wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 08:57 PM EST

PDB ID	:	7MQ8
EMDB ID	:	EMD-23936
Title	:	Cryo-EM structure of the human SSU processome, state pre-A1
Authors	:	Vanden Broeck, A.; Singh, S.; Klinge, S.
Deposited on	:	2021-05-05
Resolution	:	3.60 Å(reported)
Based on initial models	:	5FAI, 5WLC, 2OZB, 6ZOJ, 6G4S, 6ZQD, 2IPX, 6G18, 4JXM

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:

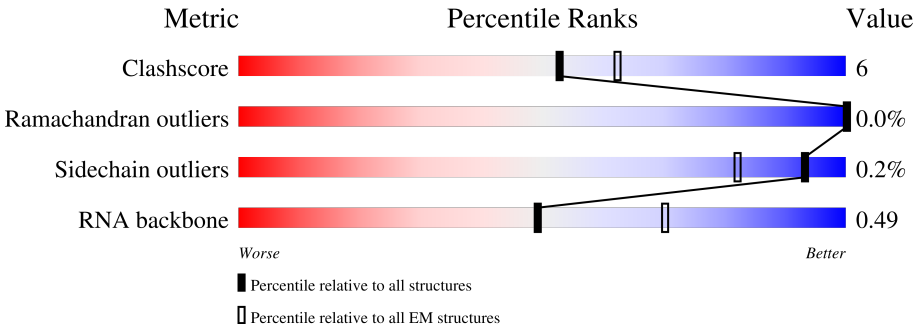
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.60 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	L0	3617	93%
2	L1	1869	9%, 37%, 27%, 5%, 30%
3	L2	217	18%, 46%, 43%, 10%
4	L3	116	53%, 75%, 24%
5	L4	263	10%, 89%, 11%
6	L5	204	82%, 11%, 7%
7	L6	249	76%, 13%, 10%

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Mol	Chain	Length	Quality of chain
8	L7	194	24% 65% 22% 13%
9	L8	208	72% 14% 13%
10	L9	194	76% 12% 12%
11	LA	132	91% 69% 22% 9%
12	LC	146	85% 10% 5%
13	LD	158	6% 82% 11% 7%
14	LF	133	6% 62% 17% 22%
15	LG	69	83% 7% 10%
16	LH	830	8% 76% 14% 10%
17	LI	678	65% 68% 11% 21%
18	LJ	518	74% 16% 9%
19	LK	677	11% 13% 5% 83%
19	LL	677	8% 63% 12% 25%
20	LM	2144	32% 75% 19% 6%
21	LN	686	6% 79% 18%
22	LO	919	79% 13% 8%
23	LP	597	85% 10% 5%
24	LQ	943	6% 74% 14% 12%
25	LR	808	77% 19%
26	LS	556	67% 14% 19%
27	LT	951	79% 13% 9%
28	LU	445	82% 18%
29	LW	610	66% 8% 26%
30	LZ	184	92% 7%
31	N0	22	36% 100%

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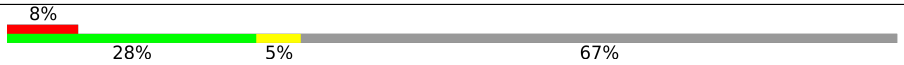
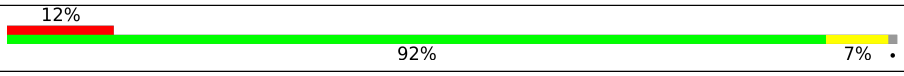
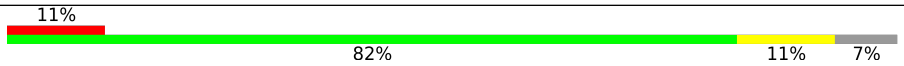
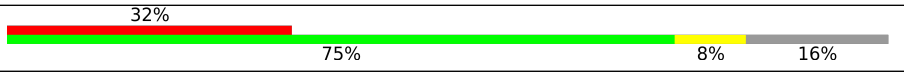
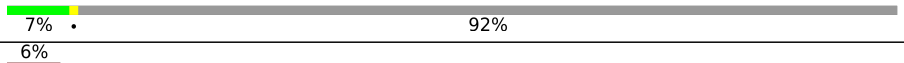
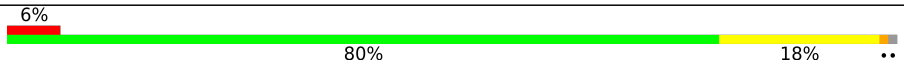
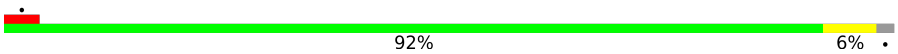
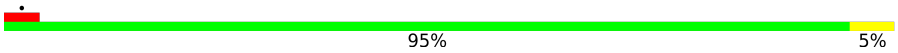
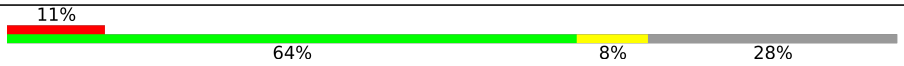
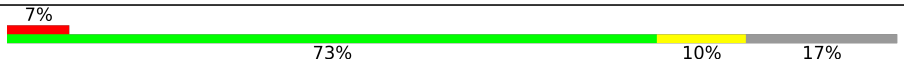
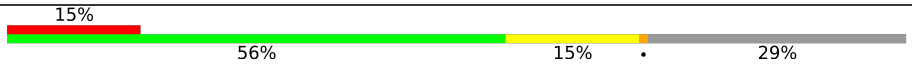
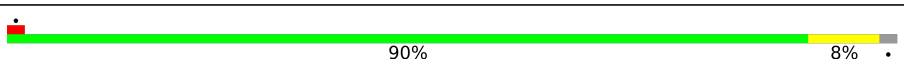
Mol	Chain	Length	Quality of chain
32	NA	681	
33	NB	479	
34	NC	315	
35	ND	257	
36	NE	293	
37	NF	151	
38	NG	151	
39	NH	1146	
40	NI	280	
41	NJ	1025	
41	NK	1025	
42	NM	264	
43	NN	560	
44	NO	130	
45	NQ	84	
46	NR	861	
47	NT	156	
48	NU	135	
49	NW	688	
50	NY	381	
51	SA	594	
52	SB	529	
53	SC	321	
53	SD	321	
54	SE	128	

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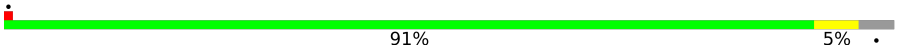
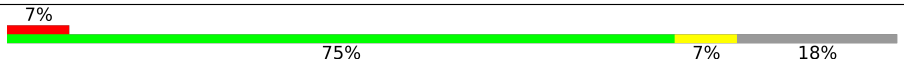
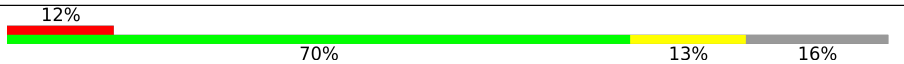
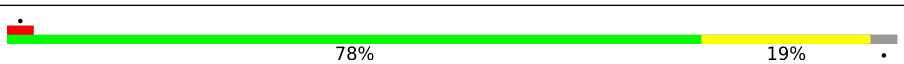
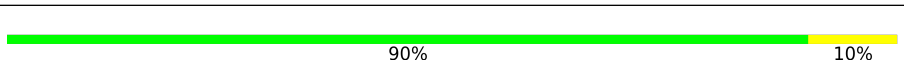
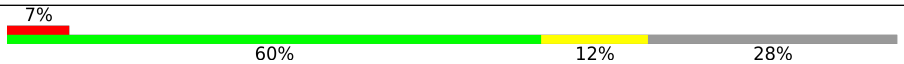
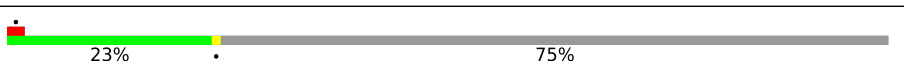
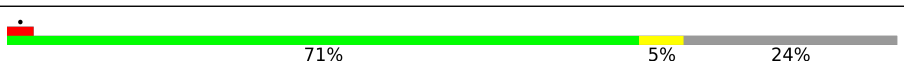
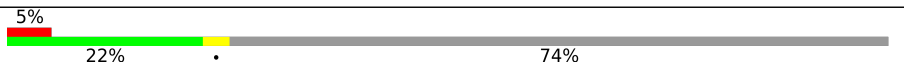
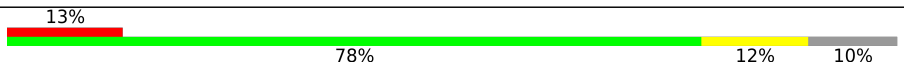
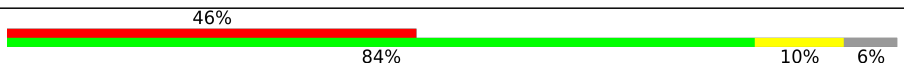
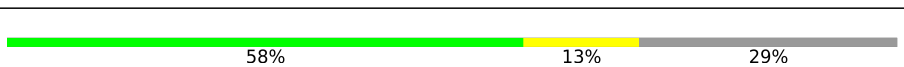
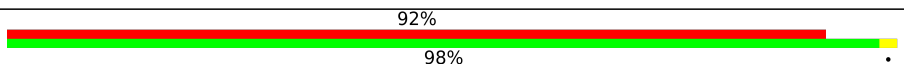
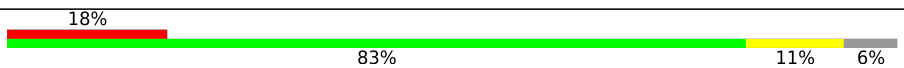
Mol	Chain	Length	Quality of chain
54	SF	128	
55	SG	475	
56	SH	373	
57	SI	1282	
58	SJ	244	
58	SK	244	
59	SL	198	
60	SM	291	
61	SP	2785	
62	SQ	756	
63	SR	143	
64	SS	771	
65	ST	632	
66	SU	472	
67	SW	252	
68	SX	177	
69	SY	253	
70	SZ	304	

2 Entry composition (i)

There are 75 unique types of molecules in this entry. The entry contains 245114 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5'ETS rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L0	242	5152	2289	908	1713	242	0	0

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L1	1301	27777	12396	5002	9078	1301	0	0

- Molecule 3 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L2	215	4589	2047	809	1518	215	0	0

- Molecule 4 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L3	115	854	538	164	151	1	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L4	262	2076	1324	386	358	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L5	190	1501	939	285	270	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L6	223	Total	C	N	O	S	0	0
			1811	1133	361	311	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L7	168	Total	C	N	O	S	0	0
			1346	862	239	244	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L8	180	Total	C	N	O	S	0	0
			1474	925	294	250	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L9	171	Total	C	N	O	S	0	0
			1425	908	284	232	1		

- Molecule 11 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LA	120	Total	C	N	O	S	0	0
			931	584	164	174	9		

- Molecule 12 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LC	139	Total	C	N	O	S	0	0
			1098	699	207	189	3		

- Molecule 13 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LD	147	Total	C	N	O	S	0	0
			1204	767	225	206	6		

- Molecule 14 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LF	104	Total	C	N	O	S	0	0
			851	543	158	145	5		

- Molecule 15 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LG	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 16 is a protein called WD repeat-containing protein 75.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH	746	Total	C	N	O	S	0	0
			5987	3846	1005	1101	35		

- Molecule 17 is a protein called Nucleolar protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LI	537	Total	C	N	O	S	0	0
			3889	2508	654	706	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LJ	469	Total	C	N	O	S	0	0
			3711	2372	637	688	14		

- Molecule 19 is a protein called WD repeat-containing protein 43.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LK	118	Total	C	N	O	S	0	0
			943	612	163	163	5		
19	LL	510	Total	C	N	O	S	0	0
			3982	2538	686	731	27		

- Molecule 20 is a protein called HEAT repeat-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LM	2005	Total	C	N	O	S	0	0
			15820	10259	2597	2883	81		

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LN	671	Total	C	N	O	S	0	0
			5299	3394	925	956	24		

- Molecule 22 is a protein called Periodic tryptophan protein 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LO	848	Total	C	N	O	S	0	0
			6676	4258	1151	1234	33		

- Molecule 23 is a protein called U3 small nucleolar RNA-associated protein 6 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LP	567	Total	C	N	O	S	0	0
			4705	3022	808	847	28		

- Molecule 24 is a protein called WD repeat-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LQ	828	Total	C	N	O	S	0	0
			6438	4103	1108	1194	33		

- Molecule 25 is a protein called Transducin beta-like protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LR	773	Total	C	N	O	S	0	0
			6015	3789	1079	1116	31		

- Molecule 26 is a protein called U3 small nucleolar RNA-associated protein 18 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LS	453	Total	C	N	O	S	0	0
			3560	2235	631	671	23		

- Molecule 27 is a protein called WD repeat-containing protein 36.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LT	869	Total	C	N	O	S	0	0
			6756	4321	1158	1244	33		

- Molecule 28 is a protein called DDB1- and CUL4-associated factor 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LU	445	Total	C	N	O	S	0	0
			3611	2282	653	651	25		

- Molecule 29 is a protein called WD repeat-containing protein 46.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LW	453	Total	C	N	O	S	0	0
			3519	2221	637	646	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LZ	183	Total	C	N	O	S	0	0
			1532	966	292	270	4		

- Molecule 31 is a RNA chain called 5'ETS rRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	N0	22	Total	C	O	P	0	0
			264	110	132	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	NA	249	Total	C	N	O	S	0	0
			2055	1299	359	391	6		

- Molecule 33 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	NB	73	Total	C	N	O	0	0
			617	379	140	98		

- Molecule 34 is a protein called Neuroguidin.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	NC	94	Total	C	N	O	S	0	0
			779	469	160	147	3		

- Molecule 35 is a protein called Nucleolar protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	ND	84	Total	C	N	O	S	0	0
			696	438	143	114	1		

- Molecule 36 is a protein called Uncharacterized protein C1orf131.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NE	100	Total	C	N	O	S	0	0
			799	509	143	146	1		

- Molecule 37 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	NF	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 38 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NG	116	Total	C	N	O	S	0	0
			861	531	159	165	6		

- Molecule 39 is a protein called Nucleolar protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	NH	1066	Total	C	N	O	S	0	0
			8374	5345	1491	1506	32		

- Molecule 40 is a protein called Ribosomal RNA-processing protein 7 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	NI	234	Total	C	N	O	S	0	0
			1840	1171	329	336	4		

- Molecule 41 is a protein called RNA cytidine acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	NJ	827	Total	C	N	O	S	0	0
			6526	4187	1126	1178	35		
41	NK	815	Total	C	N	O	S	0	0
			6419	4118	1109	1160	32		

- Molecule 42 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	NM	233	Total	C	N	O	S	0	0
			1873	1186	339	334	14		

- Molecule 43 is a protein called Protein AATF.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	NN	42	Total	C	N	O	S	0	0
			340	215	63	60	2		

- Molecule 44 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	NO	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 45 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	NQ	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 46 is a protein called RRP12-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	NR	861	Total	C	N	O	0	0
			4305	2583	861	861		

- Molecule 47 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	NT	58	Total	C	N	O	S	0	0
			470	295	89	79	7		

- Molecule 48 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	NU	60	Total	C	N	O	S	0	0
			495	314	98	81	2		

- Molecule 49 is a protein called Nucleolar protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	NW	311	Total	C	N	O	S	0	0
			2498	1599	413	472	14		

- Molecule 50 is a protein called KRR1 small subunit processome component homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	NY	274	Total	C	N	O	S	0	0
			2222	1422	391	400	9		

- Molecule 51 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SA	396	Total	C	N	O	S	0	0
			3077	1948	542	575	12		

- Molecule 52 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SB	440	Total	C	N	O	S	0	0
			3439	2179	596	642	22		

- Molecule 53 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SC	229	Total	C	N	O	S	0	0
			1781	1129	322	323	7		
53	SD	237	Total	C	N	O	S	0	0
			1841	1163	337	334	7		

- Molecule 54 is a protein called NHP2-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SE	125	Total	C	N	O	S	0	0
			968	611	172	180	5		
54	SF	123	Total	C	N	O	S	0	0
			955	604	170	176	5		

- Molecule 55 is a protein called U3 small nucleolar RNA-interacting protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SG	389	Total	C	N	O	S	1	0
			2884	1809	534	528	13		

- Molecule 56 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SH	368	Total	C	N	O	S	0	0
			2832	1803	495	518	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SI	844	Total	C	N	O	S	0	0
			6803	4351	1230	1188	34		

- Molecule 58 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SJ	204	Total	C	N	O	S	0	0
			1579	1012	272	286	9		
58	SK	204	Total	C	N	O	S	0	0
			1579	1012	272	286	9		

- Molecule 59 is a protein called rRNA-processing protein FCF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SL	192	Total	C	N	O	S	0	0
			1586	1006	290	275	15		

- Molecule 60 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SM	290	Total	C	N	O	S	0	0
			2369	1485	451	424	9		

- Molecule 61 is a protein called Small subunit processome component 20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SP	1993	Total	C	N	O	S	0	0
			16078	10412	2689	2897	80		

- Molecule 62 is a protein called Deoxynucleotidyltransferase terminal-interacting protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SQ	187	Total	C	N	O	S	0	0
			1533	972	278	277	6		

- Molecule 63 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SR	108	Total	C	N	O	S	0	0
			816	521	153	140	2		

- Molecule 64 is a protein called U3 small nucleolar RNA-associated protein 14 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SS	197	Total	C	N	O	S	0	0
			1626	1039	301	285	1		

- Molecule 65 is a protein called Nucleolar protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	ST	568	Total	C	N	O	S	0	0
			4170	2634	760	755	21		

- Molecule 66 is a protein called Nucleolar complex protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SU	442	Total	C	N	O	S	0	0
			3154	2030	565	551	8		

- Molecule 67 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SW	180	Total	C	N	O	S	0	0
			1413	906	257	246	4		

- Molecule 68 is a protein called Unassigned peptides.

Mol	Chain	Residues	Atoms				AltConf	Trace
68	SX	177	Total	C	N	O	0	0
			885	531	177	177		

- Molecule 69 is a protein called Probable U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SY	238	Total	C	N	O	S	0	0
			2024	1280	385	353	6		

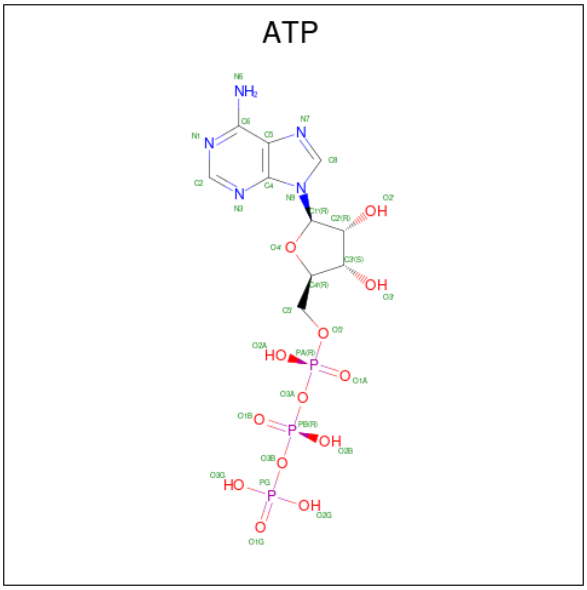
- Molecule 70 is a protein called Bystin.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SZ	290	Total	C	N	O	S	0	0
			2222	1438	392	383	9		

- Molecule 71 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
71	L1	19	Total	Mg	0
			19	19	
71	NH	1	Total	Mg	0
			1	1	
71	SI	1	Total	Mg	0
			1	1	
71	SL	1	Total	Mg	0
			1	1	

- Molecule 72 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

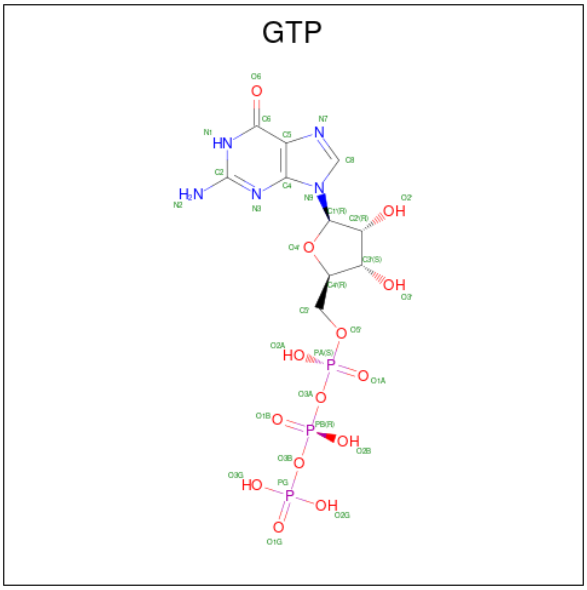


Mol	Chain	Residues	Atoms					AltConf
72	NH	1	Total	C	N	O	P	0
			31	10	5	13	3	
72	NK	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 73 is ZINC ION (three-letter code: ZN) (formula: Zn).

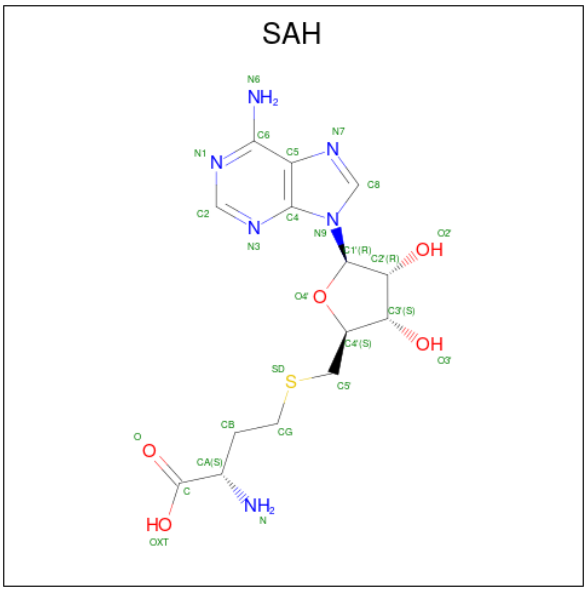
Mol	Chain	Residues	Atoms	AltConf
73	NQ	1	Total Zn 1 1	0
73	NT	1	Total Zn 1 1	0
73	SL	1	Total Zn 1 1	0

- Molecule 74 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 75 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



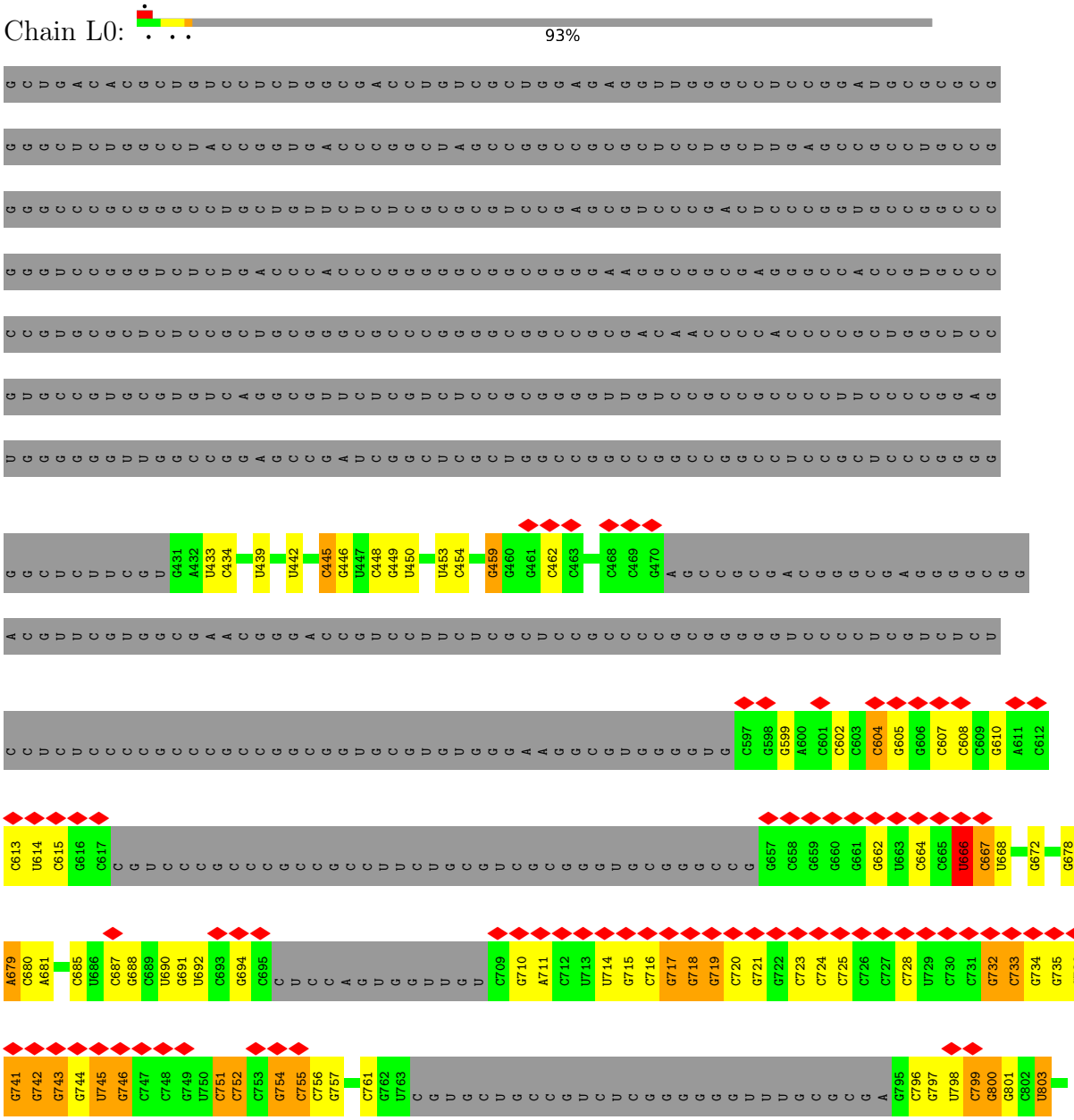
Mol	Chain	Residues	Atoms					AltConf
75	SJ	1	Total	C	N	O	S	0
			26	14	6	5	1	
75	SK	1	Total	C	N	O	S	0
			26	14	6	5	1	

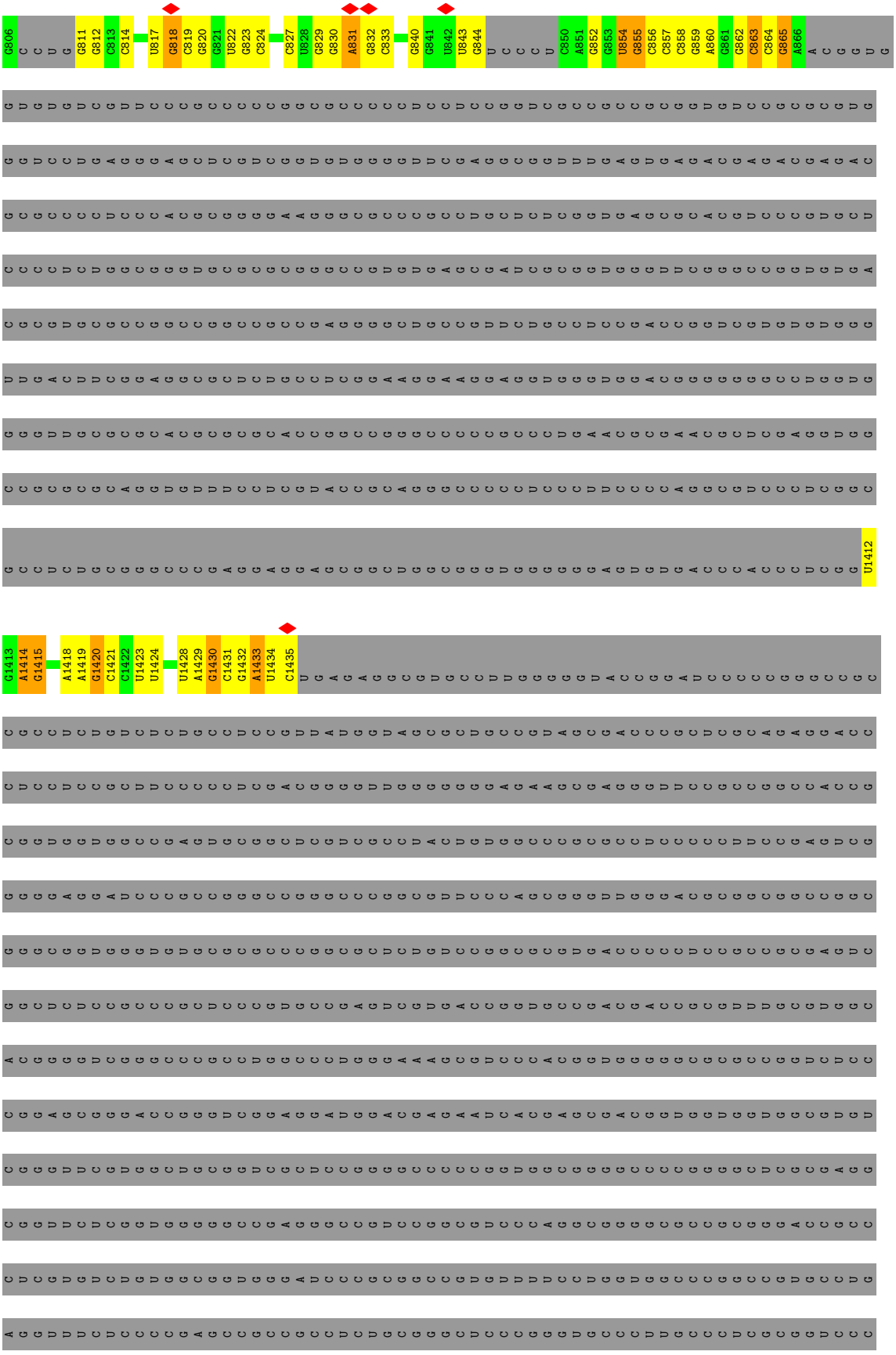
3 Residue-property plots (i)

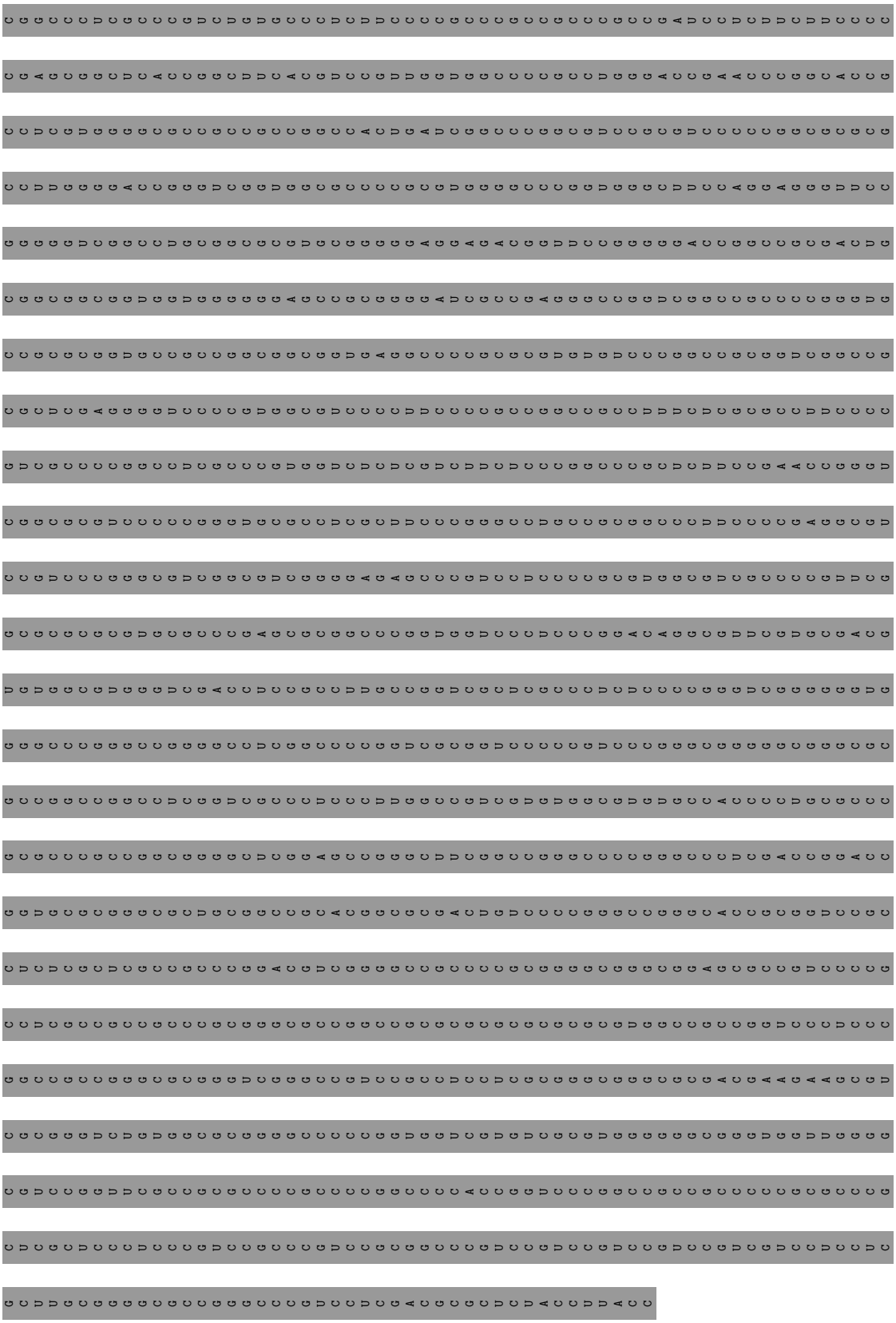
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 5'ETS rRNA

Chain L0:

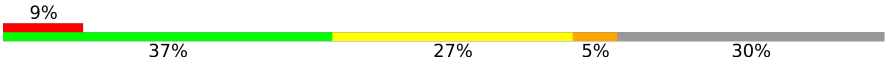


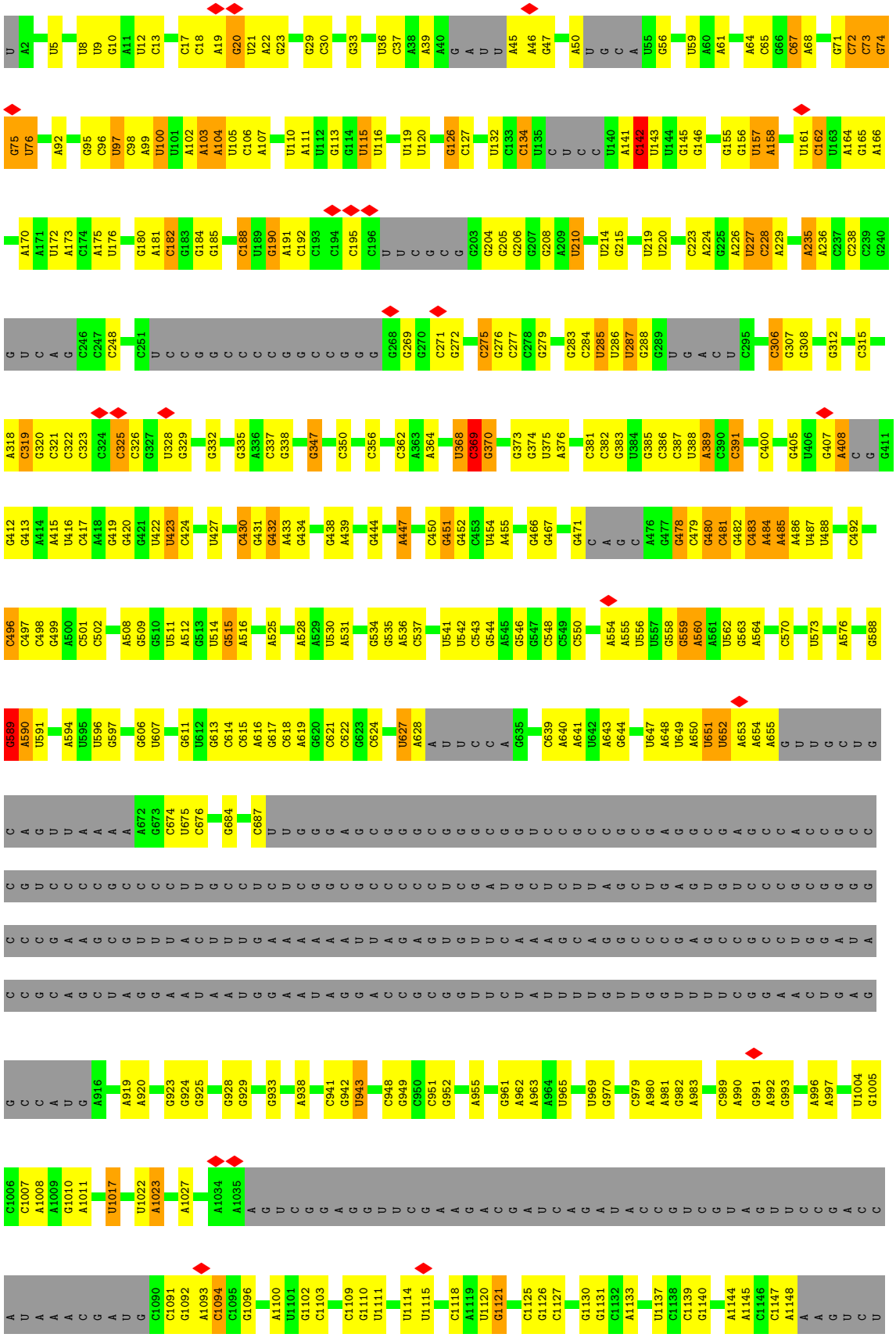

G806 C C U G G811 G812 C813 C814 U817 G818 C819 G820 G821 U822 G823 C824 C827 U828 G829 G830 A831 G832 C833 G840 G841 U842 U843 G844 U C C C U C850 A851 G852 G853 U854 G855 C856 C857 C858 G859 A860 G861 G862 C863 C864 G865 A866 A C G G U G
U1412
G1413 A1414 G1415 A1418 A1419 G1420 C1421 C1422 U1423 U1424 U1428 A1429 G1430 C1431 G1432 A1433 U1434 C1435

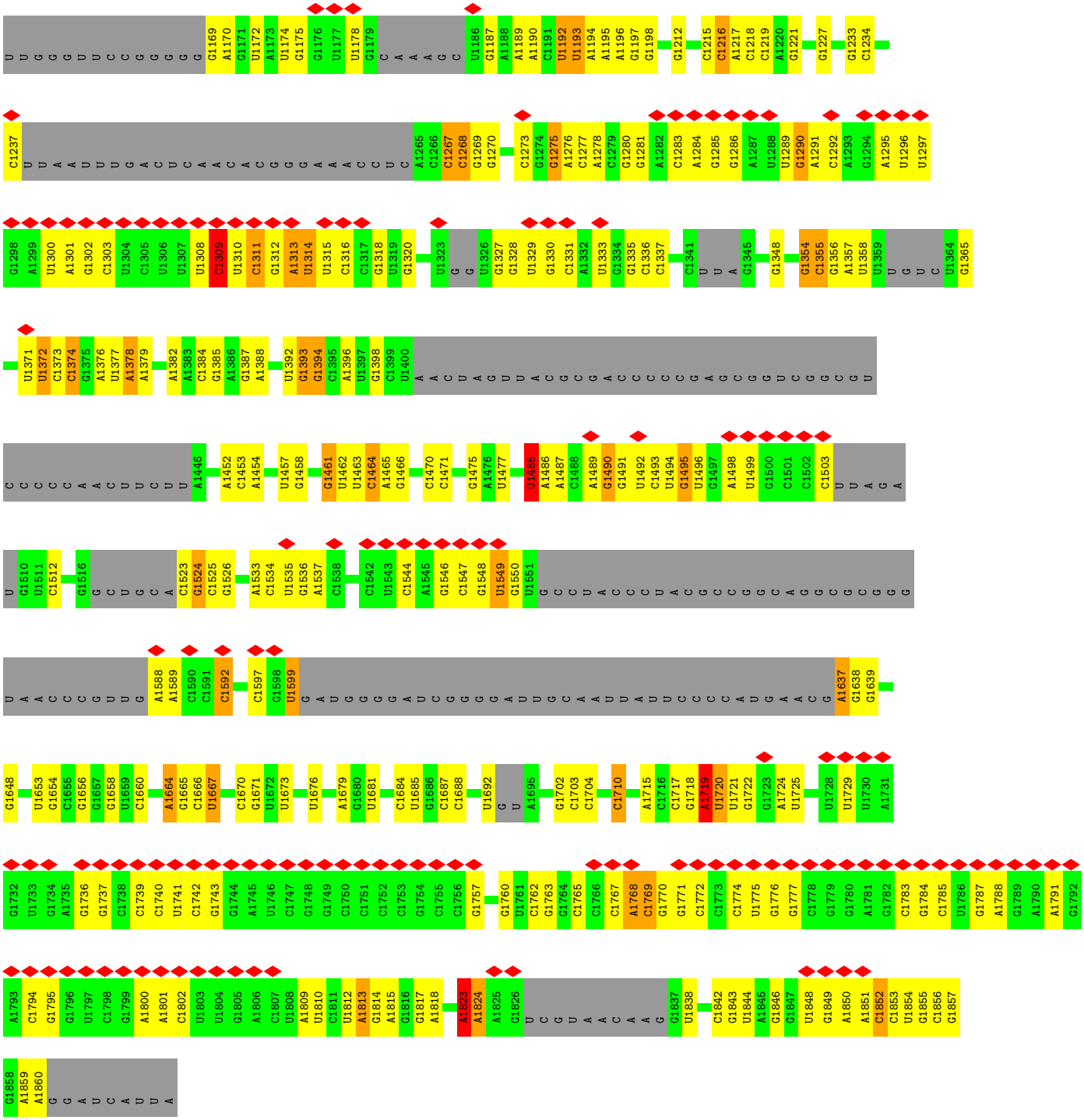


• Molecule 2: 18S rRNA

Chain L1:

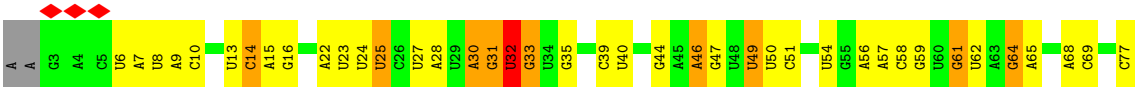


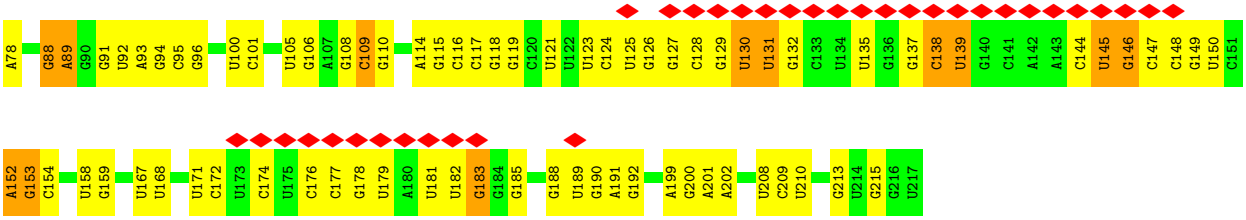




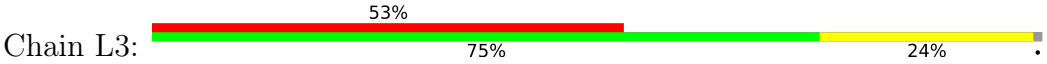
• Molecule 3: U3 snoRNA

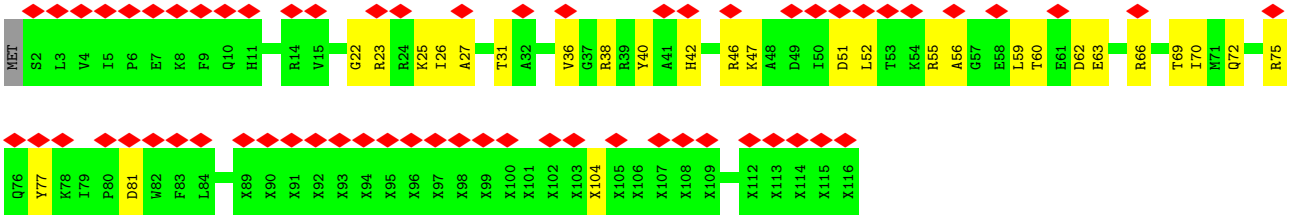
Chain L2:



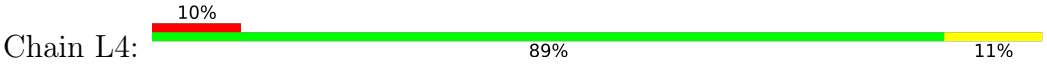


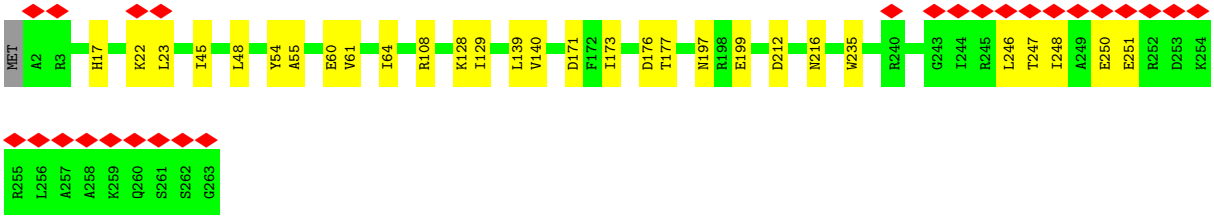
• Molecule 4: 40S ribosomal protein S18



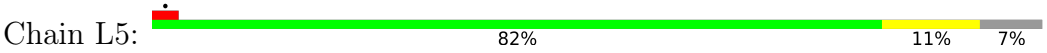


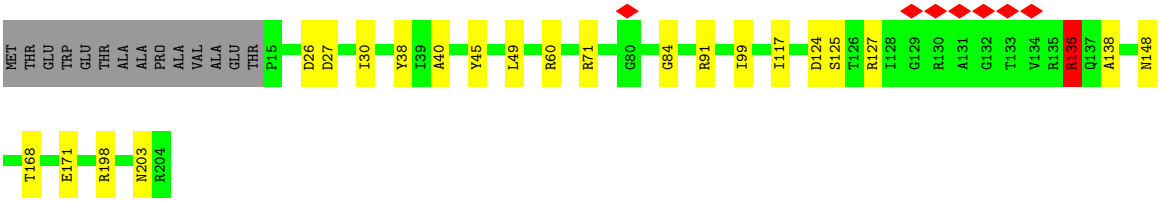
• Molecule 5: 40S ribosomal protein S4, X isoform



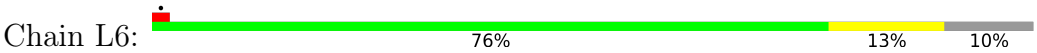


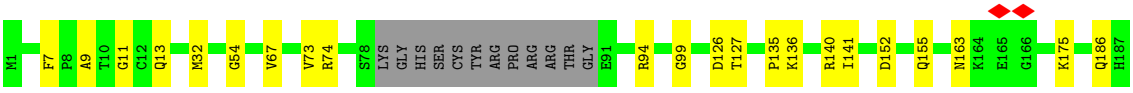
• Molecule 6: 40S ribosomal protein S5

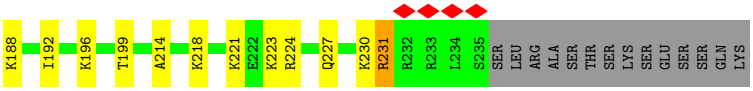




• Molecule 7: 40S ribosomal protein S6

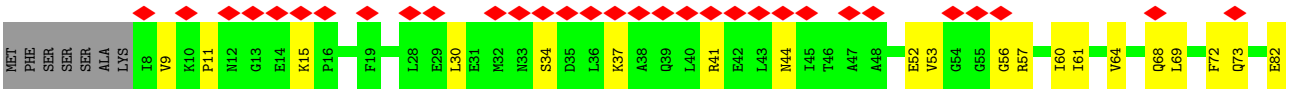


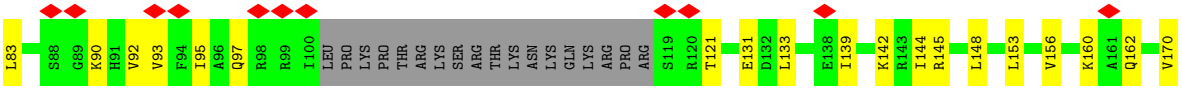


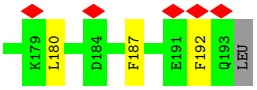


• Molecule 8: 40S ribosomal protein S7

Chain L7:

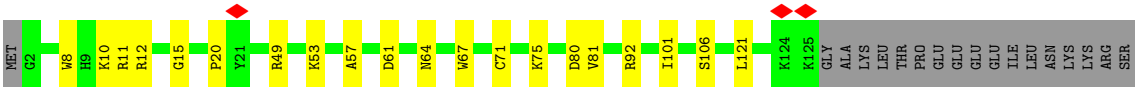


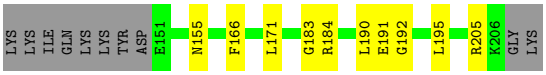




• Molecule 9: 40S ribosomal protein S8

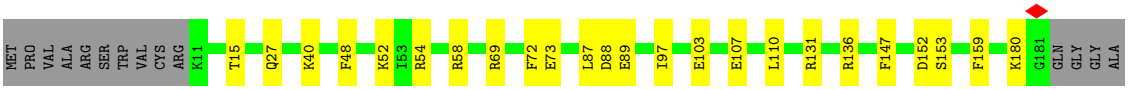
Chain L8:

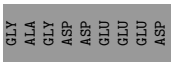




• Molecule 10: 40S ribosomal protein S9

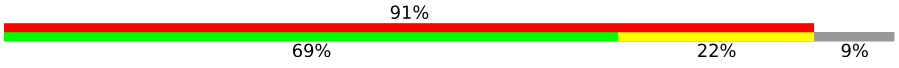
Chain L9:

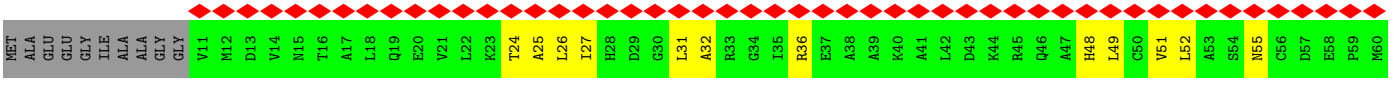


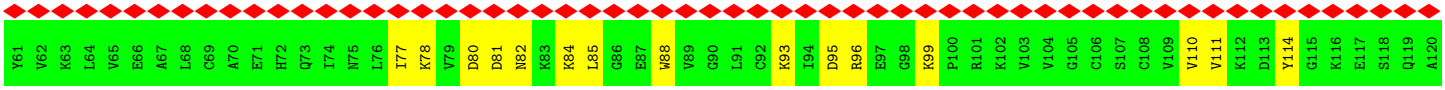


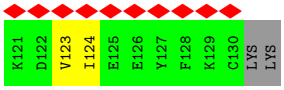
• Molecule 11: 40S ribosomal protein S12

Chain LA:



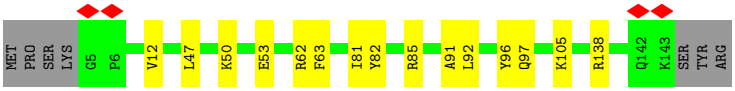






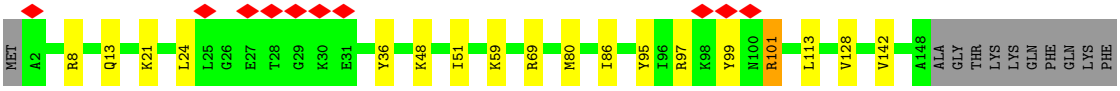
• Molecule 12: 40S ribosomal protein S16

Chain LC:



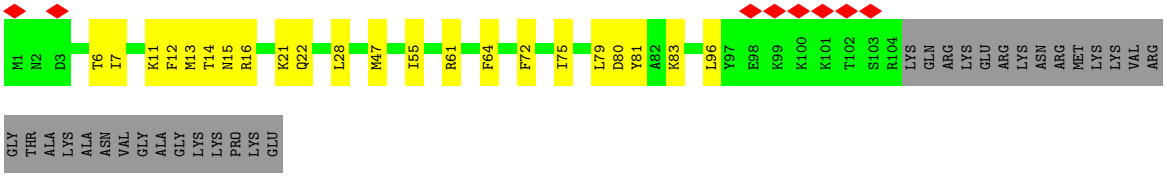
• Molecule 13: 40S ribosomal protein S11

Chain LD:



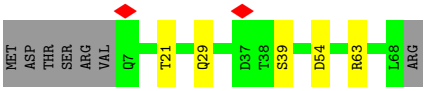
• Molecule 14: 40S ribosomal protein S24

Chain LF:



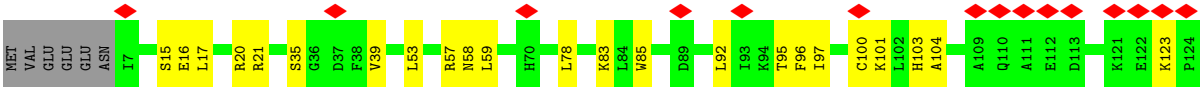
• Molecule 15: 40S ribosomal protein S28

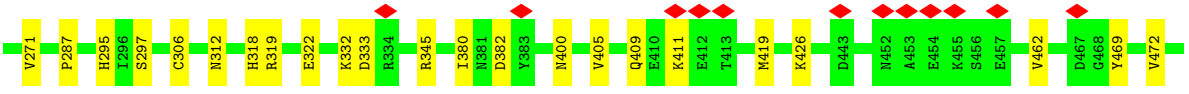
Chain LG:

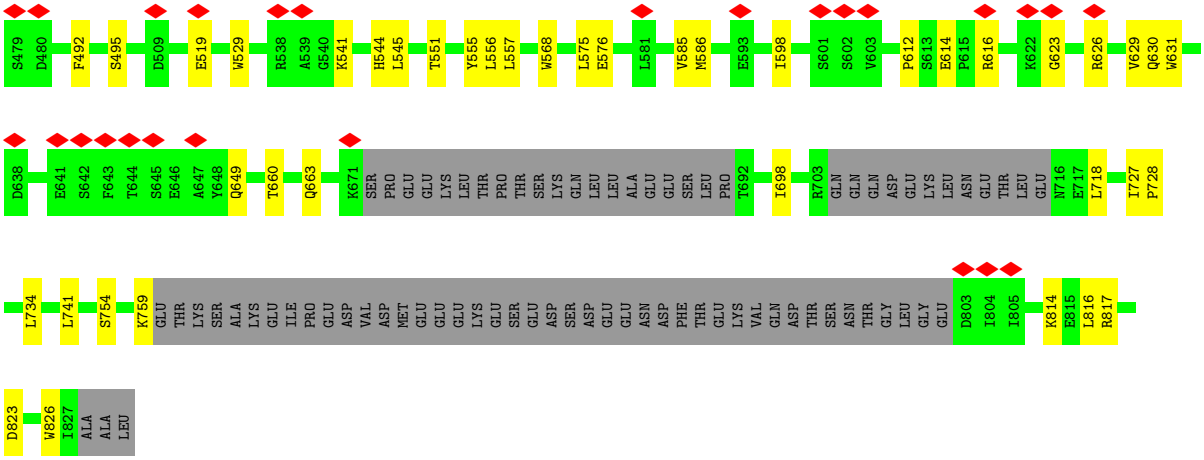


• Molecule 16: WD repeat-containing protein 75

Chain LH:

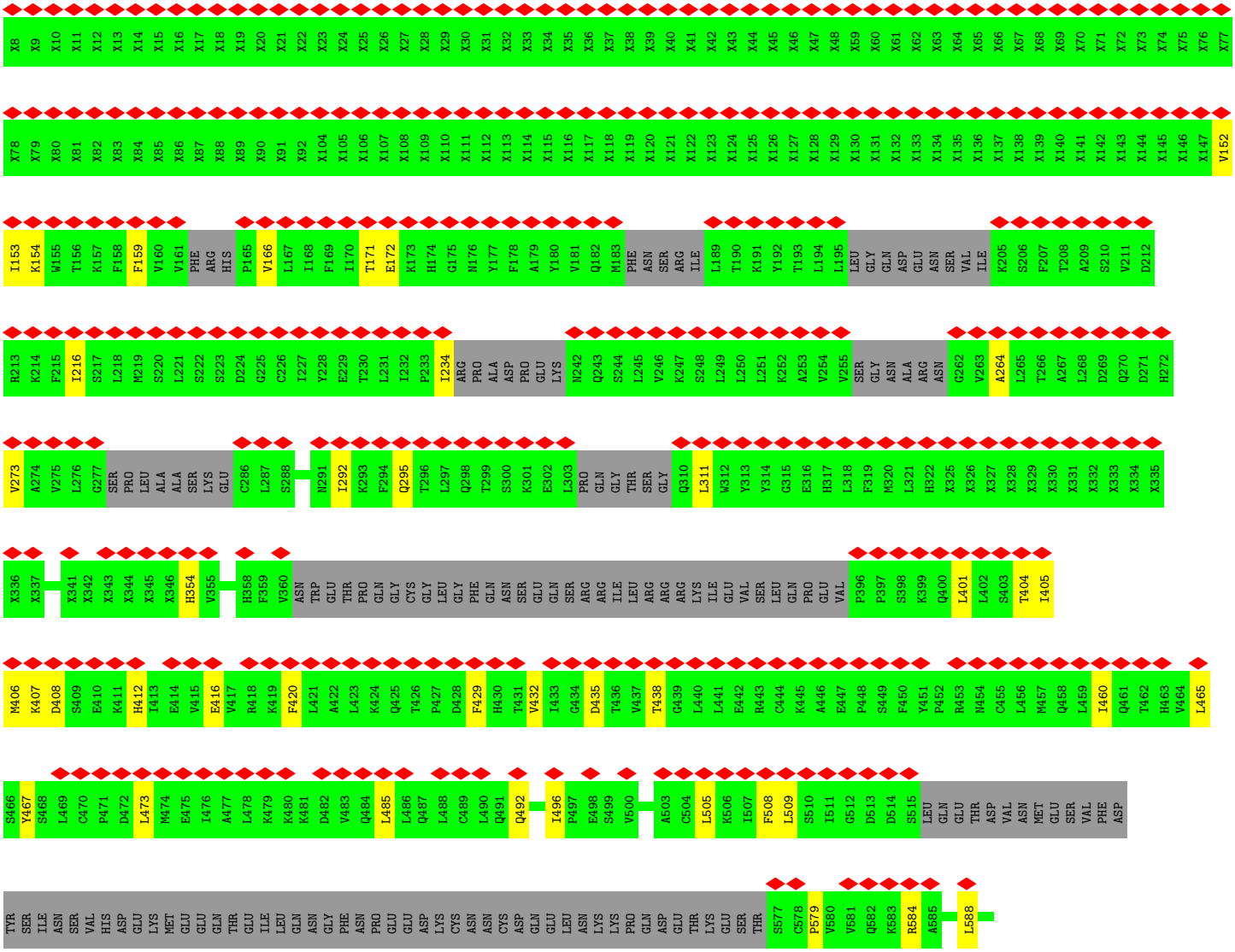


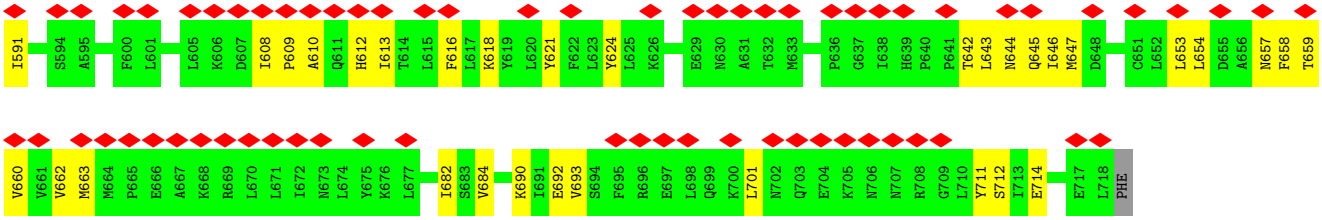




• Molecule 17: Nucleolar protein 11

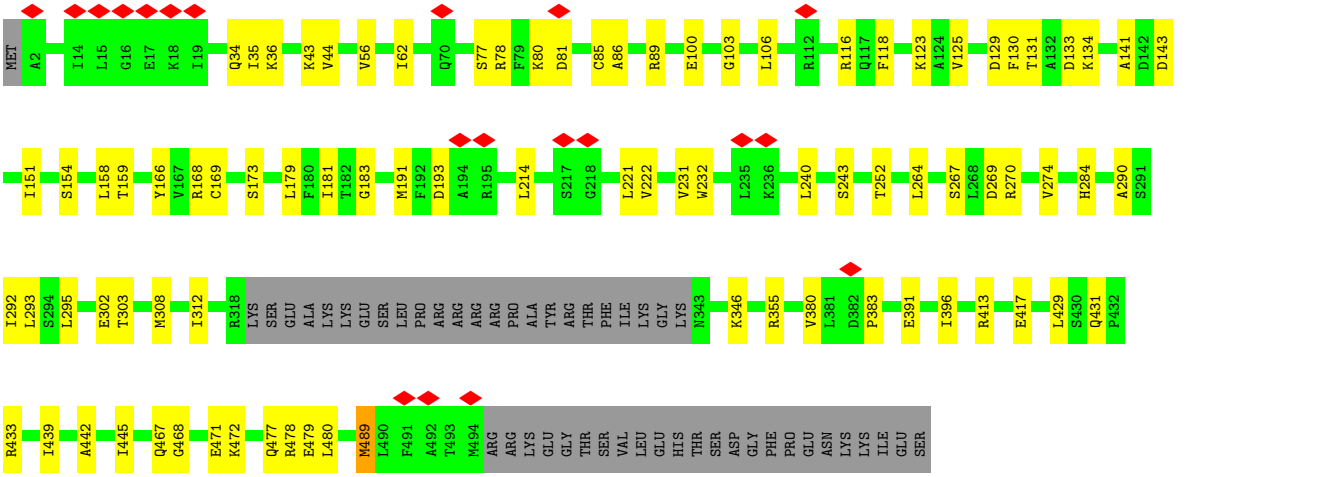
Chain LI:





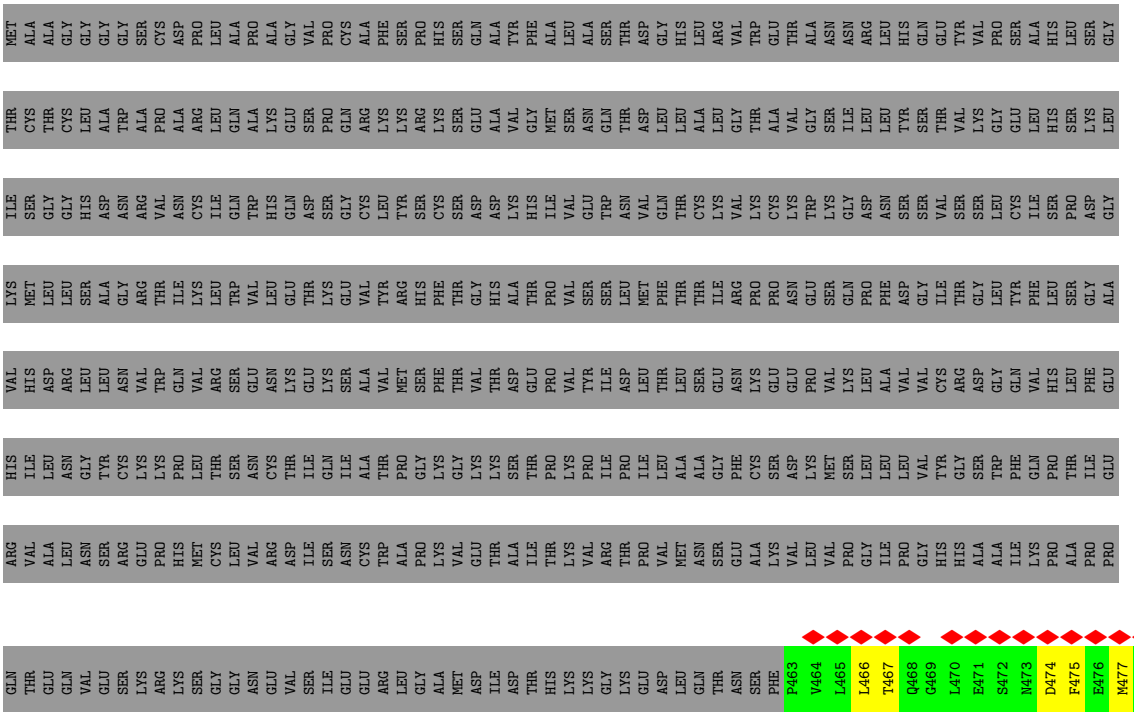
• Molecule 18: U3 small nucleolar RNA-associated protein 15 homolog

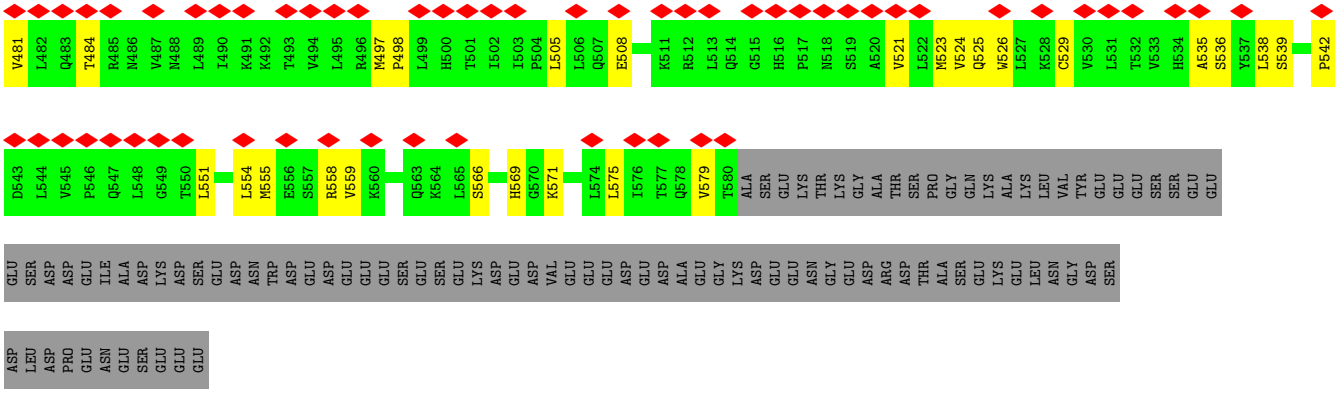
Chain LJ:



• Molecule 19: WD repeat-containing protein 43

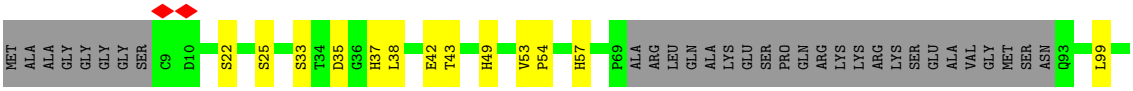
Chain LK:

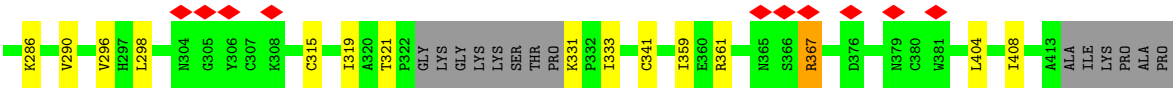


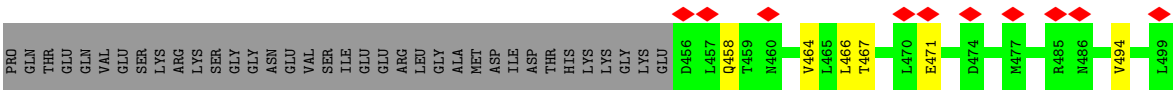


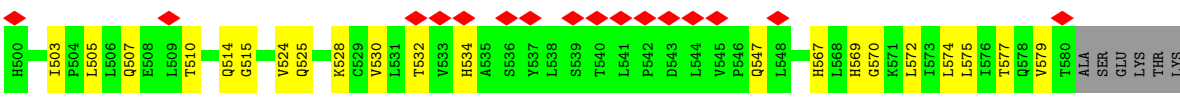
• Molecule 19: WD repeat-containing protein 43

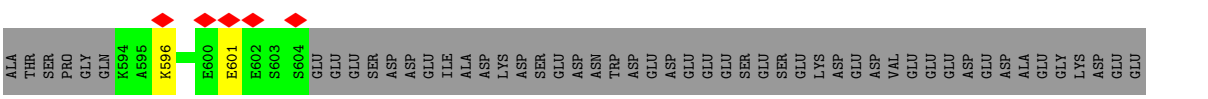
Chain LL:





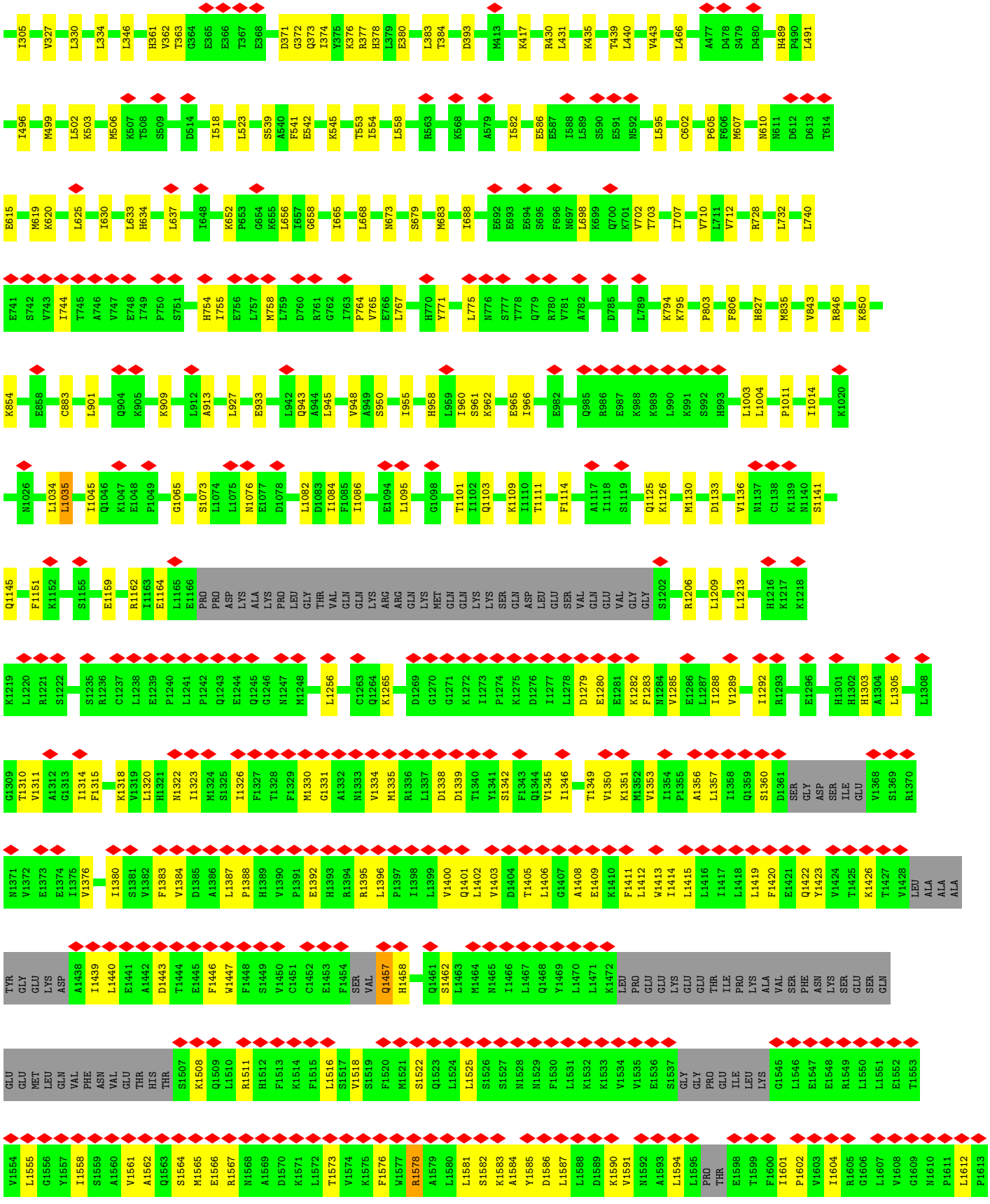


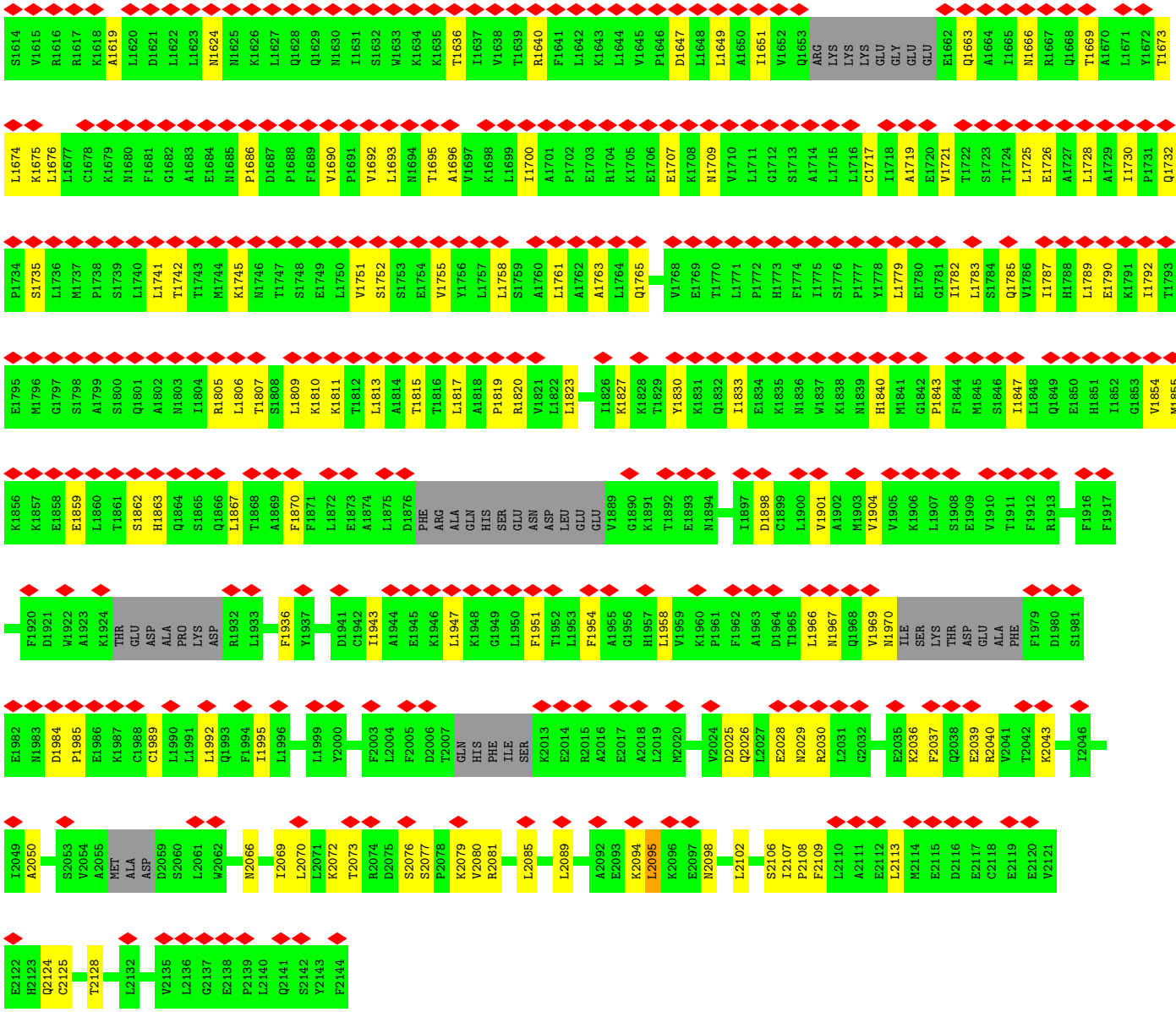




• Molecule 20: HEAT repeat-containing protein 1

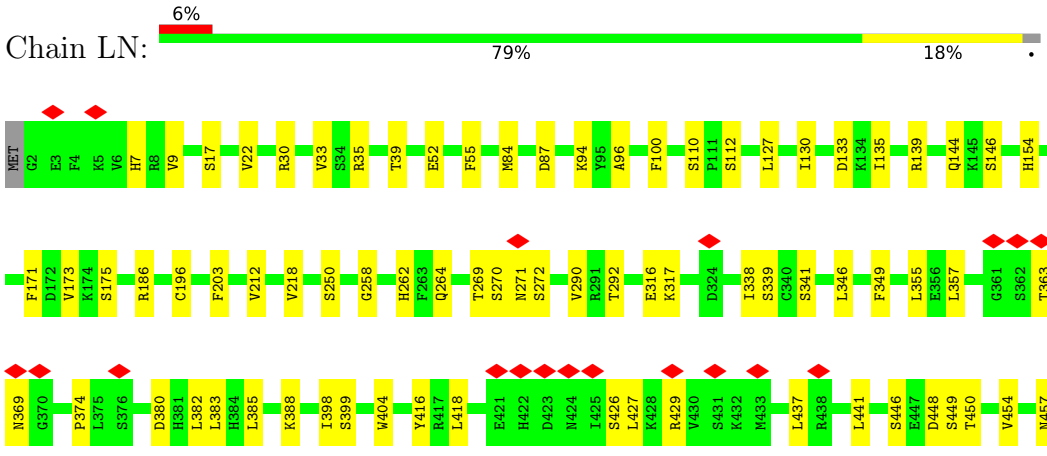
Chain LM:

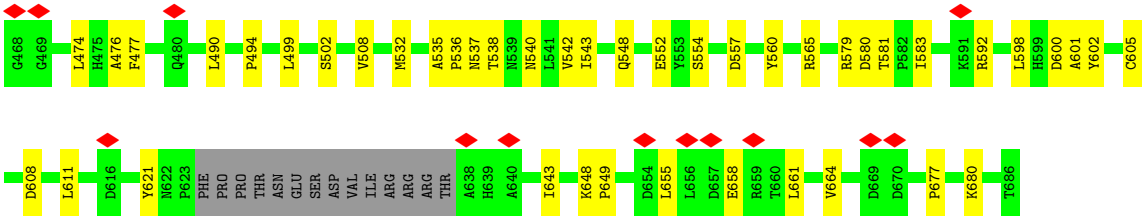

I305 V327 L330 L334 L346 H361 V362 T363 G364 E365 E366 T367 E368 D371 G372 Q373 I374 Y375 K376 R377 H378 L379 E380 L383 T384 D393 M413 K417 R430 L431 K435 T439 L440 V443 L466 A477 D478 S479 D480 H489 P490 L491
I496 M499 L502 K503 M506 K507 T508 S509 D514 I518 L523 S539 A540 F541 E542 K545 T553 I554 L558 R563 K568 A579 I582 E586 E587 I588 L589 S590 E591 N592 L595 G602 P605 F606 M607 N610 N611 D612 D613 T614
E615 M619 K620 L625 I630 L633 H634 L637 I648 K652 P653 G654 K655 L656 I657 G658 I665 L668 N673 S679 M683 I688 E692 E693 E694 S695 F696 N697 L698 K699 Q700 K701 V702 T703 I707 V710 L711 V712 R728 L732 L740
E741 S742 V743 I744 T745 A746 V747 E748 I749 P750 S751 H754 I755 E756 L757 M758 L759 D760 R761 G762 I763 P764 V765 E766 L767 H770 Y771 L775 N776 S777 T778 Q779 R780 V781 A782 D785 L789 K794 K795 P803 F806 H827 M835 V843 R846 K850
K854 E858 C883 L901 Q904 K905 K909 L912 A913 L927 E933 L942 Q943 A944 L945 V948 A949 S950 I955 H958 L959 I960 S961 K962 E965 I966 E982 Q985 R986 E987 K988 K989 L990 K991 S992 H993 L1003 L1004 P1011 I1014 K1020
N1026 L1034 L1035 I1045 Q1046 K1047 E1048 P1049 G1065 S1073 L1074 L1075 N1076 E1077 D1078 L1082 D1083 I1084 F1085 I1086 E1094 L1095 G1098 T1101 I1102 Q1103 K1109 I1110 T1111 F1114 A1117 I1118 S1119 Q1125 K1126 M1130 D1133 V1136 N1137 C1138 K1139 N1140 S1141
Q1145 F1151 K1152 S1155 E1159 R1162 I1163 E1164 L1165 E1166 PRO PRO ASP LYS ALA LYS PRO LEU GLY THR VAL GLN GLN LYS ARG ARG GLN LYS MET GLN GLN LYS LYS SER GLN ASP LEU GLU SER VAL GLN GLU VAL GLY GLY S1202 R1206 L1209 L1213 H1216 K1217 K1218
K1219 L1220 R1221 S1222 S1235 R1236 C1237 L1238 E1239 P1240 L1241 P1242 Q1243 E1244 Q1245 G1246 N1247 M1248 L1256 C1263 Q1264 K1265 D1269 G1270 G1271 K1272 I1273 P1274 K1275 D1276 I1277 L1278 D1279 E1280 E1281 K1282 F1283 N1284 V1285 E1286 L1287 I1288 V1289 I1292 R1293 E1296 H1301 H1302 H1303 A1304 L1305 L1308
G1309 T1310 V1311 A1312 G1313 I1314 F1315 K1318 V1319 L1320 H1321 N1322 I1323 M1324 S1325 I1326 F1327 T1328 F1329 M1330 G1331 A1332 N1333 V1334 M1335 R1336 L1337 D1338 D1339 T1340 Y1341 S1342 F1343 Q1344 V1345 I1346 T1349 V1350 K1351 M1352 V1353 I1354 P1355 A1356 L1357 I1358 Q1359 S1360 D1361 SER GLY ASP SER ILE GLU V1368 S1369 R1370
N1371 V1372 E1373 E1374 I1375 V1376 I1380 S1381 V1382 F1383 V1384 D1385 A1386 L1387 P1388 H1389 V1390 P1391 E1392 H1393 R1394 R1395 L1396 P1397 I1398 L1399 V1400 Q1401 L1402 V1403 D1404 T1405 L1406 G1407 A1408 E1409 K1410 F1411 L1412 W1413 I1414 L1415 L1416 I1417 L1418 L1419 F1420 E1421 Q1422 Y1423 V1424 T1425 K1426 T1427 V1428 LEU ALA ALA ALA
TYR GLY GLU LYS ASP A1438 I1439 L1440 E1441 A1442 D1443 T1444 E1445 F1446 W1447 F1448 S1449 V1450 C1451 C1452 E1453 F1454 SER VAL Q1457 H1458 Q1461 S1462 L1463 M1464 N1465 I1466 L1467 Q1468 Y1469 L1470 L1471 K1472 LEU PRO GLU GLU LYS GLU GLU THR ILE PRO LYS ALA VAL SER PHE ASN LYS SER GLU SER GLN
GLU GLU MET LEU GLN VAL PHE ASN VAL GLU THR HIS THR S1507 K1508 Q1509 L1510 R1511 H1512 F1513 K1514 F1515 L1516 S1517 V1518 S1519 F1520 M1521 S1522 Q1523 L1524 L1525 S1526 S1527 N1528 N1529 F1530 L1531 K1532 K1533 V1534 V1535 E1536 S1537 GLY GLY PRO GLU ILE LEU LYS G1545 L1546 E1547 E1548 R1549 L1550 L1551 E1552 T1553
V1554 L1555 G1556 Y1557 I1558 S1559 A1560 V1561 A1562 Q1563 S1564 M1565 E1566 R1567 N1568 A1569 D1570 K1571 L1572 T1573 V1574 K1575 F1576 W1577 R1578 A1579 L1580 L1581 S1582 K1583 A1584 Y1585 D1586 L1587 L1588 D1589 K1590 V1591 N1592 A1593 L1594 L1595 PRO THR E1598 T1599 F1600 I1601 P1602 V1603 I1604 R1605 G1606 L1607 V1608 G1609 N1610 P1611 L1612 P1613



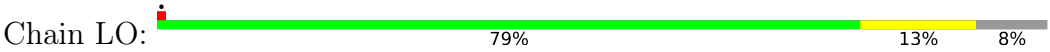
• Molecule 21: U3 small nucleolar RNA-associated protein 4 homolog

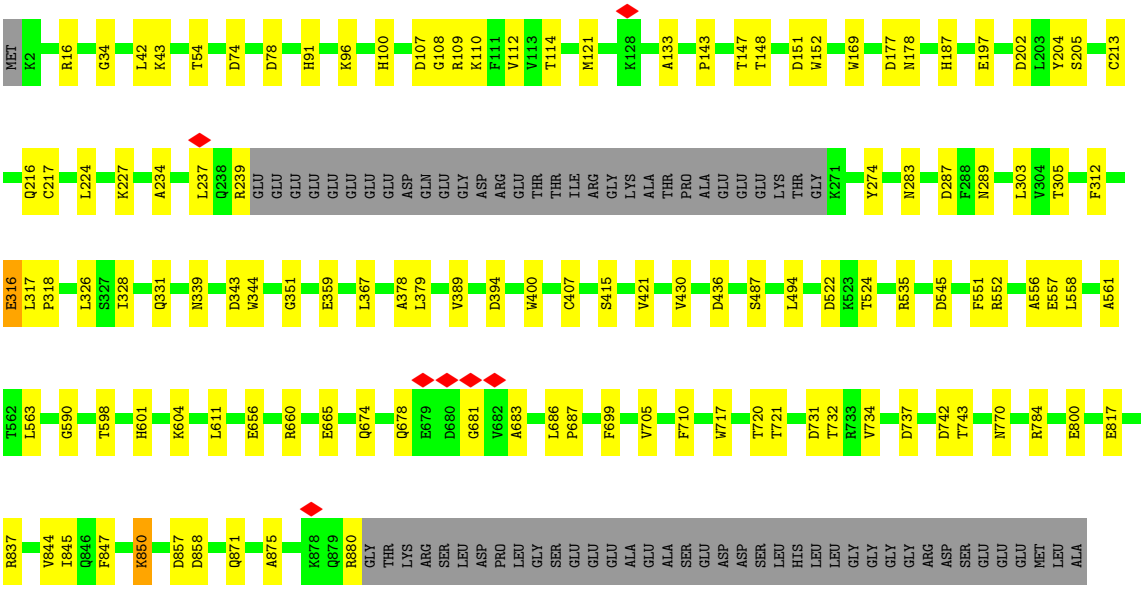
Chain LN:



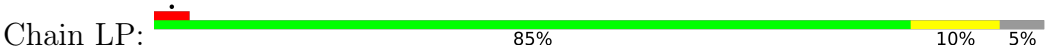


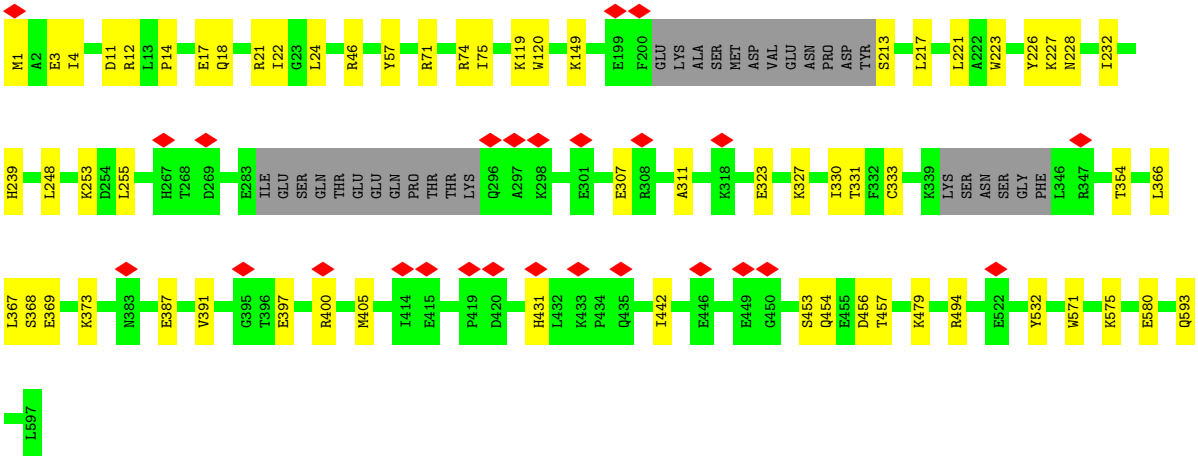
• Molecule 22: Periodic tryptophan protein 2 homolog



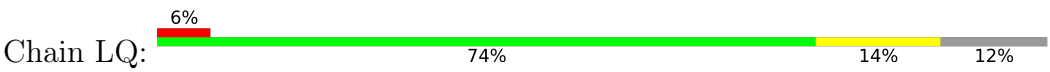


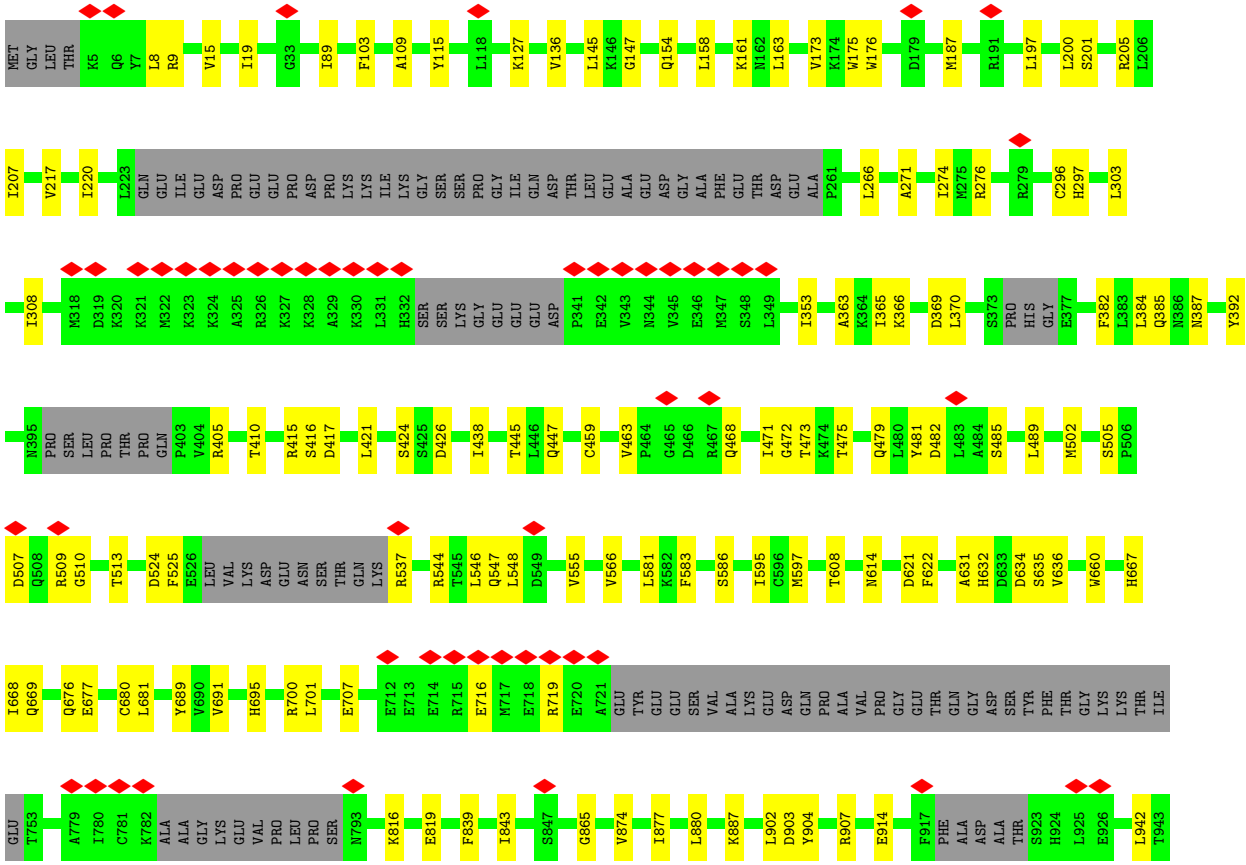
• Molecule 23: U3 small nucleolar RNA-associated protein 6 homolog





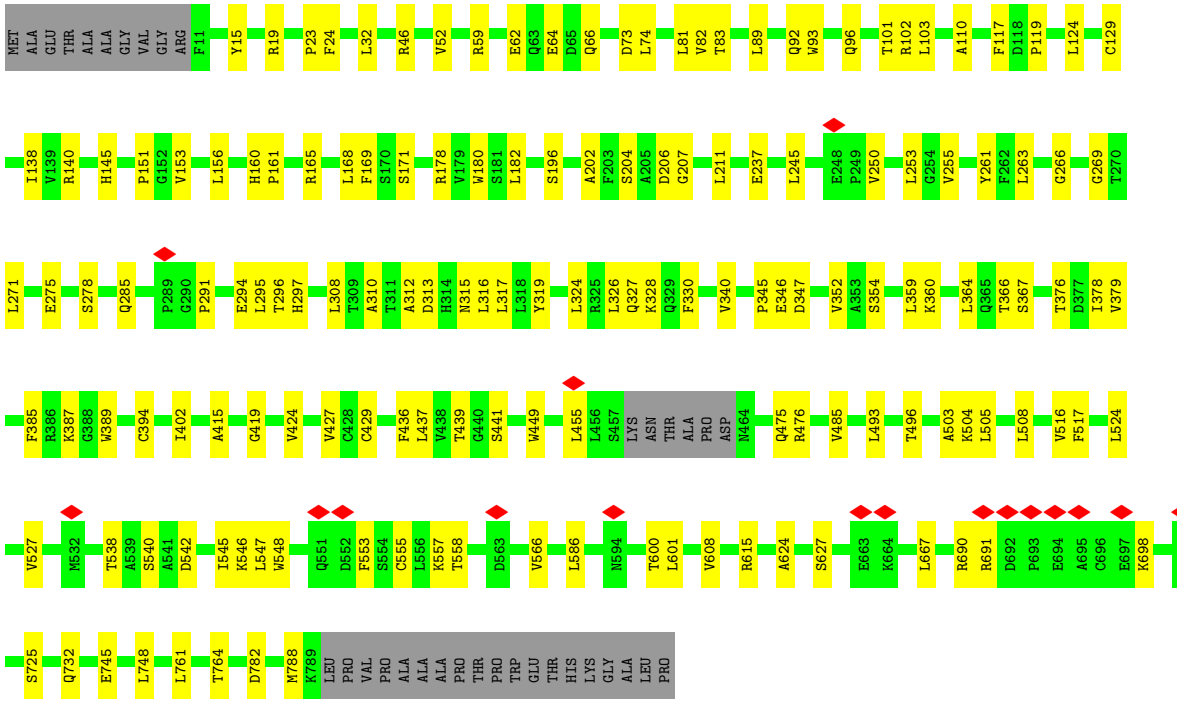
• Molecule 24: WD repeat-containing protein 3





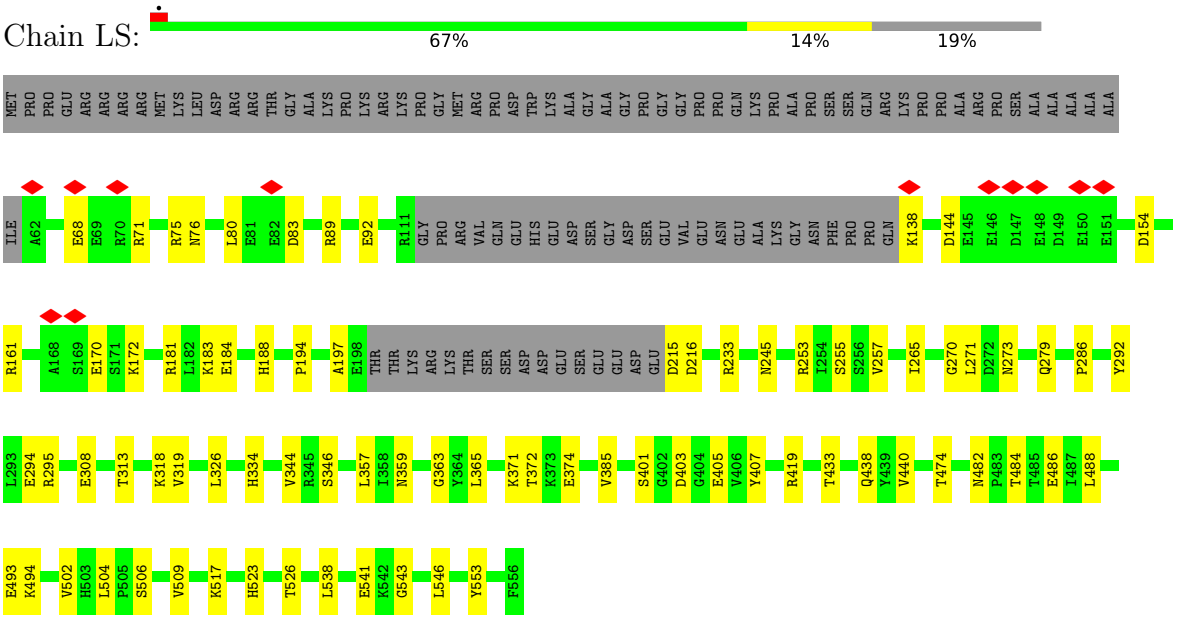
• Molecule 25: Transducin beta-like protein 3

Chain LR:



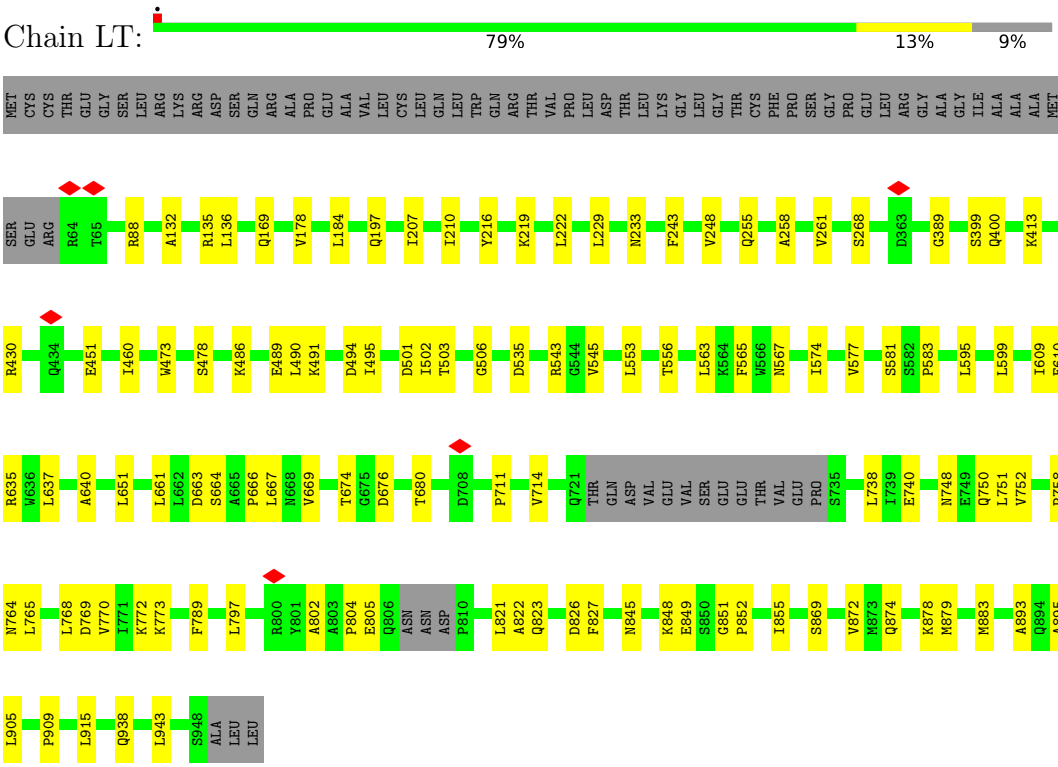
• Molecule 26: U3 small nucleolar RNA-associated protein 18 homolog

Chain LS:



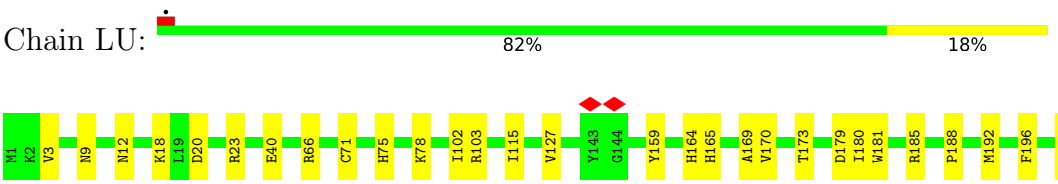
• Molecule 27: WD repeat-containing protein 36

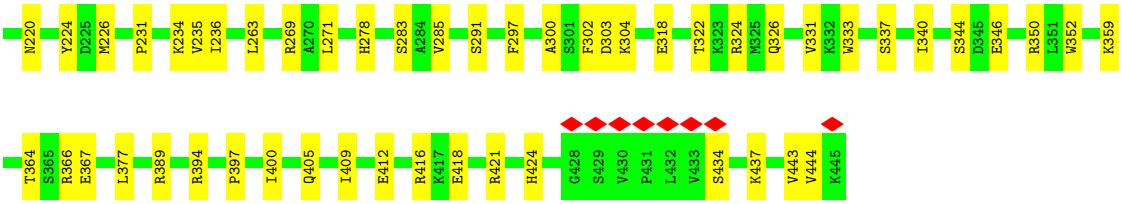
Chain LT:



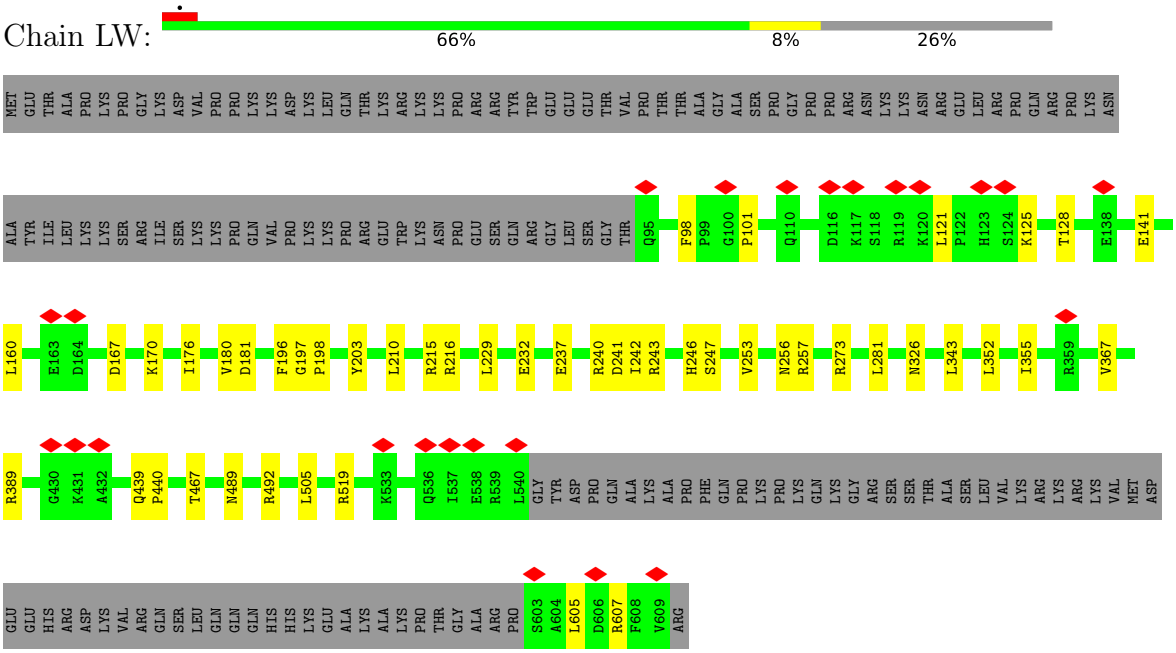
• Molecule 28: DDB1- and CUL4-associated factor 13

Chain LU:

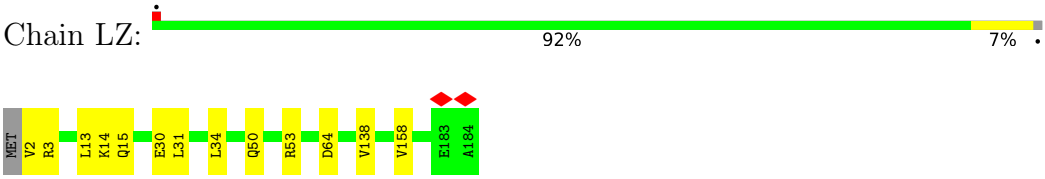




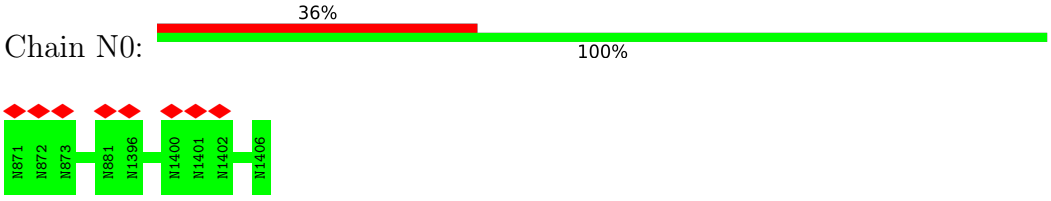
• Molecule 29: WD repeat-containing protein 46



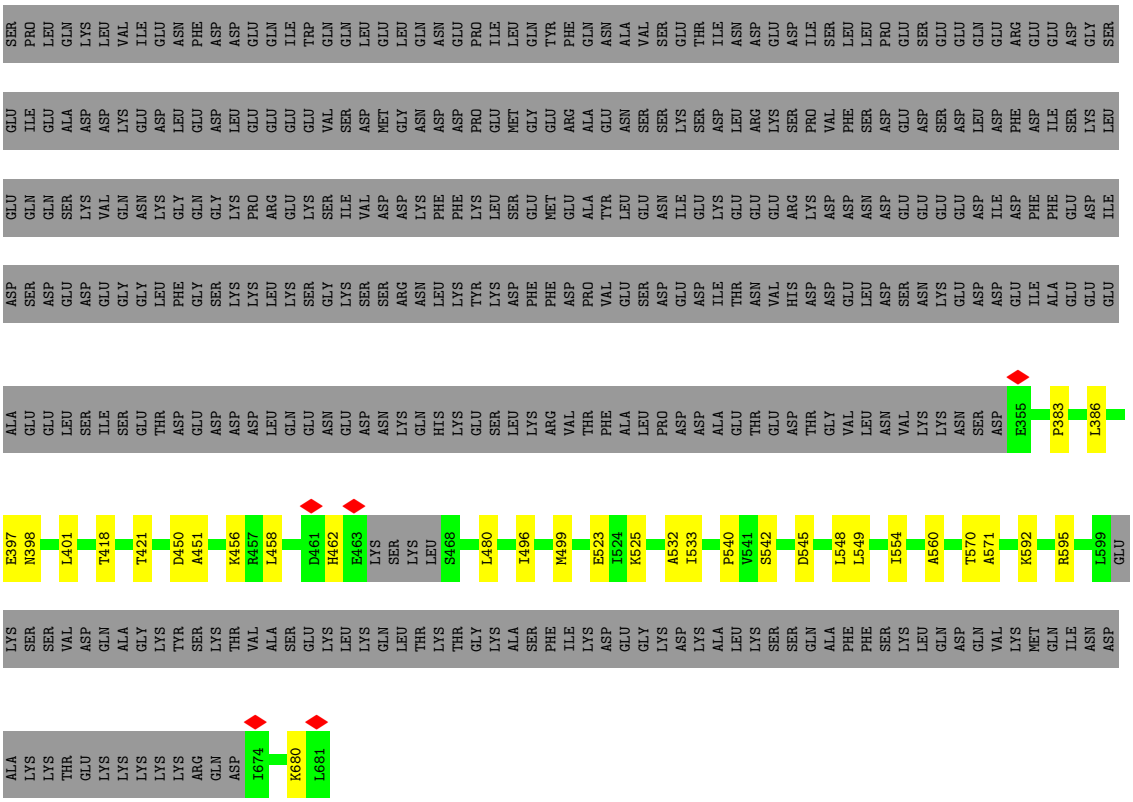
• Molecule 30: U3 small nucleolar ribonucleoprotein protein IMP3



• Molecule 31: 5'ETS rRNA



• Molecule 32: U3 small nucleolar ribonucleoprotein protein MPP10

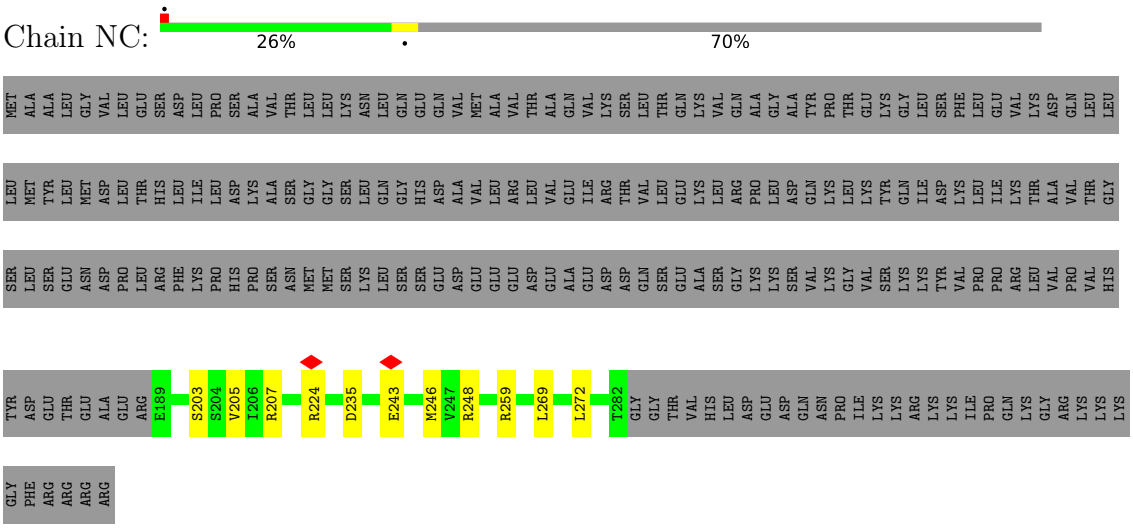


• Molecule 33: Something about silencing protein 10

Chain NB: 13% 85%

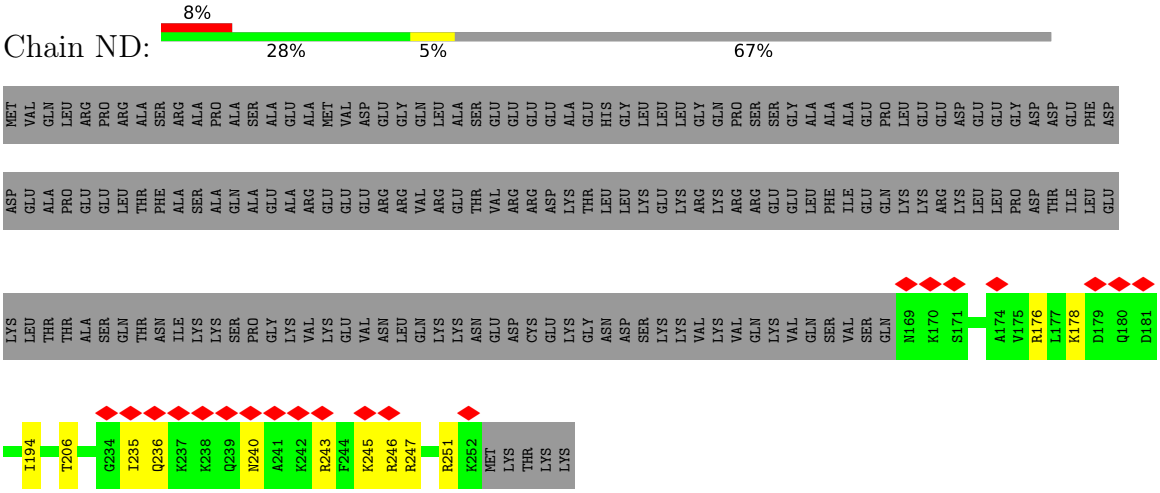
• Molecule 34: Neuroguidin

Chain NC:



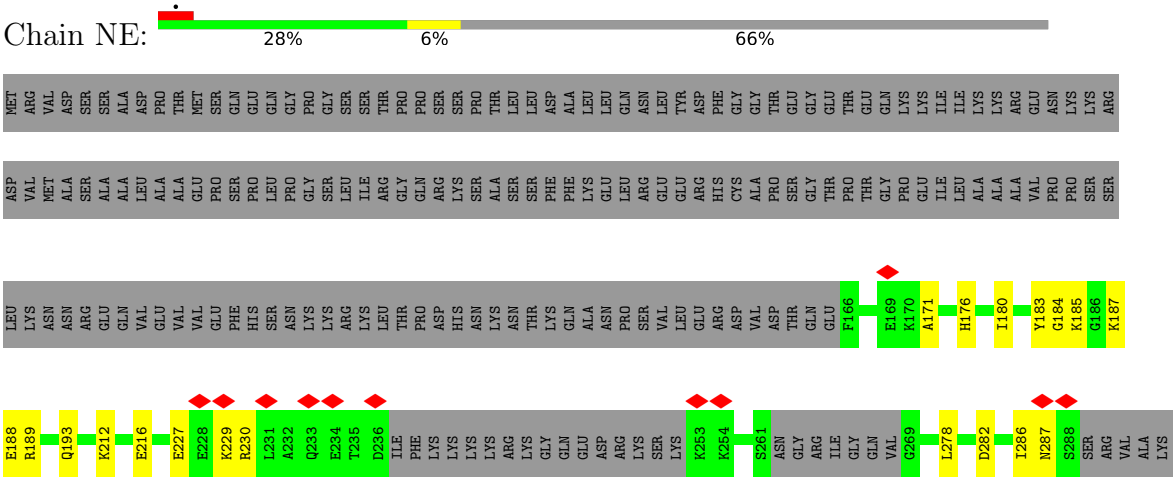
• Molecule 35: Nucleolar protein 7

Chain ND:



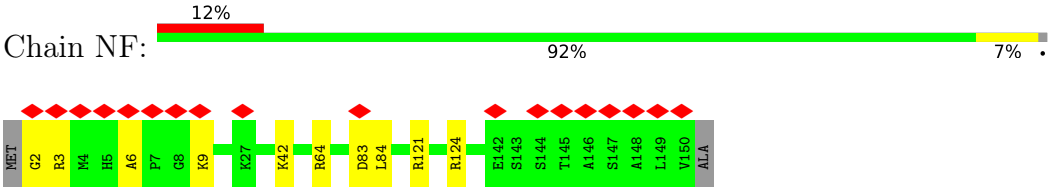
• Molecule 36: Uncharacterized protein C1orf131

Chain NE:



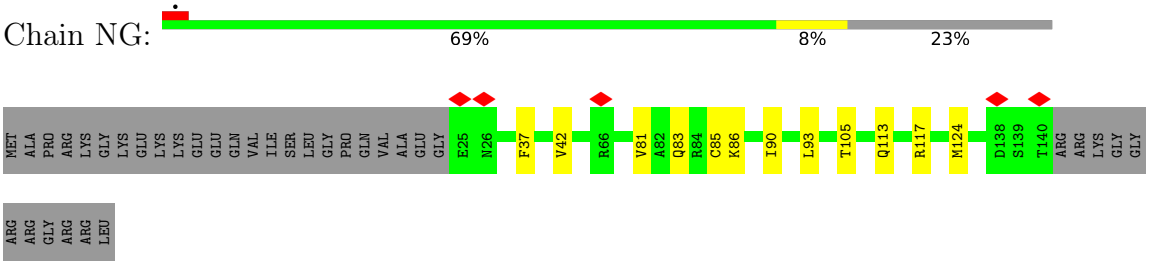
• Molecule 37: 40S ribosomal protein S13

Chain NF:



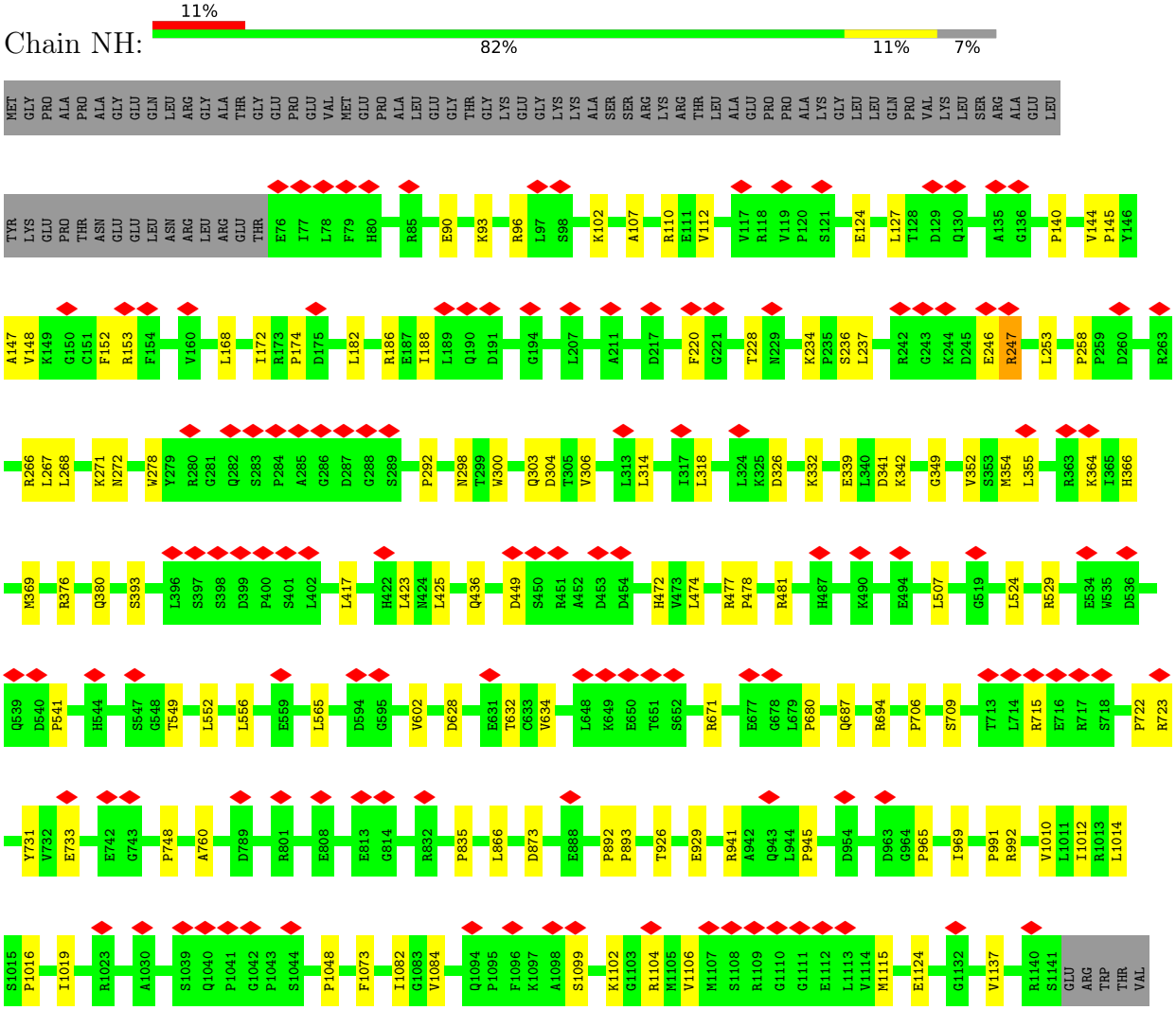
• Molecule 38: 40S ribosomal protein S14

Chain NG:



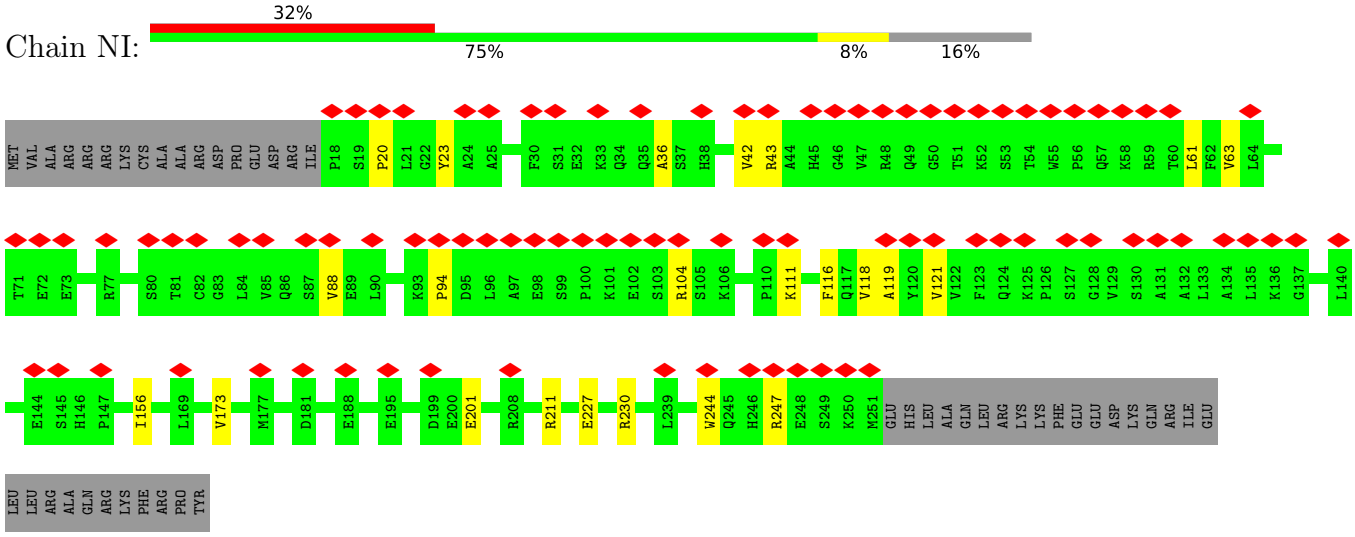
• Molecule 39: Nucleolar protein 6

Chain NH:



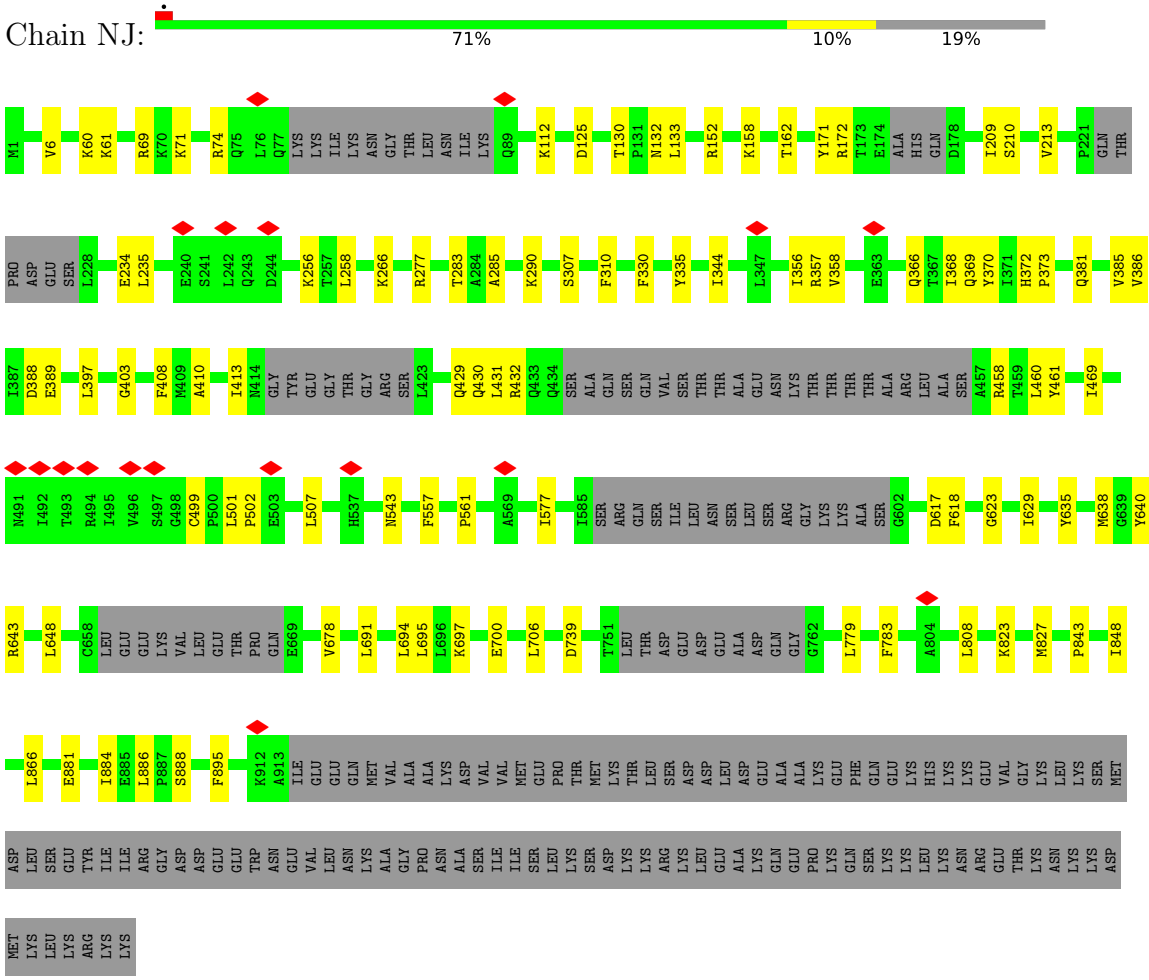
• Molecule 40: Ribosomal RNA-processing protein 7 homolog A

Chain NI:



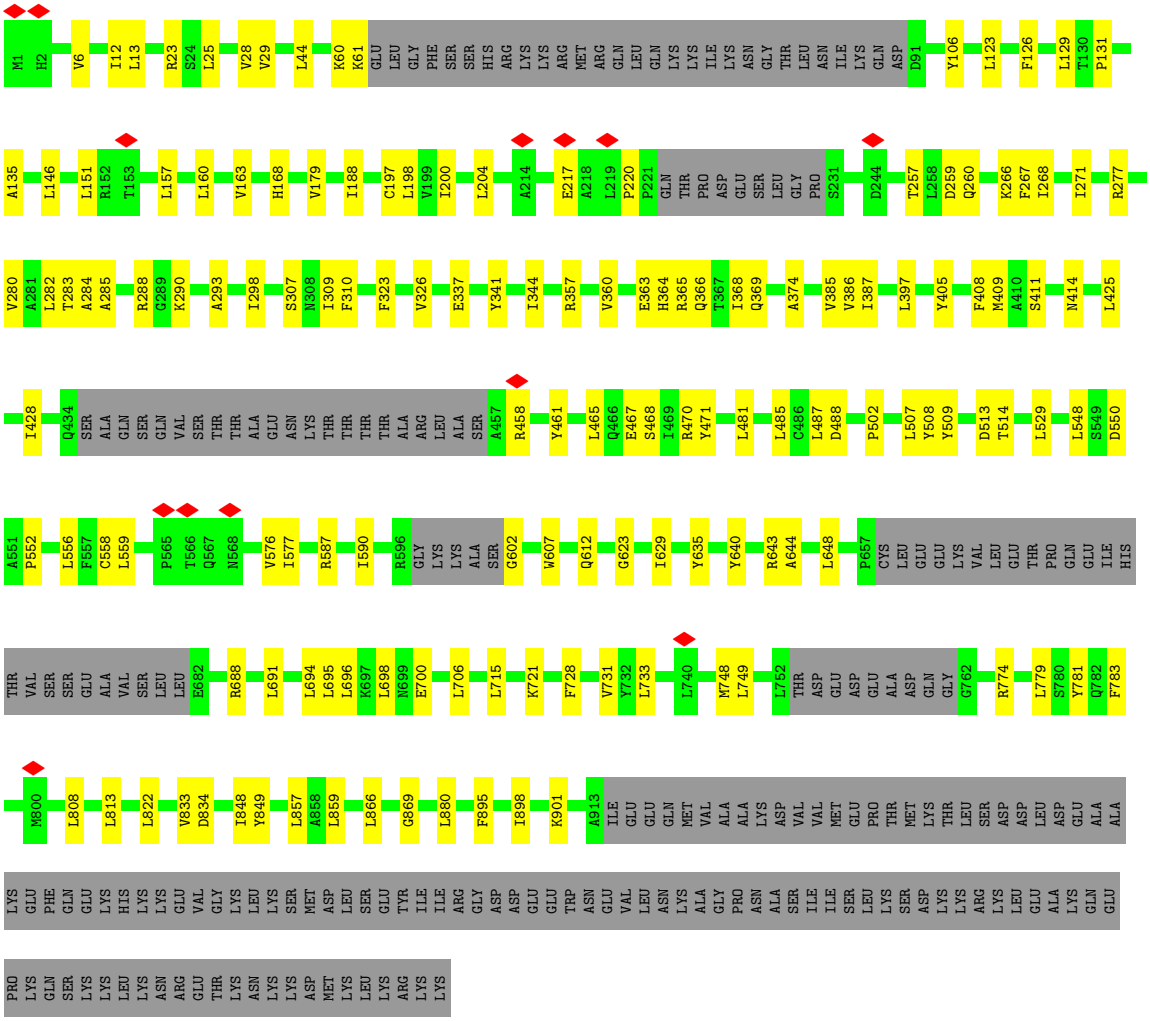
• Molecule 41: RNA cytidine acetyltransferase

Chain NJ:



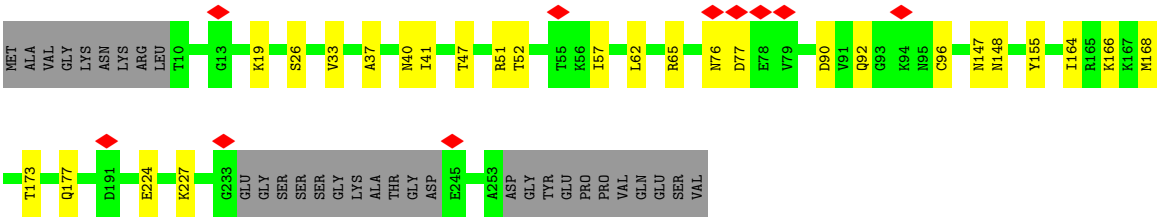
• Molecule 41: RNA cytidine acetyltransferase

Chain NK:



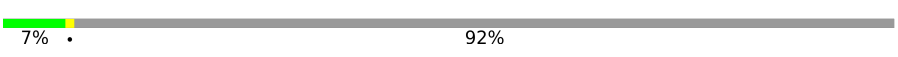
• Molecule 42: 40S ribosomal protein S3a

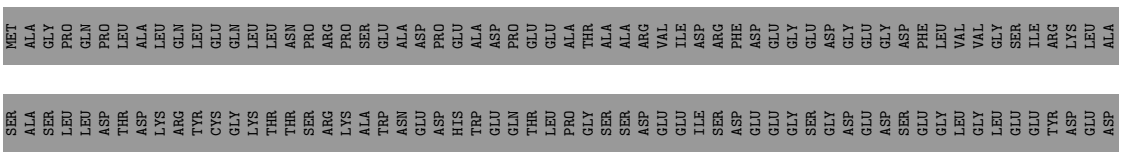
Chain NM:

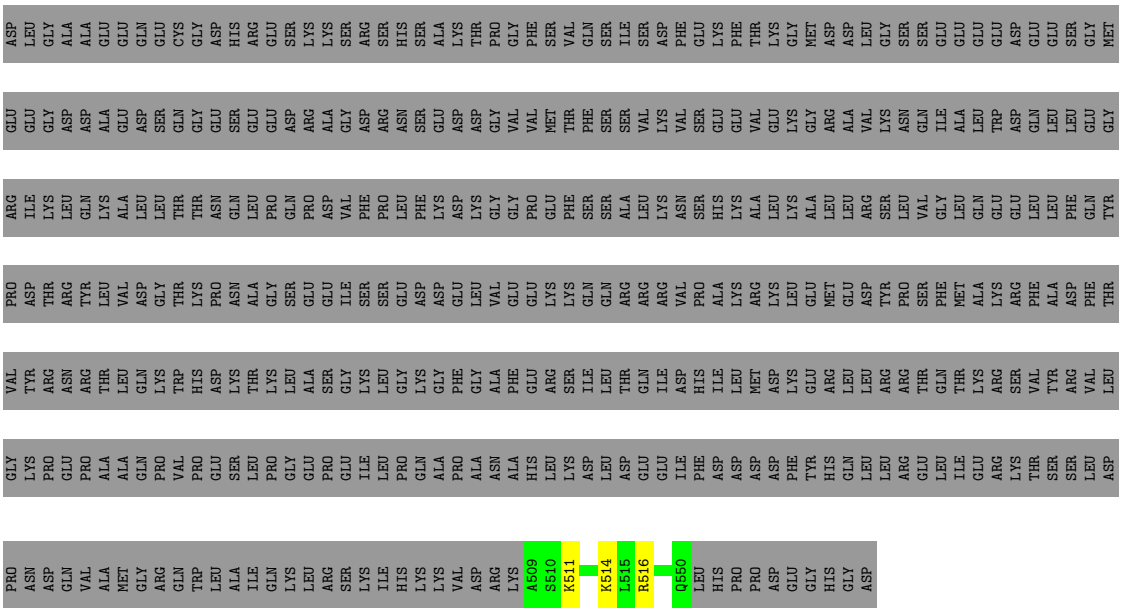


• Molecule 43: Protein AATF

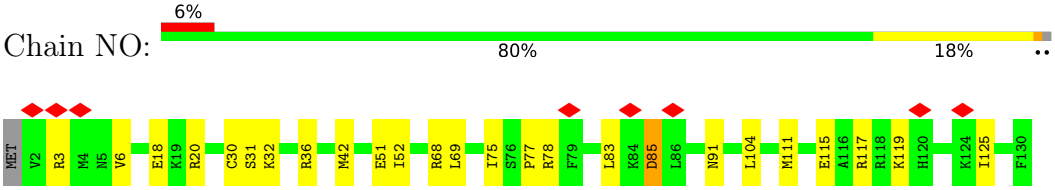
Chain NN:



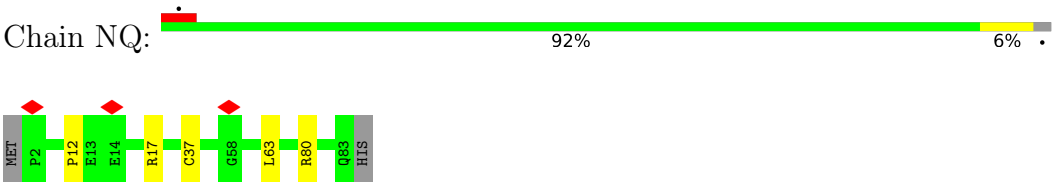




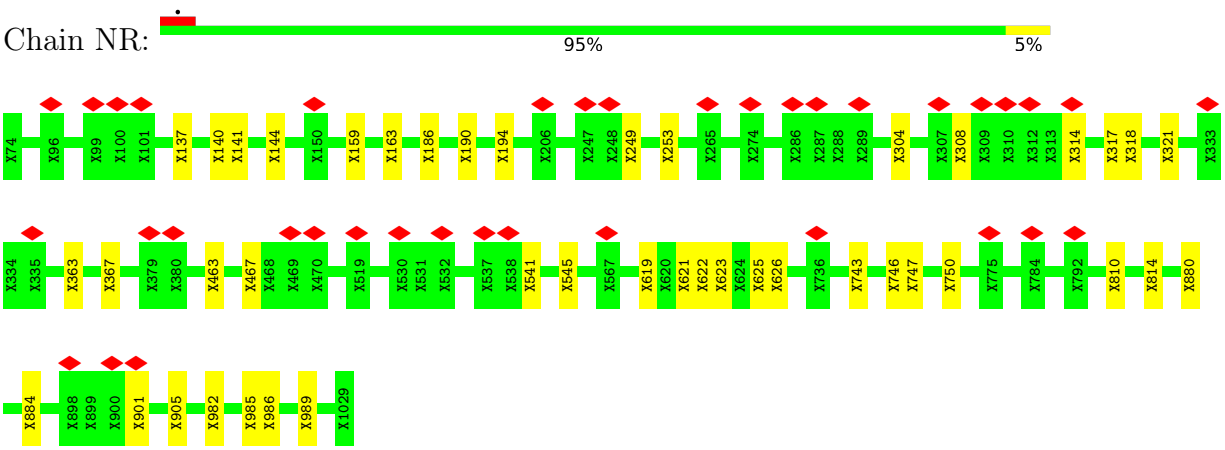
• Molecule 44: 40S ribosomal protein S15a



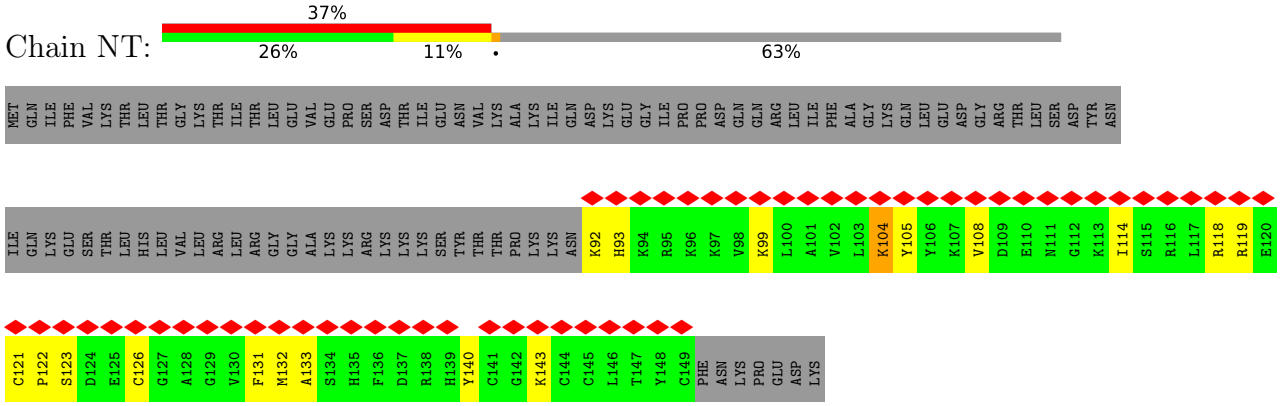
• Molecule 45: 40S ribosomal protein S27



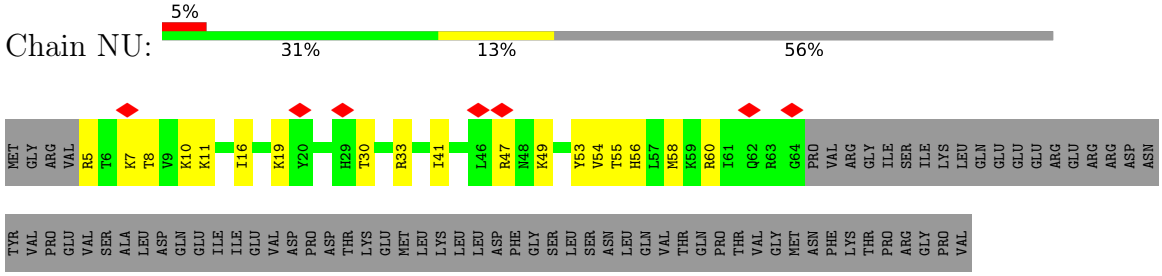
• Molecule 46: RRP12-like protein



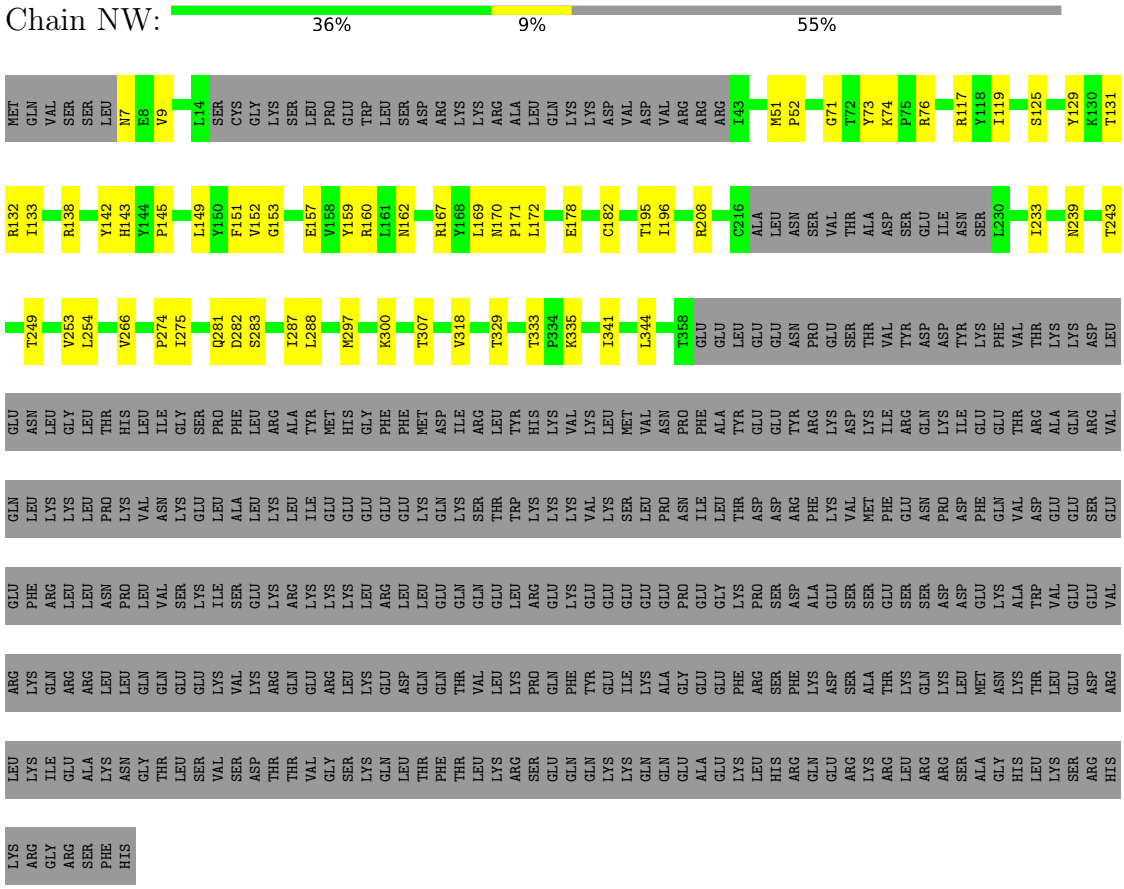
• Molecule 47: Ubiquitin-40S ribosomal protein S27a



• Molecule 48: 40S ribosomal protein S17

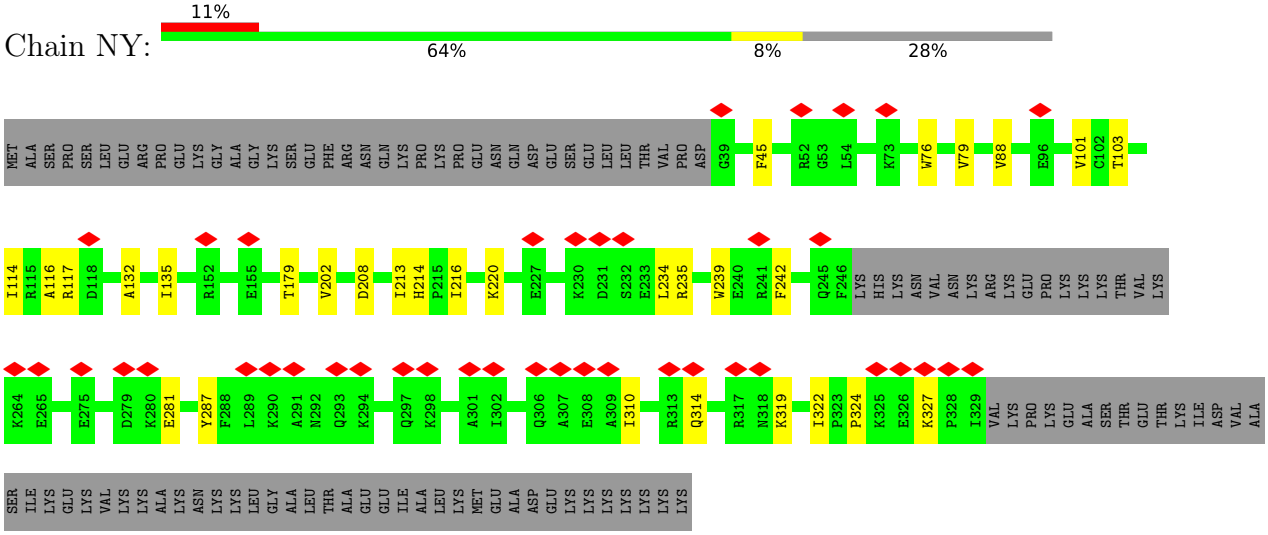


• Molecule 49: Nucleolar protein 10



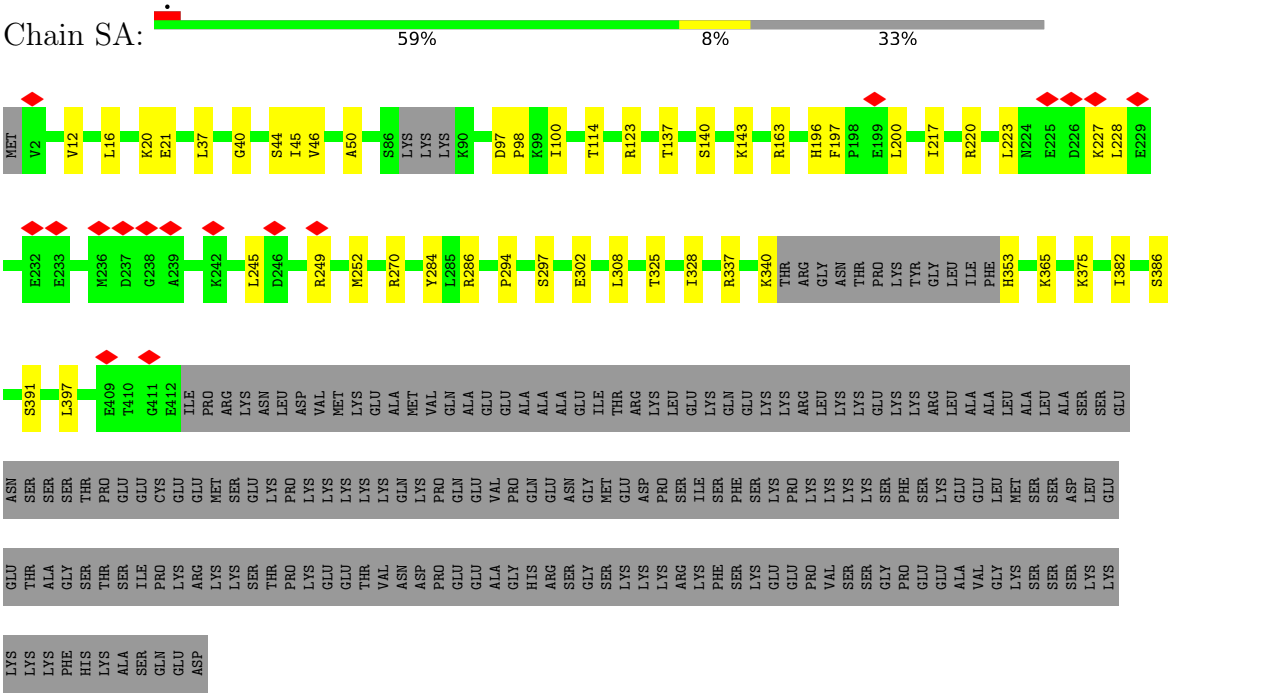
• Molecule 50: KRR1 small subunit processome component homolog

Chain NY:



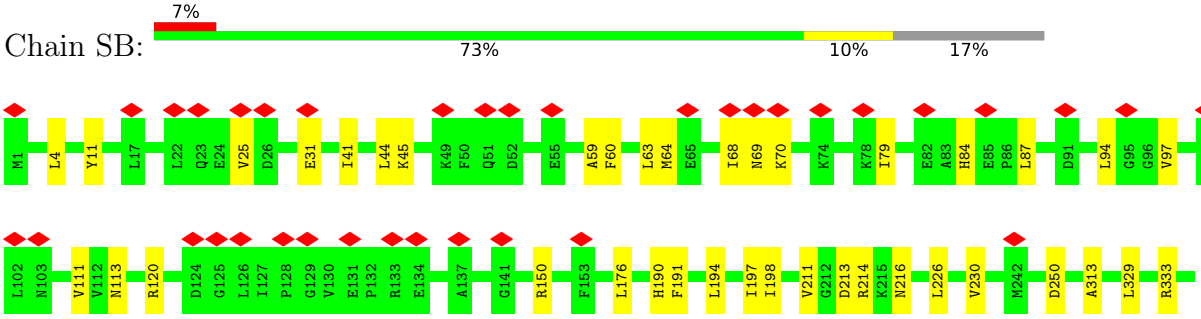
• Molecule 51: Nucleolar protein 56

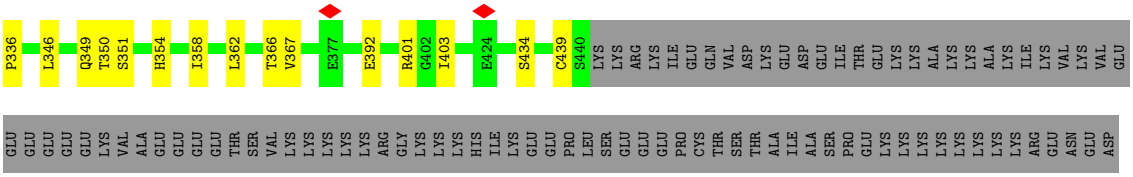
Chain SA:



• Molecule 52: Nucleolar protein 58

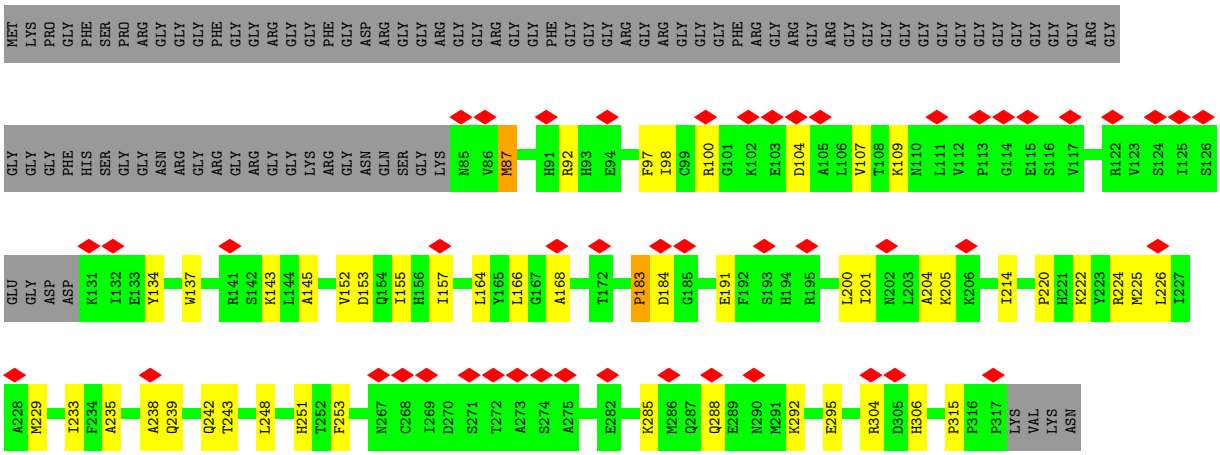
Chain SB:





• Molecule 53: rRNA 2'-O-methyltransferase fibrillarin

Chain SC:

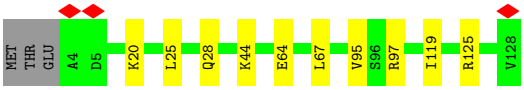


• Molecule 53: rRNA 2'-O-methyltransferase fibrillarin

Chain SD:

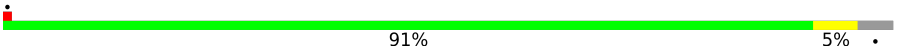
• Molecule 54: NHP2-like protein 1

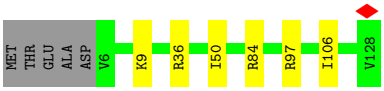
Chain SE:



• Molecule 54: NHP2-like protein 1

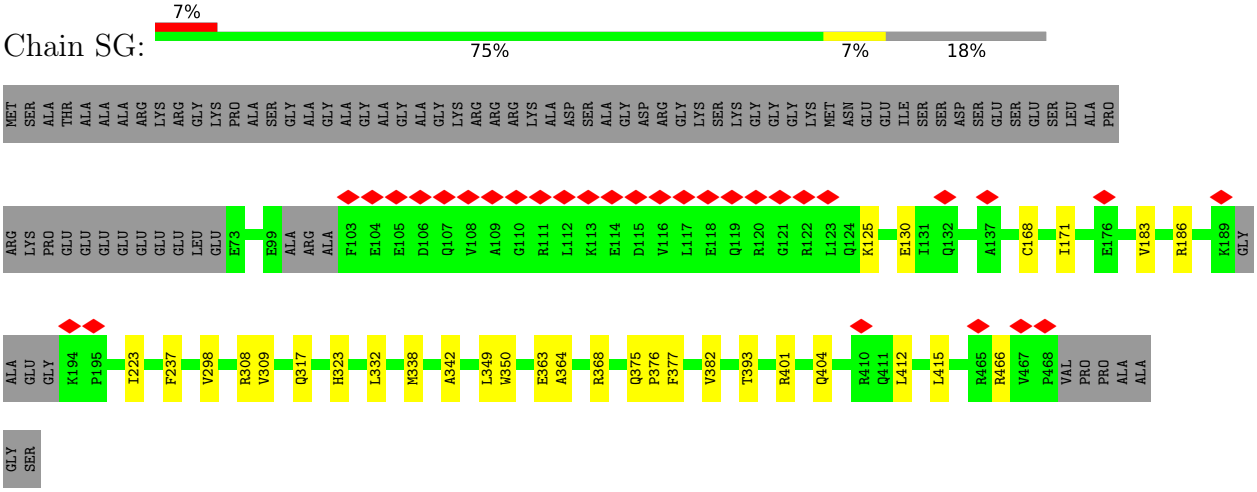
Chain SF:





• Molecule 55: U3 small nucleolar RNA-interacting protein 2

Chain SG:

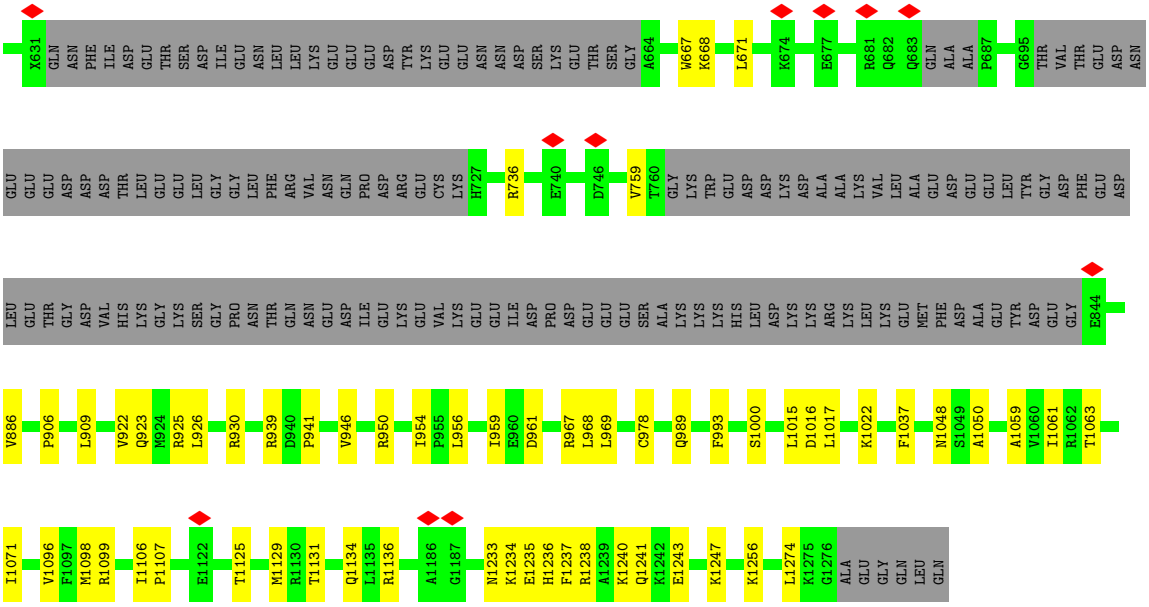


• Molecule 56: RNA 3'-terminal phosphate cyclase-like protein

Chain SH:

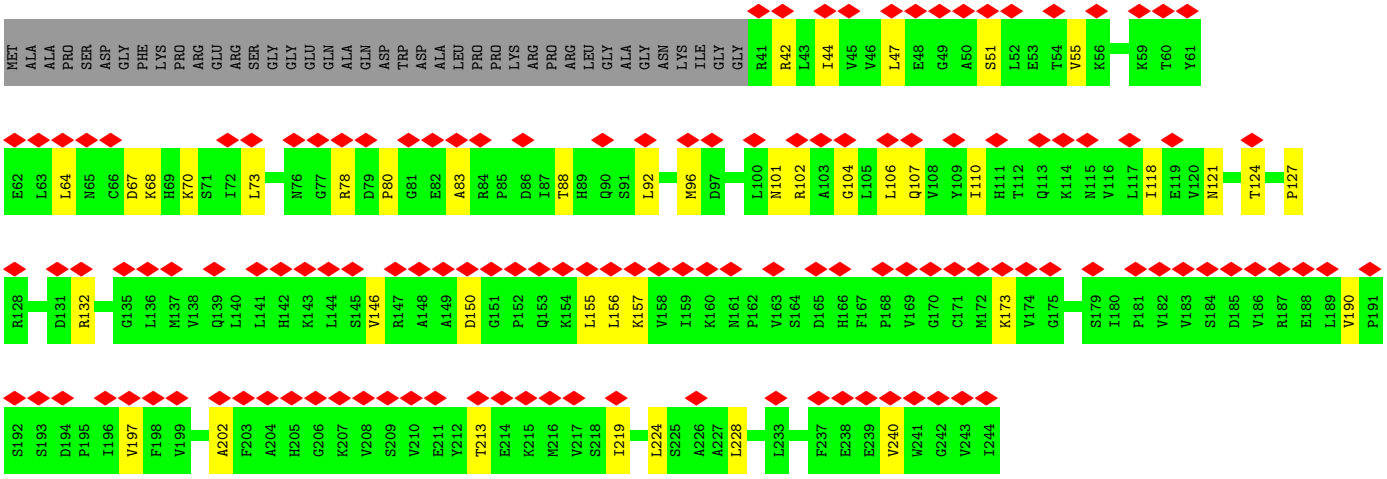
• Molecule 57: Ribosome biogenesis protein BMS1 homolog

Chain SI:



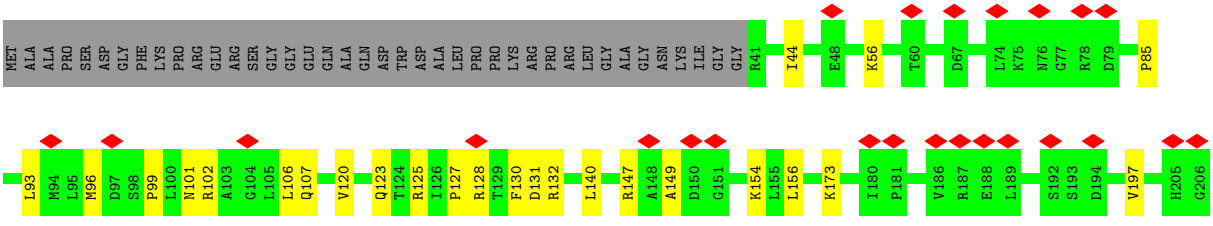
• Molecule 58: Ribosomal RNA small subunit methyltransferase NEP1

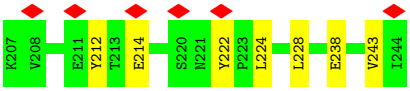
Chain SJ:



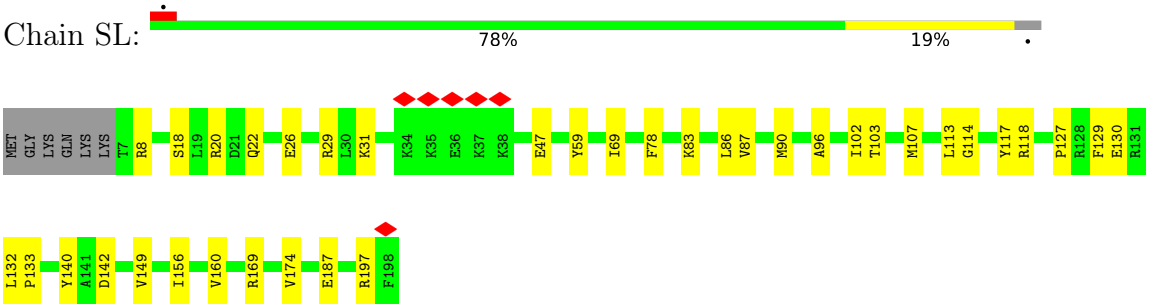
• Molecule 58: Ribosomal RNA small subunit methyltransferase NEP1

Chain SK:

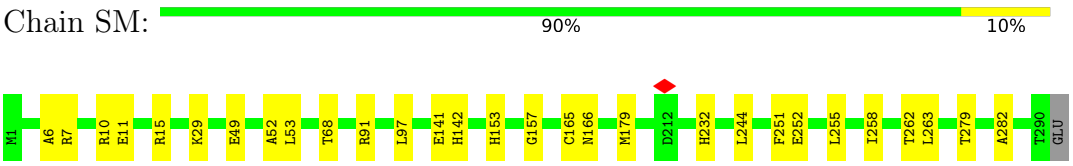




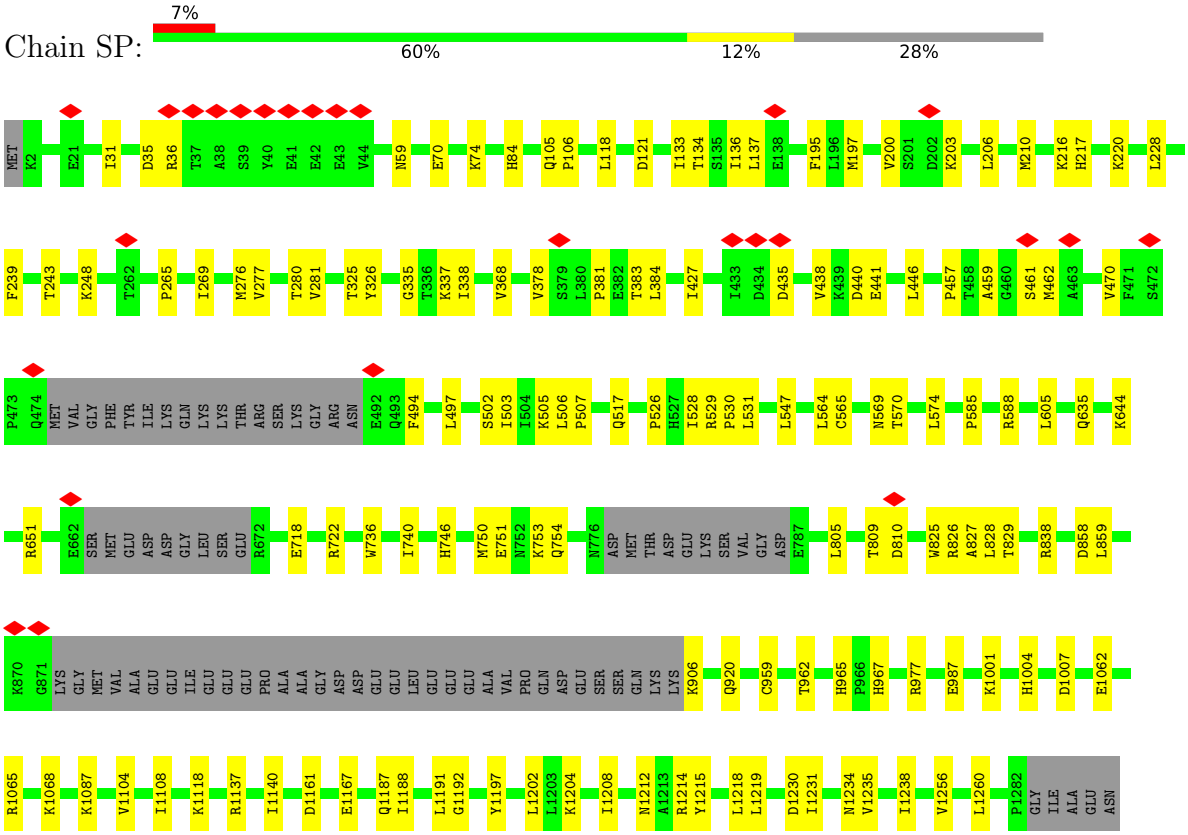
• Molecule 59: rRNA-processing protein FCF1 homolog

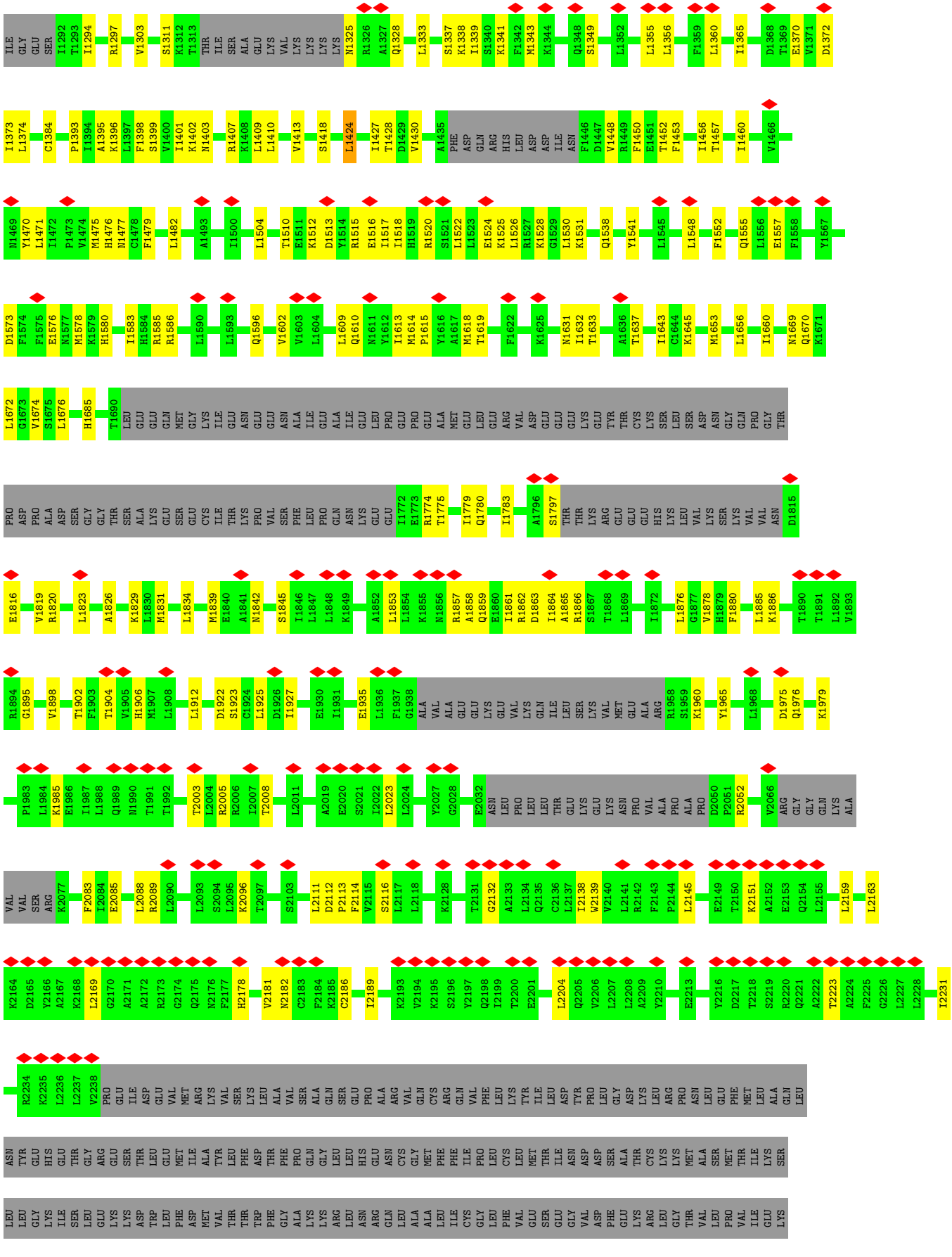


• Molecule 60: U3 small nucleolar ribonucleoprotein protein IMP4



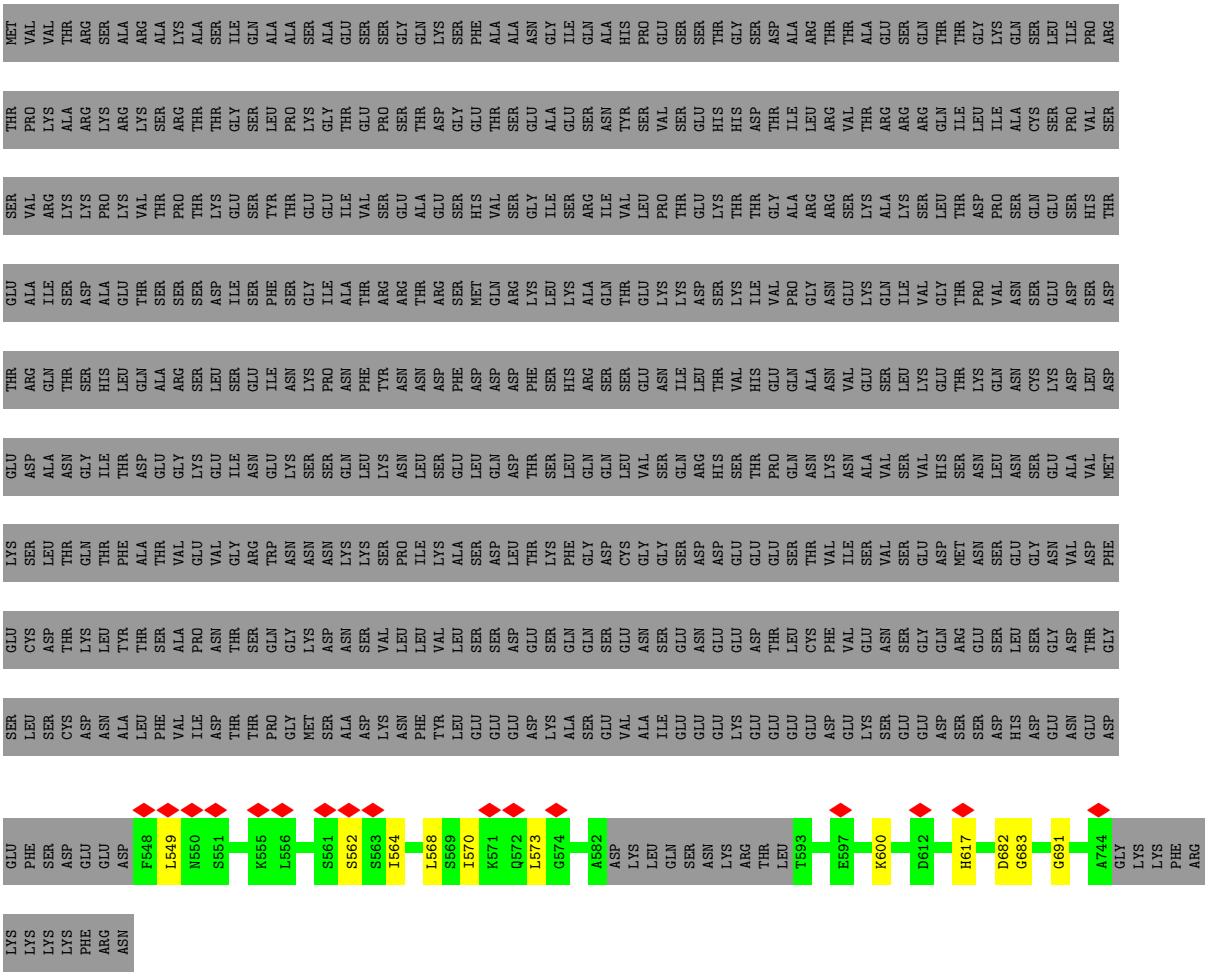
• Molecule 61: Small subunit processome component 20 homolog




ILE GLY GLU SER I1292 T1293 I1294 R1297 V1303 S1311 K1312 T1313 THR ILE SER ALA GLU LYS VAL LYS LYS LYS N1325 R1326 A1327 Q1328 L1333 S1337 K1338 I1339 S1340 K1341 F1342 M1343 K1344 Q1348 S1349 L1362 L1355 L1356 F1359 L1360 I1365 D1368 T1369 E1370 V1371 D1372
I1373 L1374 C1384 P1393 I1394 A1395 K1396 L1397 F1398 S1399 V1400 I1401 K1402 N1403 R1407 K1408 L1409 L1410 V1413 S1418 L1424 I1427 T1428 D1429 V1430 A1435 PHE ASP GLN ARG HIS LEU ASP ASP ILE ASN F1446 D1447 V1448 R1449 F1450 E1451 T1452 F1453 I1456 T1457 I1460 V1466
N1469 Y1470 L1471 I1472 P1473 V1474 M1475 H1476 N1477 C1478 F1479 L1482 A1493 I1500 L1504 T1510 E1511 K1512 D1513 Y1514 R1515 E1516 I1517 I1518 H1519 R1520 S1521 L1522 L1523 E1524 K1525 L1526 R1527 K1528 G1529 L1530 K1531 Q1538 Y1541 L1545 L1548 F1552 Q1555 L1556 E1557 F1558 Y1567
D1573 F1574 F1575 E1576 N1577 M1578 K1579 H1580 I1583 H1584 R1585 R1586 L1590 L1593 Q1596 V1602 V1603 L1604 L1609 Q1610 N1611 Y1612 I1613 M1614 P1615 Y1616 A1617 M1618 T1619 F1622 K1625 N1631 I1632 T1633 A1636 T1637 I1643 C1644 K1645 M1653 L1656 I1660 N1669 Q1670 K1671
L1672 G1673 V1674 S1675 L1676 H1685 T1690 LEU GLU GLU GLN MET GLY LYS ILE GLU ASN GLU GLU ASN ALA ILE GLU ALA ILE GLU LEU PRO GLU PRO GLU ALA MET GLU LEU GLU ARG VAL ASP GLU GLU GLU LYS GLU TYR THR CYS LYS SER LEU SER ASP ASN GLY GLN PRO GLY THR
PRO ASP PRO ALA ASP SER GLY GLY THR SER ALA LYS GLU SER GLU CYS ILE THR LYS PRO VAL SER PHE LEU PRO GLN ASN LYS GLU GLU I1772 E1773 R1774 T1775 I1779 Q1780 I1783 A1796 S1797 THR THR LYS ARG GLU GLU GLU HIS LYS LEU VAL LYS SER LYS VAL VAL ASN D1815
E1816 V1819 R1820 L1823 A1826 K1829 L1830 M1831 L1834 M1839 E1840 A1841 N1842 S1845 I1846 L1847 L1848 K1849 A1852 L1853 L1854 K1855 N1856 R1857 A1858 Q1859 E1860 I1861 R1862 D1863 I1864 A1865 R1866 S1867 T1868 L1869 I1872 L1876 G1877 V1878 H1879 F1880 L1885 K1886 T1890 T1891 L1892 V1893
R1894 G1895 V1898 T1902 F1903 T1904 V1905 H1906 M1907 L1908 L1912 D1922 S1923 C1924 L1925 D1926 I1927 E1930 I1931 E1935 L1936 F1937 G1938 ALA VAL ALA GLU GLU LYS GLU VAL LYS GLN ILE LEU SER LYS VAL MET GLU ALA ARG R1958 S1959 K1960 Y1965 L1968 D1975 Q1976 K1979
P1983 L1984 K1985 E1986 I1987 L1988 Q1989 N1990 T1991 T1992 T2003 L2004 R2005 R2006 I2007 T2008 L2011 A2019 E2020 S2021 I2022 L2023 L2024 Y2027 G2028 E2032 ASN LEU PRO LEU LEU THR GLU LYS GLU LYS ASN PRO VAL ALA PRO ALA PRO D2050 P2051 R2052 V2066 ARG GLY GLY GLN LYS ALA
VAL VAL SER ARG K2077 F2083 I2084 E2085 L2088 R2089 L2090 L2093 S2094 L2095 K2096 T2097 S2103 L2111 D2112 P2113 F2114 V2115 S2116 L2117 L2118 K2128 T2131 G2132 A2133 L2134 Q2135 C2136 L2137 I2138 W2139 V2140 L2141 R2142 F2143 P2144 L2145 E2149 T2150 K2151 A2152 E2153 Q2154 L2155 L2159 L2163
K2164 D2165 Y2166 A2167 K2168 L2169 G2170 A2171 A2172 R2173 G2174 Q2175 N2176 F2177 H2178 V2181 N2182 C2183 F2184 K2185 C2186 I2189 K2193 V2194 K2195 S2196 Y2197 Q2198 I2199 T2200 E2201 L2204 Q2205 V2206 L2207 L2208 A2209 Y2210 E2213 Y2216 D2217 T2218 S2219 R2220 Q2221 A2222 T2223 A2224 F2225 G2226 L2227 L2228 I2231
R2234 K2235 L2236 L2237 V2238 PRO GLU ILE ASP GLU VAL MET ARG LYS VAL SER LYS LEU ALA VAL SER ALA GLN SER GLU PRO ALA ARG VAL GLN CYS ARG GLN VAL PHE LEU LYS TYR ILE LEU ASP TYR PRO LEU GLY ASP LYS LEU ARG PRO ASN LEU GLU LEU MET PHE MET LEU ALA GLN LEU
ASN TYR GLU HIS GLU THR GLY ARG GLU SER THR LEU GLU MET ILE ALA TYR LEU PHE ASP THR PHE PRO GLN GLY LEU LEU HIS GLU ARG GLN ASN CYS GLY MET PHE PHE ILE PRO LEU CYS LEU MET THR ILE ASN ASP ASP SER ALA THR CYS LYS LYS MET ALA LEU SER MET THR ILE LYS SER
LEU LEU GLY LYS ILE SER LEU GLU LYS ASP TRP LEU PHE ASP MET VAL THR THR TRP PHE GLY ALA LYS LYS ARG LEU ASN ARG GLN LEU ALA ALA LEU ILE CYS GLY LEU PHE VAL GLU SER GLU GLY VAL ASP PHE GLU LYS ARG LEU GLY THR VAL LEU PRO VAL ILE ILE GLU LYS

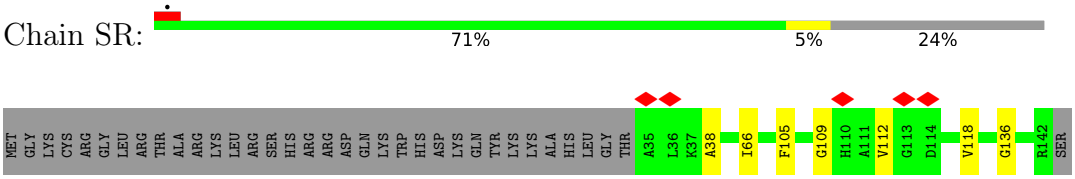
• Molecule 62: Deoxynucleotidyltransferase terminal-interacting protein 2

Chain SQ:



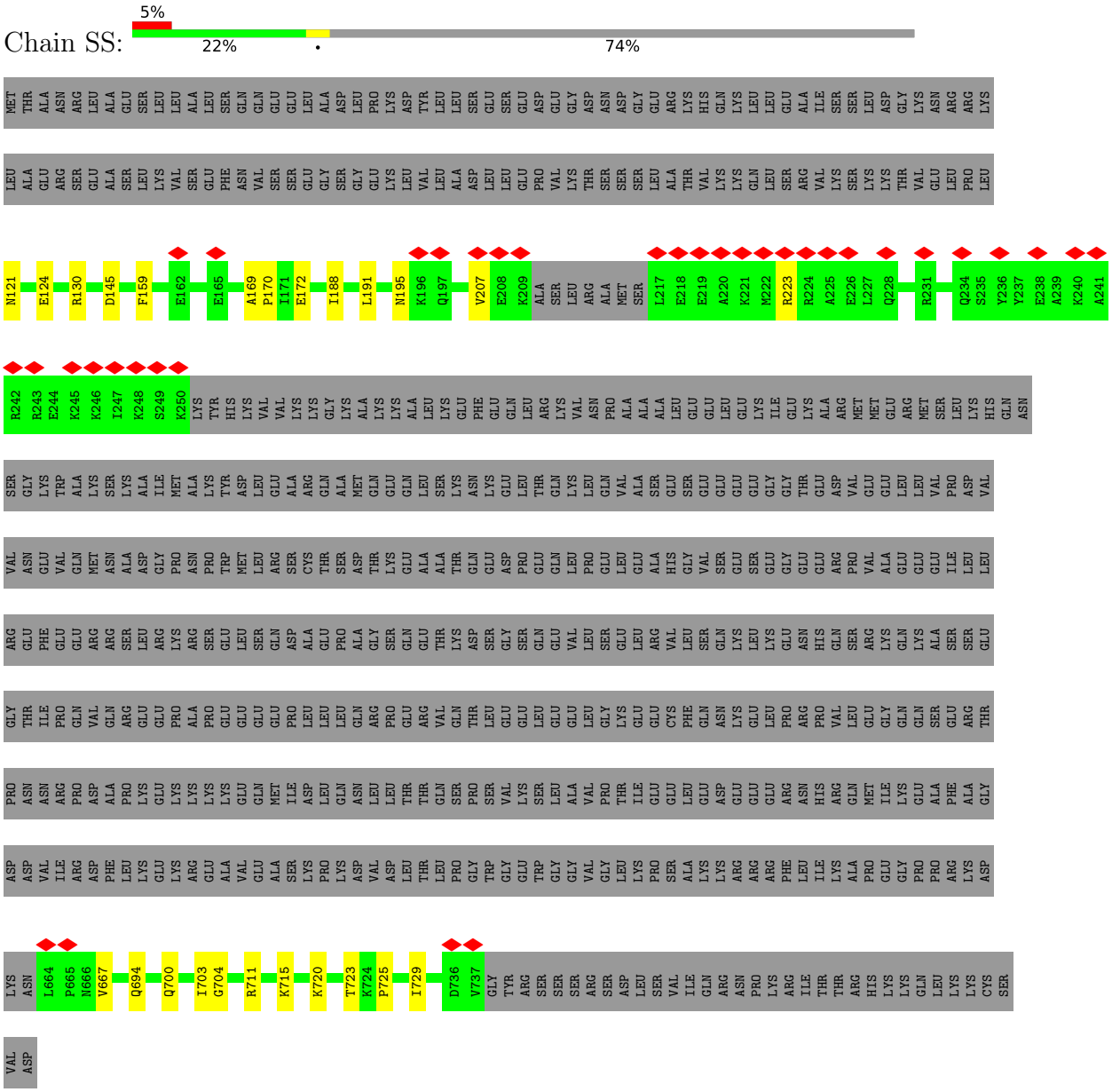
• Molecule 63: 40S ribosomal protein S23

Chain SR:



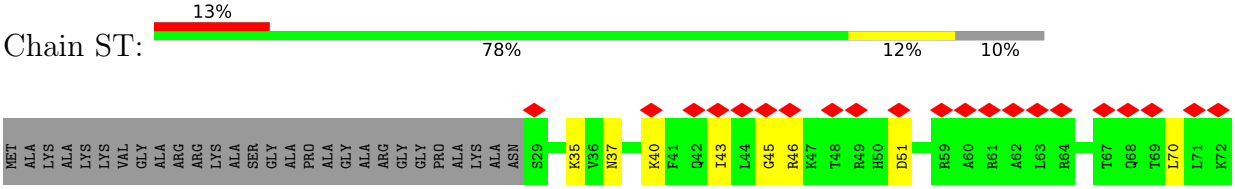
• Molecule 64: U3 small nucleolar RNA-associated protein 14 homolog A

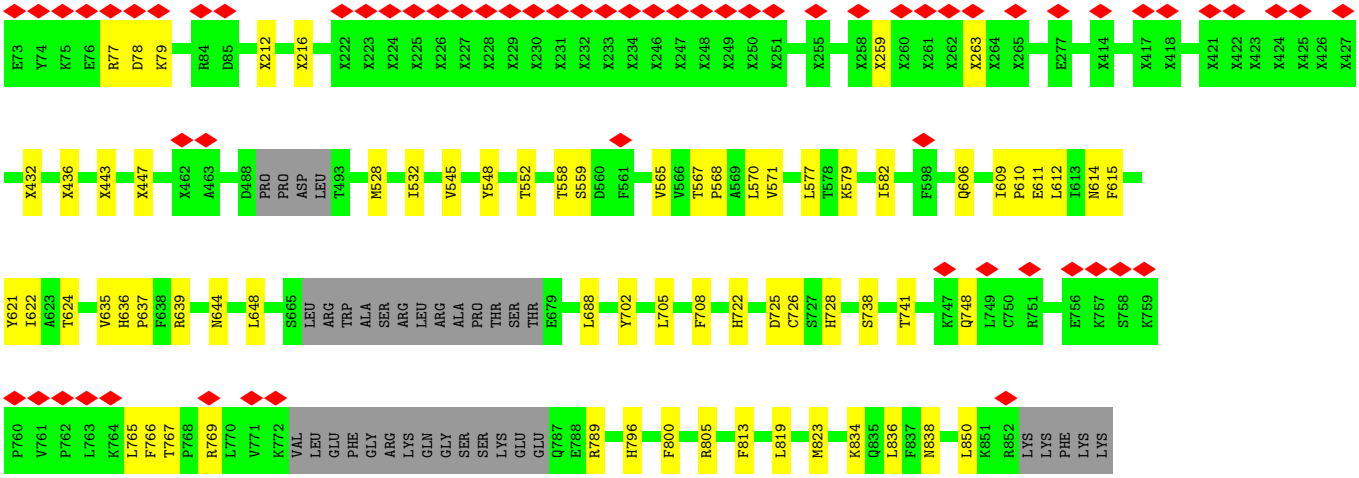
Chain SS:



• Molecule 65: Nucleolar protein 14

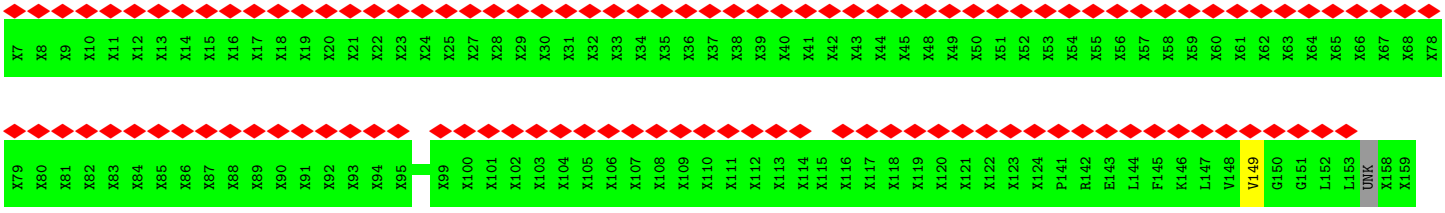
Chain ST:





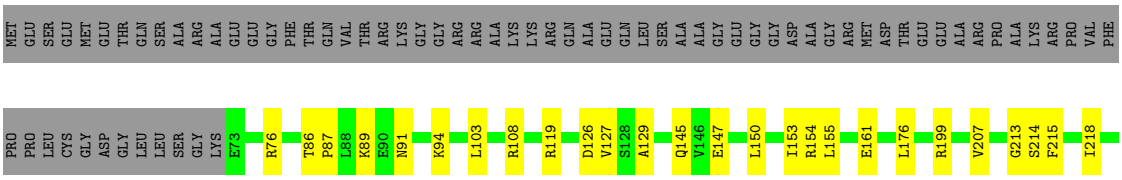
• Molecule 66: Nucleolar complex protein 4 homolog

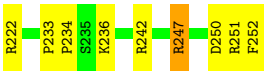
Chain SU:



• Molecule 67: RNA-binding protein PNO1

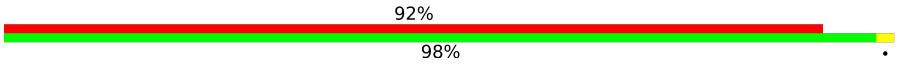
Chain SW:

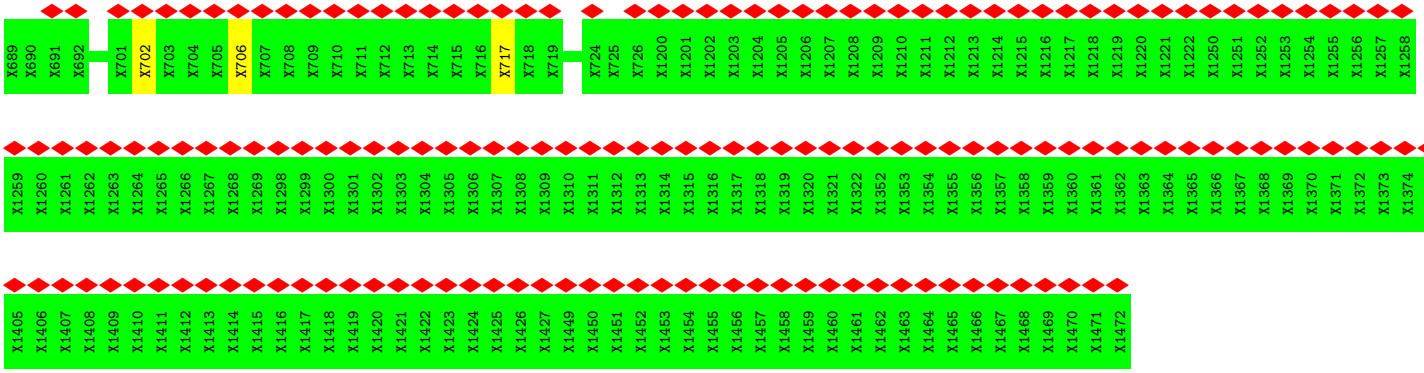




• Molecule 68: Unassigned peptides

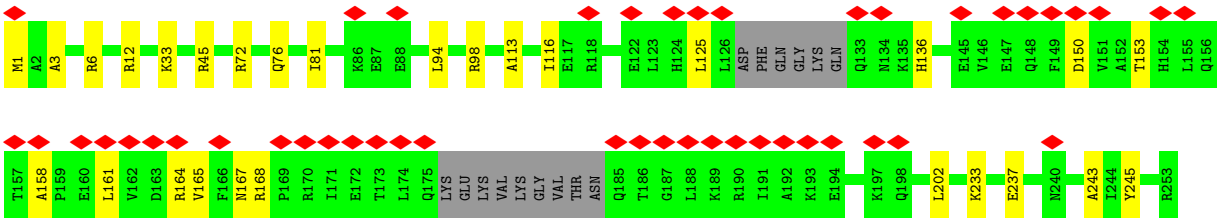
Chain SX:





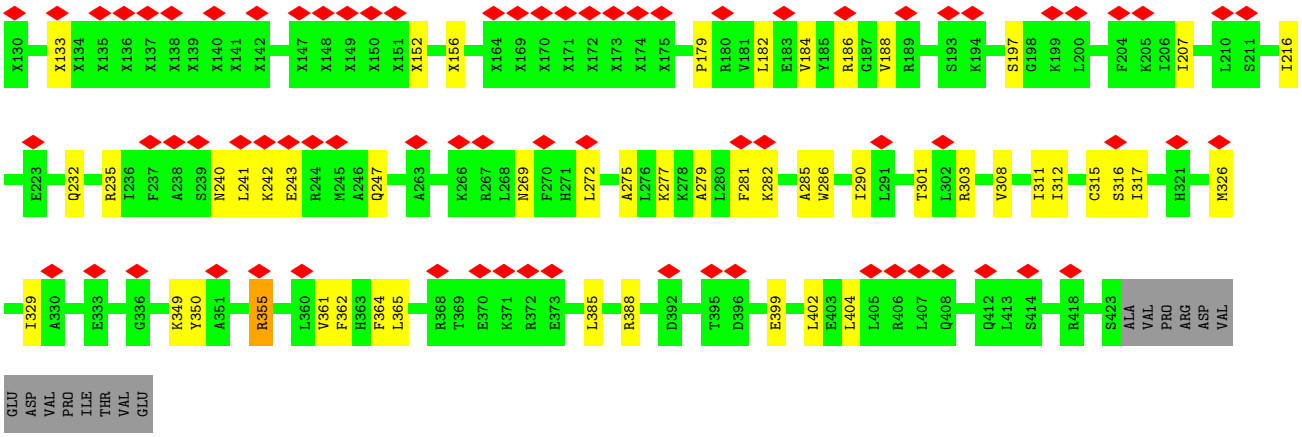
• Molecule 69: Probable U3 small nucleolar RNA-associated protein 11

Chain SY:



• Molecule 70: Bystin

Chain SZ:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42142	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 ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	20.935	Depositor
Minimum map value	-14.456	Depositor
Average map value	0.024	Depositor
Map value standard deviation	0.682	Depositor
Recommended contour level	2.68	Depositor
Map size (Å)	604.80005, 604.80005, 604.80005	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	L0	0.19	0/5739	0.85	2/8931 (0.0%)
2	L1	0.19	0/31039	0.85	66/48327 (0.1%)
3	L2	0.18	0/5130	0.81	5/7996 (0.1%)
4	L3	0.26	0/720	0.61	0/970
5	L4	0.25	0/2118	0.56	0/2849
6	L5	0.26	0/1523	0.56	2/2048 (0.1%)
7	L6	0.27	0/1830	0.59	0/2434
8	L7	0.29	0/1365	0.56	0/1830
9	L8	0.26	0/1500	0.57	0/2002
10	L9	0.25	0/1447	0.56	0/1930
11	LA	0.28	0/941	0.54	0/1264
12	LC	0.27	0/1115	0.56	0/1494
13	LD	0.26	0/1225	0.60	0/1640
14	LF	0.25	0/868	0.54	0/1159
15	LG	0.24	0/490	0.62	0/656
16	LH	0.25	0/6127	0.50	0/8292
17	LI	0.26	0/3245	0.48	0/4386
18	LJ	0.27	0/3788	0.56	2/5128 (0.0%)
19	LK	0.29	0/959	0.58	1/1302 (0.1%)
19	LL	0.24	0/4072	0.51	0/5539
20	LM	0.26	0/16110	0.50	3/21817 (0.0%)
21	LN	0.25	0/5438	0.51	1/7377 (0.0%)
22	LO	0.26	0/6835	0.55	0/9256
23	LP	0.25	0/4806	0.47	0/6455
24	LQ	0.24	0/6548	0.51	0/8839
25	LR	0.25	0/6141	0.53	0/8348
26	LS	0.25	0/3621	0.51	0/4876
27	LT	0.25	0/6907	0.50	0/9359
28	LU	0.24	0/3695	0.52	0/4986
29	LW	0.28	1/3594 (0.0%)	0.57	3/4867 (0.1%)
30	LZ	0.25	0/1560	0.56	0/2104
32	NA	0.26	0/2084	0.50	1/2789 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	NB	0.25	0/622	0.64	0/816
34	NC	0.24	0/788	0.57	0/1049
35	ND	0.25	0/708	0.54	0/947
36	NE	0.25	0/807	0.46	0/1069
37	NF	0.23	0/1226	0.49	0/1649
38	NG	0.25	0/873	0.52	0/1177
39	NH	0.25	0/8580	0.51	0/11685
40	NI	0.25	0/1887	0.52	0/2558
41	NJ	0.25	0/6652	0.50	0/9006
41	NK	0.25	0/6545	0.52	1/8867 (0.0%)
42	NM	0.24	0/1899	0.49	0/2533
43	NN	0.25	0/346	0.59	0/462
44	NO	0.27	0/1051	0.60	1/1406 (0.1%)
45	NQ	0.24	0/653	0.49	0/876
47	NT	0.28	0/479	0.69	1/635 (0.2%)
48	NU	0.25	0/501	0.55	0/667
49	NW	0.25	0/2556	0.54	0/3469
50	NY	0.25	0/2265	0.49	1/3045 (0.0%)
51	SA	0.24	0/3122	0.46	0/4208
52	SB	0.24	0/3491	0.48	0/4695
53	SC	0.29	0/1818	0.56	2/2463 (0.1%)
53	SD	0.24	0/1878	0.50	0/2540
54	SE	0.24	0/980	0.50	0/1323
54	SF	0.25	0/967	0.50	0/1305
55	SG	0.24	0/2941	0.51	0/3988
56	SH	0.24	0/2882	0.50	0/3887
57	SI	0.25	0/6917	0.49	0/9297
58	SJ	0.25	0/1609	0.53	0/2181
58	SK	0.25	0/1609	0.52	0/2181
59	SL	0.25	0/1619	0.53	0/2174
60	SM	0.25	0/2420	0.57	0/3264
61	SP	0.25	0/16393	0.49	2/22173 (0.0%)
62	SQ	0.25	0/1561	0.48	0/2083
63	SR	0.26	0/828	0.51	0/1110
64	SS	0.24	0/1663	0.50	0/2250
65	ST	0.27	0/3597	0.51	0/4836
66	SU	0.25	0/2634	0.52	1/3581 (0.0%)
67	SW	0.27	0/1436	0.59	0/1936
69	SY	0.24	0/2051	0.49	0/2723
70	SZ	0.25	0/2043	0.52	0/2763
All	All	0.24	1/245477 (0.0%)	0.59	95/340127 (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
6	L5	0	1
22	LO	0	1
67	SW	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	LW	101	PRO	CG-CD	-7.89	1.24	1.50

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	LW	101	PRO	N-CD-CG	-10.97	86.75	103.20
2	L1	1453	C	N1-C2-O2	9.35	124.51	118.90
2	L1	1453	C	C2-N1-C1'	9.25	128.98	118.80
2	L1	1535	U	C2-N1-C1'	8.14	127.47	117.70
2	L1	1742	C	C2-N1-C1'	8.11	127.72	118.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	L5	136	ARG	Sidechain
22	LO	316	GLU	Peptide
67	SW	247	ARG	Sidechain

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	L0	5152	0	2630	49	0
2	L1	27777	0	14063	253	0
3	L2	4589	0	2306	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L3	854	0	774	24	0
5	L4	2076	0	2177	17	0
6	L5	1501	0	1557	16	0
7	L6	1811	0	1974	22	0
8	L7	1346	0	1410	30	0
9	L8	1474	0	1542	21	0
10	L9	1425	0	1541	16	0
11	LA	931	0	961	18	0
12	LC	1098	0	1168	10	0
13	LD	1204	0	1274	11	0
14	LF	851	0	894	17	0
15	LG	488	0	514	4	0
16	LH	5987	0	5953	72	0
17	LI	3889	0	3464	54	0
18	LJ	3711	0	3758	65	0
19	LK	943	0	1023	25	0
19	LL	3982	0	4031	55	0
20	LM	15820	0	16318	272	0
21	LN	5299	0	5269	78	0
22	LO	6676	0	6579	74	0
23	LP	4705	0	4720	49	0
24	LQ	6438	0	6400	75	0
25	LR	6015	0	5981	90	0
26	LS	3560	0	3570	51	0
27	LT	6756	0	6768	80	0
28	LU	3611	0	3618	59	0
29	LW	3519	0	3518	33	0
30	LZ	1532	0	1553	10	0
31	N0	264	0	178	0	0
32	NA	2055	0	2135	21	0
33	NB	617	0	685	7	0
34	NC	779	0	788	10	0
35	ND	696	0	729	10	0
36	NE	799	0	854	11	0
37	NF	1202	0	1289	9	0
38	NG	861	0	871	8	0
39	NH	8374	0	8456	77	0
40	NI	1840	0	1812	18	0
41	NJ	6526	0	6599	56	0
41	NK	6419	0	6480	87	0
42	NM	1873	0	1968	17	0
43	NN	340	0	345	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	NO	1034	0	1080	18	0
45	NQ	640	0	661	5	0
46	NR	4305	0	945	22	0
47	NT	470	0	474	14	0
48	NU	495	0	541	10	0
49	NW	2498	0	2456	34	0
50	NY	2222	0	2310	16	0
51	SA	3077	0	3139	32	0
52	SB	3439	0	3559	42	0
53	SC	1781	0	1803	37	0
53	SD	1841	0	1867	14	0
54	SE	968	0	1017	7	0
54	SF	955	0	1008	5	0
55	SG	2884	0	2751	17	0
56	SH	2832	0	2937	28	0
57	SI	6803	0	6966	63	0
58	SJ	1579	0	1646	28	0
58	SK	1579	0	1646	24	0
59	SL	1586	0	1641	31	0
60	SM	2369	0	2376	18	0
61	SP	16078	0	16633	204	0
62	SQ	1533	0	1579	8	0
63	SR	816	0	871	5	0
64	SS	1626	0	1677	19	0
65	ST	4170	0	3804	56	0
66	SU	3154	0	2736	30	0
67	SW	1413	0	1489	26	0
68	SX	885	0	192	2	0
69	SY	2024	0	2148	19	0
70	SZ	2222	0	2142	32	0
71	L1	19	0	0	0	0
71	NH	1	0	0	0	0
71	SI	1	0	0	0	0
71	SL	1	0	0	0	0
72	NH	31	0	12	2	0
72	NK	31	0	12	1	0
73	NQ	1	0	0	0	0
73	NT	1	0	0	0	0
73	SL	1	0	0	0	0
74	SI	32	0	12	0	0
75	SJ	26	0	19	3	0
75	SK	26	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	245114	0	224665	2570	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 6.

The worst 5 of 2570 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)
20:LM:1457:GLN:HE21	20:LM:1457:GLN:N	1.53	1.06
28:LU:66:ARG:HH12	59:SL:127:PRO:HD3	1.40	0.84
27:LT:748:ASN:HB3	27:LT:751:LEU:HD23	1.60	0.83
21:LN:461:LEU:HB2	21:LN:477:PHE:HB2	1.63	0.81
61:SP:1430:VAL:HG12	61:SP:1477:ASN:HD21	1.45	0.80

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	
4	L3	85/116 (73%)	84 (99%)	1 (1%)	0	100	100
5	L4	260/263 (99%)	259 (100%)	1 (0%)	0	100	100
6	L5	188/204 (92%)	182 (97%)	6 (3%)	0	100	100
7	L6	219/249 (88%)	218 (100%)	1 (0%)	0	100	100
8	L7	164/194 (84%)	160 (98%)	4 (2%)	0	100	100
9	L8	176/208 (85%)	174 (99%)	2 (1%)	0	100	100
10	L9	169/194 (87%)	168 (99%)	1 (1%)	0	100	100
11	LA	118/132 (89%)	111 (94%)	7 (6%)	0	100	100
12	LC	137/146 (94%)	136 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	LD	145/158 (92%)	141 (97%)	4 (3%)	0	100	100
14	LF	102/133 (77%)	102 (100%)	0	0	100	100
15	LG	60/69 (87%)	59 (98%)	1 (2%)	0	100	100
16	LH	738/830 (89%)	721 (98%)	17 (2%)	0	100	100
17	LI	374/678 (55%)	370 (99%)	4 (1%)	0	100	100
18	LJ	465/518 (90%)	448 (96%)	17 (4%)	0	100	100
19	LK	116/677 (17%)	113 (97%)	3 (3%)	0	100	100
19	LL	500/677 (74%)	483 (97%)	17 (3%)	0	100	100
20	LM	1977/2144 (92%)	1933 (98%)	44 (2%)	0	100	100
21	LN	667/686 (97%)	647 (97%)	19 (3%)	1 (0%)	51	83
22	LO	844/919 (92%)	826 (98%)	18 (2%)	0	100	100
23	LP	559/597 (94%)	556 (100%)	3 (0%)	0	100	100
24	LQ	810/943 (86%)	792 (98%)	18 (2%)	0	100	100
25	LR	769/808 (95%)	748 (97%)	21 (3%)	0	100	100
26	LS	447/556 (80%)	440 (98%)	7 (2%)	0	100	100
27	LT	863/951 (91%)	847 (98%)	16 (2%)	0	100	100
28	LU	443/445 (100%)	435 (98%)	8 (2%)	0	100	100
29	LW	449/610 (74%)	436 (97%)	13 (3%)	0	100	100
30	LZ	181/184 (98%)	179 (99%)	2 (1%)	0	100	100
32	NA	243/681 (36%)	242 (100%)	1 (0%)	0	100	100
33	NB	71/479 (15%)	69 (97%)	2 (3%)	0	100	100
34	NC	92/315 (29%)	90 (98%)	2 (2%)	0	100	100
35	ND	82/257 (32%)	81 (99%)	1 (1%)	0	100	100
36	NE	94/293 (32%)	94 (100%)	0	0	100	100
37	NF	147/151 (97%)	145 (99%)	2 (1%)	0	100	100
38	NG	114/151 (76%)	113 (99%)	1 (1%)	0	100	100
39	NH	1064/1146 (93%)	1044 (98%)	20 (2%)	0	100	100
40	NI	232/280 (83%)	229 (99%)	3 (1%)	0	100	100
41	NJ	809/1025 (79%)	783 (97%)	26 (3%)	0	100	100
41	NK	801/1025 (78%)	782 (98%)	19 (2%)	0	100	100
42	NM	229/264 (87%)	226 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	NN	40/560 (7%)	39 (98%)	1 (2%)	0	100	100
44	NO	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
45	NQ	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
47	NT	56/156 (36%)	55 (98%)	1 (2%)	0	100	100
48	NU	58/135 (43%)	57 (98%)	1 (2%)	0	100	100
49	NW	305/688 (44%)	293 (96%)	12 (4%)	0	100	100
50	NY	270/381 (71%)	270 (100%)	0	0	100	100
51	SA	390/594 (66%)	388 (100%)	2 (0%)	0	100	100
52	SB	438/529 (83%)	437 (100%)	1 (0%)	0	100	100
53	SC	225/321 (70%)	219 (97%)	6 (3%)	0	100	100
53	SD	233/321 (73%)	227 (97%)	6 (3%)	0	100	100
54	SE	123/128 (96%)	122 (99%)	1 (1%)	0	100	100
54	SF	121/128 (94%)	119 (98%)	2 (2%)	0	100	100
55	SG	383/475 (81%)	374 (98%)	9 (2%)	0	100	100
56	SH	366/373 (98%)	362 (99%)	4 (1%)	0	100	100
57	SI	825/1282 (64%)	812 (98%)	13 (2%)	0	100	100
58	SJ	202/244 (83%)	200 (99%)	2 (1%)	0	100	100
58	SK	202/244 (83%)	200 (99%)	2 (1%)	0	100	100
59	SL	190/198 (96%)	186 (98%)	4 (2%)	0	100	100
60	SM	288/291 (99%)	280 (97%)	8 (3%)	0	100	100
61	SP	1967/2785 (71%)	1933 (98%)	34 (2%)	0	100	100
62	SQ	183/756 (24%)	182 (100%)	1 (0%)	0	100	100
63	SR	106/143 (74%)	104 (98%)	2 (2%)	0	100	100
64	SS	191/771 (25%)	187 (98%)	4 (2%)	0	100	100
65	ST	432/632 (68%)	424 (98%)	8 (2%)	0	100	100
66	SU	316/472 (67%)	311 (98%)	5 (2%)	0	100	100
67	SW	178/252 (71%)	175 (98%)	3 (2%)	0	100	100
69	SY	232/253 (92%)	230 (99%)	2 (1%)	0	100	100
70	SZ	244/304 (80%)	237 (97%)	7 (3%)	0	100	100
All	All	24774/33986 (73%)	24292 (98%)	481 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	LN	175	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L3	76/77 (99%)	76 (100%)	0	100	100
5	L4	224/225 (100%)	224 (100%)	0	100	100
6	L5	160/170 (94%)	160 (100%)	0	100	100
7	L6	195/218 (89%)	194 (100%)	1 (0%)	88	95
8	L7	149/174 (86%)	149 (100%)	0	100	100
9	L8	155/180 (86%)	155 (100%)	0	100	100
10	L9	152/168 (90%)	151 (99%)	1 (1%)	84	93
11	LA	102/108 (94%)	100 (98%)	2 (2%)	55	79
12	LC	114/121 (94%)	114 (100%)	0	100	100
13	LD	133/142 (94%)	131 (98%)	2 (2%)	65	84
14	LF	92/115 (80%)	92 (100%)	0	100	100
15	LG	55/62 (89%)	55 (100%)	0	100	100
16	LH	670/748 (90%)	667 (100%)	3 (0%)	91	97
17	LI	368/497 (74%)	368 (100%)	0	100	100
18	LJ	412/456 (90%)	412 (100%)	0	100	100
19	LK	112/594 (19%)	112 (100%)	0	100	100
19	LL	456/594 (77%)	454 (100%)	2 (0%)	91	97
20	LM	1783/1943 (92%)	1779 (100%)	4 (0%)	93	98
21	LN	582/597 (98%)	582 (100%)	0	100	100
22	LO	726/783 (93%)	725 (100%)	1 (0%)	93	98
23	LP	499/527 (95%)	499 (100%)	0	100	100
24	LQ	690/828 (83%)	690 (100%)	0	100	100
25	LR	648/672 (96%)	648 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	LS	393/476 (83%)	392 (100%)	1 (0%)	92	97
27	LT	744/823 (90%)	743 (100%)	1 (0%)	93	98
28	LU	399/399 (100%)	399 (100%)	0	100	100
29	LW	373/512 (73%)	373 (100%)	0	100	100
30	LZ	166/167 (99%)	166 (100%)	0	100	100
32	NA	229/626 (37%)	229 (100%)	0	100	100
33	NB	63/413 (15%)	63 (100%)	0	100	100
34	NC	87/282 (31%)	87 (100%)	0	100	100
35	ND	72/222 (32%)	72 (100%)	0	100	100
36	NE	86/253 (34%)	85 (99%)	1 (1%)	71	87
37	NF	130/131 (99%)	130 (100%)	0	100	100
38	NG	92/119 (77%)	92 (100%)	0	100	100
39	NH	917/984 (93%)	916 (100%)	1 (0%)	93	98
40	NI	193/246 (78%)	193 (100%)	0	100	100
41	NJ	707/899 (79%)	705 (100%)	2 (0%)	92	97
41	NK	692/899 (77%)	690 (100%)	2 (0%)	92	97
42	NM	207/231 (90%)	207 (100%)	0	100	100
43	NN	37/484 (8%)	37 (100%)	0	100	100
44	NO	112/113 (99%)	112 (100%)	0	100	100
45	NQ	74/76 (97%)	74 (100%)	0	100	100
47	NT	51/140 (36%)	50 (98%)	1 (2%)	55	79
48	NU	53/122 (43%)	53 (100%)	0	100	100
49	NW	282/635 (44%)	280 (99%)	2 (1%)	84	93
50	NY	245/340 (72%)	244 (100%)	1 (0%)	91	97
51	SA	334/511 (65%)	334 (100%)	0	100	100
52	SB	372/455 (82%)	371 (100%)	1 (0%)	92	97
53	SC	192/234 (82%)	191 (100%)	1 (0%)	88	95
53	SD	198/234 (85%)	198 (100%)	0	100	100
54	SE	108/111 (97%)	108 (100%)	0	100	100
54	SF	107/111 (96%)	107 (100%)	0	100	100
55	SG	287/382 (75%)	287 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
56	SH	315/318 (99%)	315 (100%)	0	100 100
57	SI	738/1114 (66%)	738 (100%)	0	100 100
58	SJ	181/209 (87%)	179 (99%)	2 (1%)	73 88
58	SK	181/209 (87%)	181 (100%)	0	100 100
59	SL	177/182 (97%)	177 (100%)	0	100 100
60	SM	253/254 (100%)	253 (100%)	0	100 100
61	SP	1822/2522 (72%)	1818 (100%)	4 (0%)	93 98
62	SQ	165/676 (24%)	165 (100%)	0	100 100
63	SR	85/115 (74%)	85 (100%)	0	100 100
64	SS	177/686 (26%)	176 (99%)	1 (1%)	86 94
65	ST	389/439 (89%)	388 (100%)	1 (0%)	92 97
66	SU	269/303 (89%)	269 (100%)	0	100 100
67	SW	152/208 (73%)	151 (99%)	1 (1%)	84 93
69	SY	219/232 (94%)	219 (100%)	0	100 100
70	SZ	214/227 (94%)	213 (100%)	1 (0%)	88 95
All	All	21892/29323 (75%)	21852 (100%)	40 (0%)	93 98

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	SB	70	LYS
61	SP	2052	ARG
53	SC	87	MET
61	SP	36	ARG
65	ST	789	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
64	SS	195	ASN
65	ST	37	ASN
65	ST	796	HIS
24	LQ	632	HIS
23	LP	267	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L0	234/3617 (6%)	101 (43%)	6 (2%)
2	L1	1275/1869 (68%)	346 (27%)	23 (1%)
3	L2	214/217 (98%)	80 (37%)	4 (1%)
31	N0	0/22	-	-
All	All	1723/5725 (30%)	527 (30%)	33 (1%)

5 of 527 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L0	434	C
1	L0	439	U
1	L0	442	U
1	L0	445	C
1	L0	446	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L1	1823	A
3	L2	14	C
3	L2	188	G
2	L1	423	U
2	L1	369	C

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 25 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
74	GTP	SI	2001	71	26,34,34	1.13	2 (7%)	32,54,54	1.54	6 (18%)
72	ATP	NK	1101	-	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
72	ATP	NH	3000	71	26,33,33	0.58	0	31,52,52	0.81	2 (6%)
75	SAH	SK	301	-	24,28,28	1.19	3 (12%)	25,40,40	1.71	5 (20%)
75	SAH	SJ	301	-	24,28,28	1.20	3 (12%)	25,40,40	1.70	5 (20%)

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
74	GTP	SI	2001	71	-	7/18/38/38	0/3/3/3
72	ATP	NK	1101	-	-	7/18/38/38	0/3/3/3
72	ATP	NH	3000	71	-	6/18/38/38	0/3/3/3
75	SAH	SK	301	-	-	9/11/31/31	0/3/3/3
75	SAH	SJ	301	-	-	3/11/31/31	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	SI	2001	GTP	C5-C6	-4.16	1.39	1.47
75	SJ	301	SAH	C2-N3	3.92	1.38	1.32
75	SK	301	SAH	C2-N3	3.86	1.38	1.32
75	SK	301	SAH	C2-N1	2.47	1.38	1.33
75	SJ	301	SAH	C2-N1	2.45	1.38	1.33

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
75	SK	301	SAH	N3-C2-N1	-5.40	120.25	128.68
75	SJ	301	SAH	N3-C2-N1	-5.39	120.25	128.68
74	SI	2001	GTP	PB-O3B-PG	-3.57	120.57	132.83
75	SK	301	SAH	C5'-SD-CG	-3.42	92.02	102.27
75	SJ	301	SAH	C5'-SD-CG	-3.31	92.33	102.27

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
72	NH	3000	ATP	C5'-O5'-PA-O1A
72	NH	3000	ATP	C5'-O5'-PA-O3A
72	NK	1101	ATP	C5'-O5'-PA-O1A
74	SI	2001	GTP	C5'-O5'-PA-O1A
74	SI	2001	GTP	C5'-O5'-PA-O2A

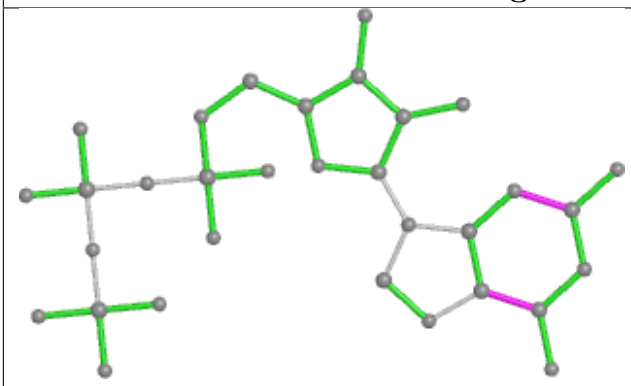
There are no ring outliers.

3 monomers are involved in 6 short contacts:

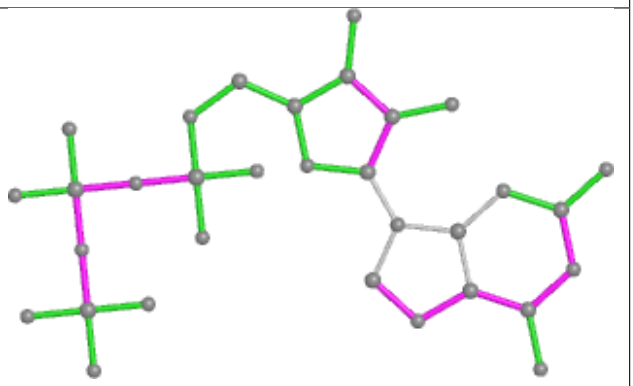
Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	NK	1101	ATP	1	0
72	NH	3000	ATP	2	0
75	SJ	301	SAH	3	0

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.

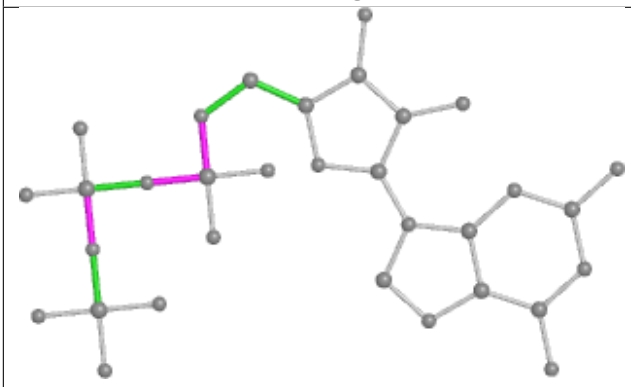
Ligand GTP SI 2001



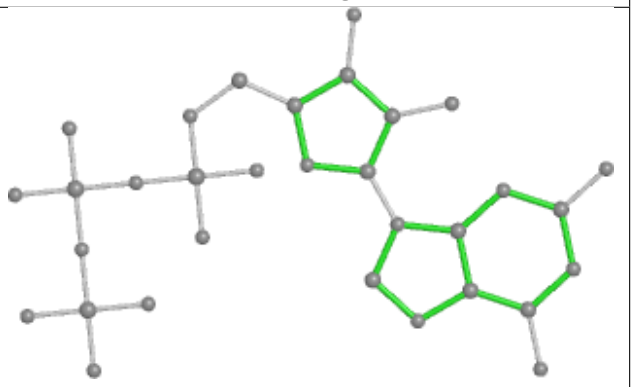
Bond lengths



Bond angles

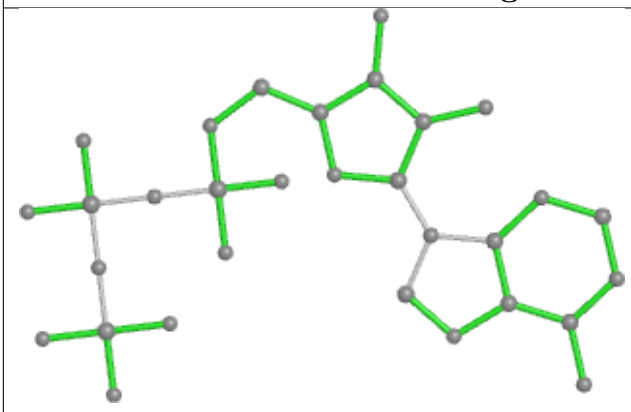


Torsions

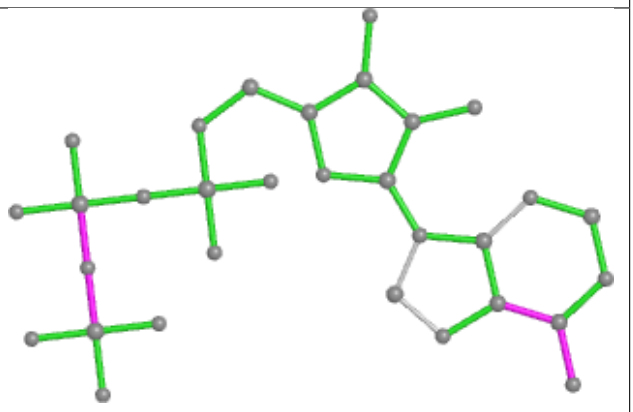


Rings

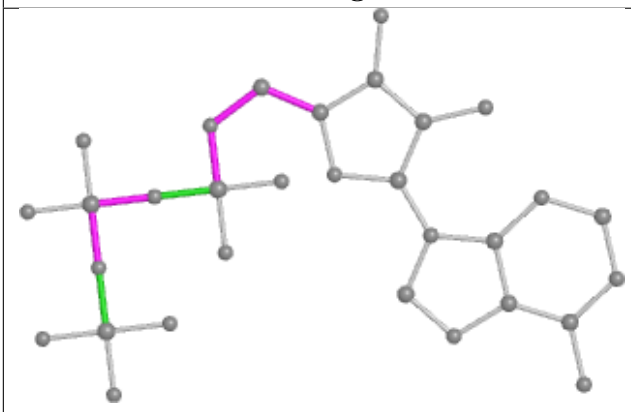
Ligand ATP NK 1101



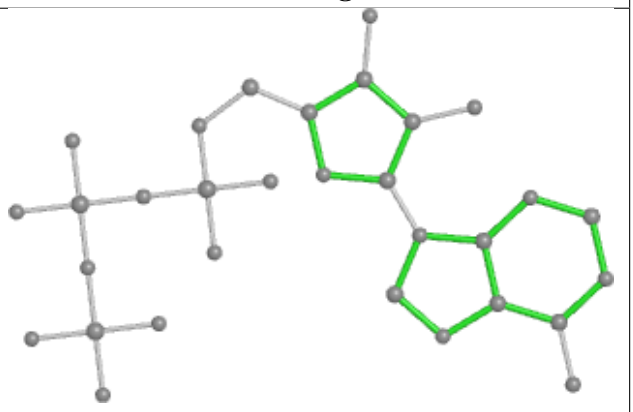
Bond lengths



Bond angles

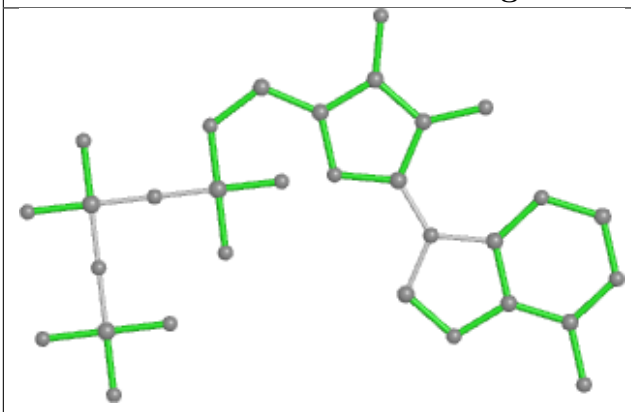


Torsions

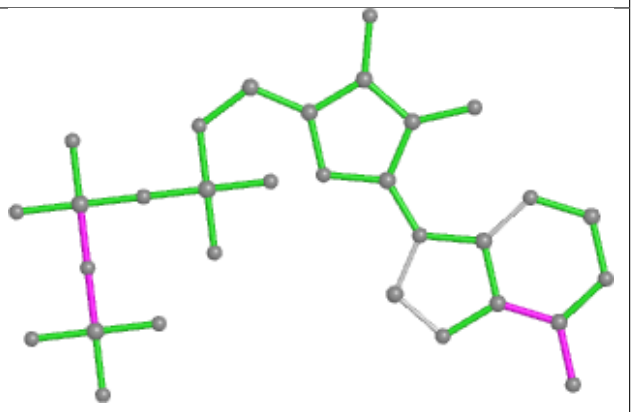


Rings

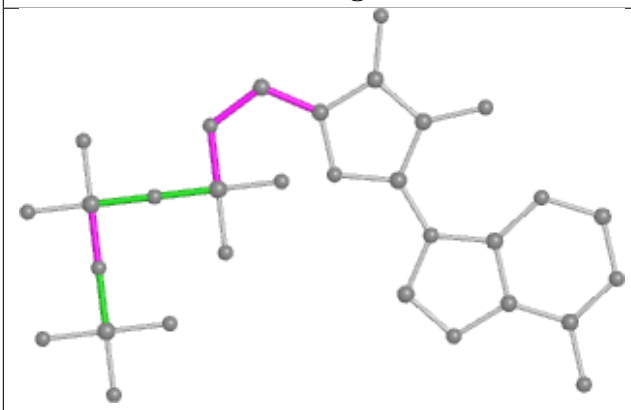
Ligand ATP NH 3000



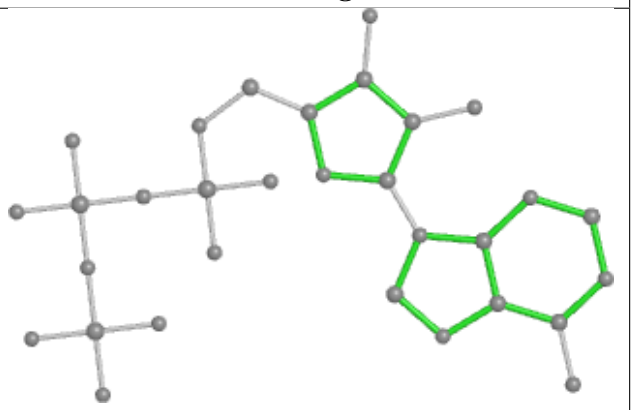
Bond lengths



Bond angles

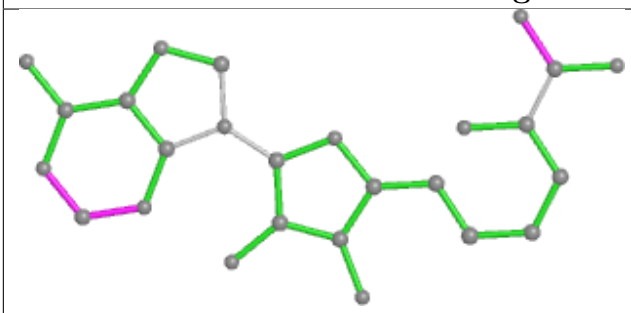


Torsions

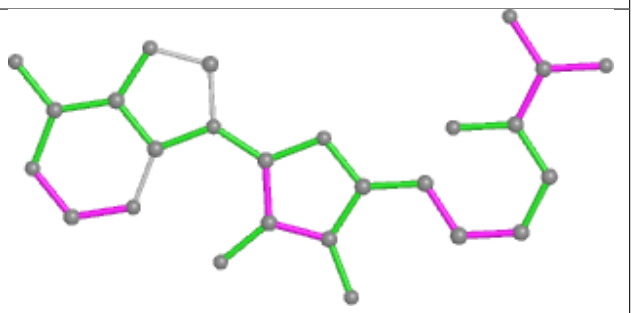


Rings

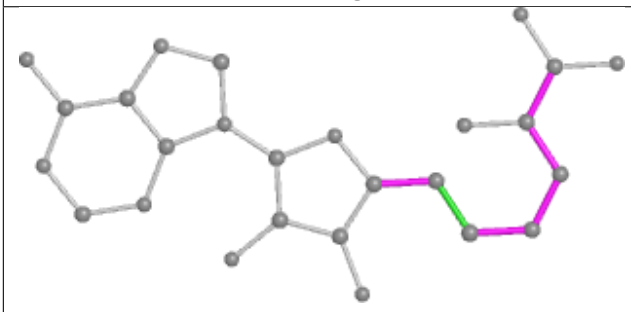
Ligand SAH SK 301



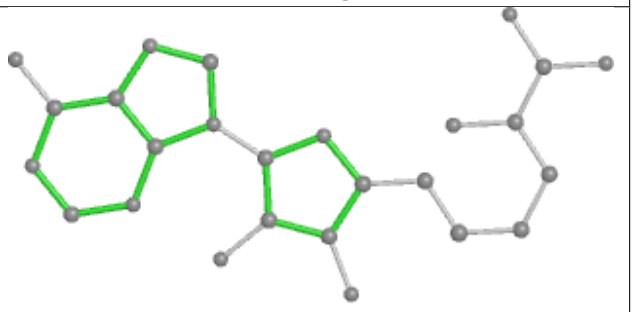
Bond lengths



Bond angles

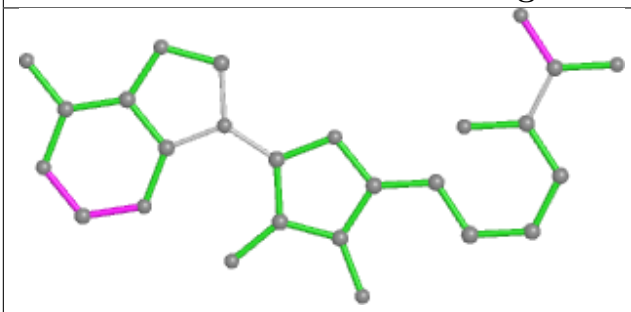


Torsions

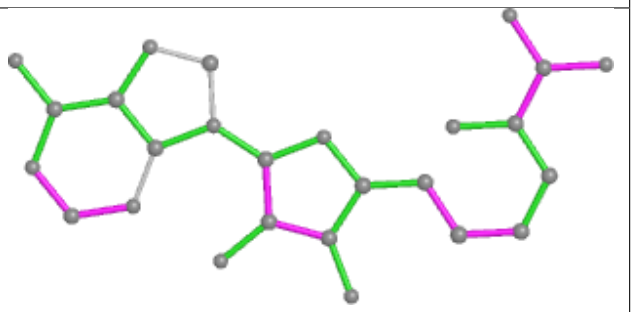


Rings

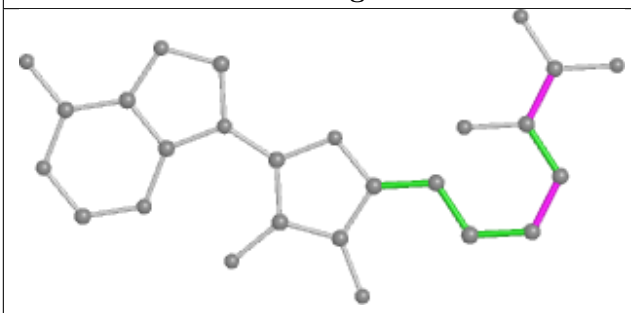
Ligand SAH SJ 301



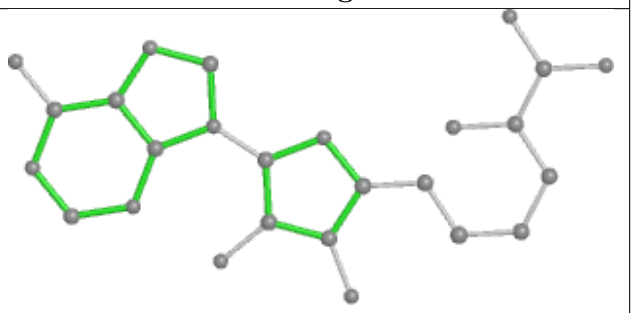
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
46	NR	41
68	SX	6
17	LI	5
66	SU	5
65	ST	3
31	N0	1
70	SZ	1

The worst 5 of 62 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SX	726:UNK	C	1200:UNK	N	185.51
1	ST	298:LEU	C	414:UNK	N	52.49
1	SX	1269:UNK	C	1298:UNK	N	38.16
1	ST	86:LYS	C	186:UNK	N	37.14

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	SX	1427:UNK	C	1449:UNK	N	35.74

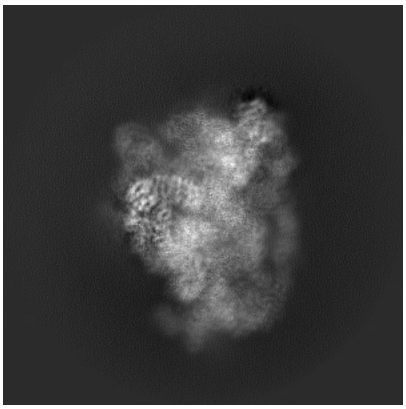
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23936. These allow visual inspection of the internal detail of the map and identification of artifacts.

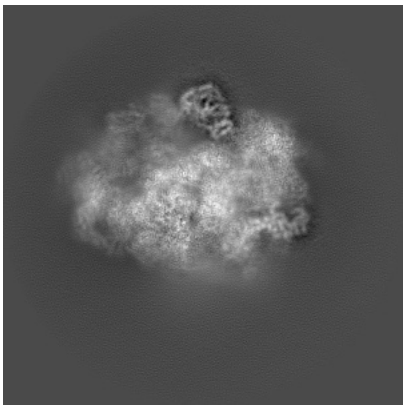
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

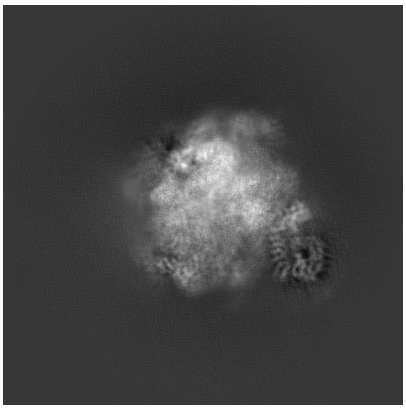
6.1.1 Primary map



X

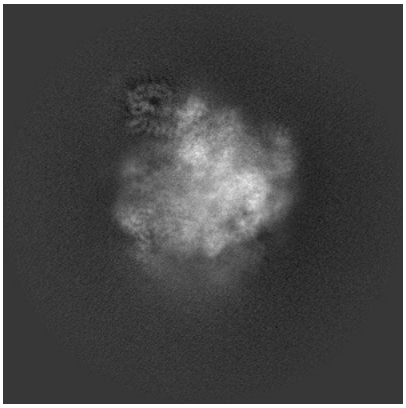


Y



Z

6.1.2 Raw map



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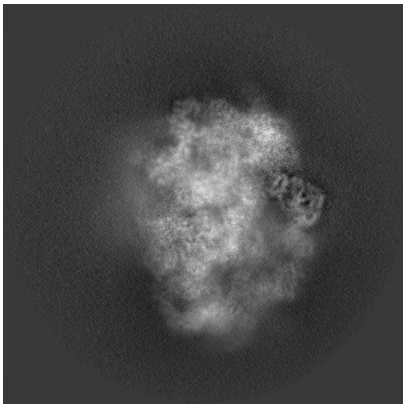
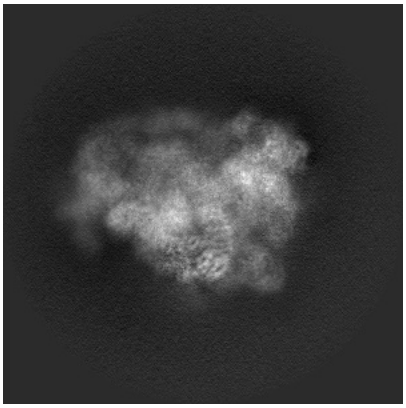


Y

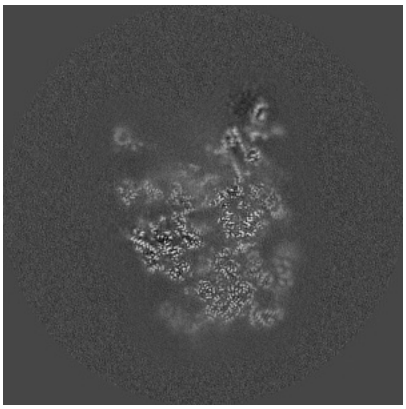


Z

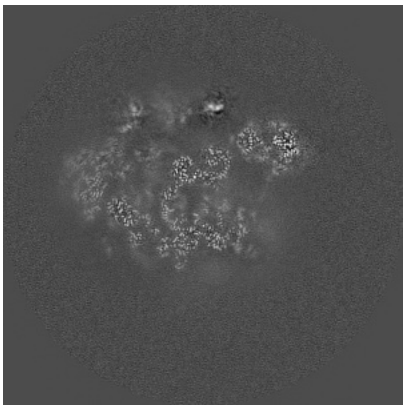
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

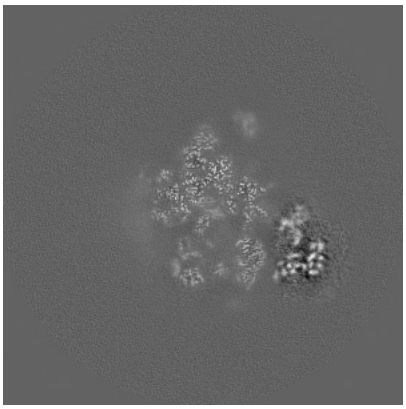
6.2.1 Primary map



X Index: 280

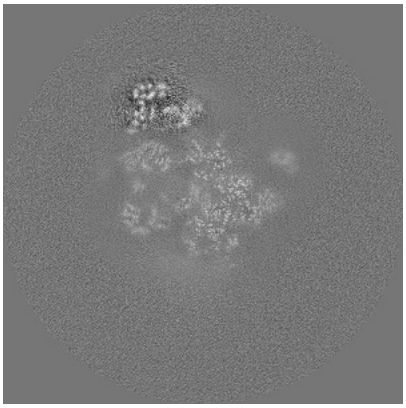


Y Index: 280

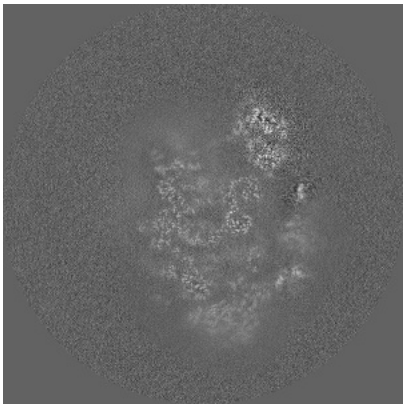


Z Index: 280

6.2.2 Raw map



X Index: 280



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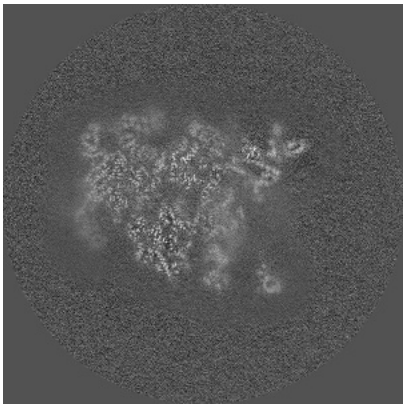
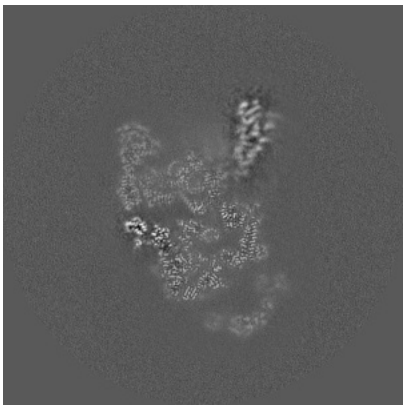


Z Index: 280

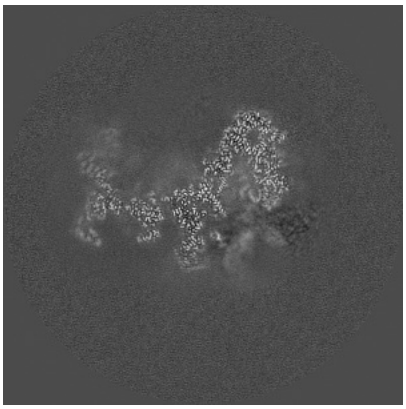
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

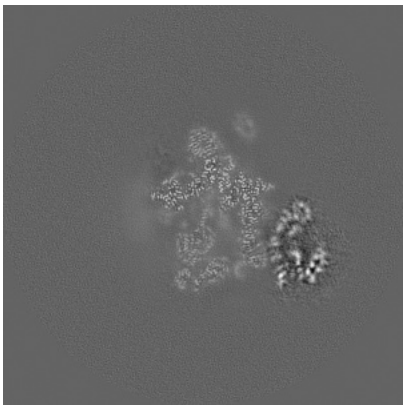
6.3.1 Primary map



X Index: 254

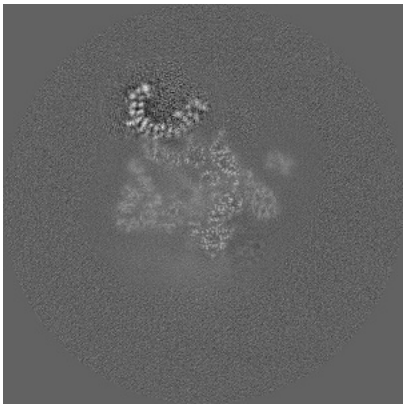


Y Index: 318

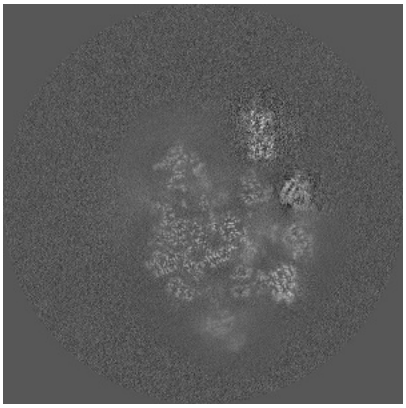


Z Index: 291

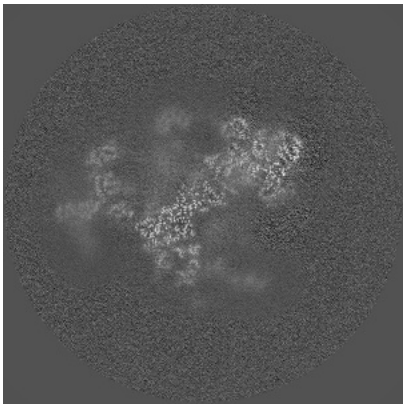
6.3.2 Raw map



X Index: 298



Y Index: 261



Z Index: 320

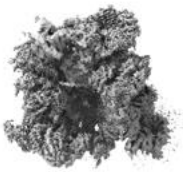
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



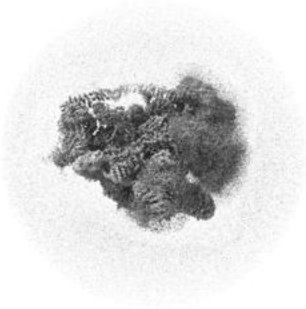
Z

The images above show the 3D surface view of the map at the recommended contour level 2.68. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X

Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

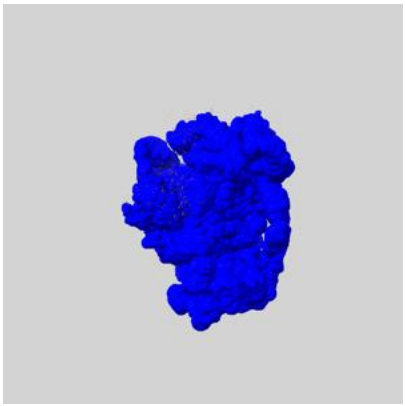
6.5 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

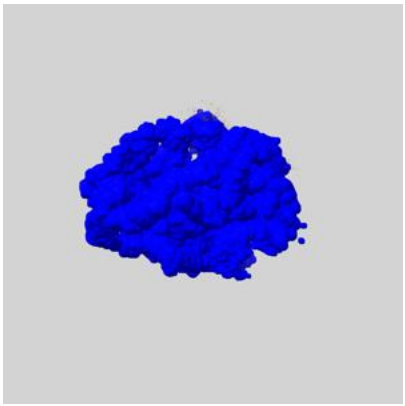
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

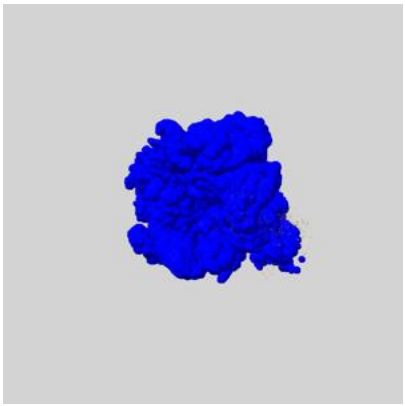
6.5.1 emd_23936_msk_1.map



X



Y

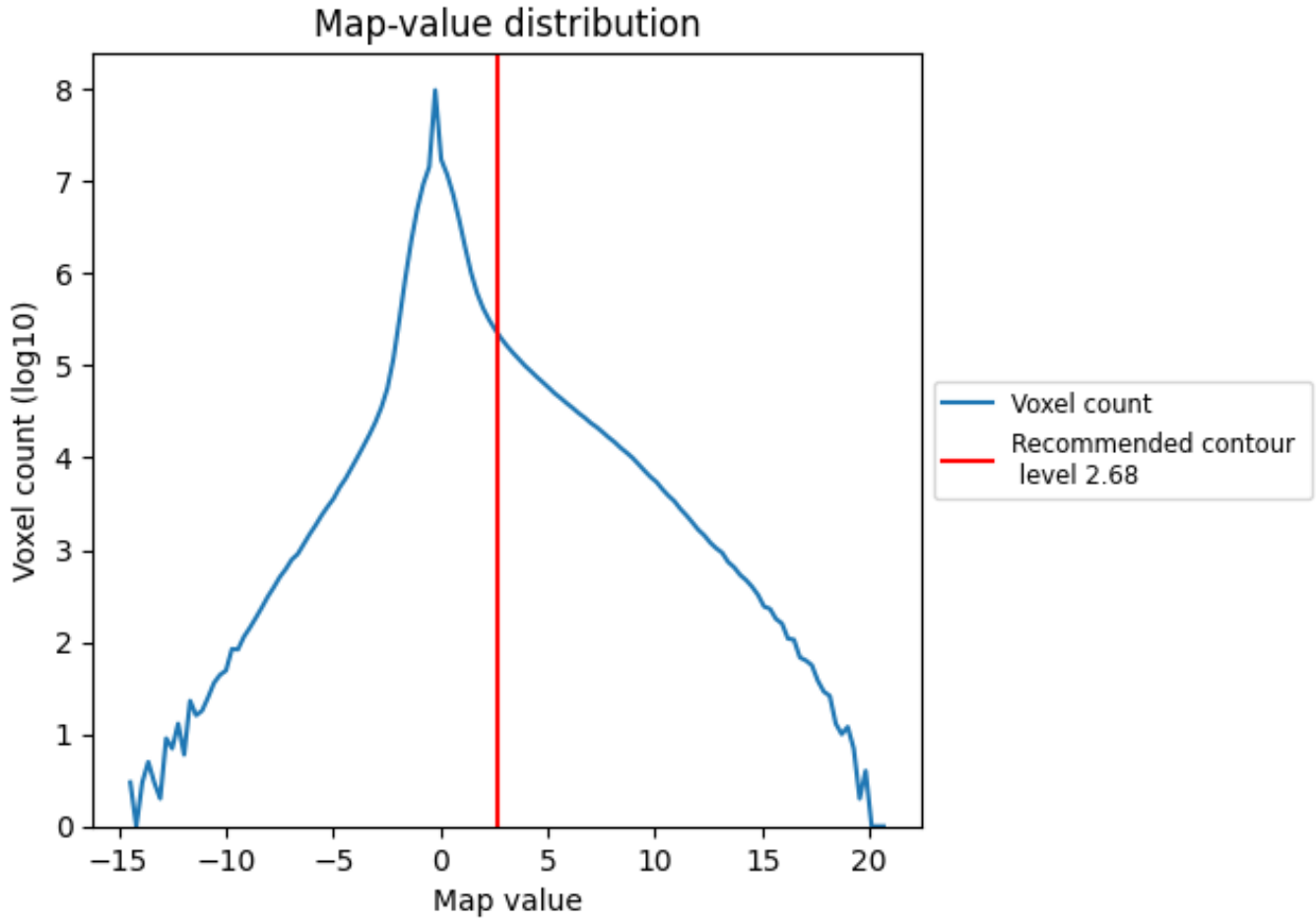


Z

7 Map analysis

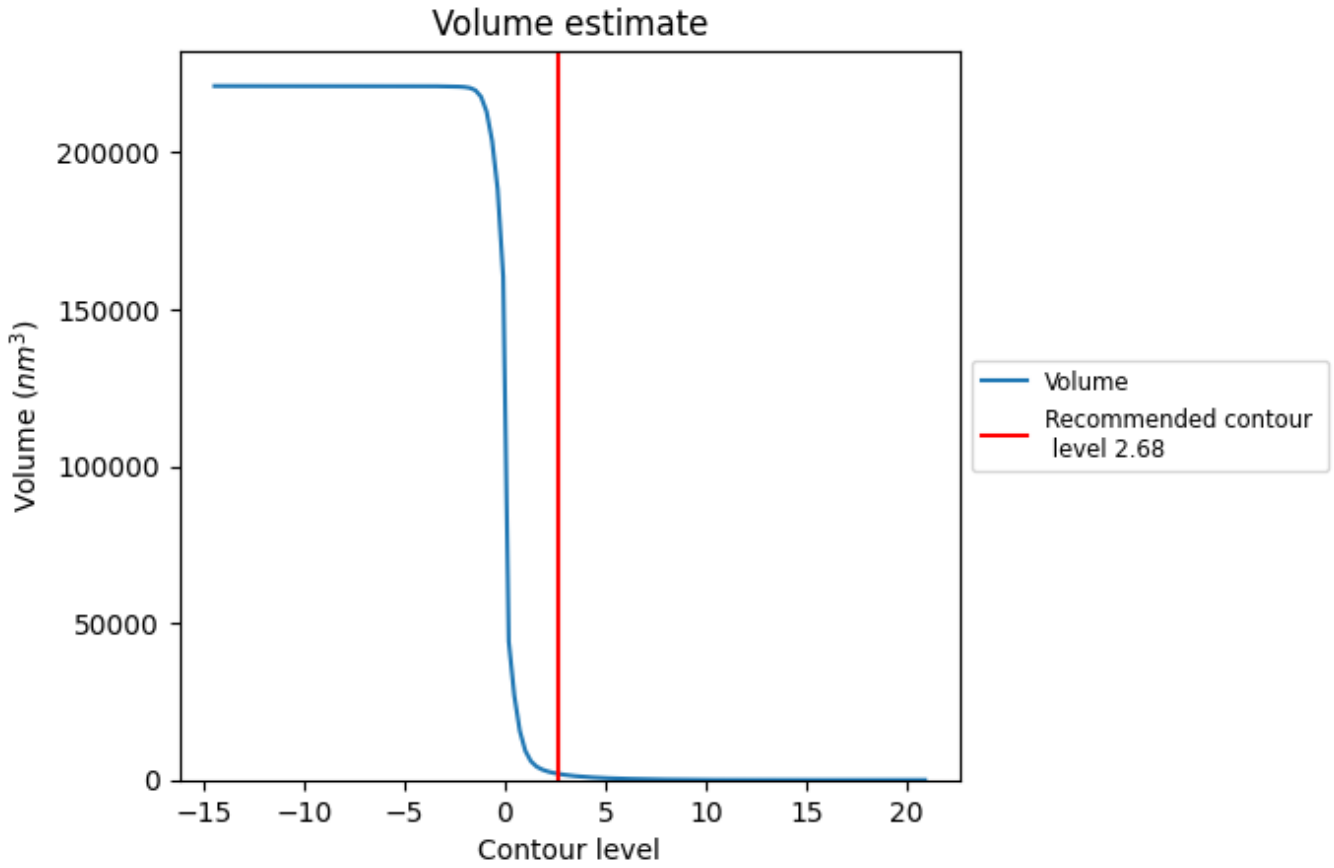
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

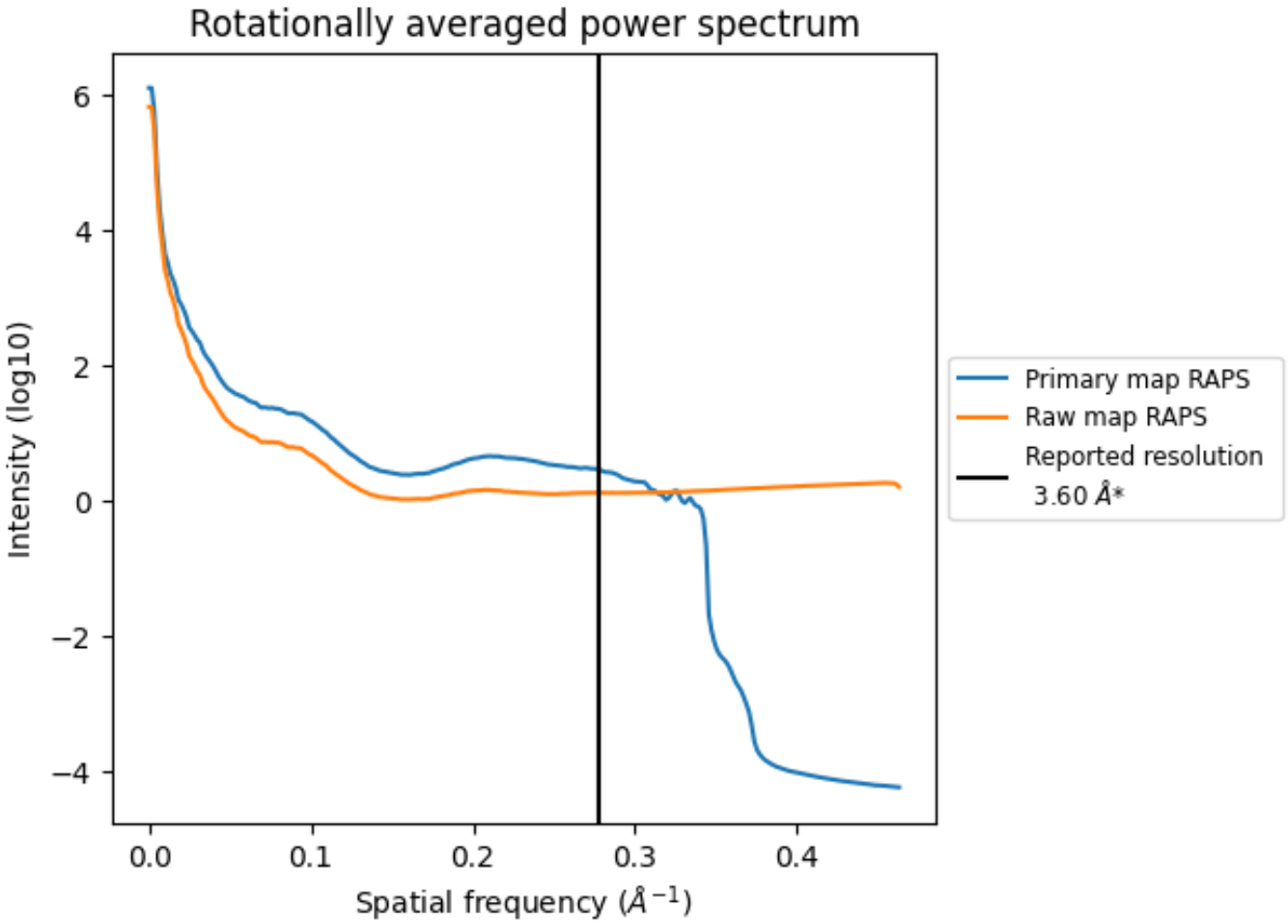
7.2 Volume estimate



The volume at the recommended contour level is 1931 nm^3; this corresponds to an approximate mass of 1744 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)

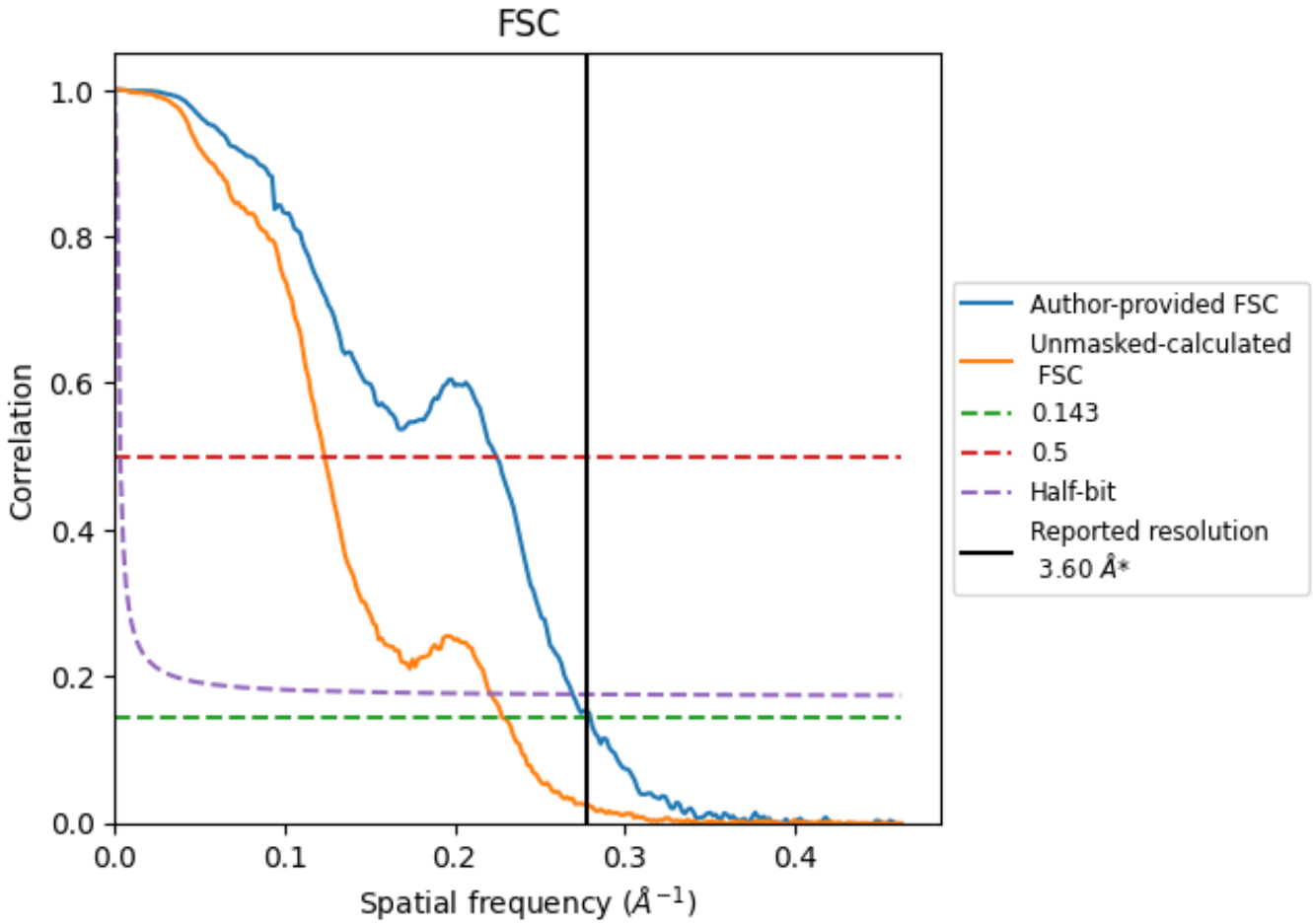


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

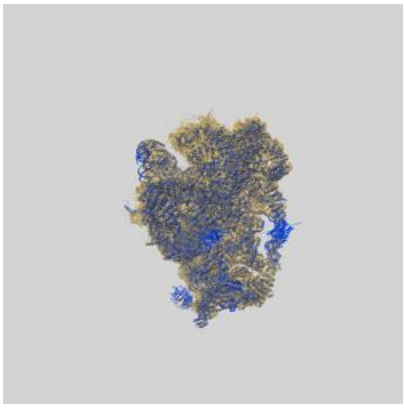
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	4.46	3.71
Unmasked-calculated*	4.38	8.10	4.52

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.38 differs from the reported value 3.6 by more than 10 %

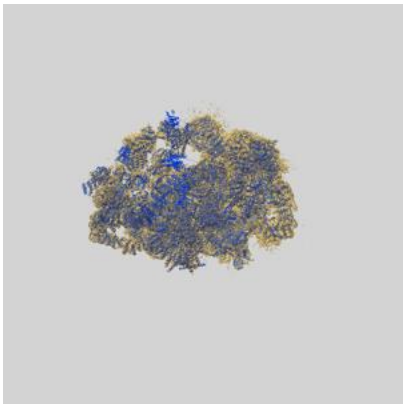
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23936 and PDB model 7MQ8. Per-residue inclusion information can be found in section 3 on page 19.

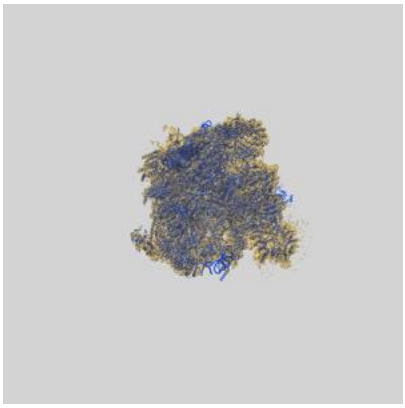
9.1 Map-model overlay



X



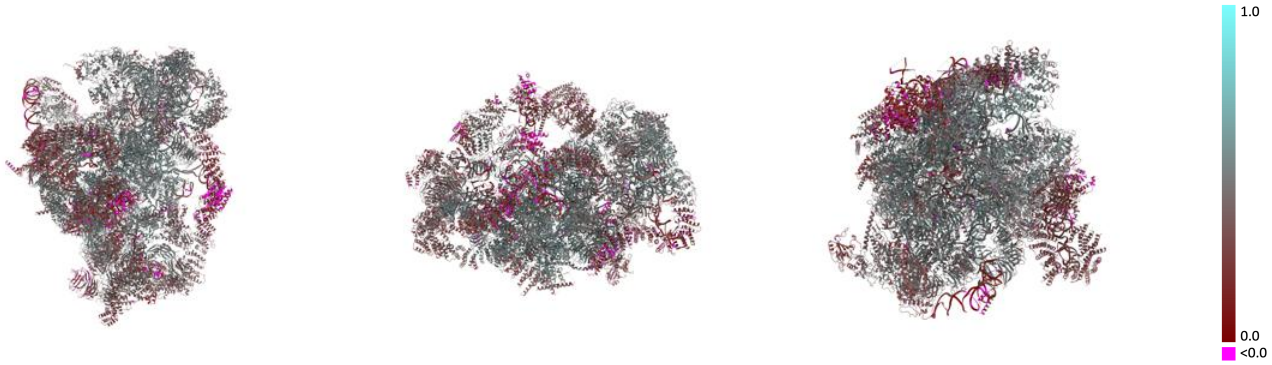
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.68 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.

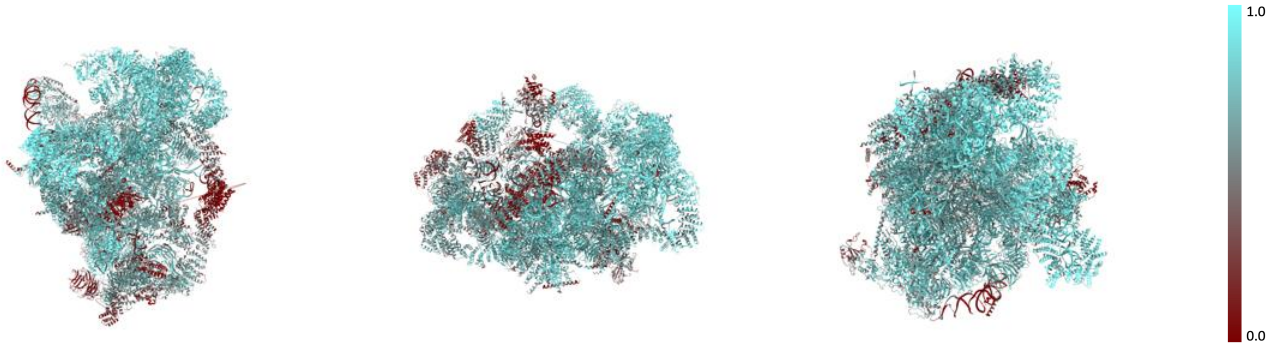
9.2 Q-score mapped to coordinate model (i)



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.

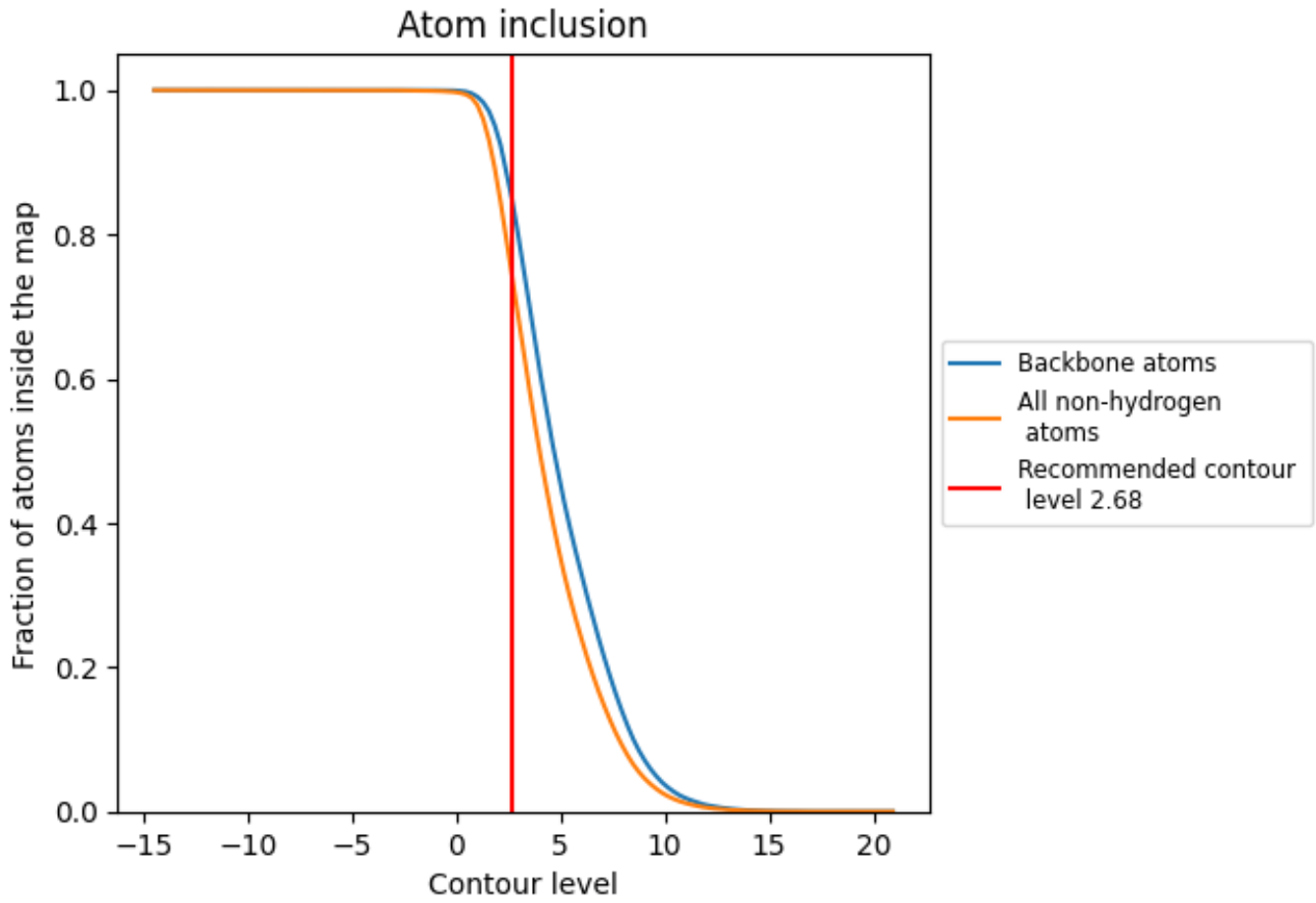
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.68).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 74% 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 (2.68) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7440	0.4170
L0	0.5928	0.3800
L1	0.8243	0.3850
L2	0.7871	0.4060
L3	0.3730	0.3330
L4	0.8267	0.4270
L5	0.8644	0.5070
L6	0.8726	0.4700
L7	0.5343	0.3320
L8	0.9090	0.4960
L9	0.9007	0.5360
LA	0.0022	0.0770
LC	0.8592	0.5180
LD	0.8340	0.4070
LF	0.8154	0.4490
LG	0.8574	0.5030
LH	0.7380	0.4450
LI	0.1925	0.2410
LJ	0.7516	0.4570
LK	0.3240	0.3190
LL	0.7275	0.4550
LM	0.5094	0.2910
LN	0.7617	0.4500
LO	0.8737	0.5190
LP	0.7729	0.4530
LQ	0.7595	0.4540
LR	0.7838	0.4430
LS	0.8284	0.5170
LT	0.8667	0.5220
LU	0.8528	0.5120
LW	0.8219	0.5080
LZ	0.8780	0.5340
N0	0.5303	0.3920
NA	0.7893	0.4960
NB	0.9142	0.5630

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
NC	0.7543	0.4330
ND	0.6012	0.4040
NE	0.6565	0.4580
NF	0.6801	0.4240
NG	0.7666	0.4680
NH	0.6655	0.3730
NI	0.4705	0.3110
NJ	0.8628	0.4660
NK	0.8895	0.4630
NM	0.7034	0.4540
NN	0.8550	0.4880
NO	0.7099	0.4780
NQ	0.7711	0.5090
NR	0.9115	0.2750
NT	0.0350	0.1220
NU	0.7071	0.2240
NW	0.8851	0.4900
NY	0.6540	0.4250
SA	0.8384	0.4900
SB	0.7290	0.4540
SC	0.6166	0.3780
SD	0.9279	0.5620
SE	0.8615	0.5220
SF	0.8798	0.5270
SG	0.7847	0.4290
SH	0.8555	0.5200
SI	0.8631	0.5100
SJ	0.3445	0.2800
SK	0.5872	0.4270
SL	0.8709	0.5300
SM	0.8863	0.5350
SP	0.7814	0.3450
SQ	0.7577	0.4580
SR	0.8755	0.5290
SS	0.6782	0.4560
ST	0.7307	0.3820
SU	0.4610	0.3320
SW	0.8379	0.3510
SX	0.0814	0.0890
SY	0.6789	0.4100
SZ	0.5934	0.2680