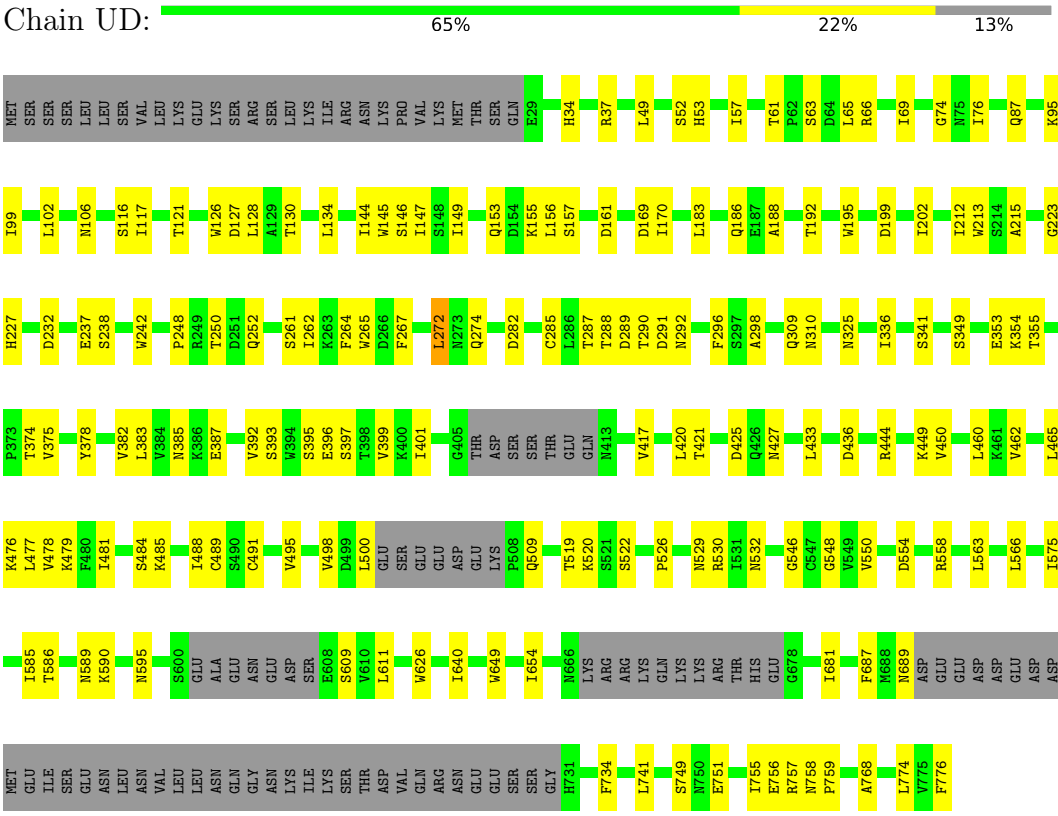
• Molecule 6: Something about silencing protein 10

Chain UC: 18% 79%



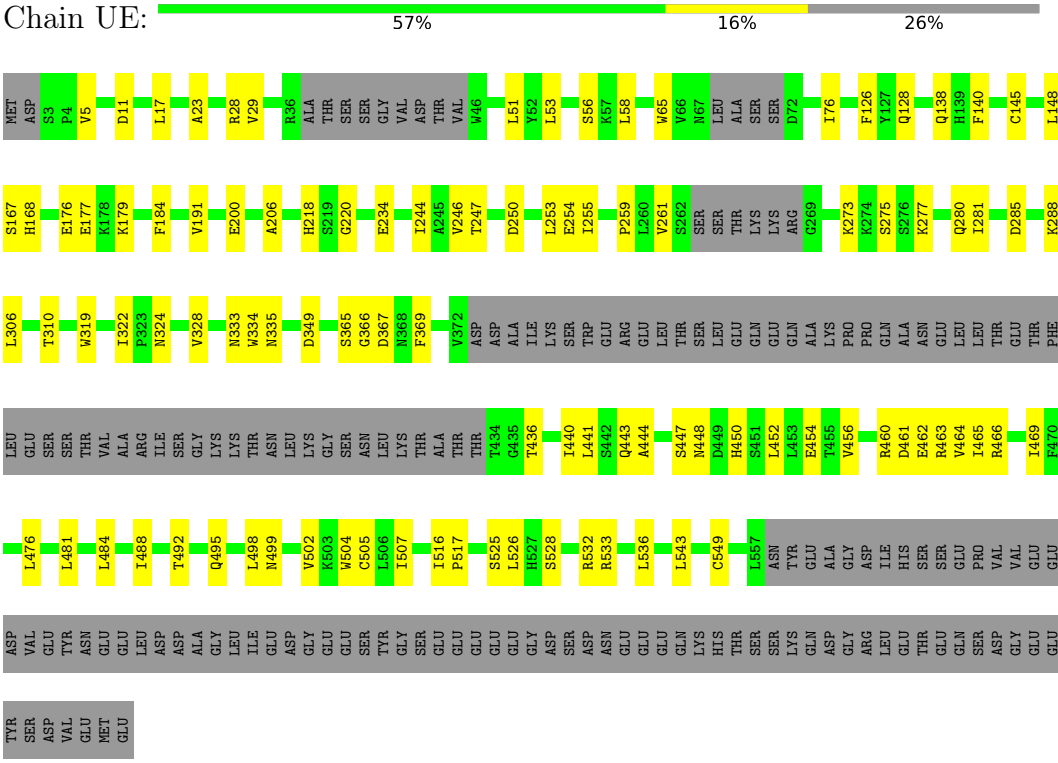
• Molecule 7: U3 small nucleolar RNA-associated protein 4

Chain UD:



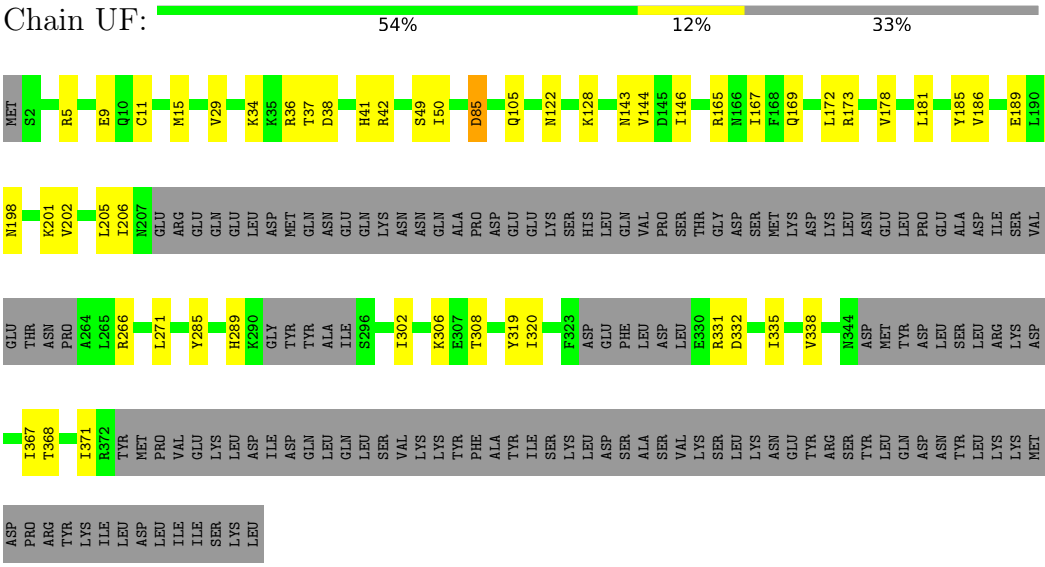
• Molecule 8: U3 small nucleolar RNA-associated protein 5

Chain UE:



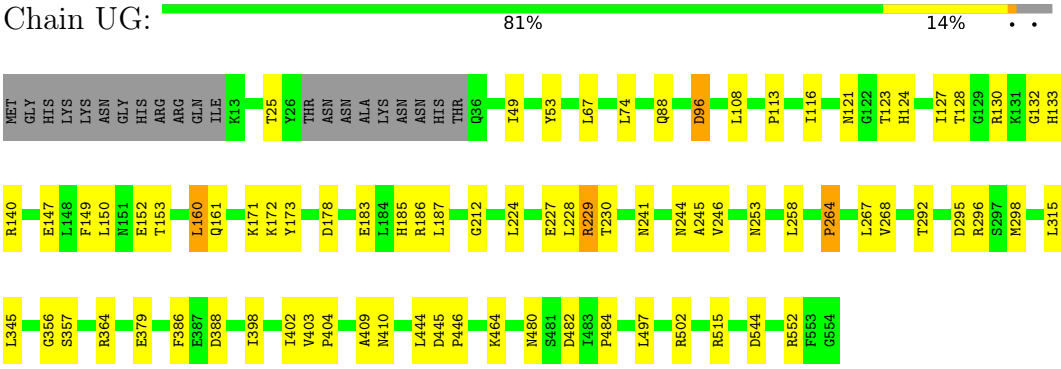
• Molecule 9: U3 small nucleolar RNA-associated protein 6

Chain UF:



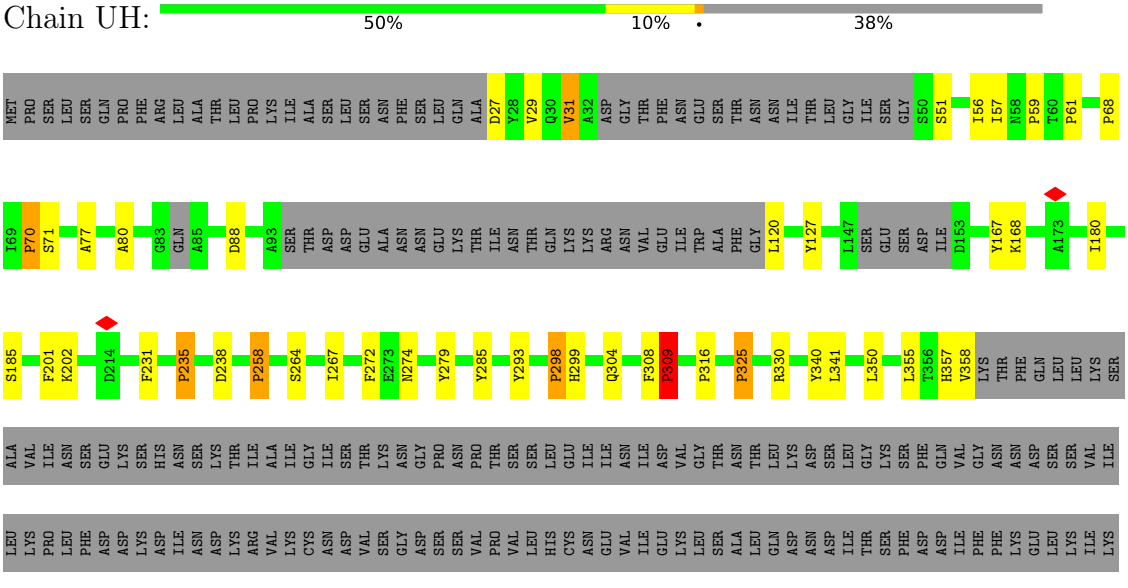
• Molecule 10: U3 small nucleolar RNA-associated protein 7

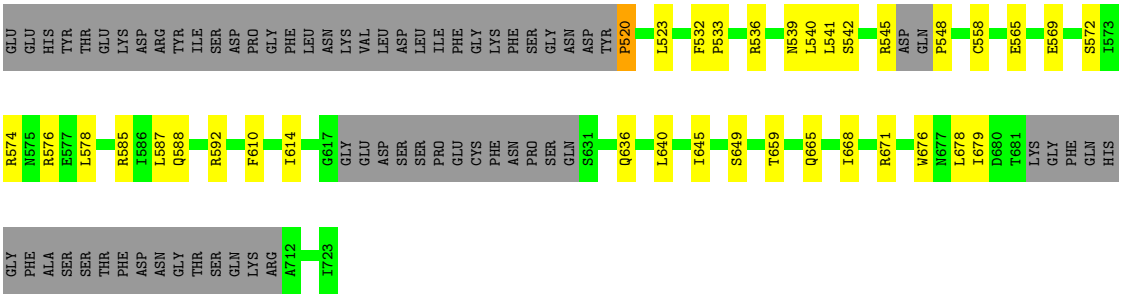
Chain UG:



• Molecule 11: U3 small nucleolar RNA-associated protein 8

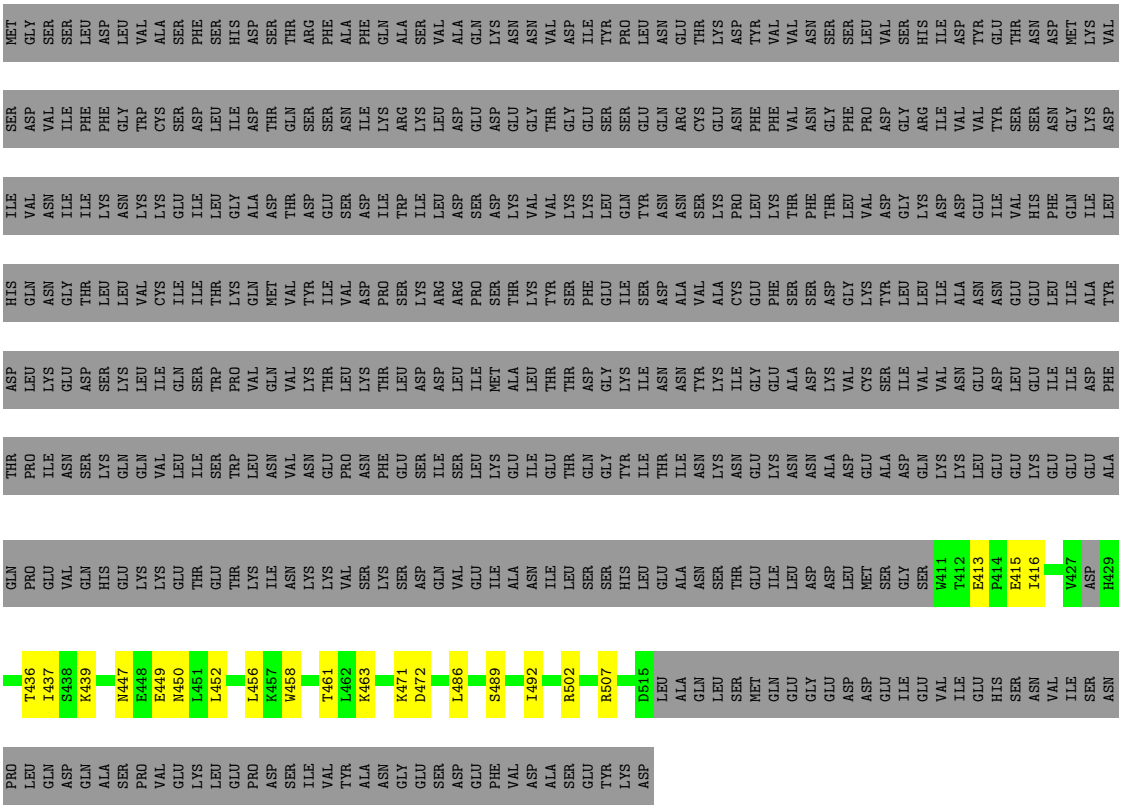
Chain UH:





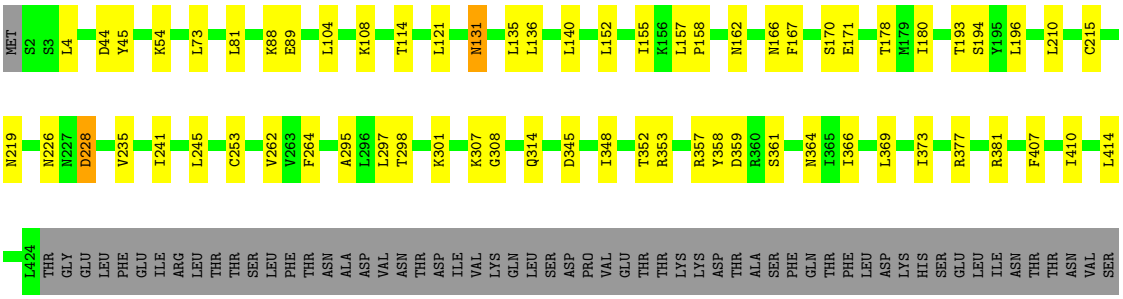
• Molecule 12: U3 small nucleolar RNA-associated protein 9

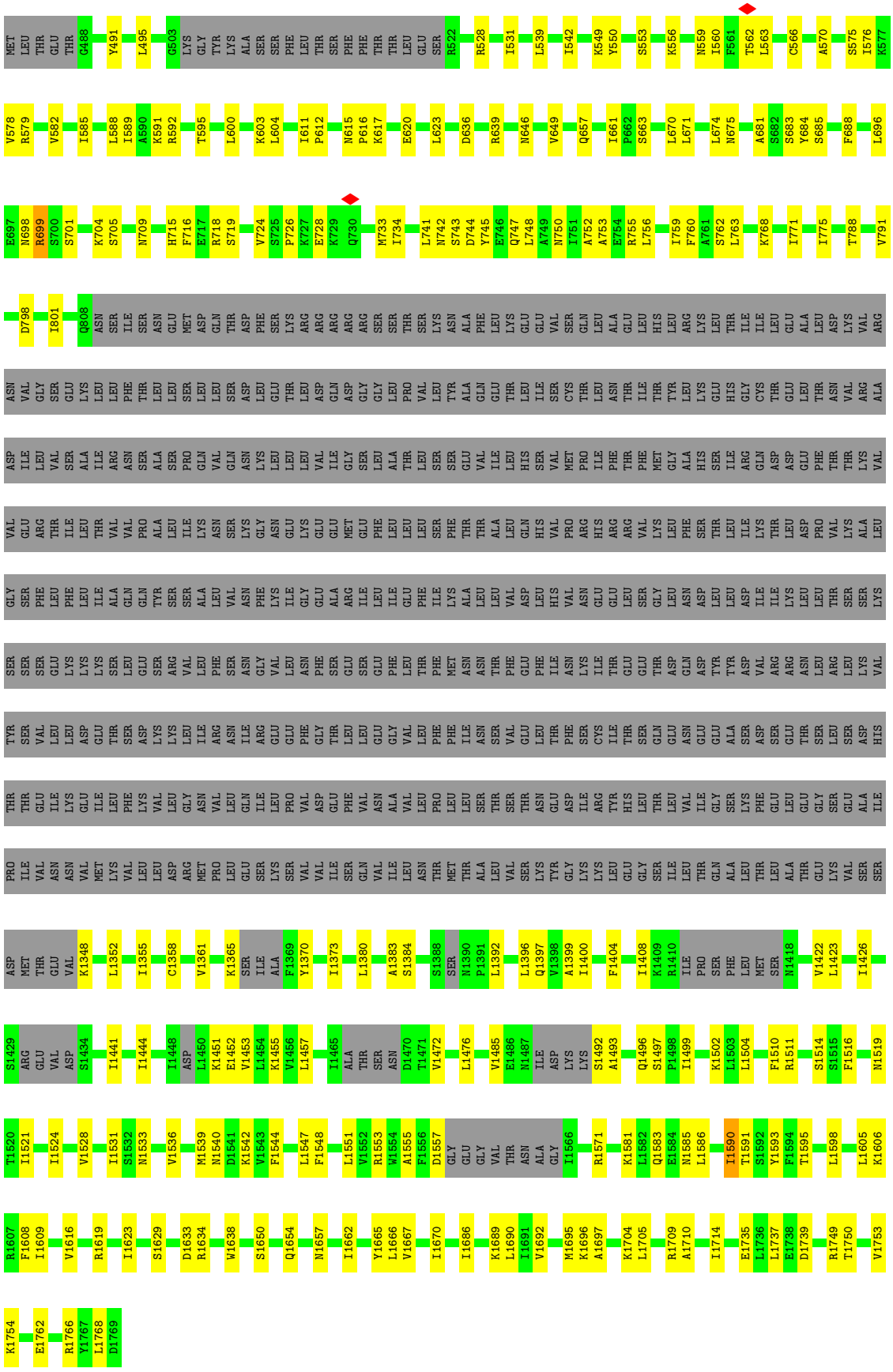
Chain UI:



• Molecule 13: U3 small nucleolar RNA-associated protein 10

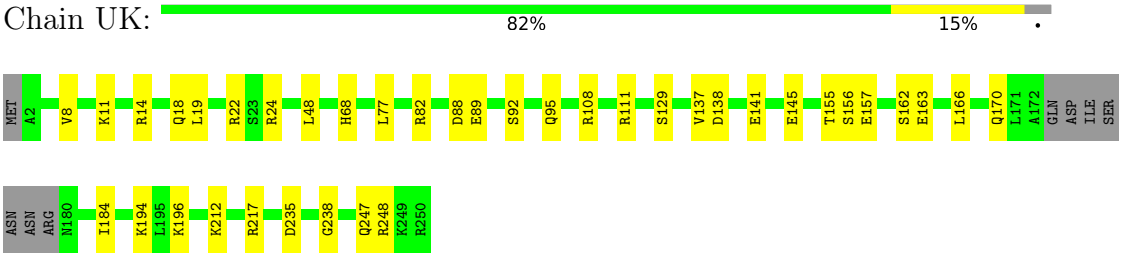
Chain UJ:





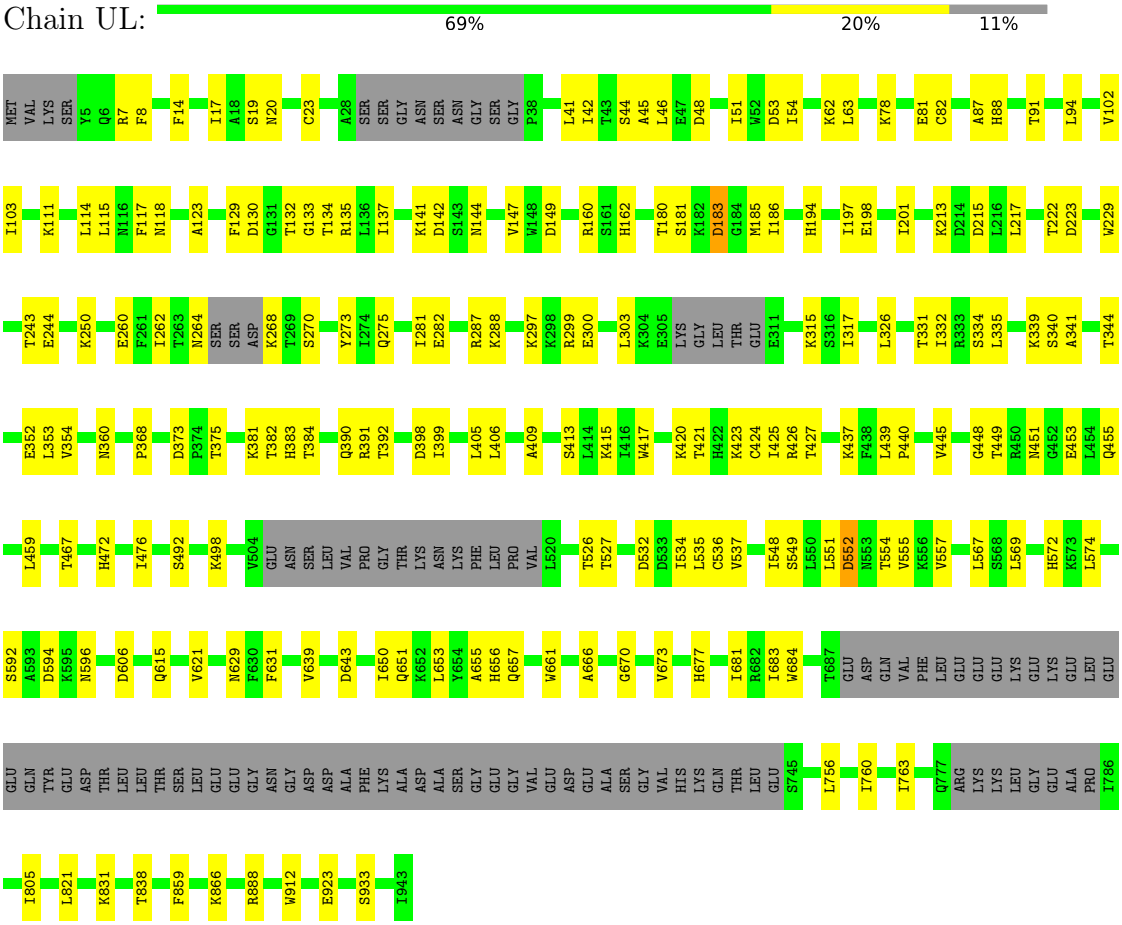
• Molecule 14: U3 small nucleolar RNA-associated protein 11

Chain UK:



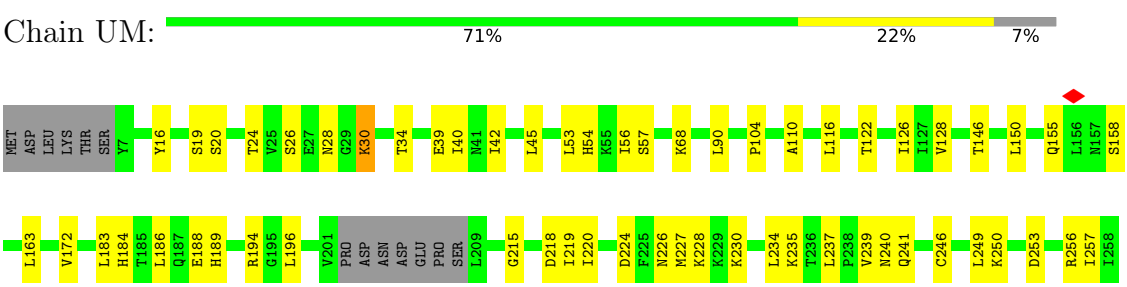
• Molecule 15: U3 small nucleolar RNA-associated protein 12

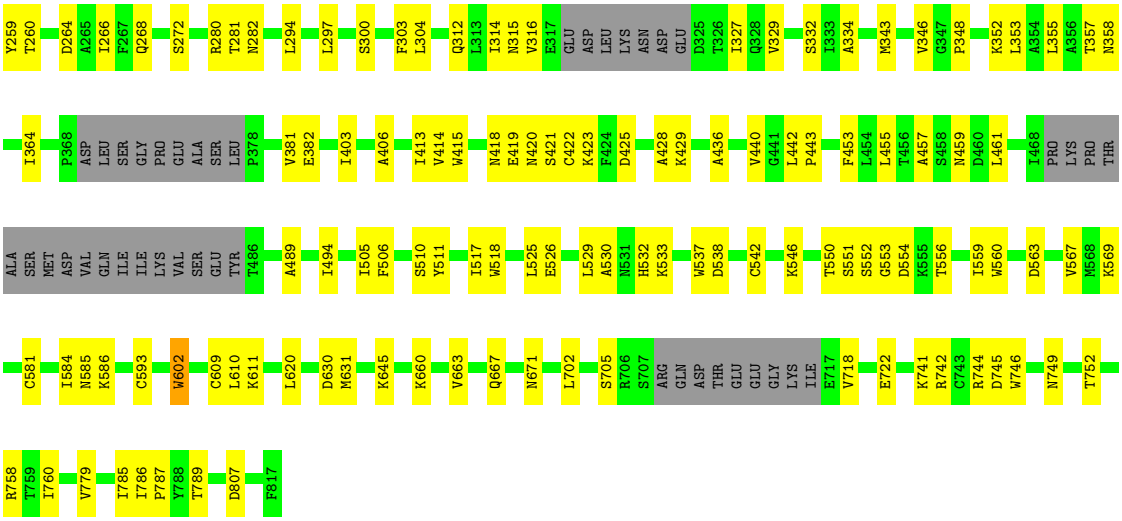
Chain UL:



• Molecule 16: U3 small nucleolar RNA-associated protein 13

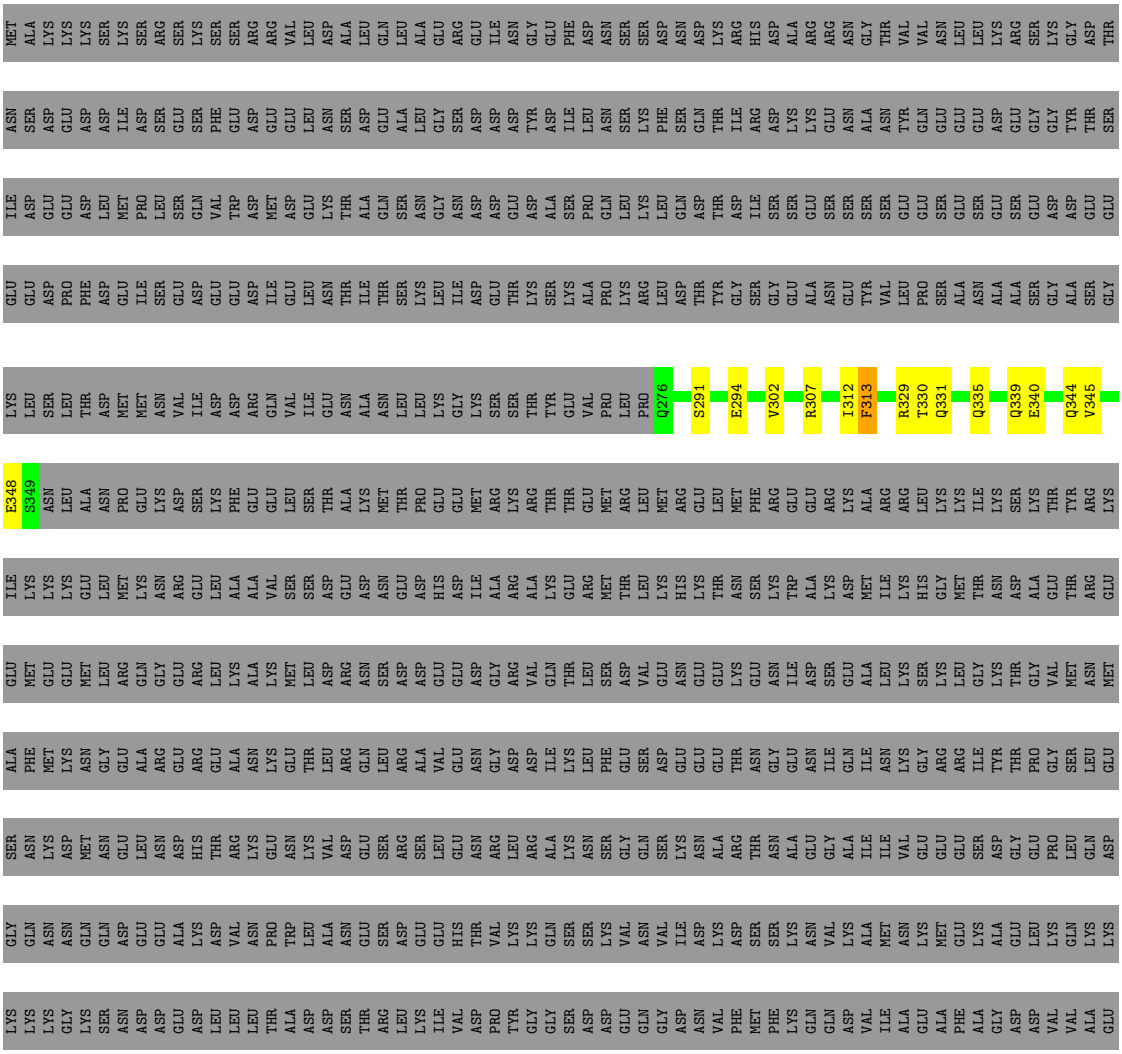
Chain UM:

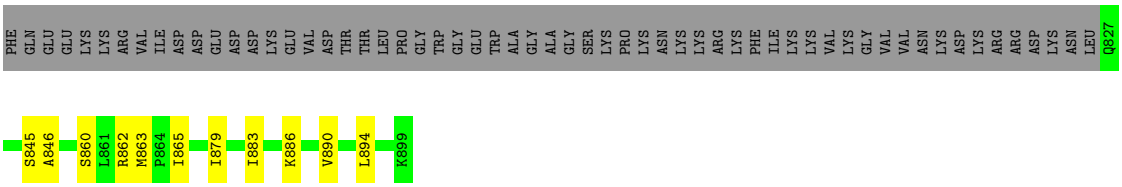




• Molecule 17: U3 small nucleolar RNA-associated protein 14

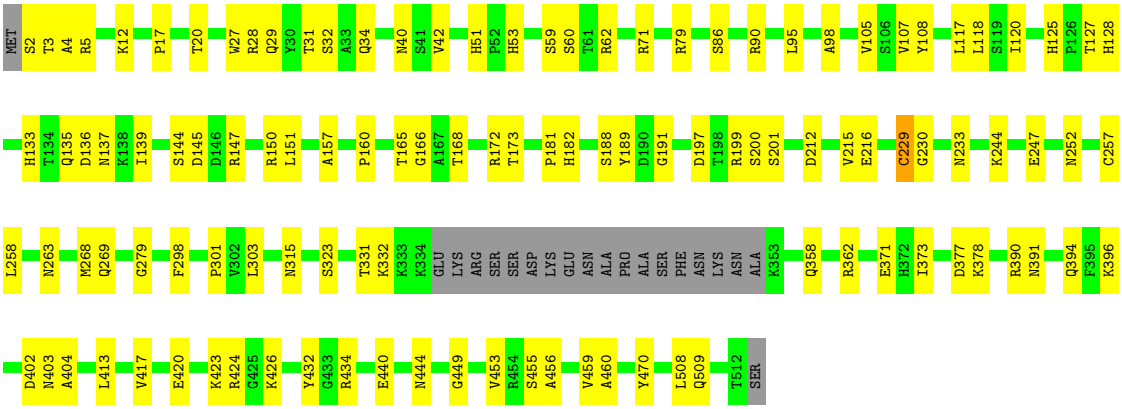
Chain UN:





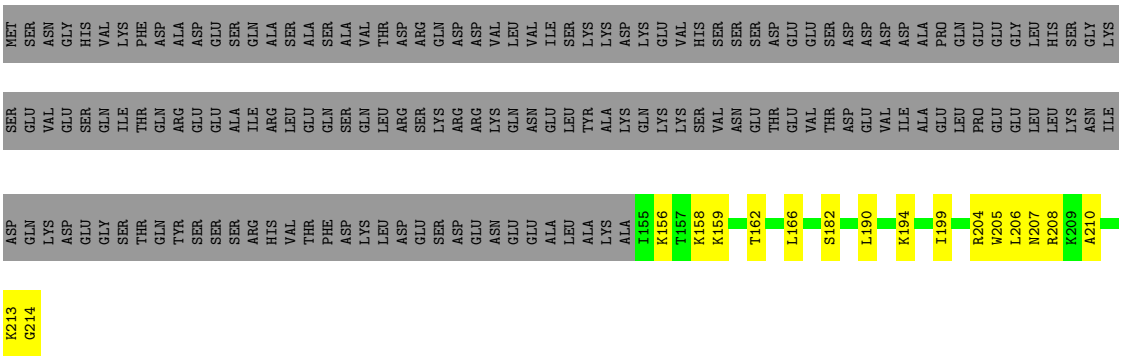
• Molecule 18: U3 small nucleolar RNA-associated protein 15

Chain UO:



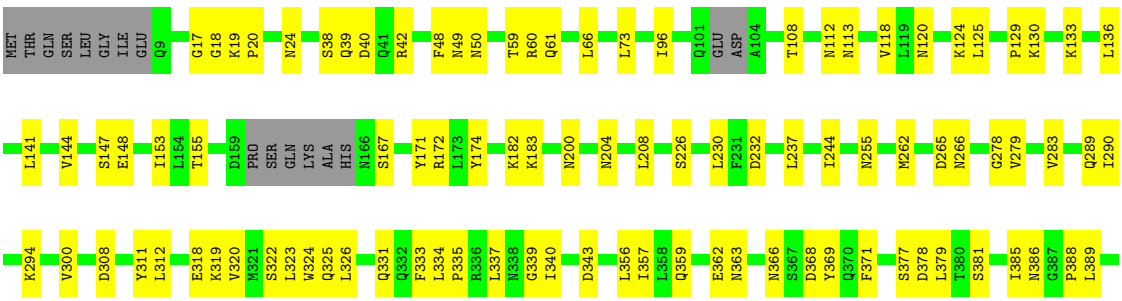
• Molecule 19: Bud site selection protein 21

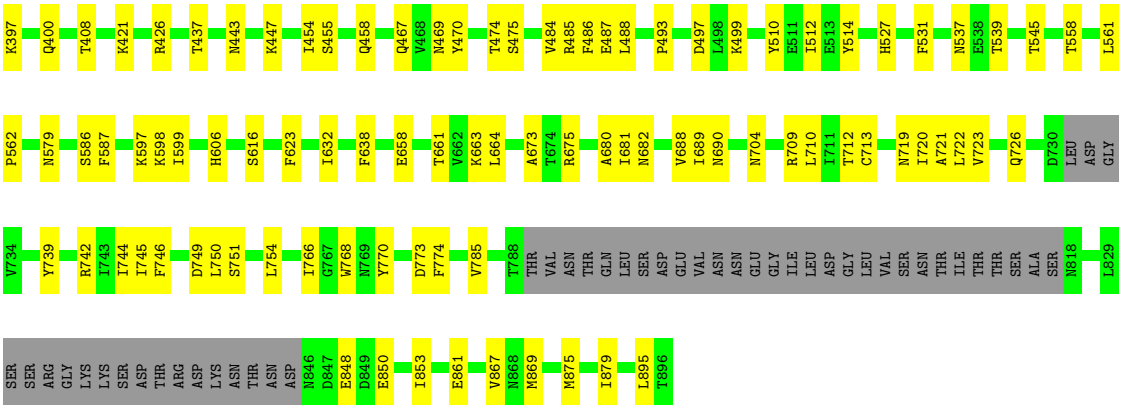
Chain UP:



• Molecule 20: NET1-associated nuclear protein 1

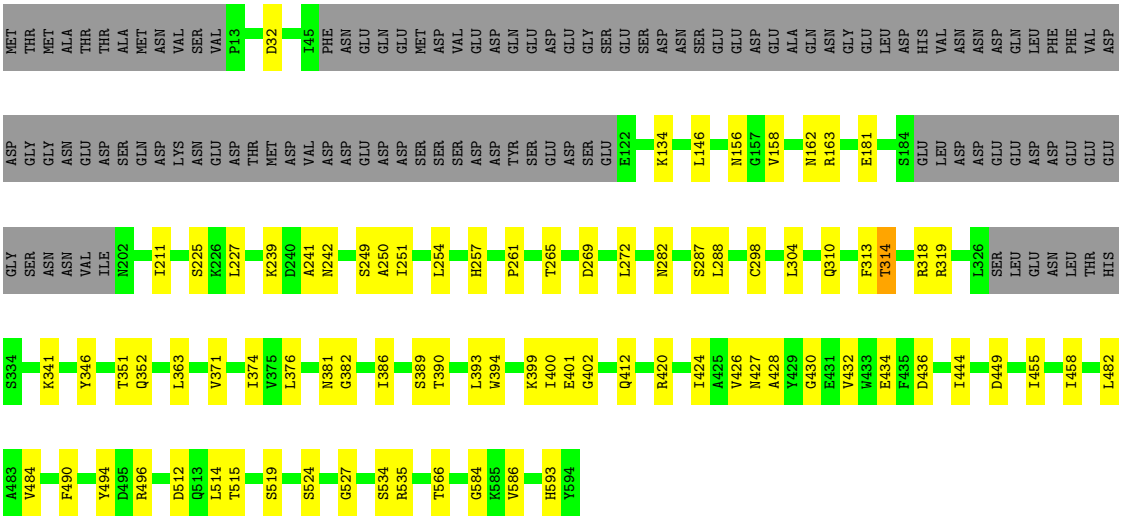
Chain UQ:





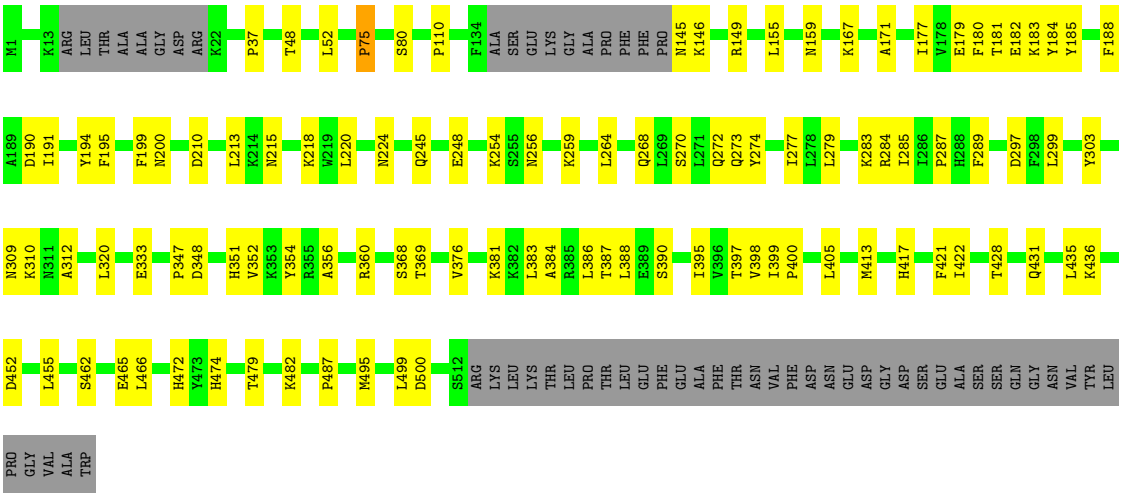
• Molecule 21: U3 small nucleolar RNA-associated protein 18

Chain UR:



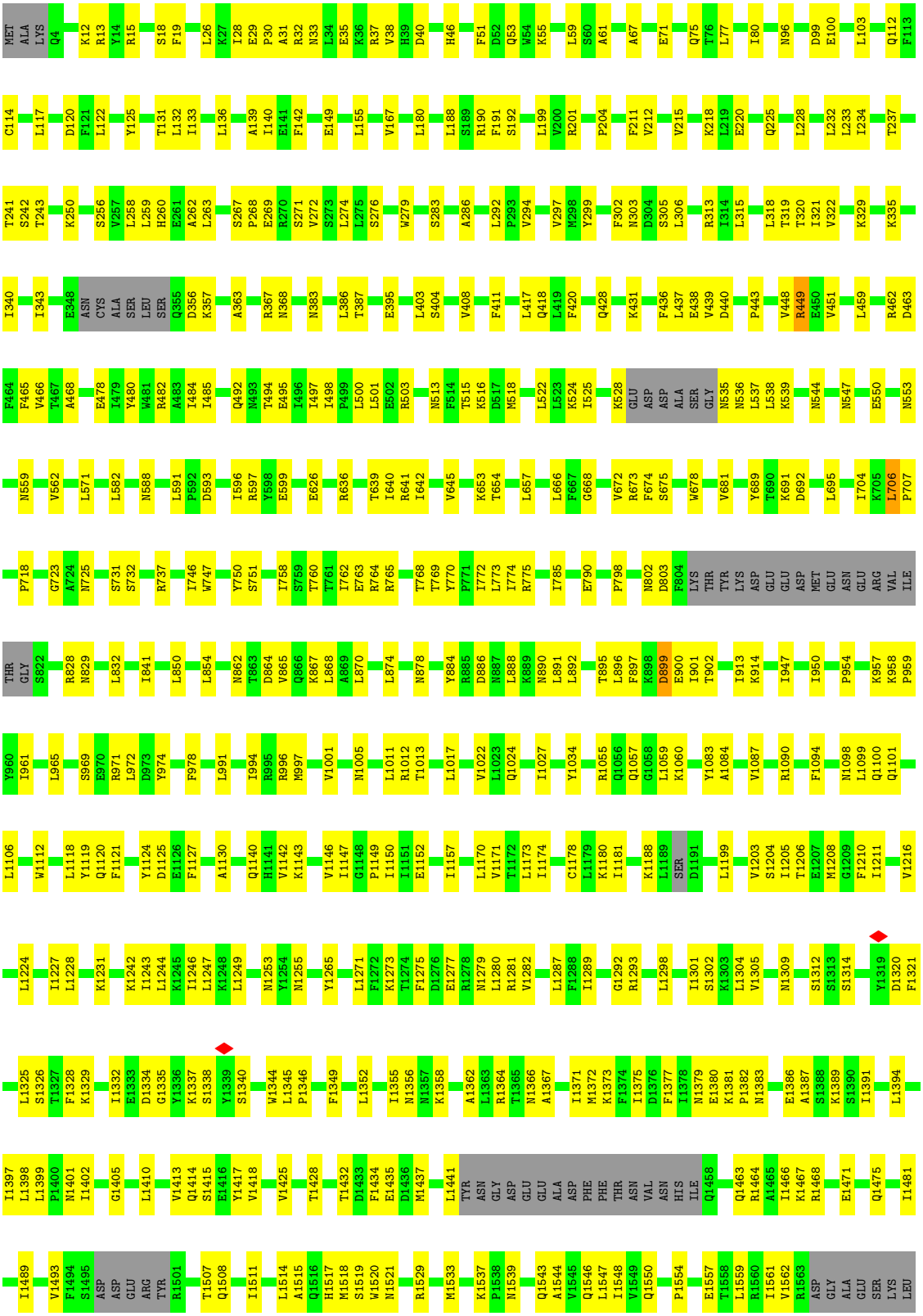
• Molecule 22: Nucleolar complex protein 4

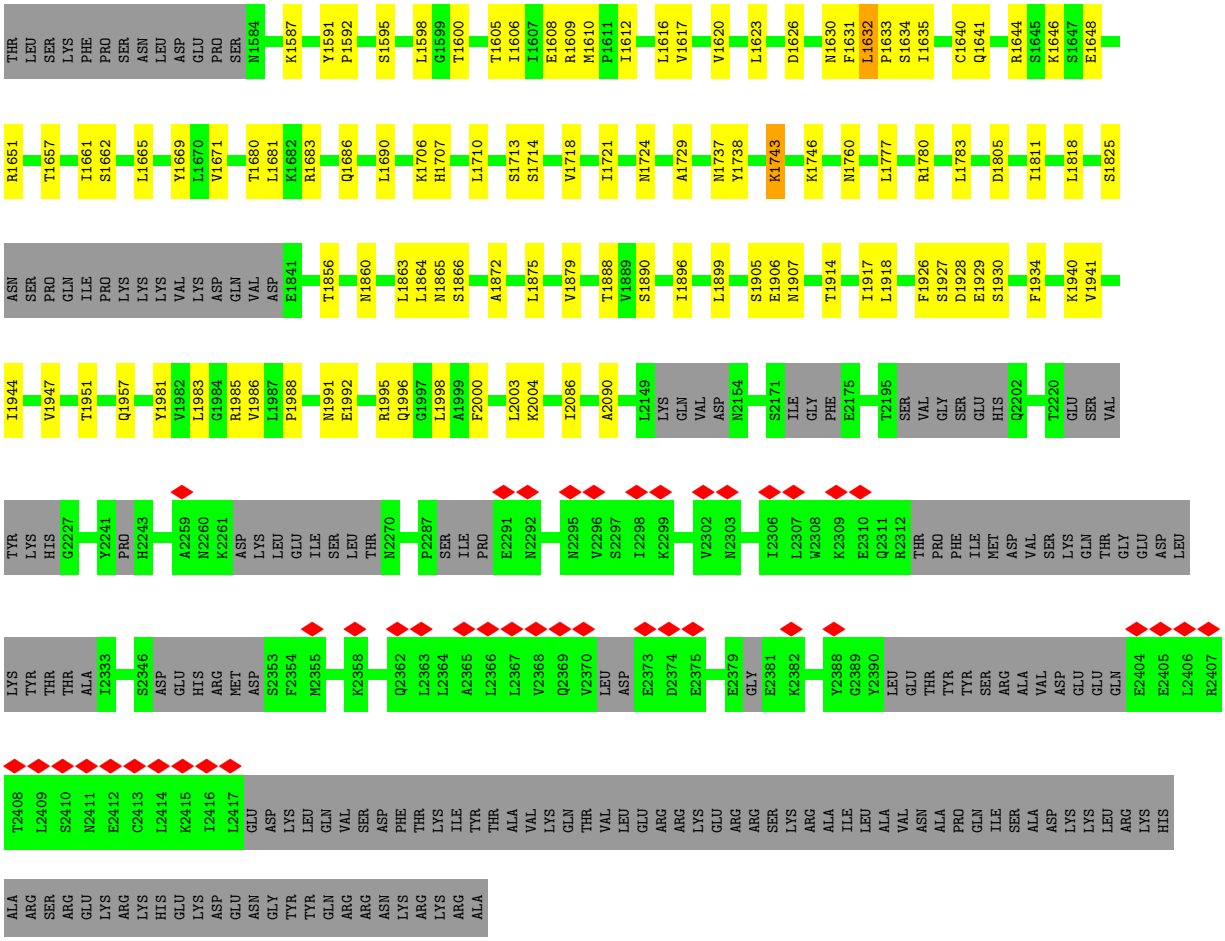
Chain US:



• Molecule 23: U3 small nucleolar RNA-associated protein 20

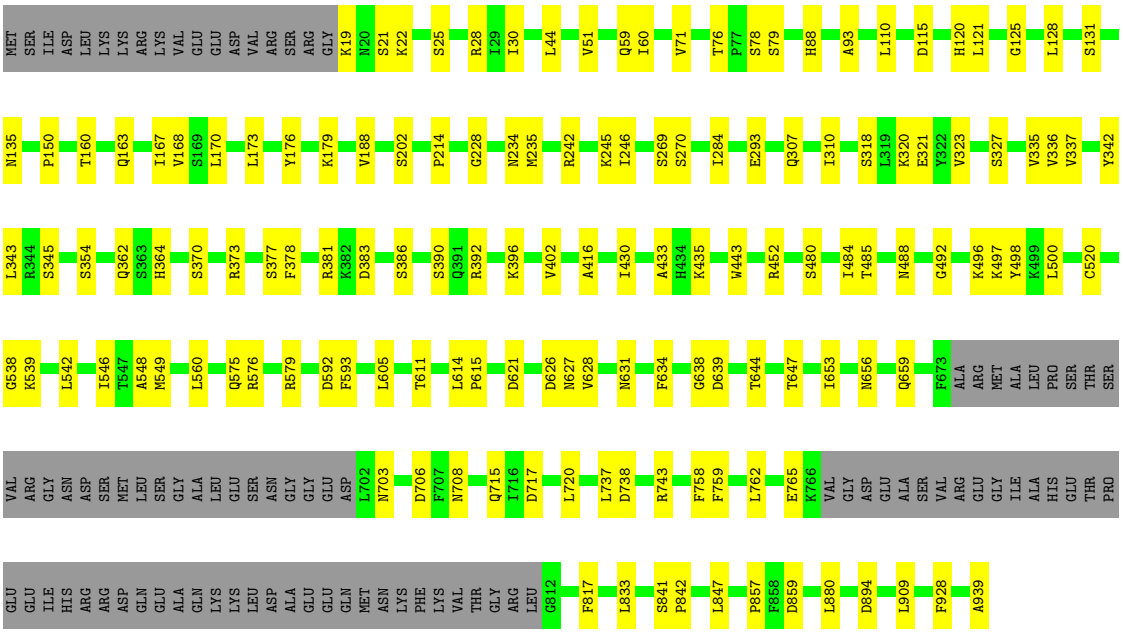
Chain UT:





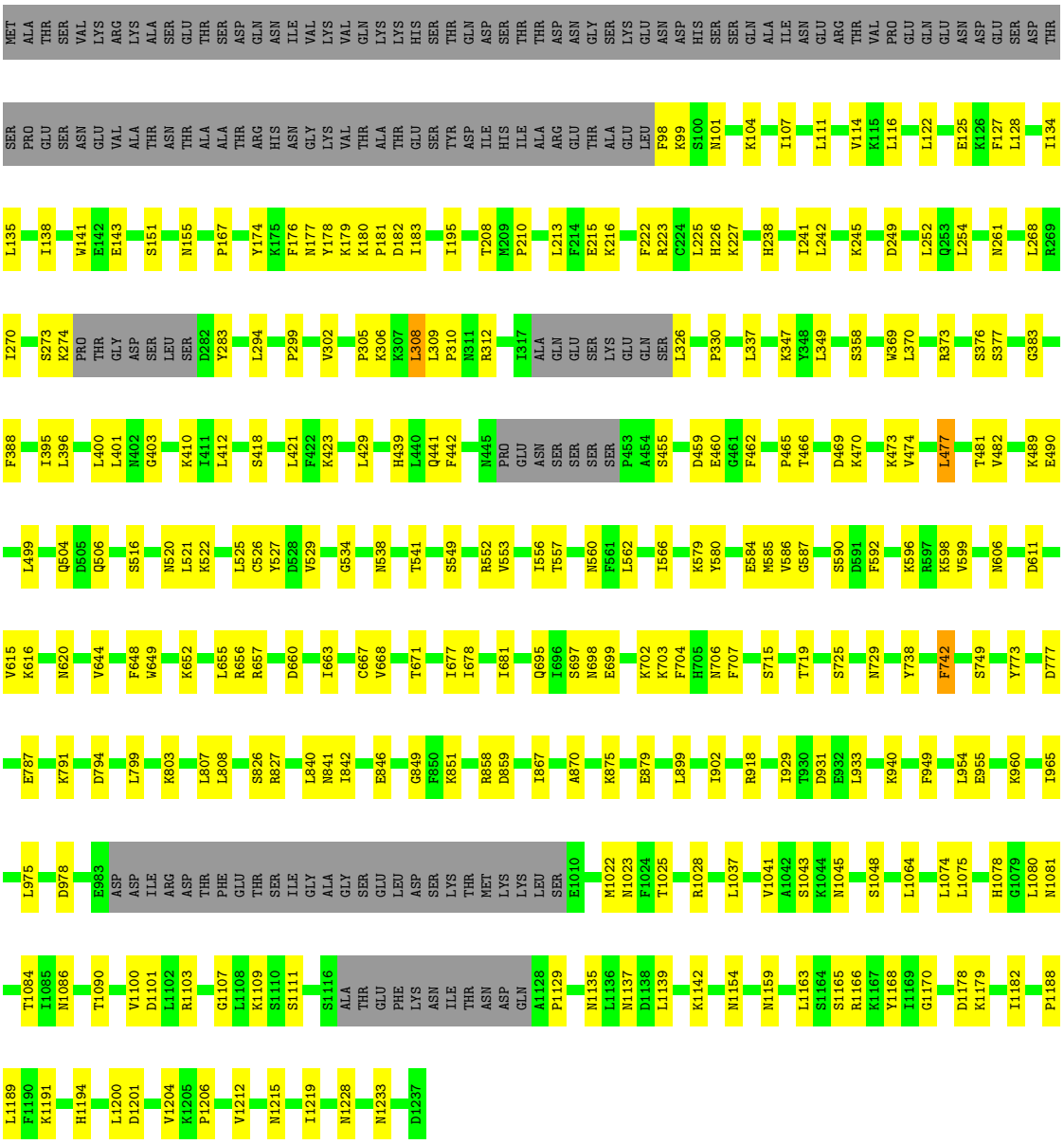
• Molecule 24: U3 small nucleolar RNA-associated protein 21

Chain UU:



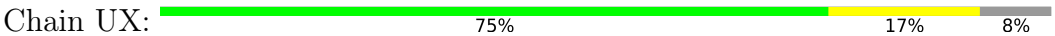
• Molecule 25: U3 small nucleolar RNA-associated protein 22

Chain UV:

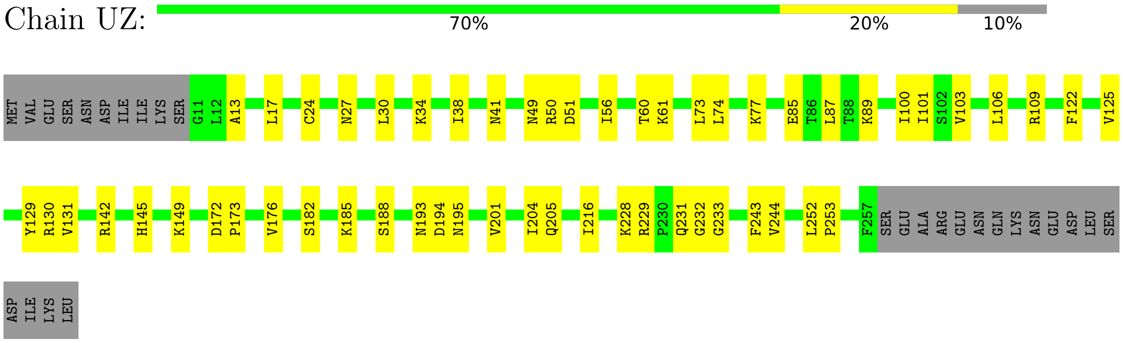


• Molecule 26: rRNA-processing protein FCF1

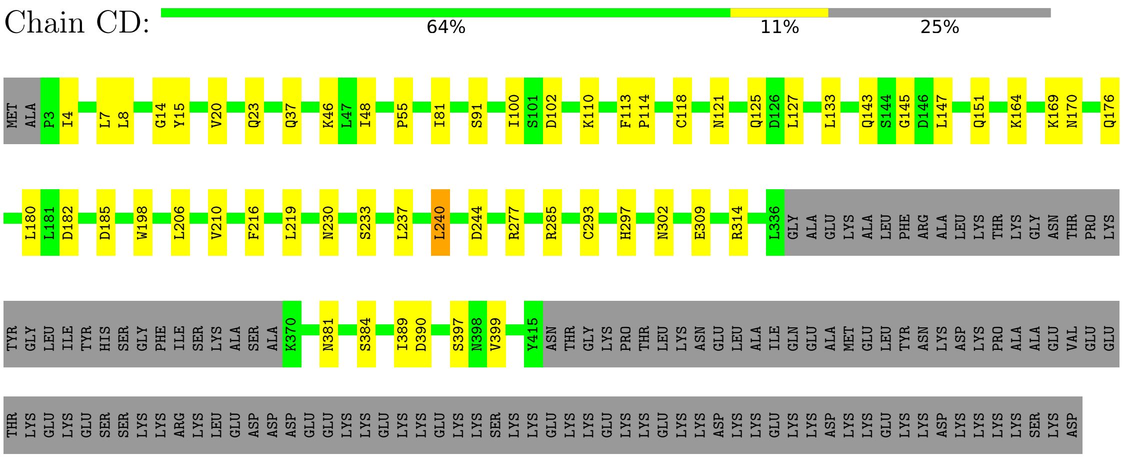
Chain UX:



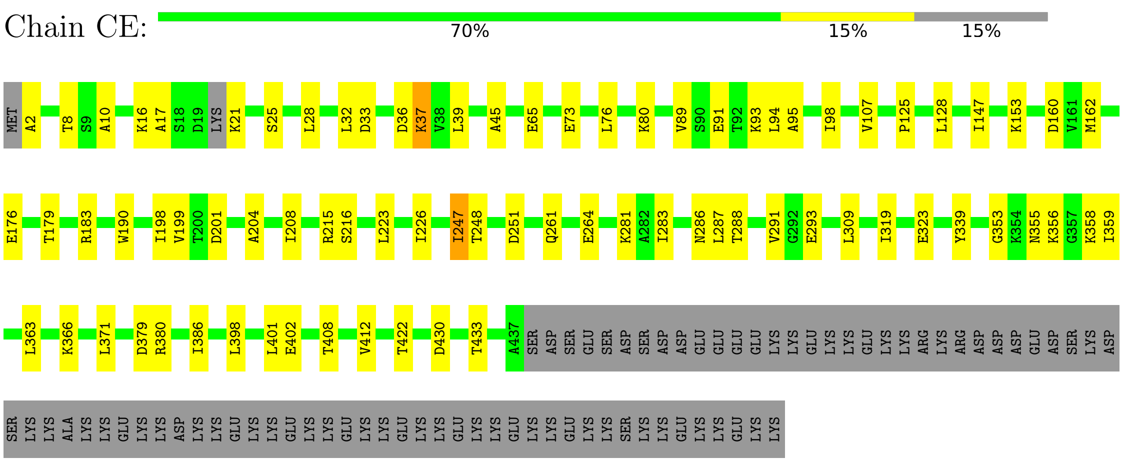
• Molecule 27: Ribosome biogenesis protein UTP30



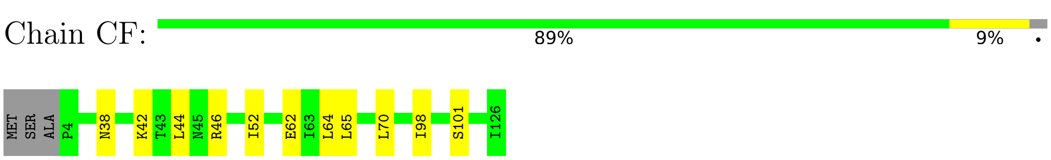
• Molecule 28: Nucleolar protein 56



• Molecule 29: Nucleolar protein 58

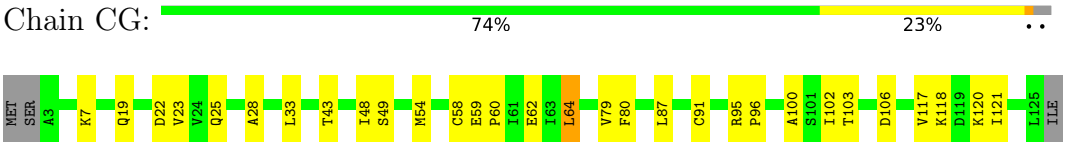


• Molecule 30: 13 kDa ribonucleoprotein-associated protein



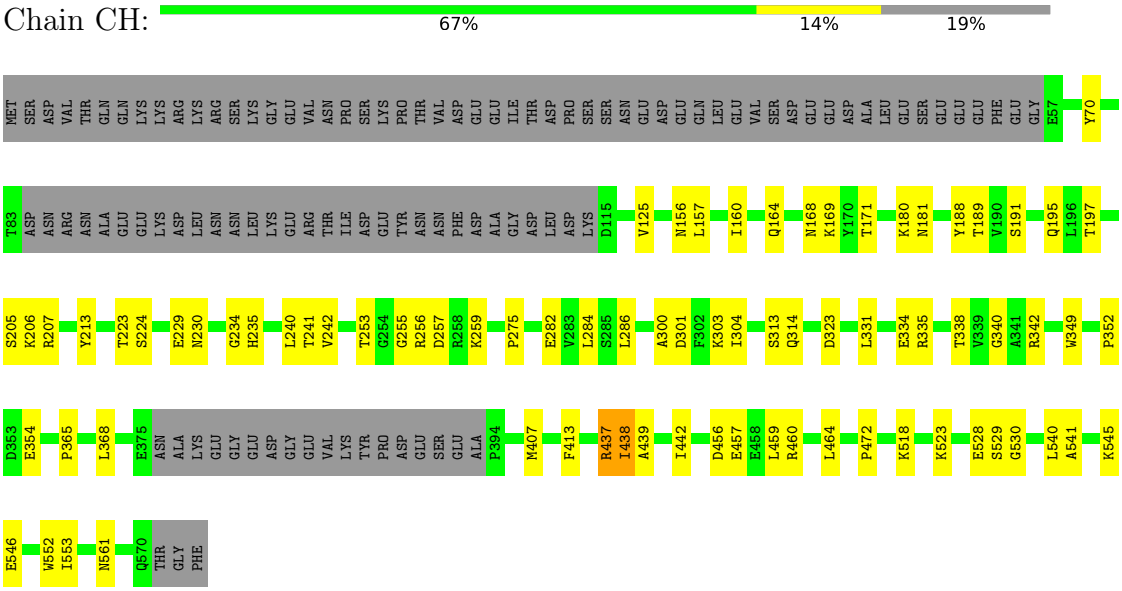
• Molecule 30: 13 kDa ribonucleoprotein-associated protein

Chain CG:



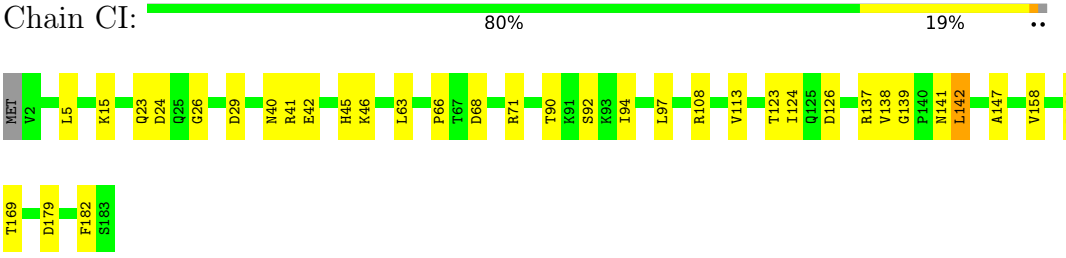
• Molecule 31: Ribosomal RNA-processing protein 9

Chain CH:



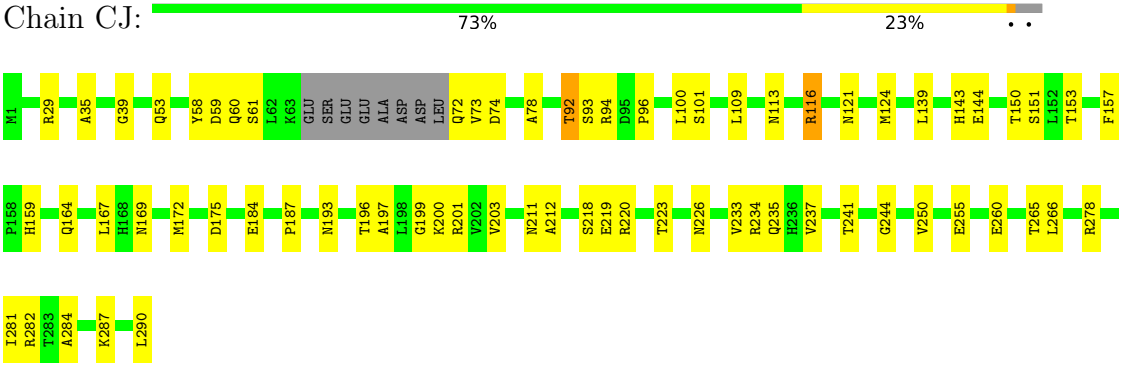
• Molecule 32: U3 small nucleolar ribonucleoprotein protein IMP3

Chain CI:



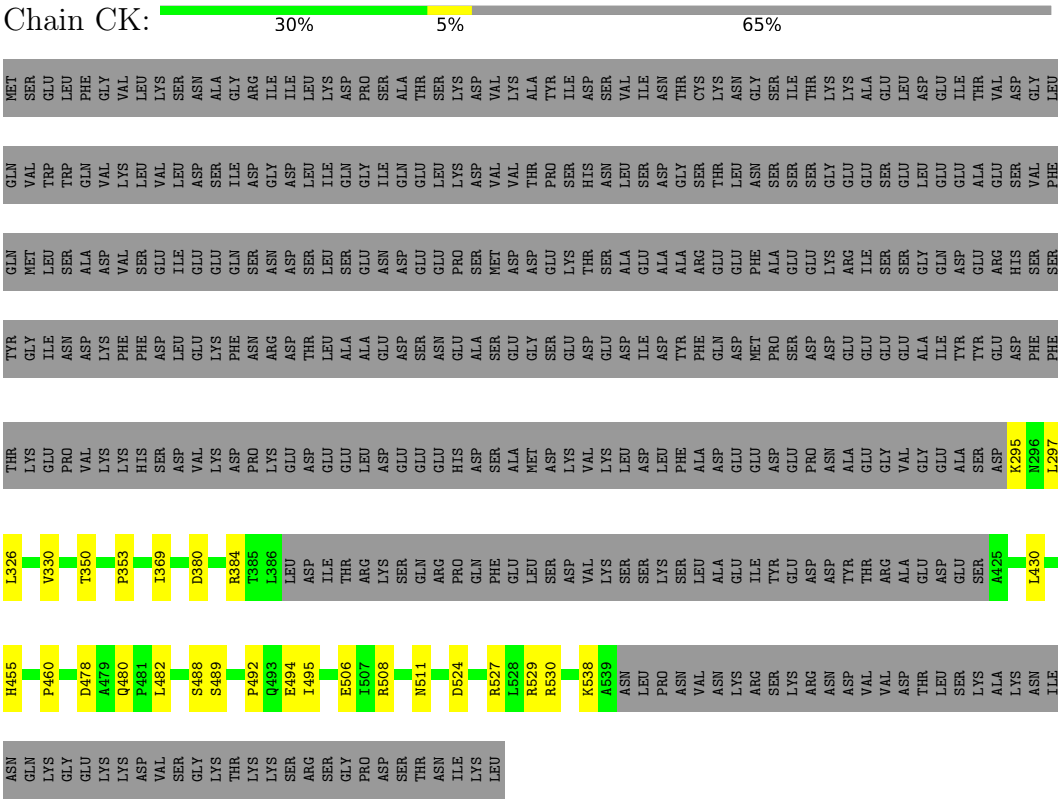
• Molecule 33: U3 small nucleolar ribonucleoprotein protein IMP4

Chain CJ:



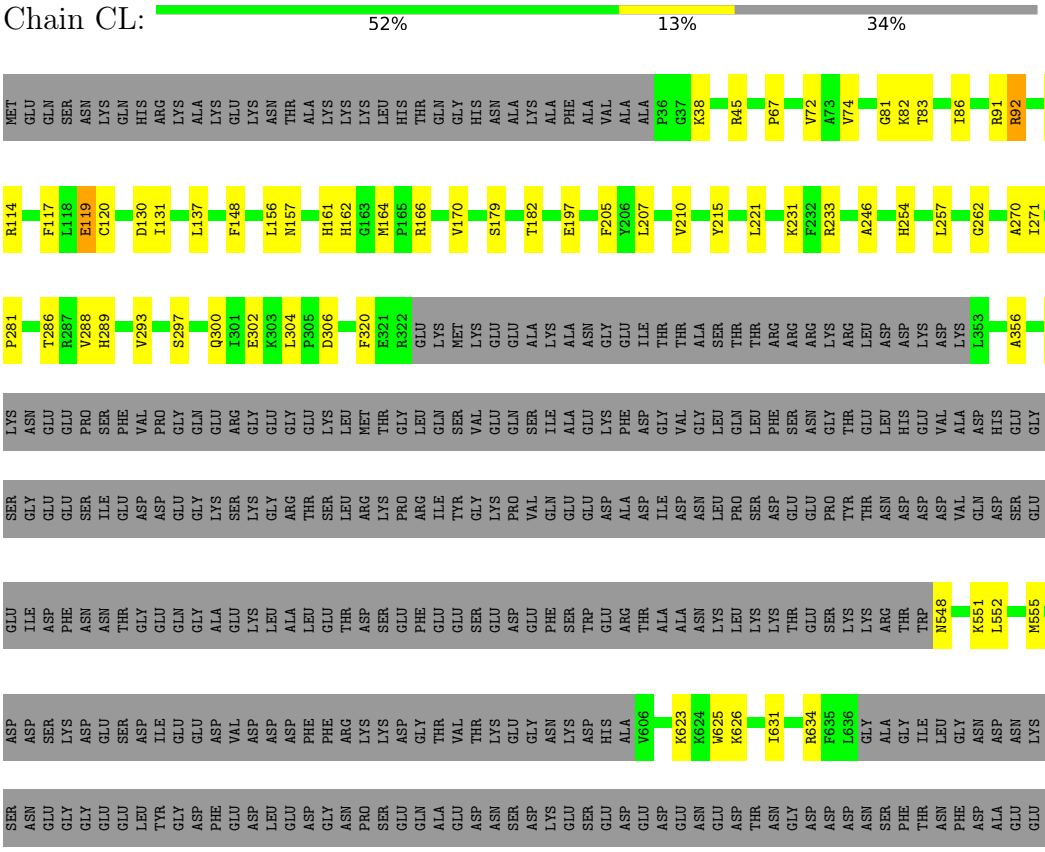
• Molecule 34: U3 small nucleolar RNA-associated protein MPP10

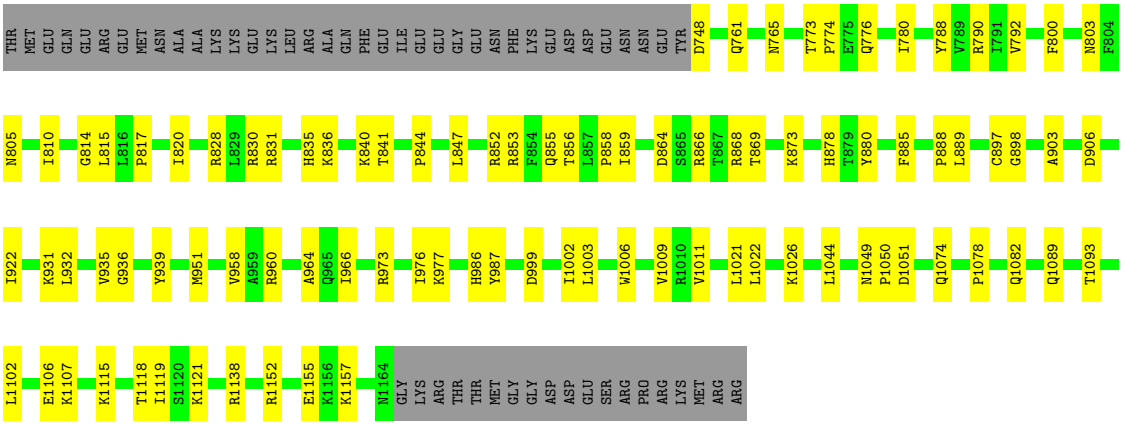
Chain CK:



• Molecule 35: Ribosome biogenesis protein BMS1

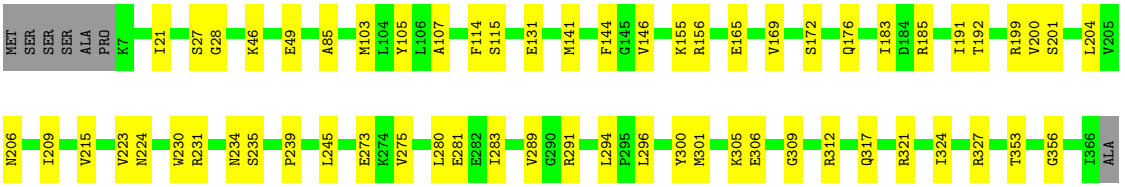
Chain CL:





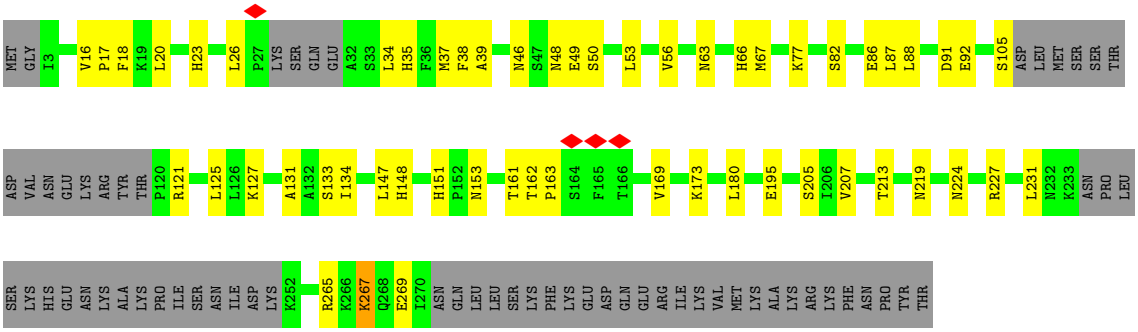
• Molecule 36: RNA 3'-terminal phosphate cyclase-like protein

Chain CM:



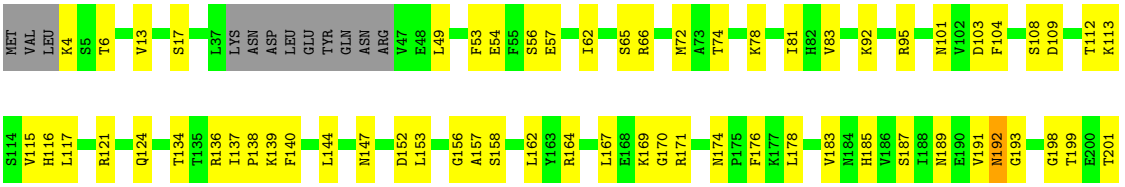
• Molecule 37: Ribosomal RNA-processing protein 7

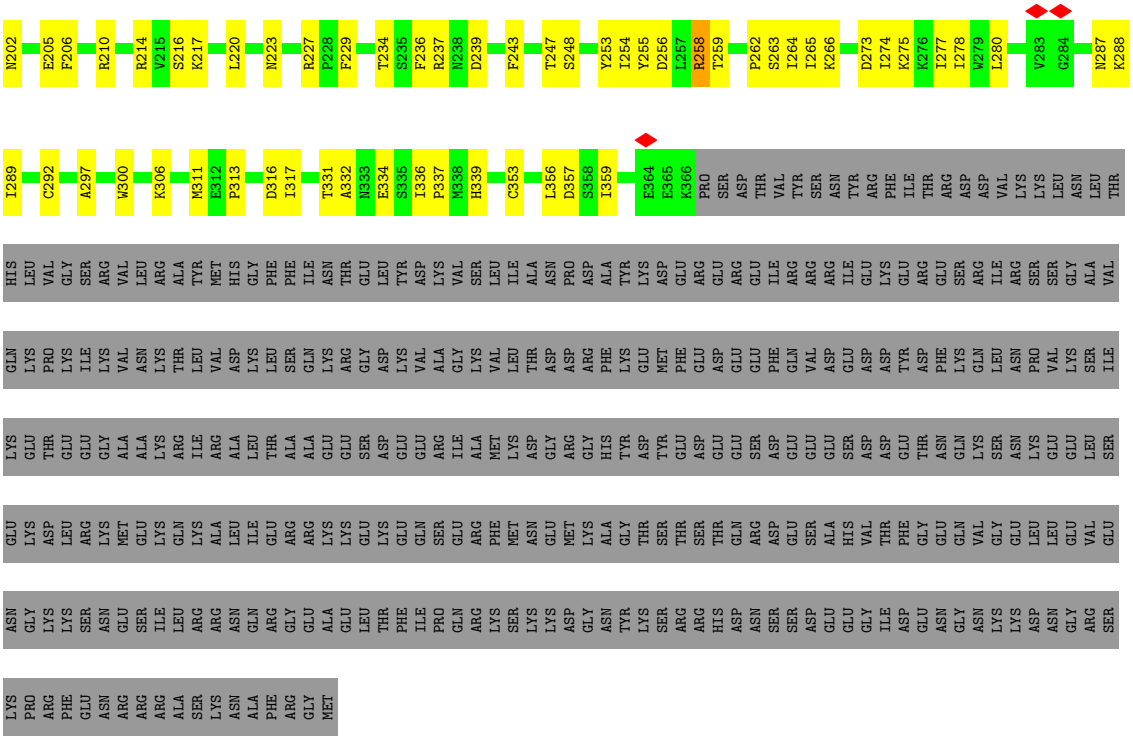
Chain CN:



• Molecule 38: Ribosome biogenesis protein ENP2

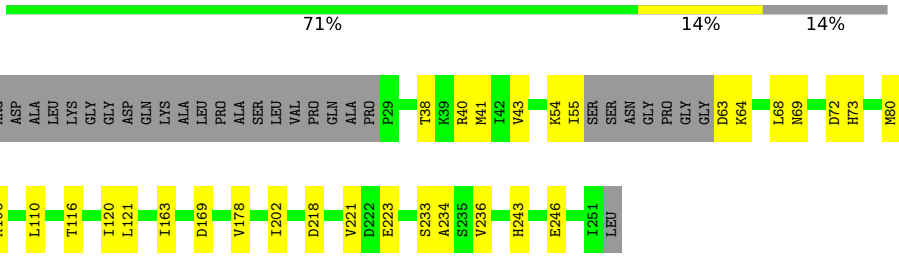
Chain JC:





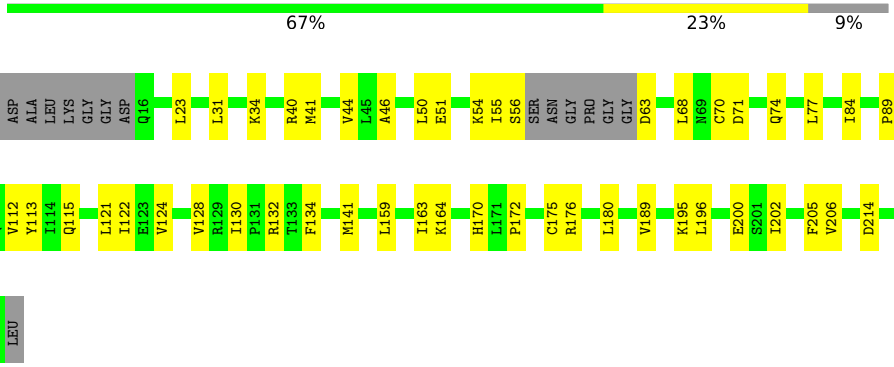
• Molecule 39: Ribosomal RNA small subunit methyltransferase NEP1

Chain JF:



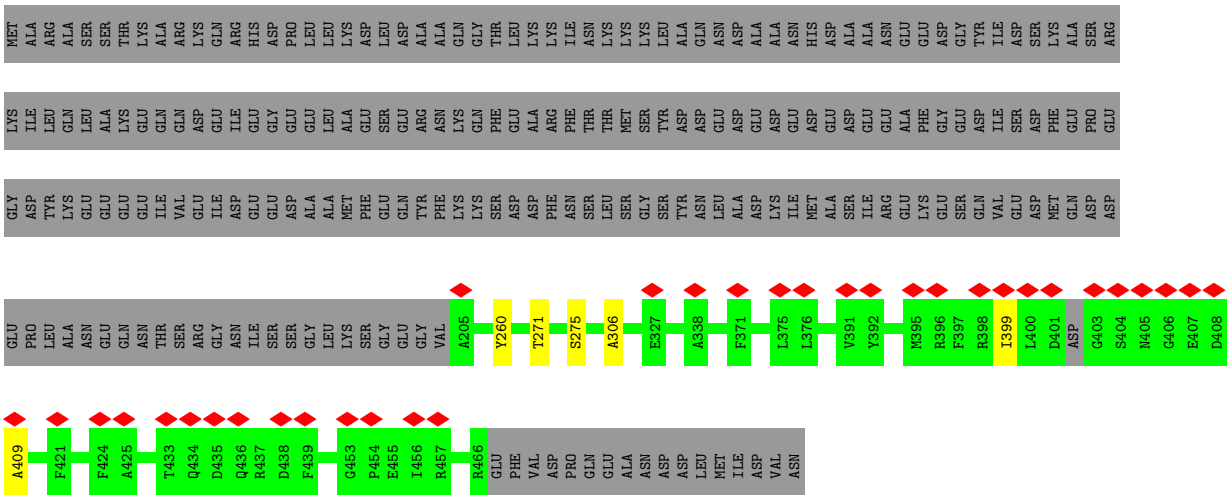
• Molecule 39: Ribosomal RNA small subunit methyltransferase NEP1

Chain JG:

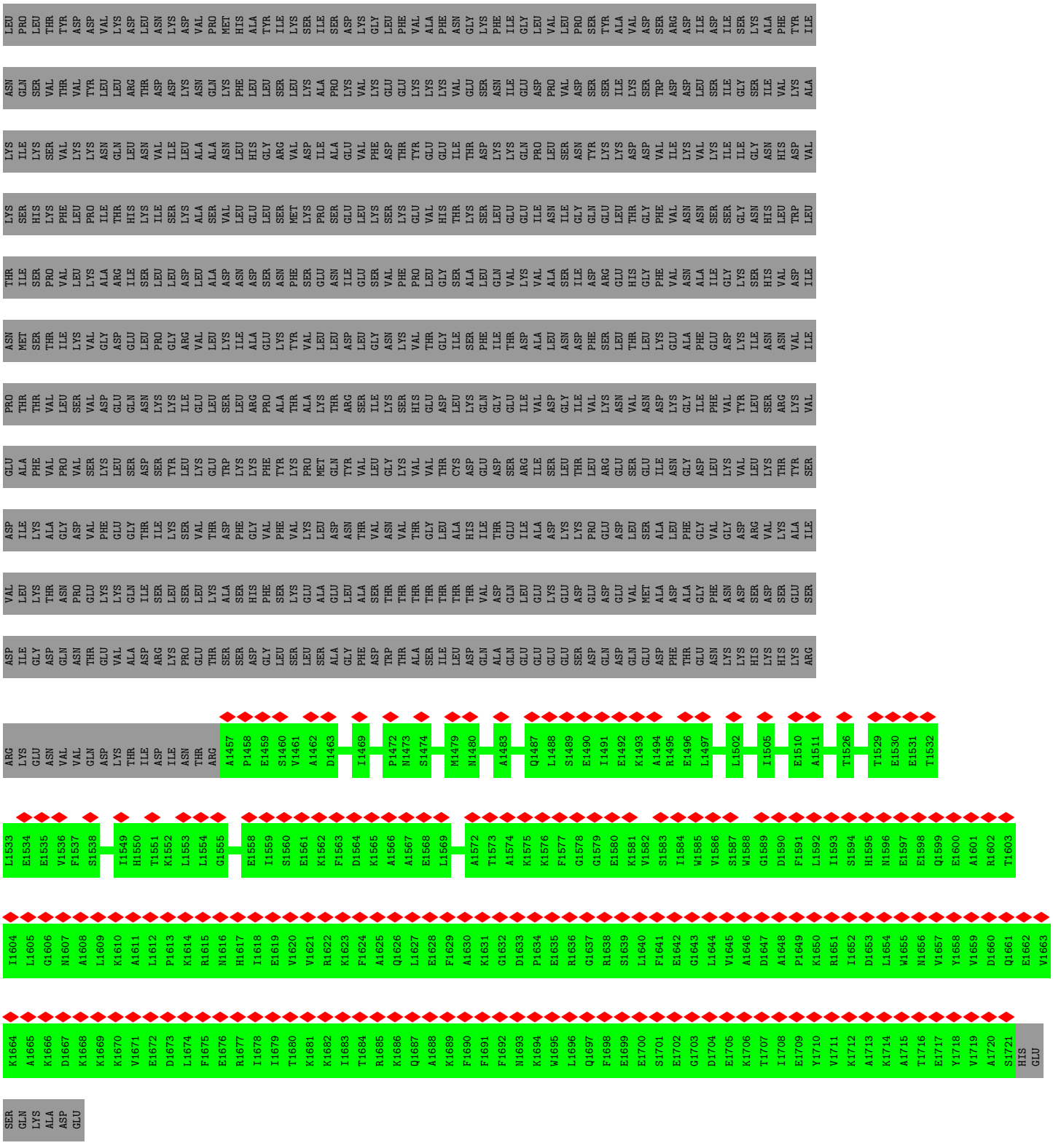


• Molecule 40: Essential nuclear protein 1

Chain JH:

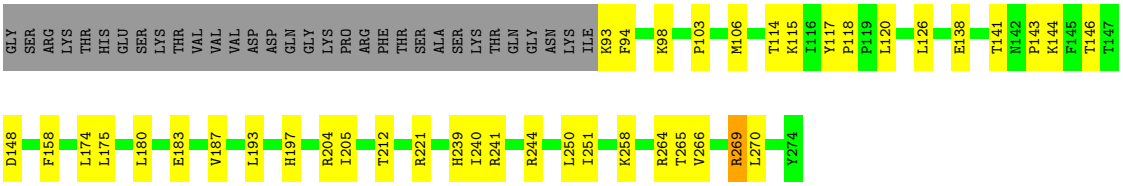


- Molecule 41: rRNA biogenesis protein RRP5



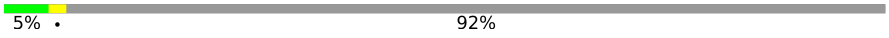
• Molecule 42: Pre-rRNA-processing protein PNO1

Chain JJ:



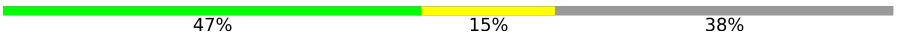
• Molecule 43: Protein BFR2

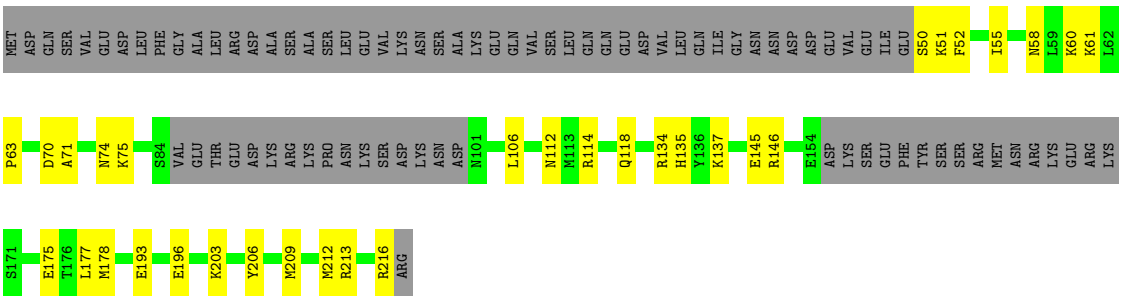
Chain JK:



• Molecule 44: rRNA-processing protein FCF2

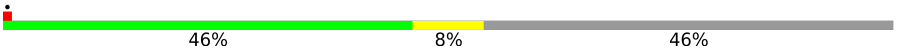
Chain JM:

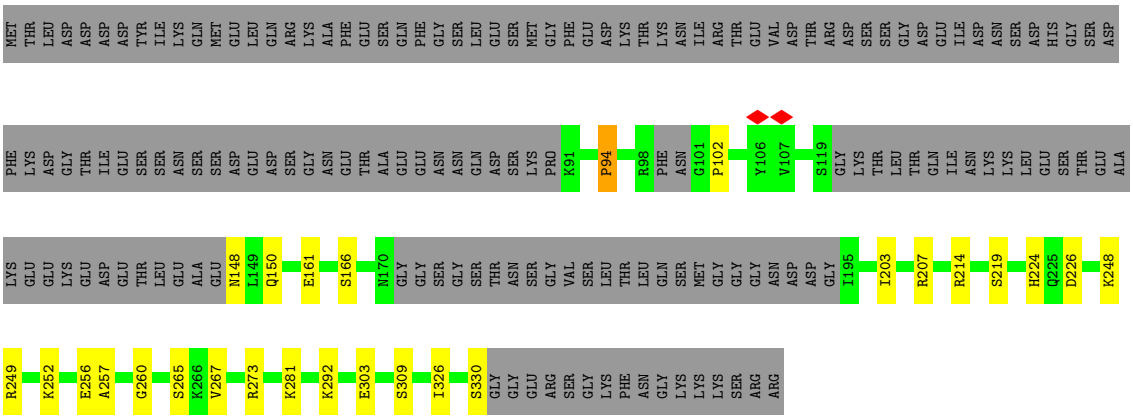




• Molecule 45: Protein FAF1

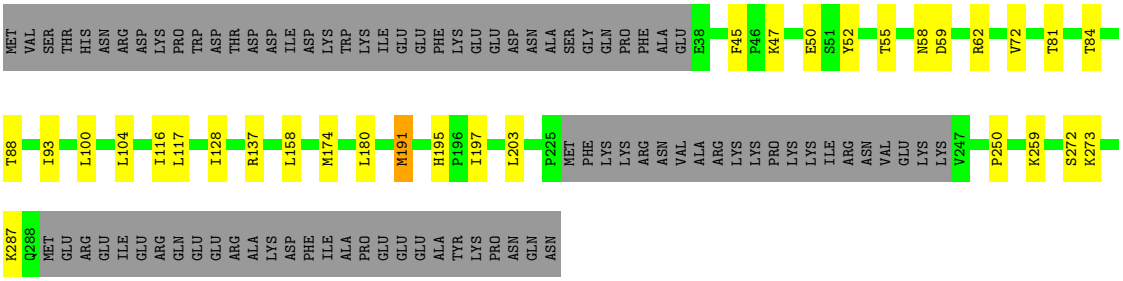
Chain JN:





• Molecule 46: KRR1 small subunit processome component

Chain JO:

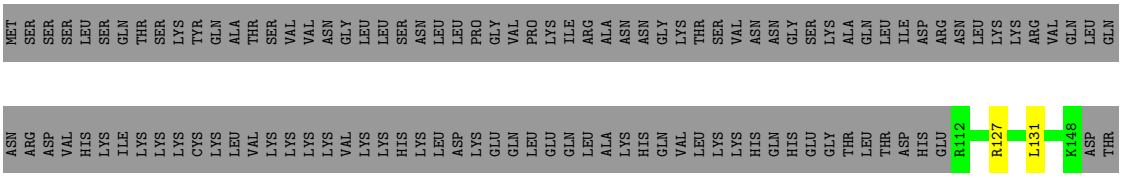


• Molecule 47: Protein SOF1

Chain JP:

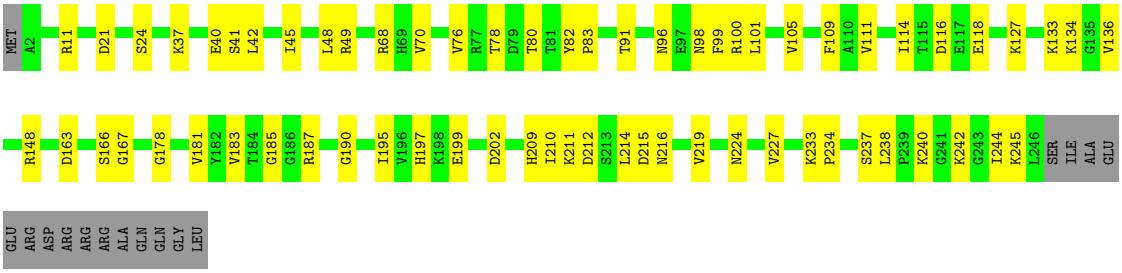
• Molecule 48: Regulator of rDNA transcription protein 14

Chain JQ:



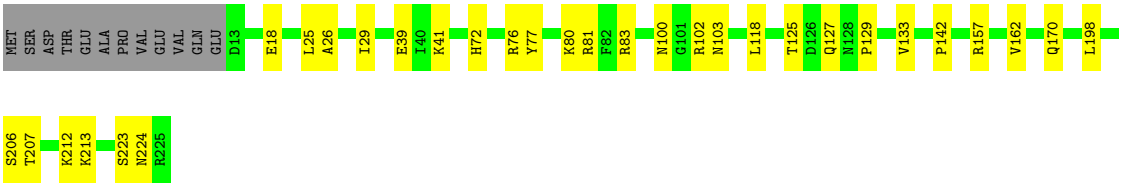
• Molecule 49: 40S ribosomal protein S4-A

Chain DE:



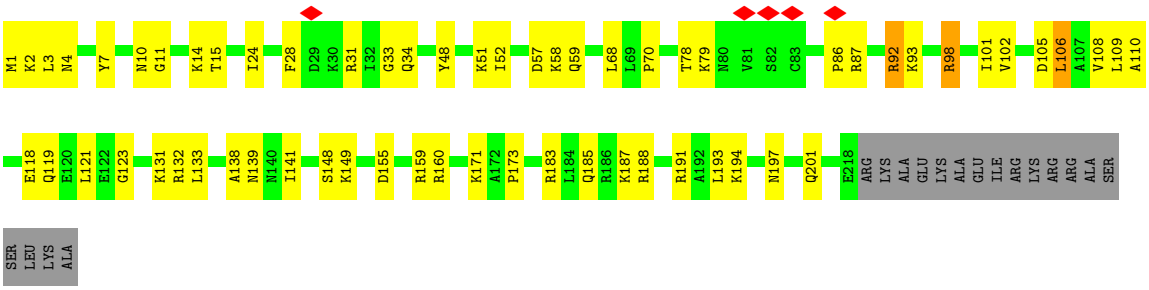
• Molecule 50: 40S ribosomal protein S5

Chain DF:



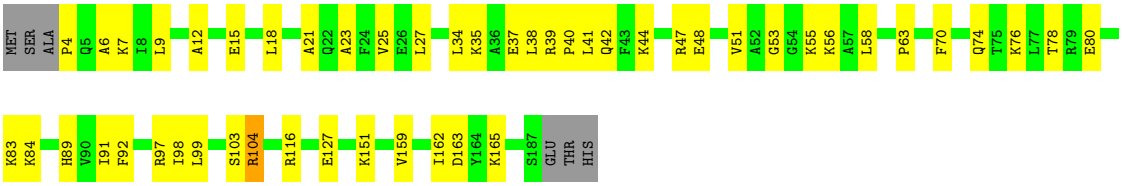
• Molecule 51: 40S ribosomal protein S6-A

Chain DG:



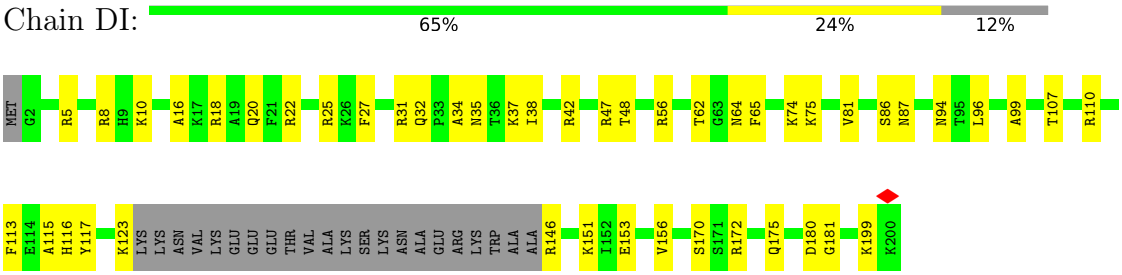
• Molecule 52: 40S ribosomal protein S7-A

Chain DH:



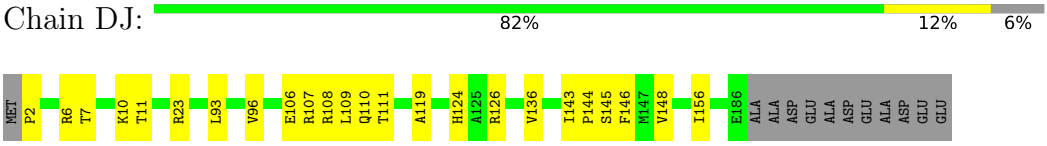
• Molecule 53: 40S ribosomal protein S8-A

Chain DI:



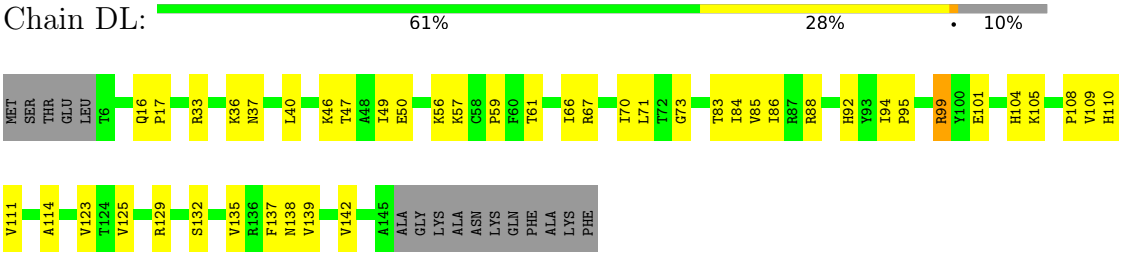
• Molecule 54: 40S ribosomal protein S9-A

Chain DJ:



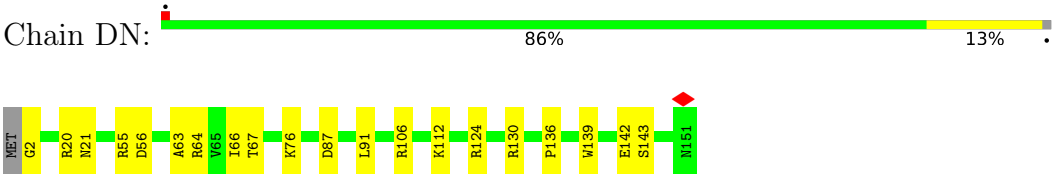
• Molecule 55: 40S ribosomal protein S11-A

Chain DL:



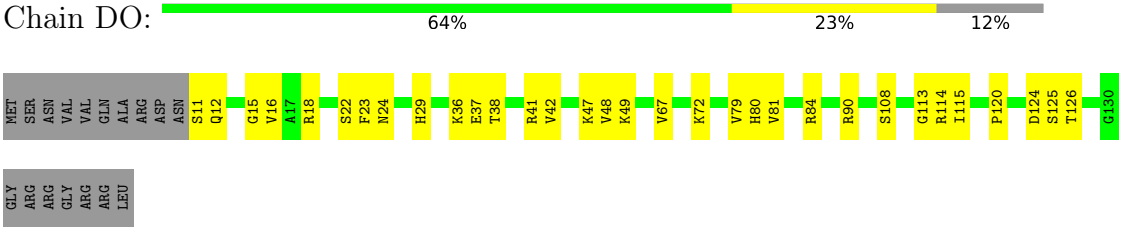
• Molecule 56: 40S ribosomal protein S13

Chain DN:



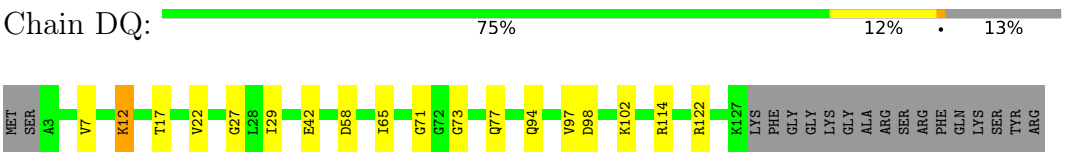
• Molecule 57: 40S ribosomal protein S14-A

Chain DO:



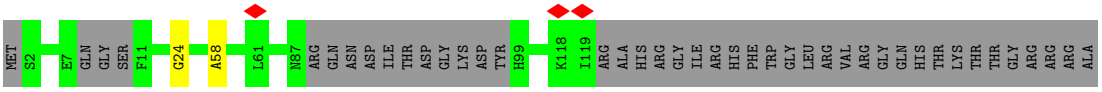
• Molecule 58: 40S ribosomal protein S16-A

Chain DQ:



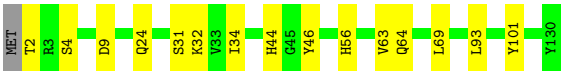
• Molecule 59: 40S ribosomal protein S18-A

Chain DS:



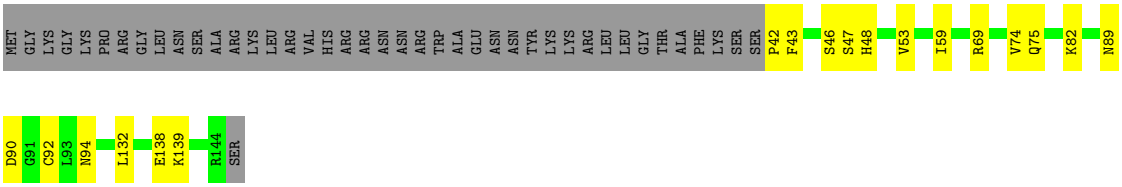
• Molecule 60: 40S ribosomal protein S22-A

Chain DW:



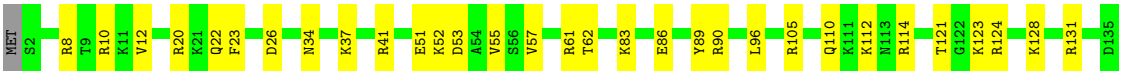
• Molecule 61: 40S ribosomal protein S23-A

Chain DX:



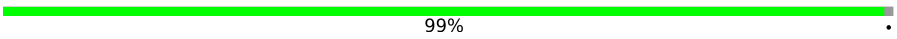
• Molecule 62: 40S ribosomal protein S24-A

Chain DY:



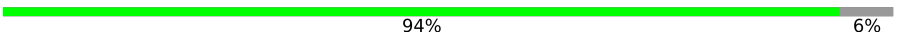
• Molecule 63: 40S ribosomal protein S27-A

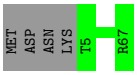
Chain Db:



• Molecule 64: 40S ribosomal protein S28-A

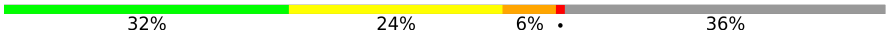
Chain Dc:

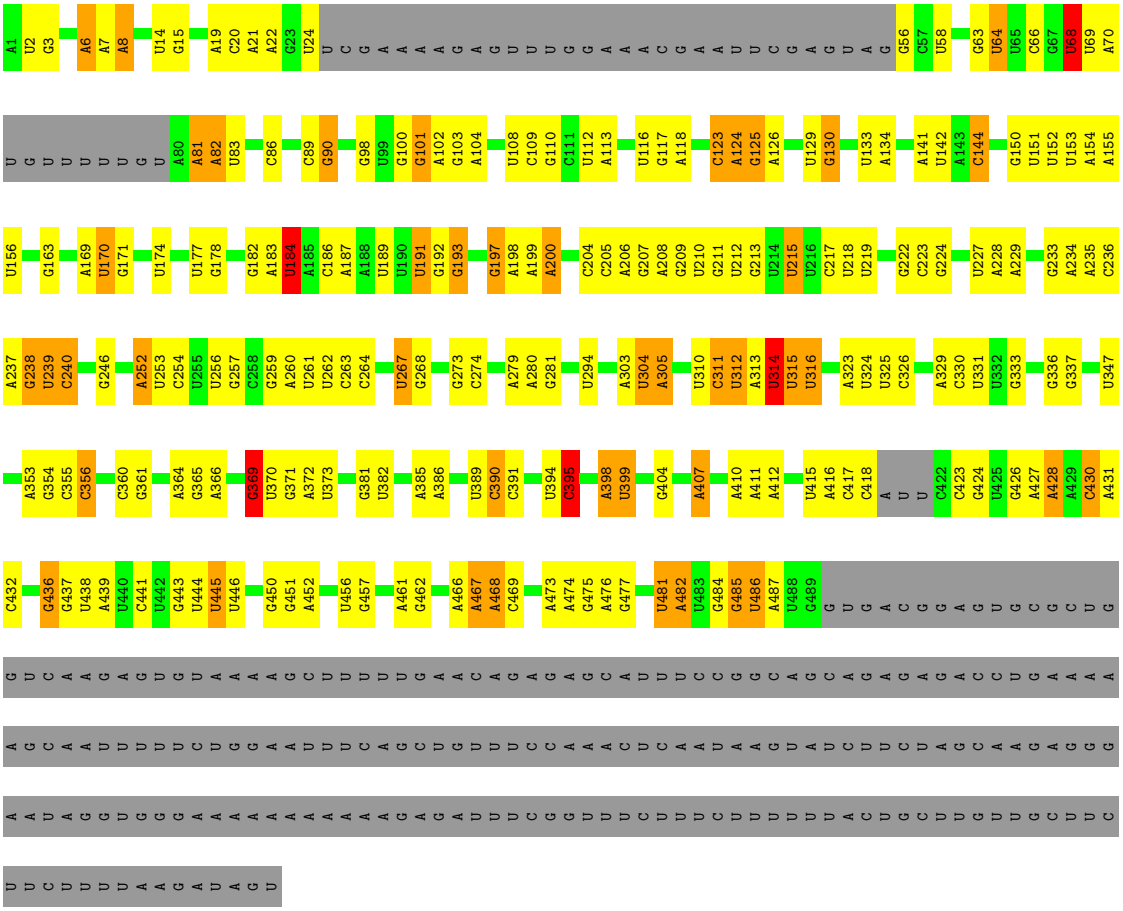




• Molecule 65: 5ETS RNA

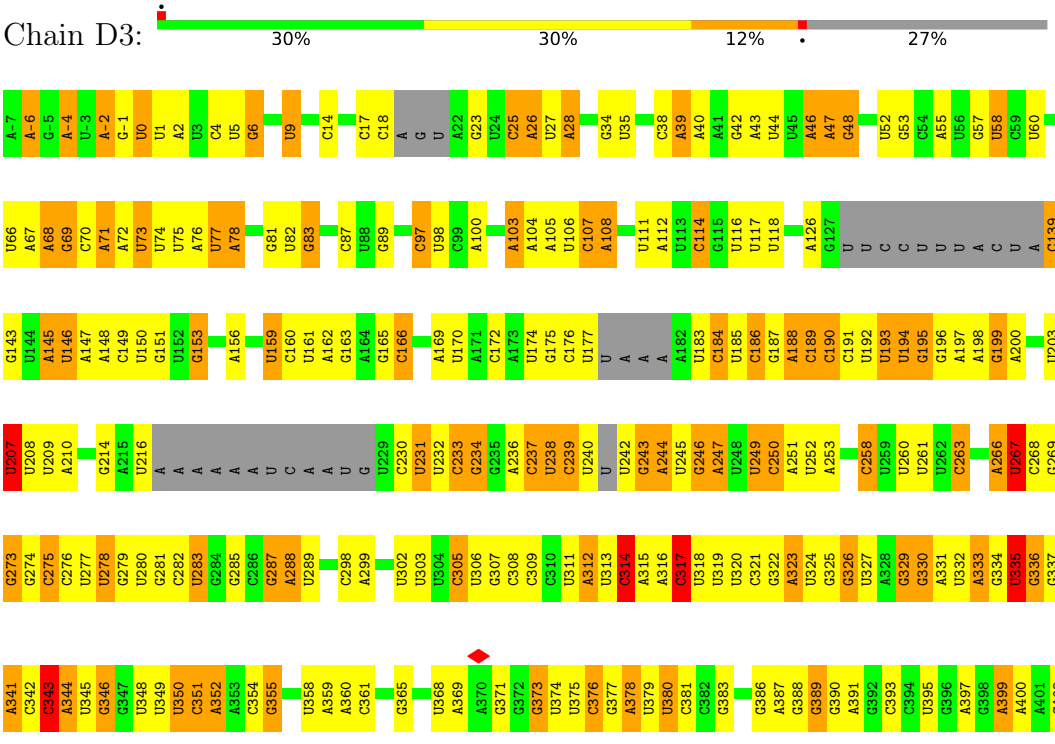
Chain D2:

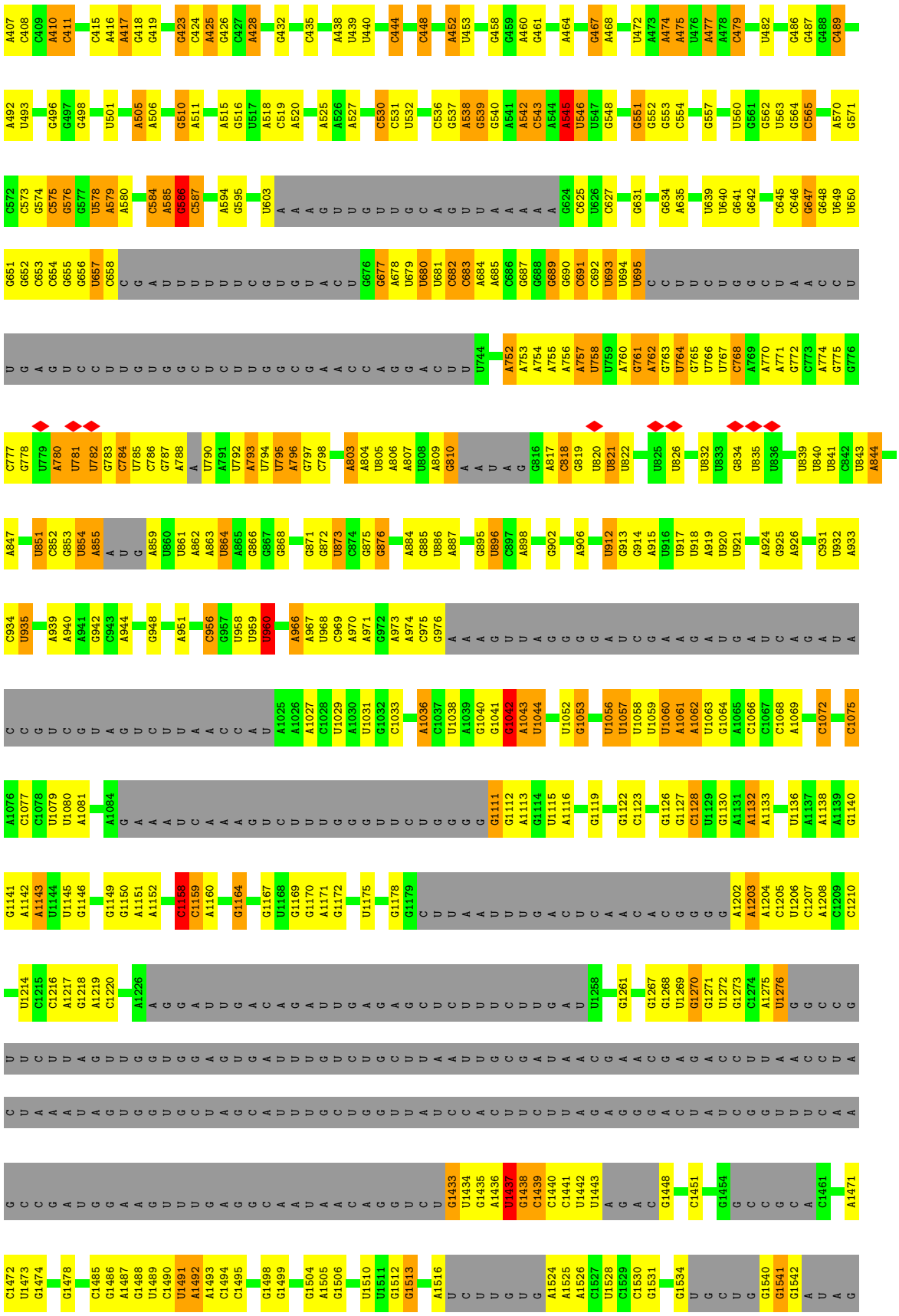


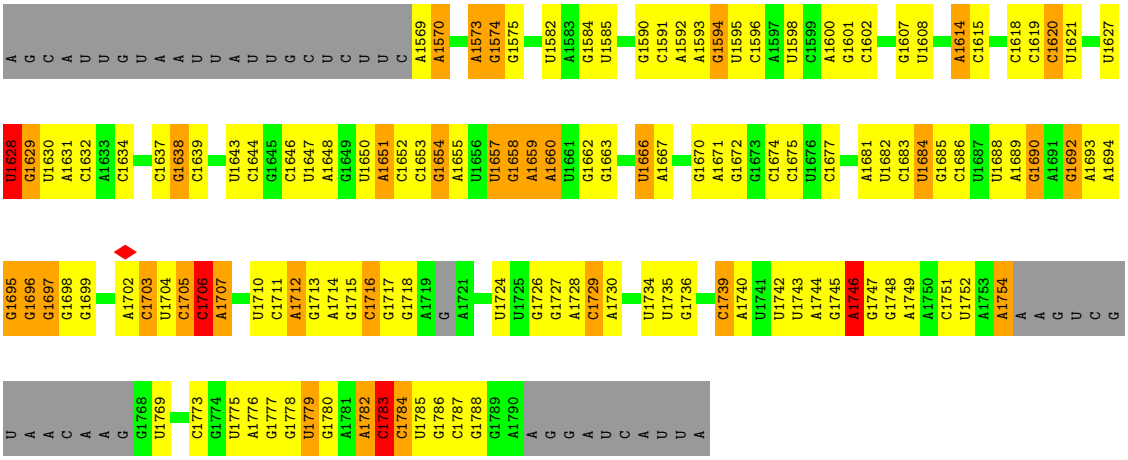


• Molecule 66: 18S rRNA

Chain D3:

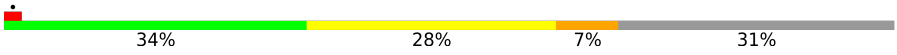


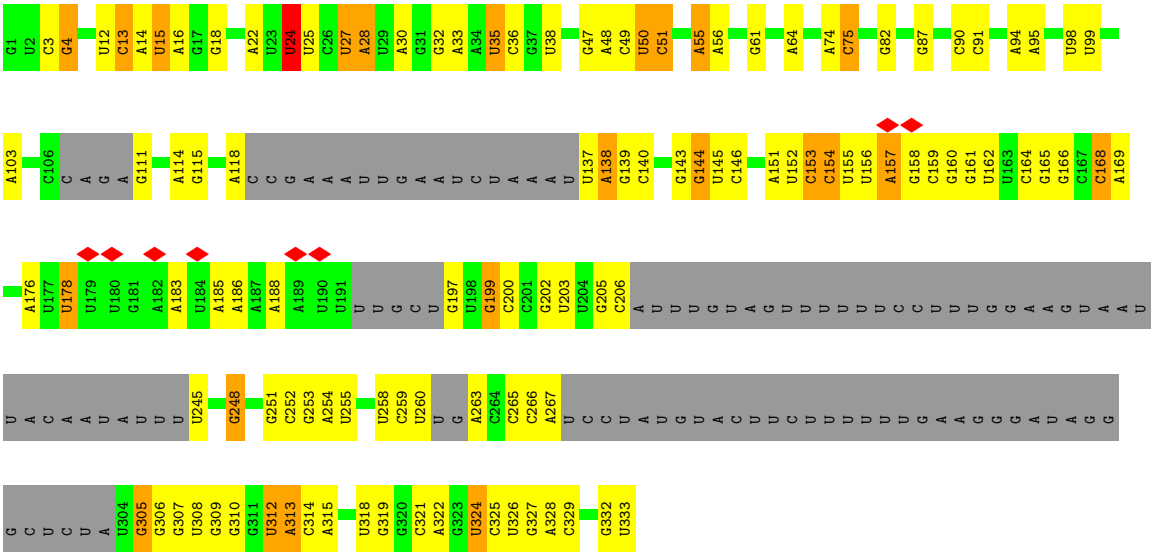




• Molecule 67: U3 snoRNA

Chain D4:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43601	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	0.212	Depositor
Minimum map value	-0.128	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	508.32, 508.32, 508.32	wwPDB
Map dimensions	480, 480, 480	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: ZN, MG, GTP

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	0.55	0/1917	0.60	1/2588 (0.0%)
1	CB	0.38	0/1815	0.56	0/2448
2	DA	0.44	0/1937	0.57	0/2593
3	JA	0.29	0/6021	0.59	3/8176 (0.0%)
3	JB	0.26	0/4128	0.53	0/5747
4	UA	0.62	0/6780	0.64	3/9175 (0.0%)
5	UB	0.30	0/3787	0.55	5/5126 (0.1%)
6	UC	0.44	0/1034	0.52	0/1365
7	UD	0.39	0/5461	0.59	3/7395 (0.0%)
8	UE	0.43	0/3840	0.59	2/5208 (0.0%)
9	UF	0.40	0/2538	0.51	1/3405 (0.0%)
10	UG	0.59	0/4302	0.64	2/5805 (0.0%)
11	UH	0.29	0/2716	0.55	7/3721 (0.2%)
12	UI	0.27	0/875	0.55	0/1176
13	UJ	0.36	0/9111	0.58	2/12323 (0.0%)
14	UK	0.44	0/2047	0.53	0/2711
15	UL	0.36	0/6857	0.57	0/9253
16	UM	0.35	0/6070	0.58	1/8216 (0.0%)
17	UN	0.48	0/1252	0.55	0/1688
18	UO	0.43	0/3993	0.57	0/5413
19	UP	0.29	0/499	0.55	0/659
20	UQ	0.38	0/6794	0.57	2/9203 (0.0%)
21	UR	0.54	0/3883	0.61	0/5265
22	US	0.32	0/3703	0.55	4/5053 (0.1%)
23	UT	0.30	0/17584	0.56	5/23824 (0.0%)
24	UU	0.56	0/6815	0.60	0/9213
25	UV	0.32	0/8945	0.53	1/12097 (0.0%)
26	UX	0.55	0/1418	0.63	0/1906
27	UZ	0.34	0/2041	0.54	0/2745
28	CD	0.41	0/3041	0.51	1/4098 (0.0%)
29	CE	0.38	0/3362	0.56	1/4533 (0.0%)
30	CF	0.47	0/944	0.57	0/1284

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	CG	0.48	0/941	0.59	0/1281
31	CH	0.40	0/3798	0.57	0/5113
32	CI	0.66	0/1559	0.68	1/2097 (0.0%)
33	CJ	0.54	0/2337	0.64	0/3148
34	CK	0.43	0/1685	0.57	0/2261
35	CL	0.47	0/6471	0.56	1/8708 (0.0%)
36	CM	0.38	0/2832	0.53	0/3825
37	CN	0.31	0/1934	0.49	0/2604
38	JC	0.30	0/2908	0.59	0/3938
39	JF	0.30	0/1727	0.53	0/2329
39	JG	0.36	0/1828	0.55	0/2470
40	JH	0.24	0/1293	0.36	0/1801
41	JI	0.25	0/1313	0.49	0/1830
42	JJ	0.33	0/1469	0.53	0/1980
43	JK	0.26	0/342	0.52	0/462
44	JM	0.40	0/1156	0.51	0/1536
45	JN	0.45	0/1435	0.57	1/1907 (0.1%)
46	JO	0.44	0/1910	0.55	0/2569
47	JP	0.63	0/3844	0.64	0/5174
48	JQ	0.30	0/385	0.48	0/529
49	DE	0.34	0/1985	0.54	0/2675
50	DF	0.49	0/1690	0.57	1/2285 (0.0%)
51	DG	0.30	0/1779	0.53	1/2379 (0.0%)
52	DH	0.34	0/1506	0.56	0/2028
53	DI	0.28	0/1422	0.51	0/1899
54	DJ	0.51	0/1519	0.58	0/2035
55	DL	0.28	0/1155	0.52	0/1557
56	DN	0.42	0/1215	0.53	0/1638
57	DO	0.45	0/892	0.53	0/1202
58	DQ	0.63	0/990	0.67	0/1335
59	DS	0.25	0/513	0.49	0/711
60	DW	0.50	0/1038	0.57	0/1395
61	DX	0.48	0/798	0.60	0/1065
62	DY	0.45	0/1087	0.52	0/1449
63	Db	0.42	0/620	0.55	0/838
64	Dc	0.46	0/499	0.59	0/670
65	D2	0.76	0/10633	1.13	50/16564 (0.3%)
66	D3	0.70	5/31617 (0.0%)	1.19	263/49213 (0.5%)
67	D4	0.78	0/5436	1.16	36/8446 (0.4%)
All	All	0.49	5/243071 (0.0%)	0.75	398/338358 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	JA	0	1
4	UA	0	1
11	UH	0	1
15	UL	0	2
16	UM	0	6
17	UN	0	1
23	UT	0	2
24	UU	0	1
25	UV	0	1
28	CD	0	1
31	CH	0	1
34	CK	0	1
46	JO	0	1
47	JP	0	2
58	DQ	0	1
All	All	0	23

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	D3	1164	G	C6-O6	-7.57	1.17	1.24
66	D3	1158	C	N3-C4	-7.56	1.28	1.33
66	D3	553	G	C2-N3	-6.93	1.27	1.32
66	D3	1158	C	C4-N4	-6.11	1.28	1.33
66	D3	355	G	C2-N3	-5.13	1.28	1.32

The worst 5 of 398 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
66	D3	1158	C	N3-C4-N4	-25.45	100.18	118.00
66	D3	1164	G	N1-C6-O6	-24.31	105.32	119.90
66	D3	1158	C	C5-C4-N4	18.09	132.87	120.20
66	D3	1158	C	N3-C4-C5	11.86	126.64	121.90
65	D2	356	C	N3-C2-O2	-11.72	113.69	121.90

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	JA	46	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	UA	289	LEU	Peptide
11	UH	532	PHE	Peptide
15	UL	183	ASP	Peptide
15	UL	552	ASP	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	25	0
1	CB	1782	0	1826	29	0
2	DA	1912	0	2023	35	0
3	JA	5916	0	5463	134	0
3	JB	4132	0	1819	12	0
4	UA	6635	0	6525	107	0
5	UB	3734	0	3432	50	0
6	UC	1026	0	1080	18	0
7	UD	5361	0	5364	119	0
8	UE	3772	0	3806	72	0
9	UF	2487	0	2533	36	0
10	UG	4218	0	4222	58	0
11	UH	2701	0	1951	53	0
12	UI	860	0	922	14	0
13	UJ	8961	0	9273	179	0
14	UK	2021	0	2098	31	0
15	UL	6726	0	6764	121	0
16	UM	5969	0	6006	114	0
17	UN	1227	0	1223	20	0
18	UO	3911	0	3906	76	0
19	UP	495	0	561	13	0
20	UQ	6662	0	6588	137	0
21	UR	3799	0	3783	60	0
22	US	3622	0	3214	69	0
23	UT	17290	0	16616	374	0
24	UU	6678	0	6652	98	0
25	UV	8736	0	8850	160	0
26	UX	1395	0	1473	24	0
27	UZ	2006	0	2118	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	CD	2994	0	3018	41	0
29	CE	3325	0	3414	52	0
30	CF	931	0	983	7	0
30	CG	928	0	976	20	0
31	CH	3725	0	3746	49	0
32	CI	1530	0	1572	29	0
33	CJ	2296	0	2325	42	0
34	CK	1667	0	1701	28	0
35	CL	6332	0	6515	139	0
36	CM	2781	0	2878	35	0
37	CN	1893	0	1875	35	0
38	JC	2845	0	2761	85	0
39	JF	1701	0	1767	22	0
39	JG	1799	0	1872	44	0
40	JH	1295	0	570	3	0
41	JI	1314	0	610	0	0
42	JJ	1442	0	1513	28	0
43	JK	334	0	313	11	0
44	JM	1137	0	1188	22	0
45	JN	1428	0	1425	19	0
46	JO	1876	0	1968	22	0
47	JP	3765	0	3714	65	0
48	JQ	381	0	255	5	0
49	DE	1944	0	2030	43	0
50	DF	1669	0	1723	21	0
51	DG	1755	0	1846	47	0
52	DH	1481	0	1572	42	0
53	DI	1399	0	1431	40	0
54	DJ	1494	0	1573	17	0
55	DL	1129	0	1196	31	0
56	DN	1192	0	1255	17	0
57	DO	881	0	910	24	0
58	DQ	973	0	1029	14	0
59	DS	516	0	222	1	0
60	DW	1021	0	1060	13	0
61	DX	786	0	843	14	0
62	DY	1073	0	1132	24	0
63	Db	610	0	631	0	0
64	Dc	497	0	535	0	0
65	D2	9508	0	4781	119	0
66	D3	28287	0	14259	496	0
67	D4	4872	0	2469	65	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	Db	1	0	0	0	0
68	UX	1	0	0	0	0
69	CL	1	0	0	0	0
69	UX	1	0	0	0	0
70	CL	32	0	12	26	0
All	All	234757	0	209487	3712	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 8.

The worst 5 of 3712 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)
35:CL:210:VAL:HG21	70:CL:2001:GTP:C5	1.53	1.43
35:CL:210:VAL:CG2	70:CL:2001:GTP:C5	2.05	1.39
52:DH:27:LEU:CD2	52:DH:84:LYS:NZ	1.88	1.35
4:UA:77:GLY:HA3	4:UA:95:PHE:O	1.30	1.32
10:UG:132:GLY:HA3	10:UG:150:LEU:O	1.20	1.30

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%)	220 (92%)	18 (8%)	0	100	100
1	CB	224/327 (68%)	208 (93%)	16 (7%)	0	100	100
2	DA	236/255 (92%)	217 (92%)	19 (8%)	0	100	100
3	JA	802/1056 (76%)	735 (92%)	67 (8%)	0	100	100
3	JB	827/1056 (78%)	758 (92%)	69 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	UA	830/923 (90%)	758 (91%)	72 (9%)	0	100	100
5	UB	495/810 (61%)	470 (95%)	24 (5%)	1 (0%)	47	79
6	UC	124/610 (20%)	112 (90%)	12 (10%)	0	100	100
7	UD	663/776 (85%)	599 (90%)	64 (10%)	0	100	100
8	UE	465/643 (72%)	412 (89%)	53 (11%)	0	100	100
9	UF	283/440 (64%)	276 (98%)	7 (2%)	0	100	100
10	UG	529/554 (96%)	481 (91%)	48 (9%)	0	100	100
11	UH	426/713 (60%)	345 (81%)	58 (14%)	23 (5%)	2	22
12	UI	100/575 (17%)	97 (97%)	3 (3%)	0	100	100
13	UJ	1092/1769 (62%)	1030 (94%)	62 (6%)	0	100	100
14	UK	238/250 (95%)	219 (92%)	19 (8%)	0	100	100
15	UL	828/943 (88%)	752 (91%)	75 (9%)	1 (0%)	51	83
16	UM	750/817 (92%)	674 (90%)	74 (10%)	2 (0%)	41	74
17	UN	143/899 (16%)	132 (92%)	11 (8%)	0	100	100
18	UO	489/513 (95%)	446 (91%)	43 (9%)	0	100	100
19	UP	58/214 (27%)	55 (95%)	3 (5%)	0	100	100
20	UQ	820/896 (92%)	750 (92%)	70 (8%)	0	100	100
21	UR	474/594 (80%)	434 (92%)	40 (8%)	0	100	100
22	US	488/552 (88%)	445 (91%)	41 (8%)	2 (0%)	34	70
23	UT	2213/2493 (89%)	2086 (94%)	127 (6%)	0	100	100
24	UU	842/939 (90%)	776 (92%)	66 (8%)	0	100	100
25	UV	1069/1237 (86%)	1020 (95%)	49 (5%)	0	100	100
26	UX	170/189 (90%)	161 (95%)	9 (5%)	0	100	100
27	UZ	245/274 (89%)	225 (92%)	20 (8%)	0	100	100
28	CD	376/504 (75%)	358 (95%)	18 (5%)	0	100	100
29	CE	431/511 (84%)	397 (92%)	34 (8%)	0	100	100
30	CF	121/126 (96%)	115 (95%)	6 (5%)	0	100	100
30	CG	121/126 (96%)	116 (96%)	5 (4%)	0	100	100
31	CH	459/573 (80%)	419 (91%)	37 (8%)	3 (1%)	22	60
32	CI	180/183 (98%)	167 (93%)	13 (7%)	0	100	100
33	CJ	278/290 (96%)	249 (90%)	29 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	CK	203/593 (34%)	186 (92%)	16 (8%)	1 (0%)	29	66
35	CL	771/1183 (65%)	731 (95%)	40 (5%)	0	100	100
36	CM	358/367 (98%)	342 (96%)	16 (4%)	0	100	100
37	CN	224/297 (75%)	204 (91%)	20 (9%)	0	100	100
38	JC	350/707 (50%)	313 (89%)	37 (11%)	0	100	100
39	JF	212/252 (84%)	203 (96%)	9 (4%)	0	100	100
39	JG	226/252 (90%)	217 (96%)	9 (4%)	0	100	100
40	JH	257/483 (53%)	248 (96%)	9 (4%)	0	100	100
41	JI	263/1729 (15%)	255 (97%)	8 (3%)	0	100	100
42	JJ	180/274 (66%)	171 (95%)	9 (5%)	0	100	100
43	JK	40/534 (8%)	33 (82%)	7 (18%)	0	100	100
44	JM	129/217 (59%)	122 (95%)	7 (5%)	0	100	100
45	JN	178/346 (51%)	162 (91%)	14 (8%)	2 (1%)	14	51
46	JO	226/316 (72%)	212 (94%)	14 (6%)	0	100	100
47	JP	457/489 (94%)	427 (93%)	30 (7%)	0	100	100
48	JQ	59/206 (29%)	54 (92%)	5 (8%)	0	100	100
49	DE	243/261 (93%)	227 (93%)	16 (7%)	0	100	100
50	DF	211/225 (94%)	195 (92%)	16 (8%)	0	100	100
51	DG	216/236 (92%)	205 (95%)	11 (5%)	0	100	100
52	DH	182/190 (96%)	171 (94%)	11 (6%)	0	100	100
53	DI	173/200 (86%)	162 (94%)	11 (6%)	0	100	100
54	DJ	183/197 (93%)	172 (94%)	11 (6%)	0	100	100
55	DL	138/156 (88%)	129 (94%)	9 (6%)	0	100	100
56	DN	148/151 (98%)	140 (95%)	8 (5%)	0	100	100
57	DO	118/137 (86%)	111 (94%)	7 (6%)	0	100	100
58	DQ	123/143 (86%)	115 (94%)	8 (6%)	0	100	100
59	DS	98/146 (67%)	89 (91%)	9 (9%)	0	100	100
60	DW	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
61	DX	101/145 (70%)	89 (88%)	11 (11%)	1 (1%)	15	52
62	DY	132/135 (98%)	129 (98%)	3 (2%)	0	100	100
63	Db	79/82 (96%)	75 (95%)	4 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
64	Dc	61/67 (91%)	56 (92%)	5 (8%)	0	100 100
All	All	24593/34803 (71%)	22770 (93%)	1787 (7%)	36 (0%)	54 83

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	UH	59	PRO
11	UH	61	PRO
11	UH	68	PRO
11	UH	70	PRO
11	UH	235	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	CA	202/240 (84%)	201 (100%)	1 (0%)	88 94
1	CB	192/240 (80%)	189 (98%)	3 (2%)	62 79
2	DA	212/224 (95%)	211 (100%)	1 (0%)	88 94
3	JA	555/934 (59%)	550 (99%)	5 (1%)	78 88
4	UA	730/812 (90%)	723 (99%)	7 (1%)	76 86
5	UB	344/732 (47%)	344 (100%)	0	100 100
6	UC	107/538 (20%)	106 (99%)	1 (1%)	78 88
7	UD	615/713 (86%)	615 (100%)	0	100 100
8	UE	428/574 (75%)	427 (100%)	1 (0%)	93 97
9	UF	277/414 (67%)	275 (99%)	2 (1%)	84 91
10	UG	462/480 (96%)	457 (99%)	5 (1%)	73 85
11	UH	152/657 (23%)	152 (100%)	0	100 100
12	UI	99/533 (19%)	99 (100%)	0	100 100
13	UJ	1031/1633 (63%)	1025 (99%)	6 (1%)	86 92
14	UK	226/234 (97%)	226 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	UL	747/832 (90%)	743 (100%)	4 (0%)	88 94
16	UM	668/719 (93%)	664 (99%)	4 (1%)	86 92
17	UN	137/808 (17%)	136 (99%)	1 (1%)	84 91
18	UO	437/454 (96%)	433 (99%)	4 (1%)	78 88
19	UP	57/196 (29%)	56 (98%)	1 (2%)	59 77
20	UQ	769/826 (93%)	768 (100%)	1 (0%)	93 97
21	UR	425/529 (80%)	423 (100%)	2 (0%)	88 94
22	US	332/506 (66%)	331 (100%)	1 (0%)	92 96
23	UT	1787/2307 (78%)	1780 (100%)	7 (0%)	91 95
24	UU	743/819 (91%)	739 (100%)	4 (0%)	88 94
25	UV	986/1125 (88%)	980 (99%)	6 (1%)	86 92
26	UX	156/169 (92%)	156 (100%)	0	100 100
27	UZ	230/256 (90%)	230 (100%)	0	100 100
28	CD	326/435 (75%)	325 (100%)	1 (0%)	92 96
29	CE	353/433 (82%)	349 (99%)	4 (1%)	73 85
30	CF	102/104 (98%)	102 (100%)	0	100 100
30	CG	101/104 (97%)	99 (98%)	2 (2%)	55 75
31	CH	406/503 (81%)	406 (100%)	0	100 100
32	CI	171/172 (99%)	170 (99%)	1 (1%)	86 92
33	CJ	251/258 (97%)	246 (98%)	5 (2%)	55 75
34	CK	187/535 (35%)	186 (100%)	1 (0%)	88 94
35	CL	690/1039 (66%)	684 (99%)	6 (1%)	78 88
36	CM	307/312 (98%)	307 (100%)	0	100 100
37	CN	212/274 (77%)	211 (100%)	1 (0%)	88 94
38	JC	318/636 (50%)	316 (99%)	2 (1%)	86 92
39	JF	195/222 (88%)	195 (100%)	0	100 100
39	JG	206/222 (93%)	205 (100%)	1 (0%)	88 94
42	JJ	158/238 (66%)	156 (99%)	2 (1%)	69 82
43	JK	35/482 (7%)	35 (100%)	0	100 100
44	JM	124/200 (62%)	122 (98%)	2 (2%)	62 79
45	JN	141/304 (46%)	141 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	JO	210/289 (73%)	210 (100%)	0	100 100
47	JP	416/443 (94%)	413 (99%)	3 (1%)	84 91
48	JQ	22/192 (12%)	22 (100%)	0	100 100
49	DE	209/222 (94%)	208 (100%)	1 (0%)	88 94
50	DF	180/191 (94%)	180 (100%)	0	100 100
51	DG	187/201 (93%)	185 (99%)	2 (1%)	73 85
52	DH	165/170 (97%)	164 (99%)	1 (1%)	86 92
53	DI	142/161 (88%)	141 (99%)	1 (1%)	84 91
54	DJ	158/166 (95%)	158 (100%)	0	100 100
55	DL	125/137 (91%)	123 (98%)	2 (2%)	62 79
56	DN	127/128 (99%)	127 (100%)	0	100 100
57	DO	91/105 (87%)	90 (99%)	1 (1%)	73 85
58	DQ	105/119 (88%)	105 (100%)	0	100 100
60	DW	110/111 (99%)	110 (100%)	0	100 100
61	DX	85/120 (71%)	84 (99%)	1 (1%)	71 84
62	DY	112/113 (99%)	112 (100%)	0	100 100
63	Db	70/71 (99%)	70 (100%)	0	100 100
64	Dc	56/60 (93%)	56 (100%)	0	100 100
All	All	19959/27976 (71%)	19852 (100%)	107 (0%)	89 94

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	UU	19	LYS
29	CE	247	ILE
51	DG	92	ARG
24	UU	634	PHE
25	UV	598	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 271 such sidechains are listed below:

Mol	Chain	Res	Type
38	JC	150	ASN
44	JM	74	ASN
51	DG	197	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	UM	798	ASN
16	UM	585	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
65	D2	443/700 (63%)	121 (27%)	6 (1%)
66	D3	1303/1808 (72%)	441 (33%)	22 (1%)
67	D4	223/333 (66%)	63 (28%)	4 (1%)
All	All	1969/2841 (69%)	625 (31%)	32 (1%)

5 of 625 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
65	D2	6	A
65	D2	8	A
65	D2	14	U
65	D2	15	G
65	D2	58	U

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
67	D4	143	G
67	D4	151	A
66	D3	278	U
66	D3	139	C
67	D4	157	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
70	GTP	CL	2001	69	26,34,34	0.94	1 (3%)	32,54,54	1.56	5 (15%)

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
70	GTP	CL	2001	69	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	CL	2001	GTP	C6-N1	-2.49	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
70	CL	2001	GTP	PB-O3B-PG	-4.05	118.94	132.83
70	CL	2001	GTP	PA-O3A-PB	-3.83	119.67	132.83
70	CL	2001	GTP	C3'-C2'-C1'	3.26	105.88	100.98
70	CL	2001	GTP	C5-C6-N1	2.32	118.04	113.95
70	CL	2001	GTP	C8-N7-C5	2.31	107.40	102.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
70	CL	2001	GTP	C5'-O5'-PA-O3A
70	CL	2001	GTP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
70	CL	2001	GTP	C3'-C4'-C5'-O5'
70	CL	2001	GTP	O4'-C4'-C5'-O5'

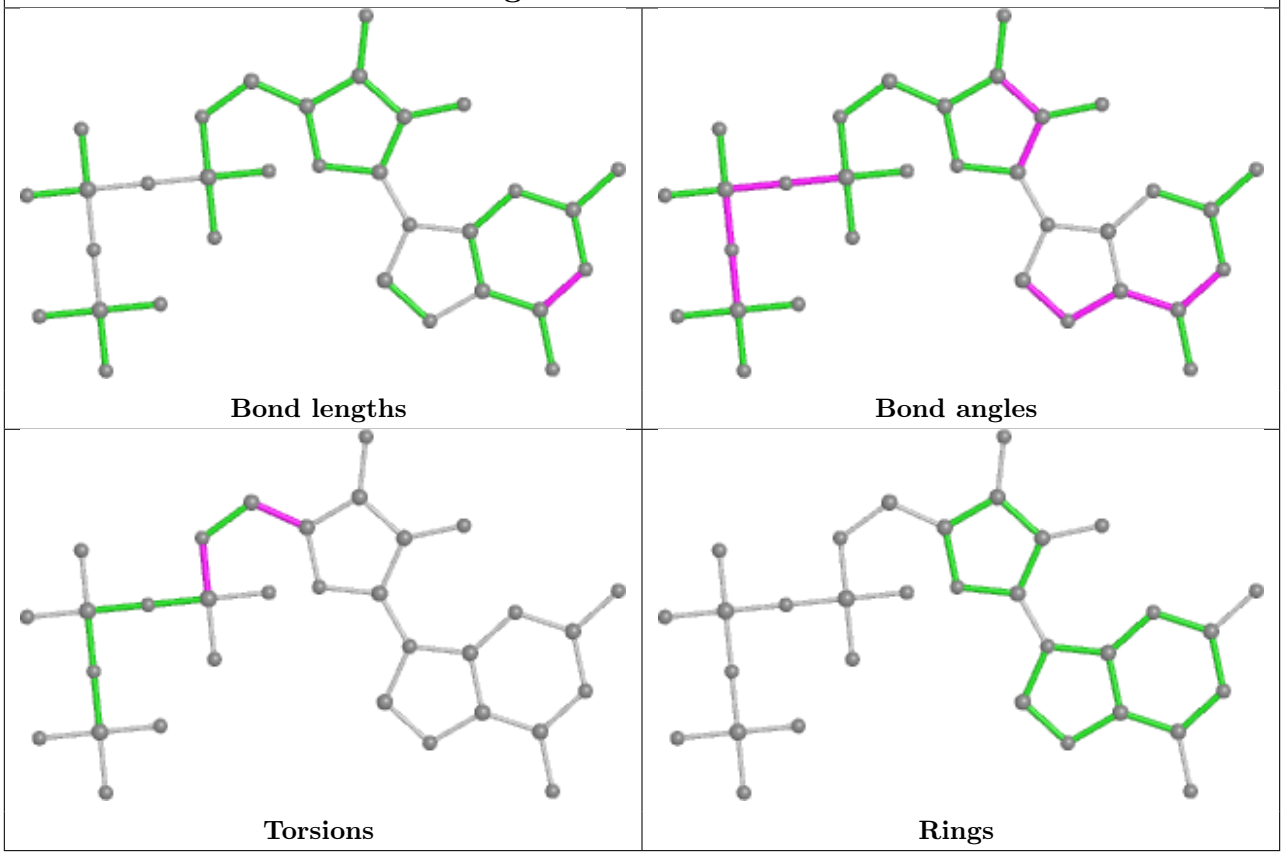
There are no ring outliers.

1 monomer is involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	CL	2001	GTP	26	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)

There are no chain breaks in this entry.

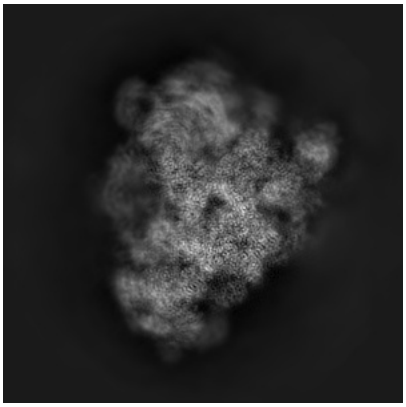
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11359. These allow visual inspection of the internal detail of the map and identification of artifacts.

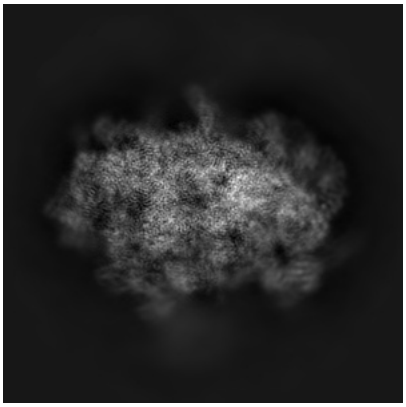
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

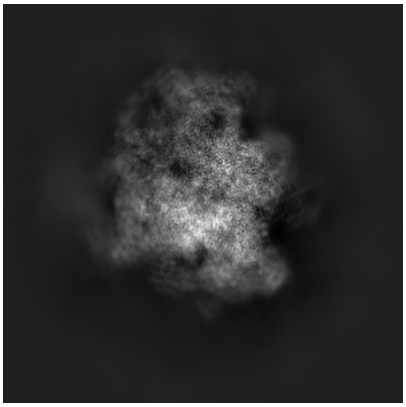
6.1.1 Primary map



X



Y

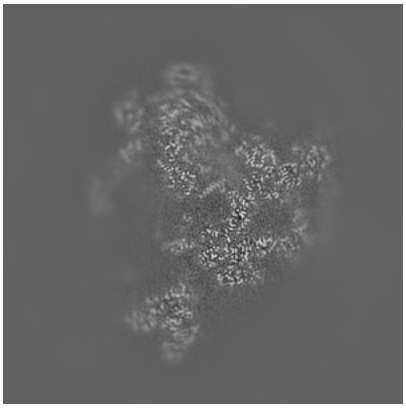


Z

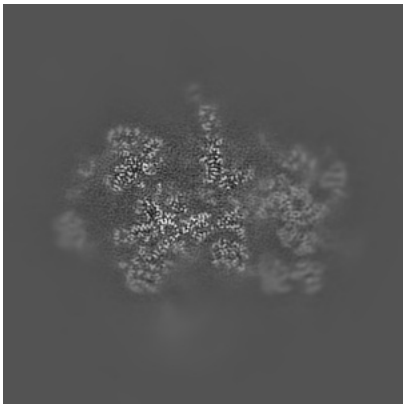
The images above show the map projected in three orthogonal directions.

6.2 Central slices

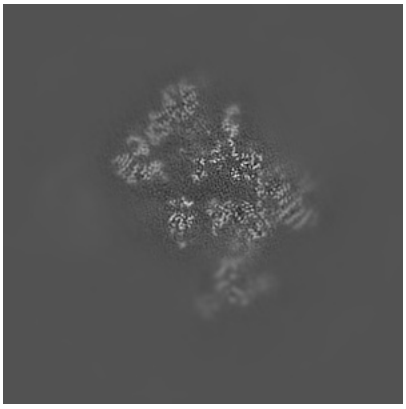
6.2.1 Primary map



X Index: 240



Y Index: 240

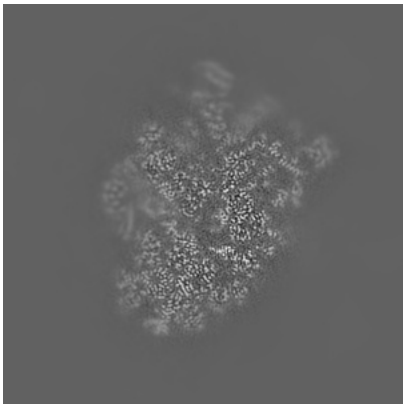


Z Index: 240

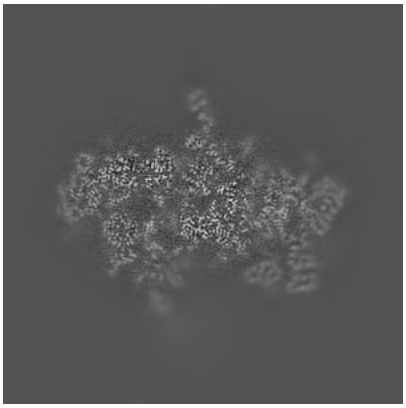
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

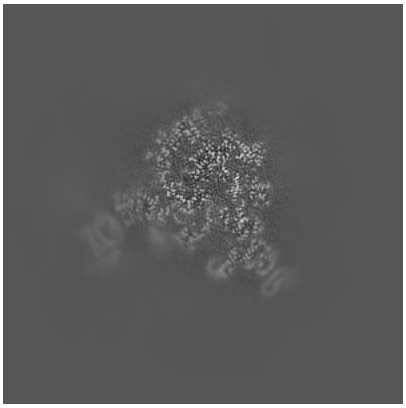
6.3.1 Primary map



X Index: 281



Y Index: 221

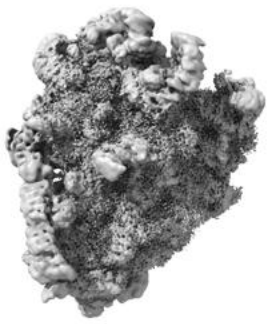


Z Index: 183

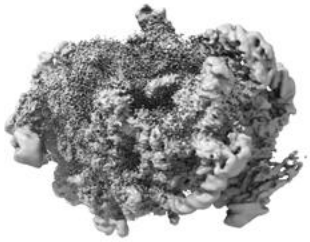
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

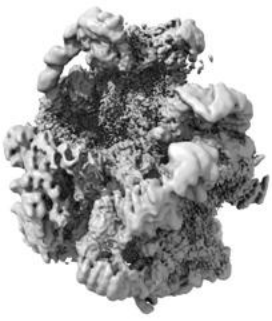
6.4.1 Primary map



X



Y



Z

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

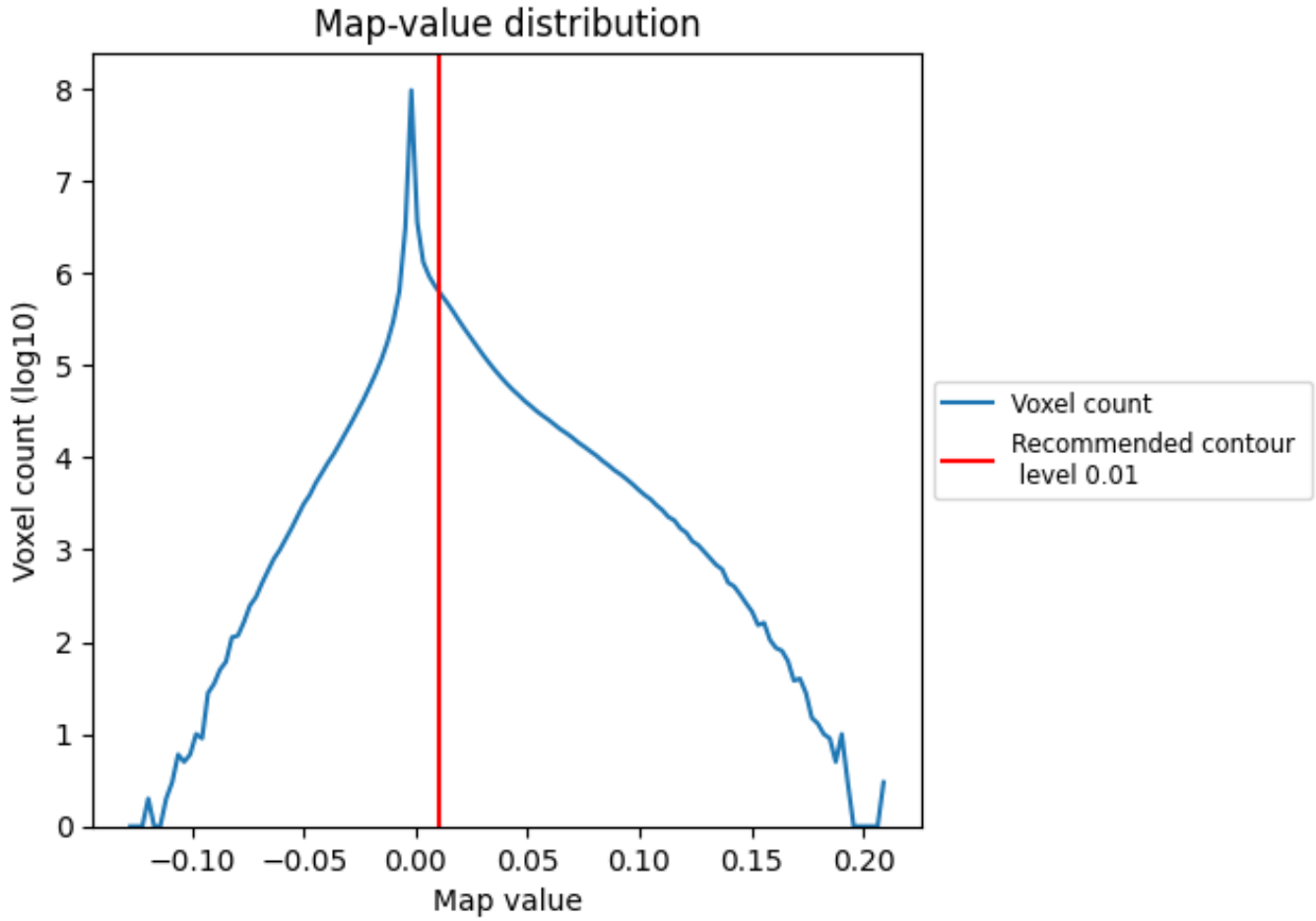
6.5 Mask visualisation (i)

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

7 Map analysis

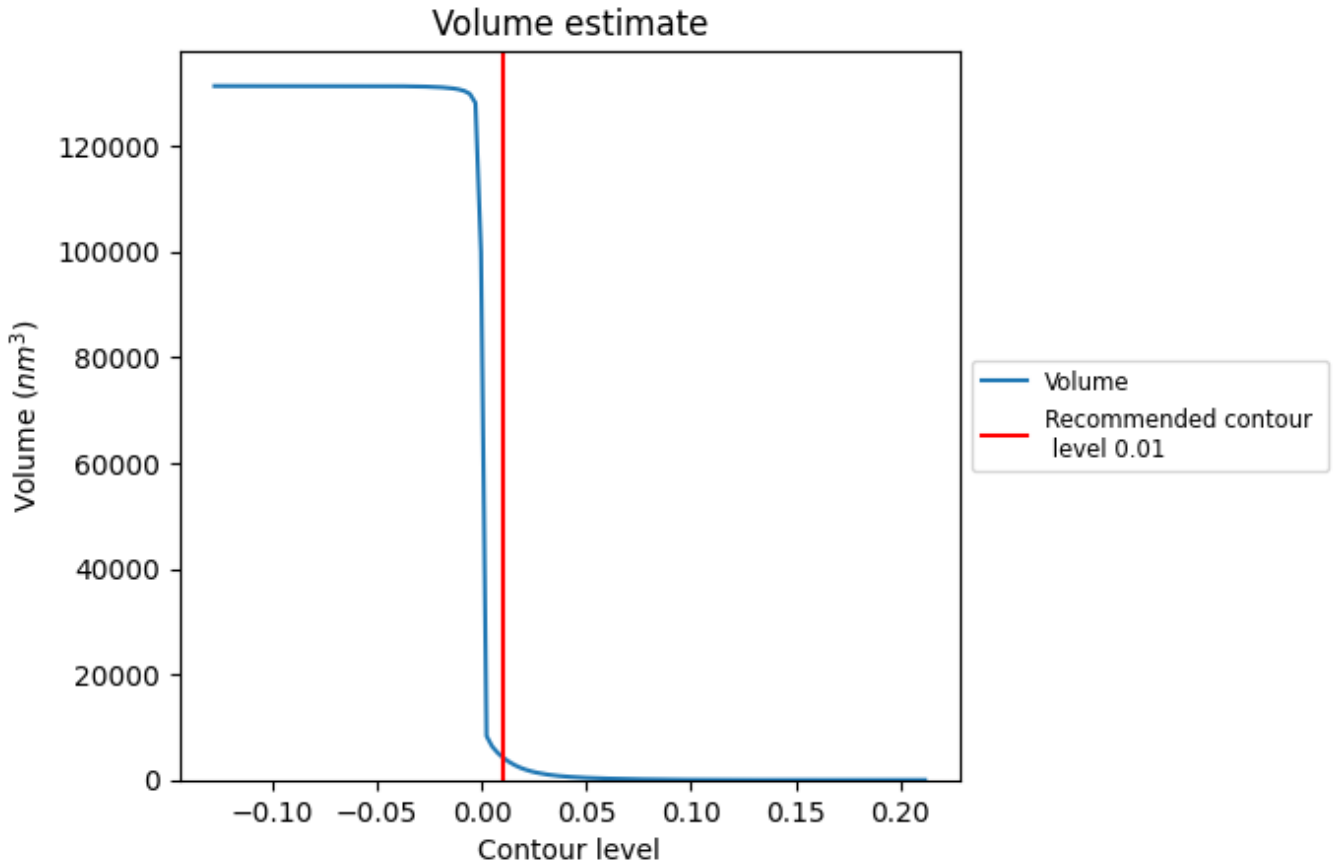
This section contains the results of statistical analysis of the map.

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.

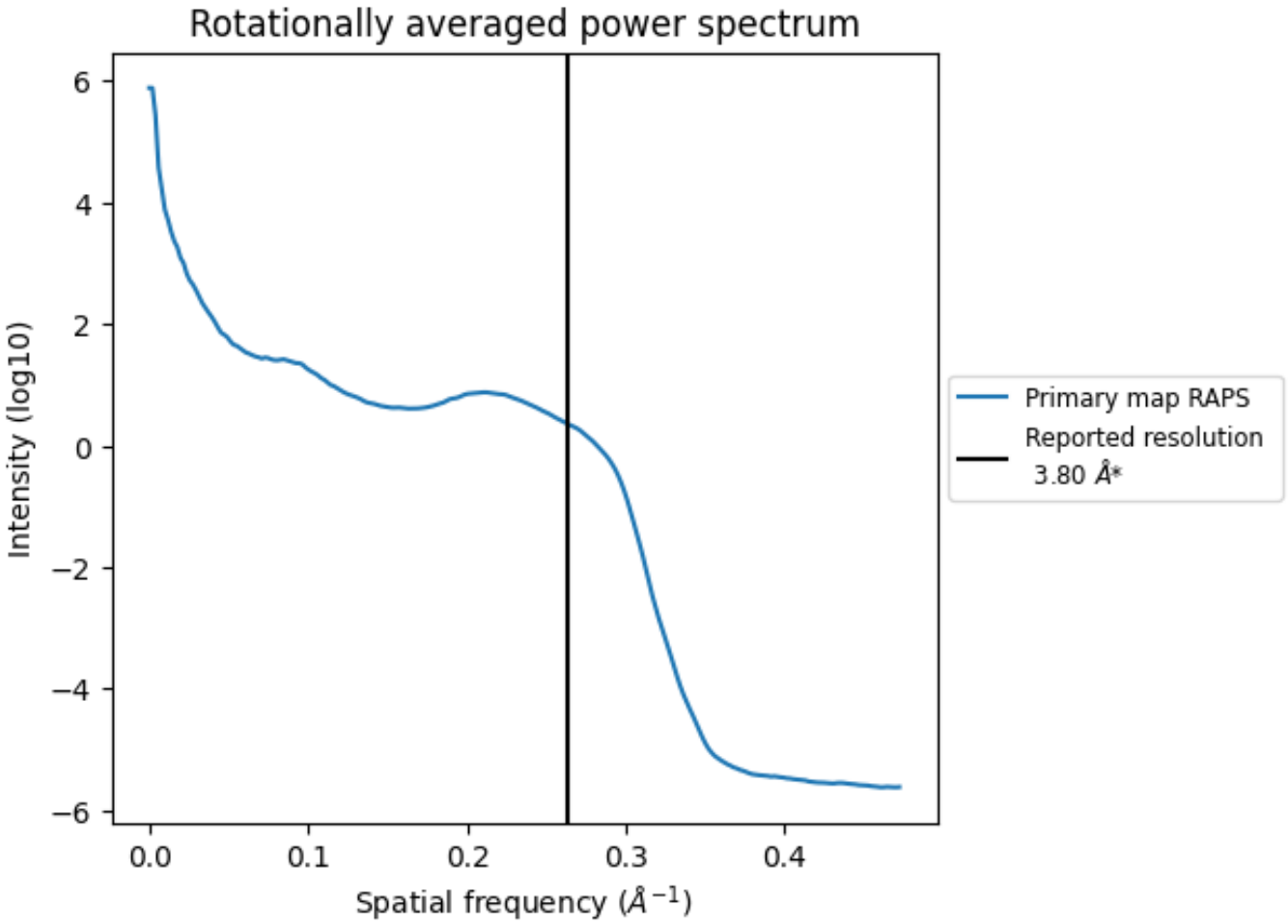
7.2 Volume estimate (i)



The volume at the recommended contour level is 4324 nm^3; this corresponds to an approximate mass of 3906 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)

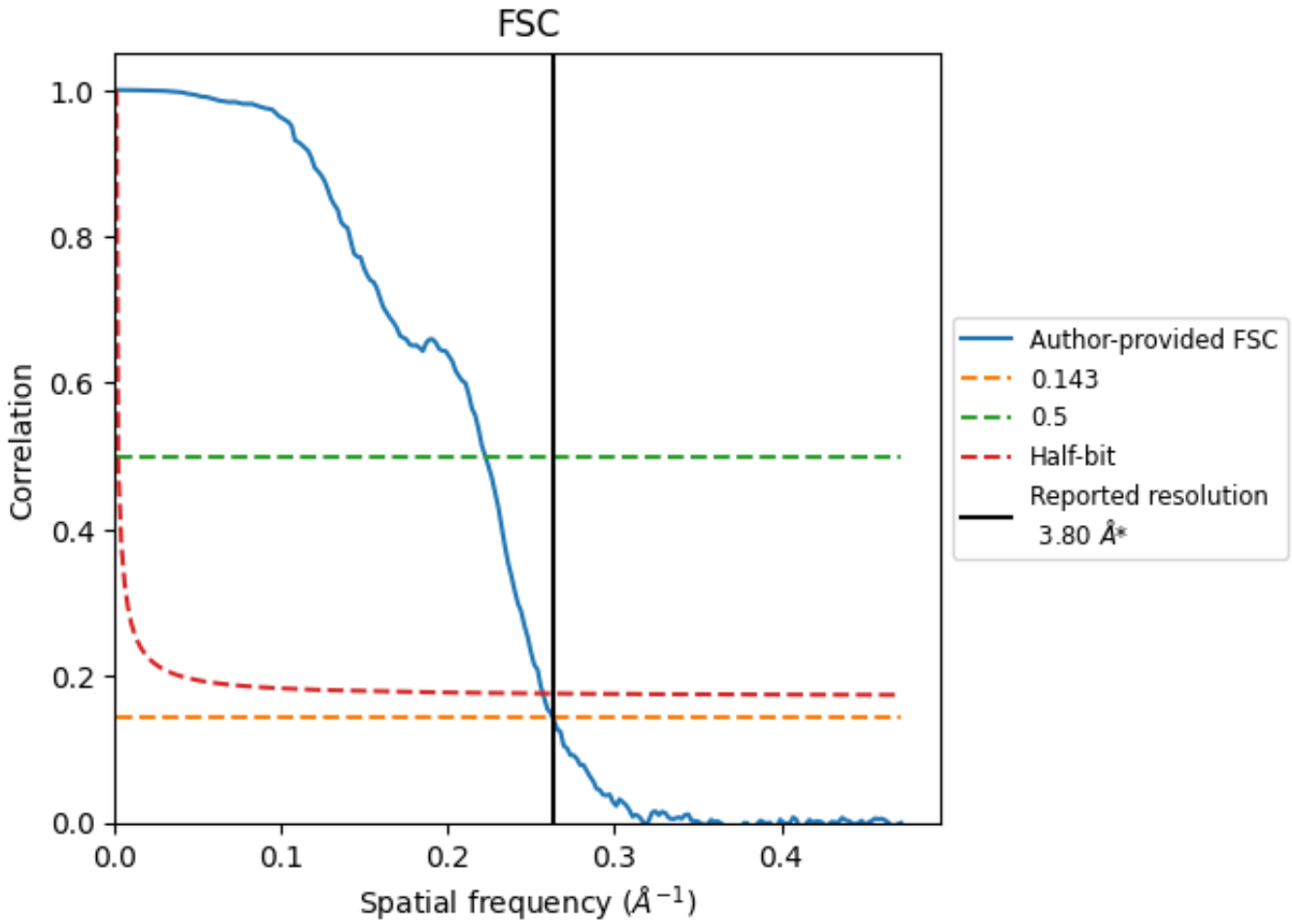


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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)

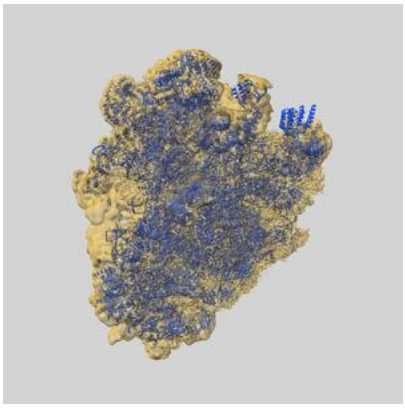
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.80	4.49	3.89
Unmasked-calculated*	-	-	-

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

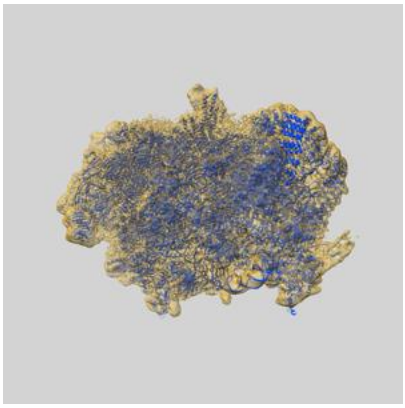
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11359 and PDB model 6ZQC. Per-residue inclusion information can be found in section 3 on page 17.

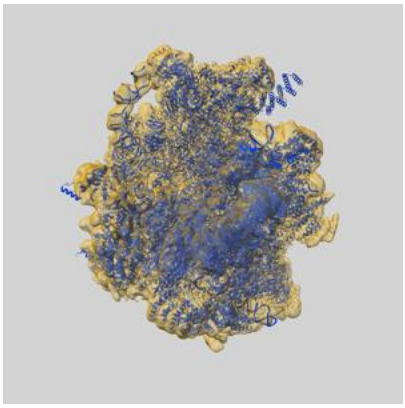
9.1 Map-model overlay



X



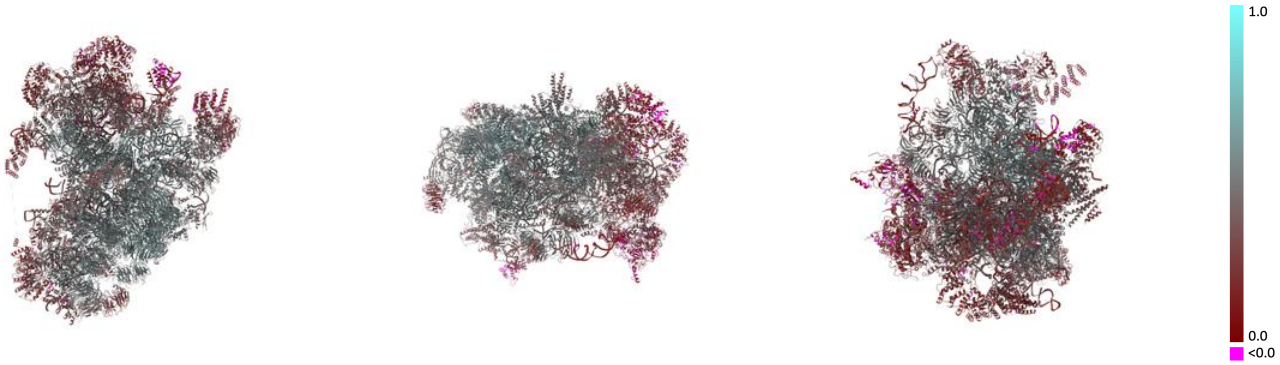
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

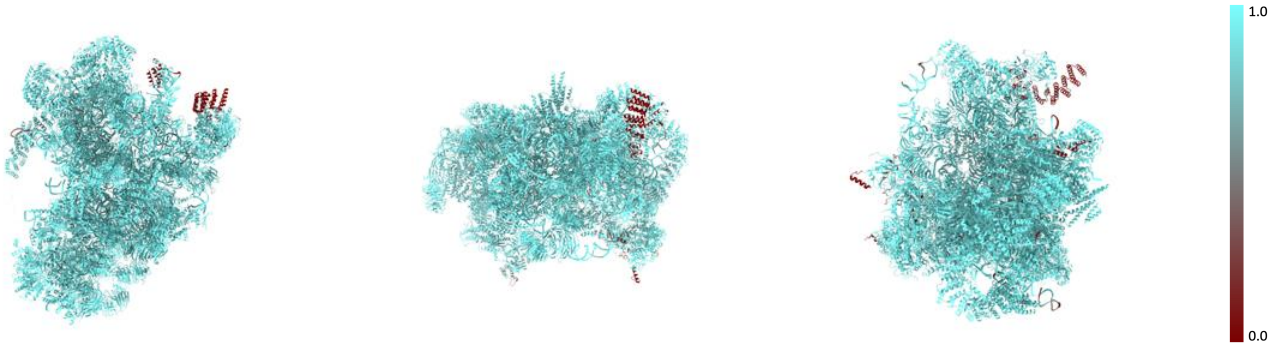
9.2 Q-score mapped to coordinate model



X Y Z

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

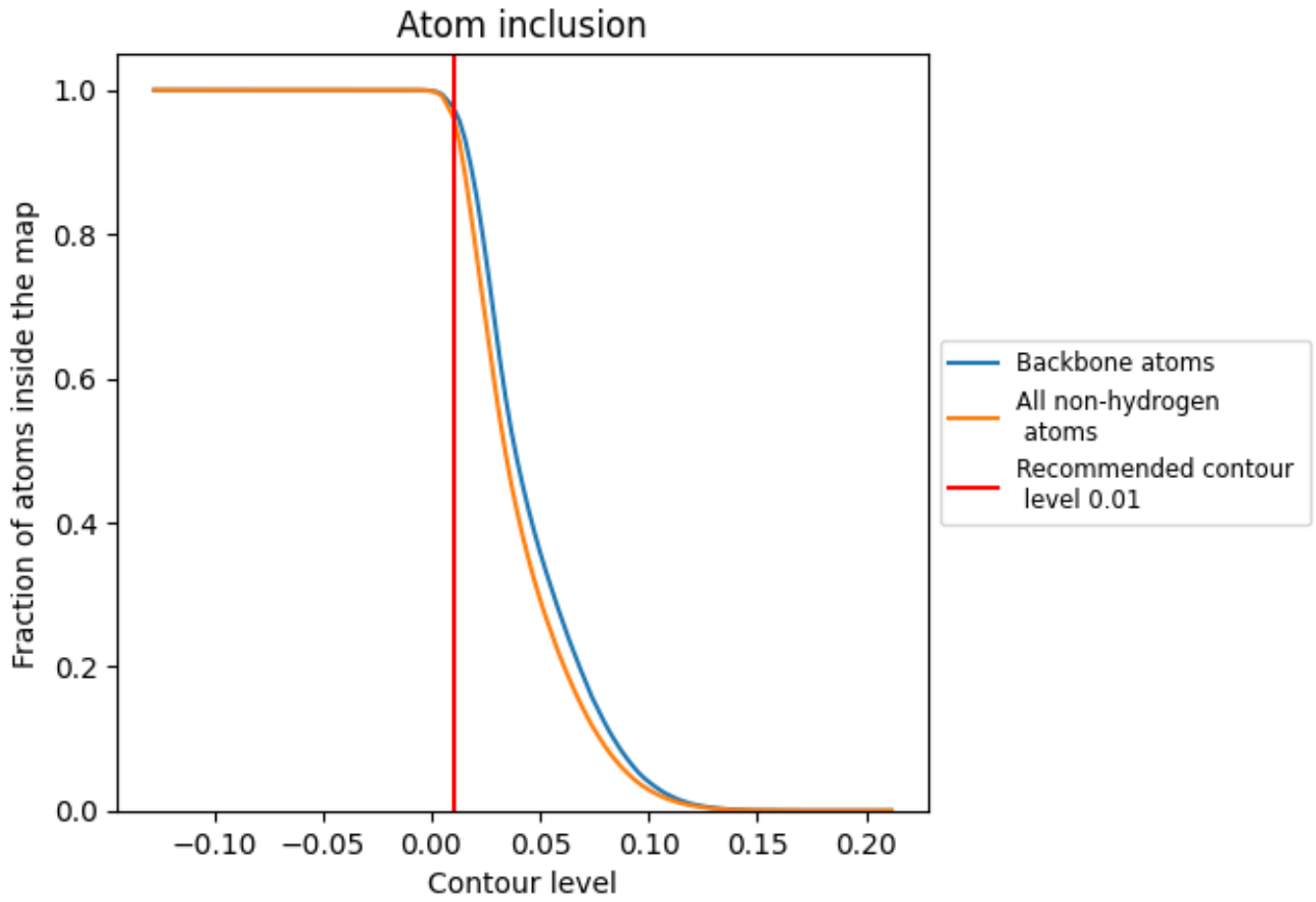
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% 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	0.9634	0.4100
CA	0.9798	0.5280
CB	0.9718	0.4530
CD	0.9790	0.4550
CE	0.9691	0.4250
CF	0.9880	0.5300
CG	0.9793	0.5190
CH	0.9841	0.4790
CI	0.9792	0.5590
CJ	0.9758	0.5240
CK	0.9693	0.4920
CL	0.9794	0.4900
CM	0.9751	0.4690
CN	0.9524	0.3260
D2	0.9823	0.4330
D3	0.9727	0.3830
D4	0.9421	0.4140
DA	0.9649	0.4940
DE	0.9679	0.4160
DF	0.9785	0.5210
DG	0.9448	0.3320
DH	0.9394	0.3600
DI	0.9622	0.2980
DJ	0.9743	0.5200
DL	0.9572	0.3380
DN	0.9680	0.4820
DO	0.9790	0.5000
DQ	0.9727	0.5490
DS	0.9380	0.3330
DW	0.9749	0.5320
DX	0.9755	0.5200
DY	0.9856	0.5030
Db	0.9867	0.5290
Dc	0.9811	0.5220
JA	0.9274	0.2550

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
JB	0.8647	0.1600
JC	0.9408	0.2480
JF	0.9659	0.3720
JG	0.9689	0.4620
JH	0.8602	0.1180
JI	0.2275	0.1810
JJ	0.9766	0.4310
JK	0.9421	0.2260
JM	0.9639	0.4550
JN	0.9712	0.5090
JO	0.9733	0.4970
JP	0.9820	0.5460
JQ	0.9841	0.4020
UA	0.9857	0.5560
UB	0.9652	0.3190
UC	0.9729	0.4750
UD	0.9797	0.4500
UE	0.9811	0.4820
UF	0.9745	0.4240
UG	0.9836	0.5410
UH	0.9798	0.2630
UI	0.9669	0.3210
UJ	0.9566	0.3340
UK	0.9792	0.4920
UL	0.9772	0.4350
UM	0.9701	0.4210
UN	0.9549	0.4720
UO	0.9814	0.4900
UP	0.9625	0.4240
UQ	0.9827	0.4610
UR	0.9810	0.5350
US	0.9710	0.3450
UT	0.9493	0.2540
UU	0.9872	0.5400
UV	0.9687	0.3510
UX	0.9824	0.5500
UZ	0.9776	0.4170