



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:03 AM UTC

PDB ID : 9N76 / pdb_00009n76
EMDB ID : EMD-49086
Title : SSU processome maturation and disassembly, State J
Authors : Buzovetsky, O.; Klinge, S.
Deposited on : 2025-02-05
Resolution : 4.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

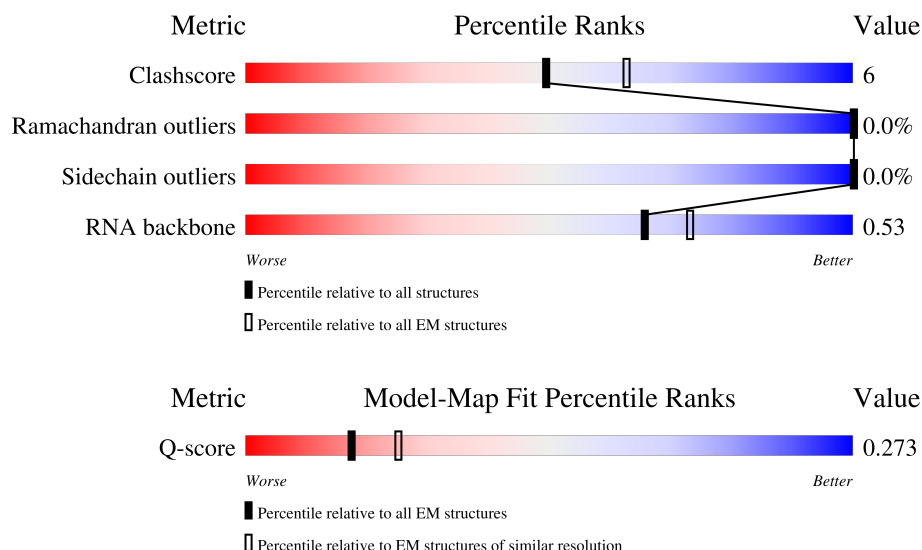
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5410 (3.70 - 4.70)

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 $\leq 5\%$. 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	700	
2	L1	1803	
3	L2	334	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	L3	146	
5	L4	261	
6	L5	225	
7	L6	236	
8	L7	190	
9	L8	200	
10	L9	197	
11	LC	143	
12	LD	156	
13	LE	130	
14	LF	135	
15	LG	67	
16	LH	896	
17	LI	713	
18	LJ	513	
19	LK	575	
20	LL	643	
21	LM	1769	
22	LN	776	
23	LO	923	
24	LP	440	
25	LQ	943	
26	LR	817	
27	LS	594	
28	LT	939	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	LZ	183	
30	NA	593	
31	NB	610	
32	ND	214	
33	NF	151	
34	NG	137	
35	NH	1237	
36	NI	297	
37	NL	318	
38	NM	255	
39	NP	144	
40	NQ	82	
41	NS	1267	
42	NV	733	
43	OH	143	
44	OU	152	
45	SA	504	
46	SB	511	
47	SC	327	
47	SD	327	
48	SE	126	
48	SF	126	
49	SG	573	
50	SH	367	
51	SI	1183	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	SJ	252	
52	SK	252	
53	SL	189	
54	SM	290	
55	SP	2493	
56	SQ	217	
57	SR	145	
58	SS	899	
59	ST	810	
60	SU	552	
61	SV	206	
62	SW	274	
63	SY	250	
64	SZ	483	

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 206690 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
1	L0	67	Total	C	N	O	P	0	0
			1437	641	258	471	67		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L1	1449	Total	C	N	O	P	0	0
			30918	13821	5521	10127	1449		

- Molecule 3 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L2	207	Total	C	N	O	P	0	0
			4394	1964	760	1462	208		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L3	106	Total	C	N	O	S	0	0
			862	545	159	156	2		

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L4	244	Total	C	N	O	S	0	0
			1936	1239	359	335	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L5	206	Total	C	N	O	S	0	0
			1635	1027	300	305	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L6	216	Total	C	N	O	S	0	0
			1740	1094	335	308	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L7	178	Total	C	N	O	S	0	0
			1427	918	251	258			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L8	170	Total	C	N	O	S	0	0
			1348	836	269	241	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L9	181	Total	C	N	O	S	0	0
			1470	930	285	254	1		

- Molecule 11 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LC	128	Total	C	N	O	S	0	0
			997	642	178	177			

- Molecule 12 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LD	137	Total	C	N	O	S	0	0
			1112	714	212	183	3		

- Molecule 13 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LE	129	Total	C	N	O	S	0	0
			1022	650	188	181	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	LF	130	Total	C	N	O		
			1046	662	204	180	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LG	62	Total	C	N	O	S		
			490	302	98	89	1	0	0

- Molecule 16 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH	806	Total	C	N	O	S		
			6449	4113	1087	1230	19	0	0

- Molecule 17 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LI	600	Total	C	N	O	S		
			3792	2375	679	733	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LJ	476	Total	C	N	O	S		
			3773	2376	675	711	11	0	0

- Molecule 19 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LK	132	Total	C	N	O	S		
			1068	681	185	199	3	0	0

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LL	487	Total	C	N	O	S		
			3871	2458	662	738	13	0	0

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LM	1599	Total	C	N	O	S	0	0
			9274	5735	1730	1797	12		

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LN	663	Total	C	N	O	S	0	0
			5263	3333	913	995	22		

- Molecule 23 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LO	792	Total	C	N	O	S	0	0
			6321	4038	1086	1179	18		

- Molecule 24 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	LP	379	Total	C	N	O	0	0
			1901	1143	379	379		

- Molecule 25 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LQ	816	Total	C	N	O	S	0	0
			6494	4152	1089	1226	27		

- Molecule 26 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LR	793	Total	C	N	O	S	0	0
			6207	3931	1044	1203	29		

- Molecule 27 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	LS	463	Total	C	N	O	P	S	0	0
			3662	2326	643	683	1	9		

- Molecule 28 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LT	871	Total	C	N	O	S	0	0
			6787	4306	1170	1289	22		

- Molecule 29 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LZ	142	Total	C	N	O	S	0	0
			1173	743	214	210	6		

- Molecule 30 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	NA	330	Total	C	N	O	S	0	0
			2426	1496	436	490	4		

- Molecule 31 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	NB	262	Total	C	N	O	S	0	0
			1645	1010	318	316	1		

- Molecule 32 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	ND	74	Total	C	N	O	0	0
			564	351	115	98		

- Molecule 33 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	NF	141	Total	C	N	O	S	0	0
			1135	725	214	194	2		

- Molecule 34 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	NG	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 35 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	NH	1077	Total	C	N	O	S	0	0
			8693	5650	1434	1585	24		

- Molecule 36 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	NI	240	Total	C	N	O	S	0	0
			1953	1248	331	366	8		

- Molecule 37 is a protein called Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	NL	285	Total	C	N	O	S	0	0
			2285	1461	405	406	13		

- Molecule 38 is a protein called Small ribosomal subunit protein eS1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	NM	237	Total	C	N	O	S	0	0
			1891	1195	350	342	4		

- Molecule 39 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	NP	134	Total	C	N	O	S	0	0
			1040	653	193	192	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	NQ	79	Total	C	N	O	S	0	0
			595	371	108	111	5		

- Molecule 41 is a protein called Probable ATP-dependent RNA helicase DHR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	NS	931	Total	C	N	O	S	0	0
			5051	3071	1001	977	2		

- Molecule 42 is a protein called Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	NV	19	Total	C	N	O	0	0
			149	94	34	21		

- Molecule 43 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	OH	120	Total	C	N	O	0	0
			594	354	120	120		

- Molecule 44 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	OU	56	Total	C	N	O	0	0
			278	166	56	56		

- Molecule 45 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SA	397	Total	C	N	O	S	1	0
			3100	1964	534	593	9		

- Molecule 46 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SB	422	Total	C	N	O	S	0	0
			3255	2056	555	634	10		

- Molecule 47 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SC	240	Total	C	N	O	S	1	0
			1865	1181	335	339	10		
47	SD	238	Total	C	N	O	S	0	0
			1850	1171	333	336	10		

- Molecule 48 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SE	121	Total	C	N	O	S	0	0
			916	583	158	171	4		
48	SF	121	Total	C	N	O	S	0	0
			916	583	158	171	4		

- Molecule 49 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SG	459	Total	C	N	O	S	0	0
			3672	2331	645	686	10		

- Molecule 50 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

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

- Molecule 51 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SI	758	Total	C	N	O	S	0	0
			6144	3946	1097	1074	27		

- Molecule 52 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	SJ	213	Total	C	N	O	0	0
			1074	648	213	213		
52	SK	229	Total	C	N	O	0	0
			1160	702	229	229		

- Molecule 53 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SL	148	Total	C	N	O	S	0	0
			1171	750	209	202	10		

- Molecule 54 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SM	247	Total	C	N	O	S	0	0
			2009	1260	379	363	7		

- Molecule 55 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SP	1852	Total	C	N	O	S	0	0
			15102	9753	2498	2804	47		

- Molecule 56 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SQ	107	Total	C	N	O	S	0	0
			885	555	165	162	3		

- Molecule 57 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SR	134	Total	C	N	O	S	0	0
			1052	668	204	178	2		

- Molecule 58 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SS	94	Total	C	N	O	S	0	0
			791	491	152	139	9		

- Molecule 59 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	ST	597	Total	C	N	O	S	0	0
			3455	2108	682	662	3		

- Molecule 60 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SU	532	Total	C	N	O		0	0
			2703	1639	532	532			

- Molecule 61 is a protein called Regulator of rDNA transcription protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SV	155	Total	C	N	O		0	0
			852	512	176	164			

- Molecule 62 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SW	213	Total	C	N	O	S	0	0
			1669	1063	303	299	4		

- Molecule 63 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SY	201	Total	C	N	O	S	0	0
			1715	1068	335	306	6		

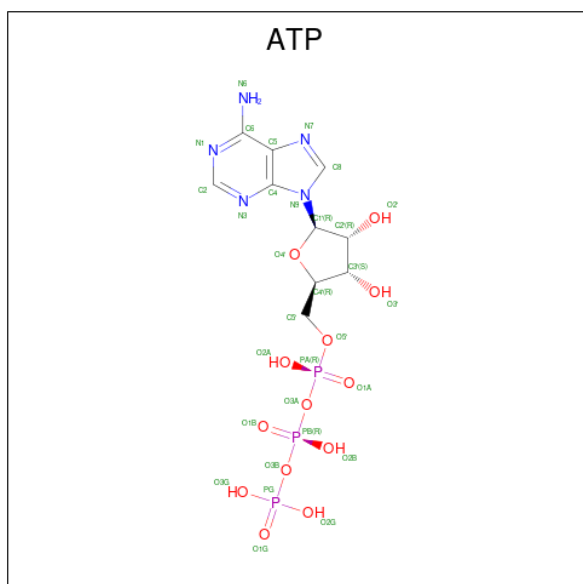
- Molecule 64 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SZ	259	Total	C	N	O		0	0
			1314	796	259	259			

- Molecule 65 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
65	L1	35	Total	Mg	0
			35	35	
65	NH	1	Total	Mg	0
			1	1	
65	NS	1	Total	Mg	0
			1	1	
65	SI	1	Total	Mg	0
			1	1	

- Molecule 66 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

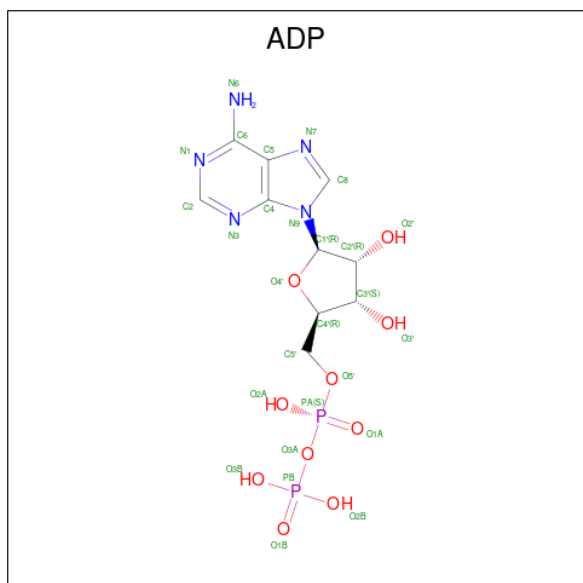


Mol	Chain	Residues	Atoms					AltConf
66	NH	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 67 is ZINC ION (CCD ID: ZN) (formula: Zn).

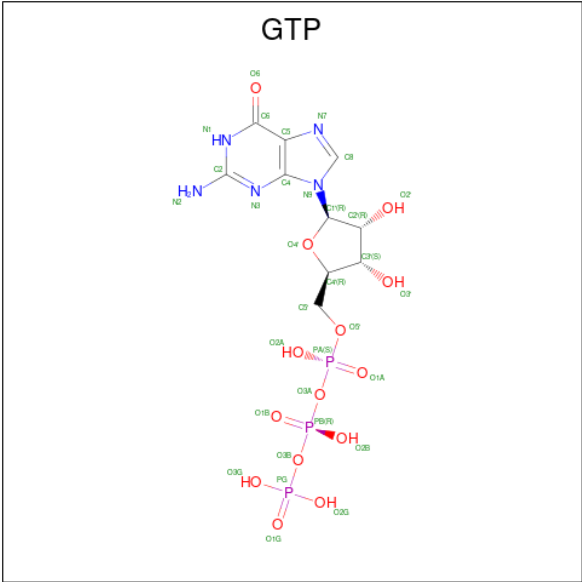
Mol	Chain	Residues	Atoms		AltConf
67	NQ	1	Total	Zn	0
			1	1	
67	SL	1	Total	Zn	0
			1	1	

- Molecule 68 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 69 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

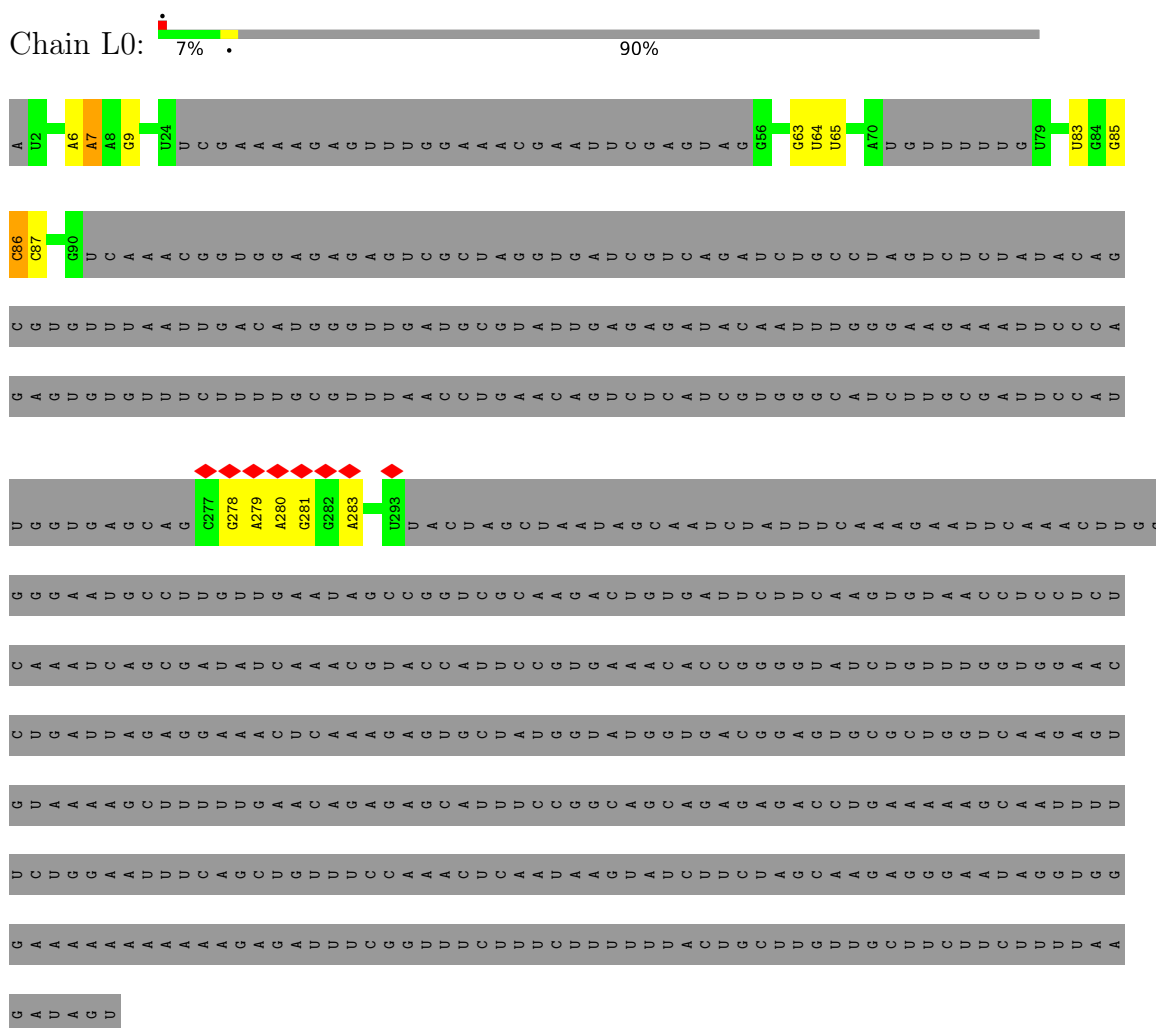


Mol	Chain	Residues	Atoms					AltConf
69	SI	1	Total	C	N	O	P	0
			32	10	5	14	3	

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



• Molecule 2: 18S rRNA

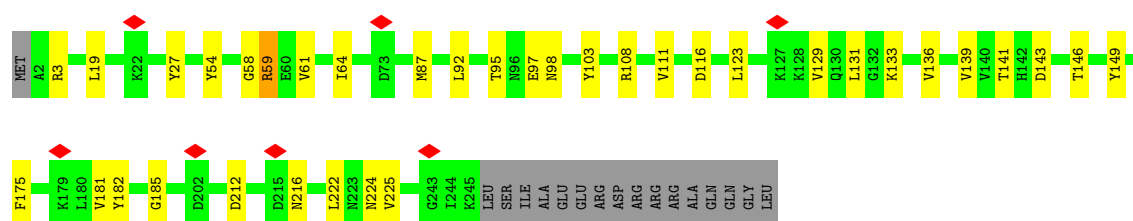




HIS
ARG
GLY
ILE
ARG
HIS
PHE
TRP
GLY
LEU
ARG
VAL
ARG
GLY
GLN
HIS
THR
LYS
THR
THR
GLY
ARG
ARG
ARG
ALA

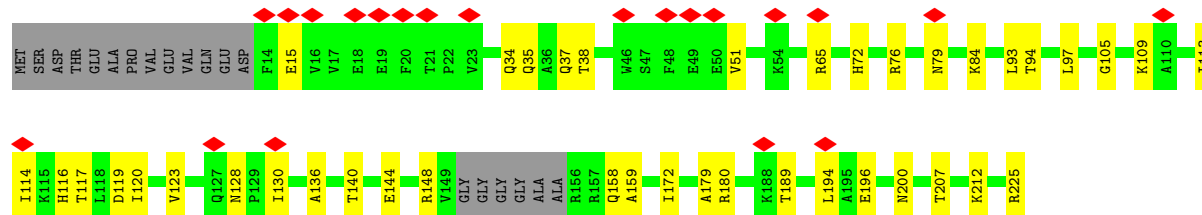
• Molecule 5: 40S ribosomal protein S4-A

Chain L4:  80% 13% 7%



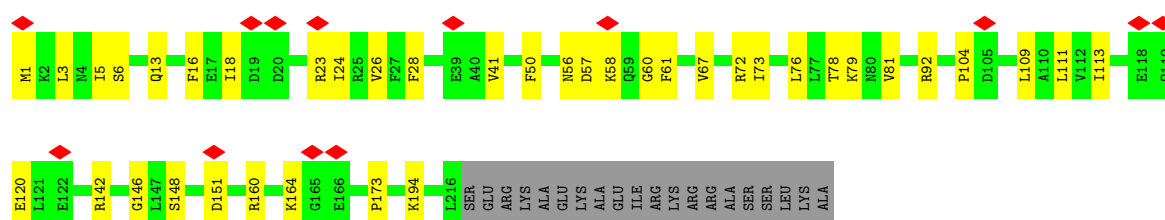
• Molecule 6: 40S ribosomal protein S5

Chain L5:  9% 73% 18% 8%



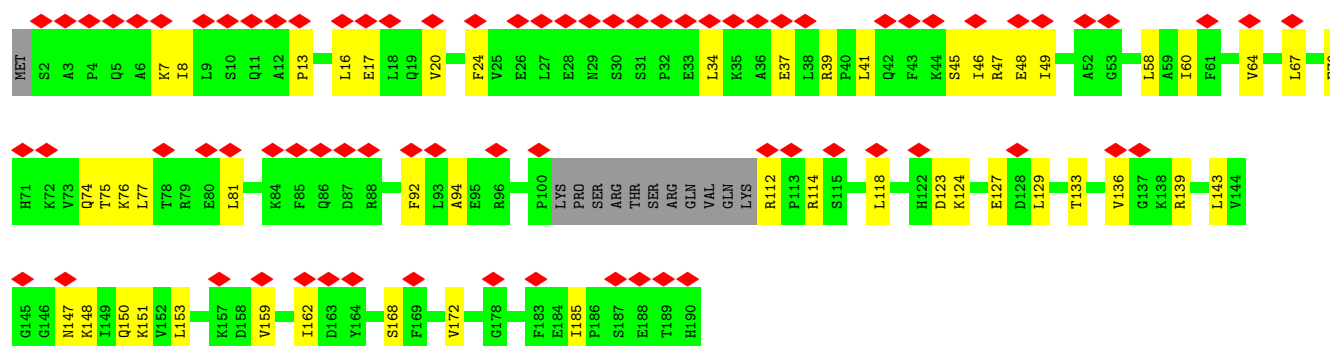
• Molecule 7: 40S ribosomal protein S6-A

Chain L6:  6% 75% 17% 8%



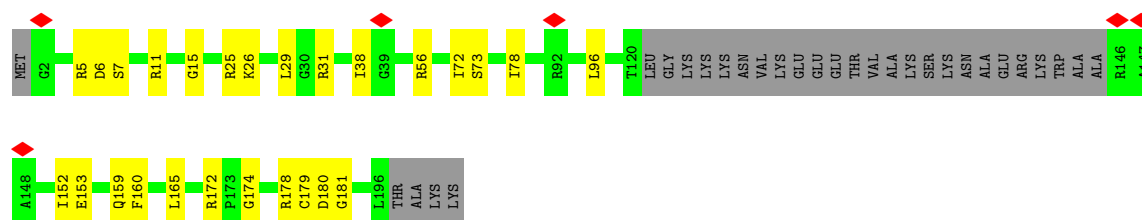
• Molecule 8: 40S ribosomal protein S7-A

Chain L7:  40% 68% 26% 6%



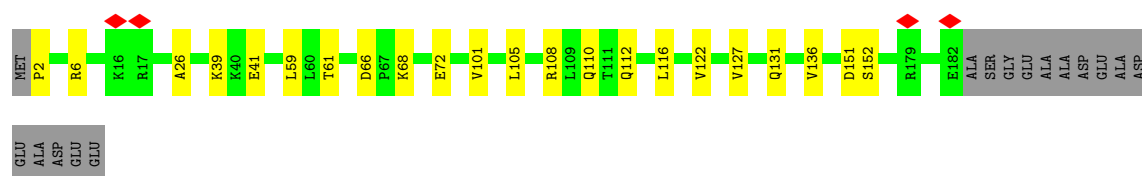
- Molecule 9: 40S ribosomal protein S8-A

Chain L8: 



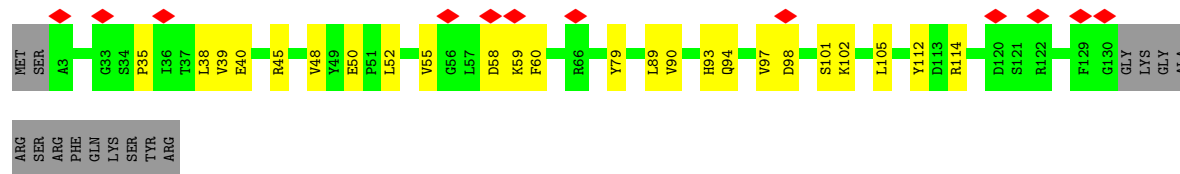
- Molecule 10: 40S ribosomal protein S9-A

Chain L9: 



- Molecule 11: 40S ribosomal protein S16-A

Chain LC: 



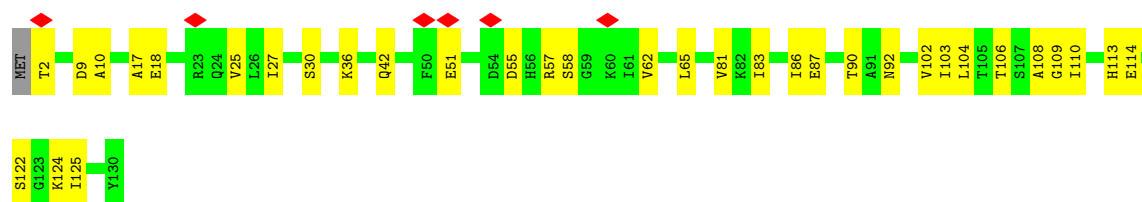
- Molecule 12: 40S ribosomal protein S11-A

Chain LD: 



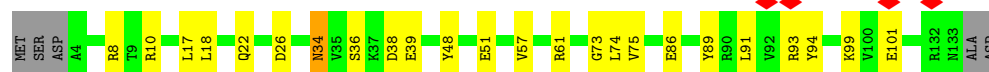
- Molecule 13: 40S ribosomal protein S22-A

Chain LE: 



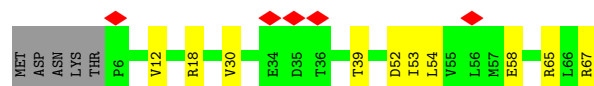
- Molecule 14: 40S ribosomal protein S24-A

Chain LF:  79% 17%



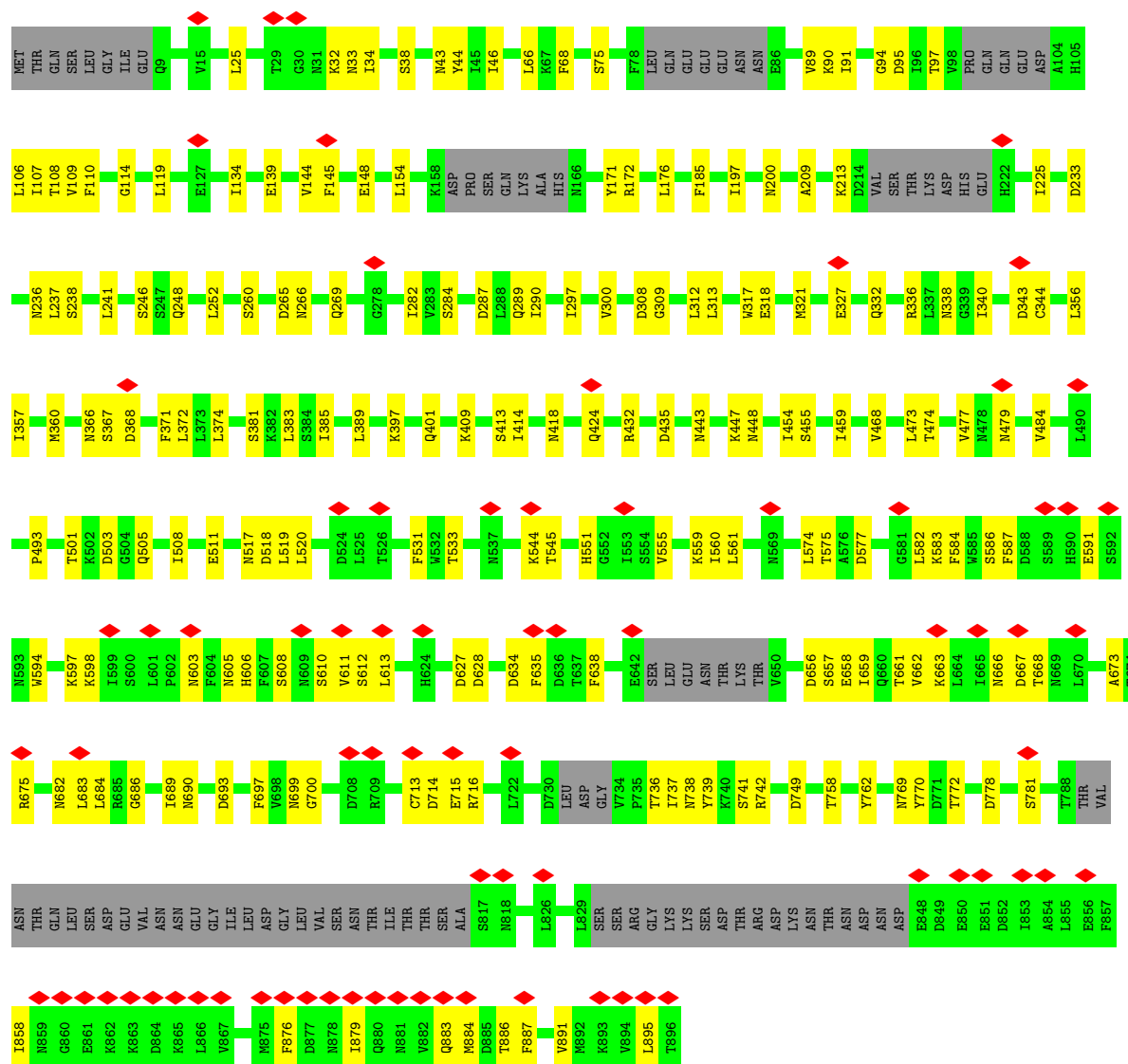
- Molecule 15: 40S ribosomal protein S28-A

Chain LG:  7% 78% 15% 7%

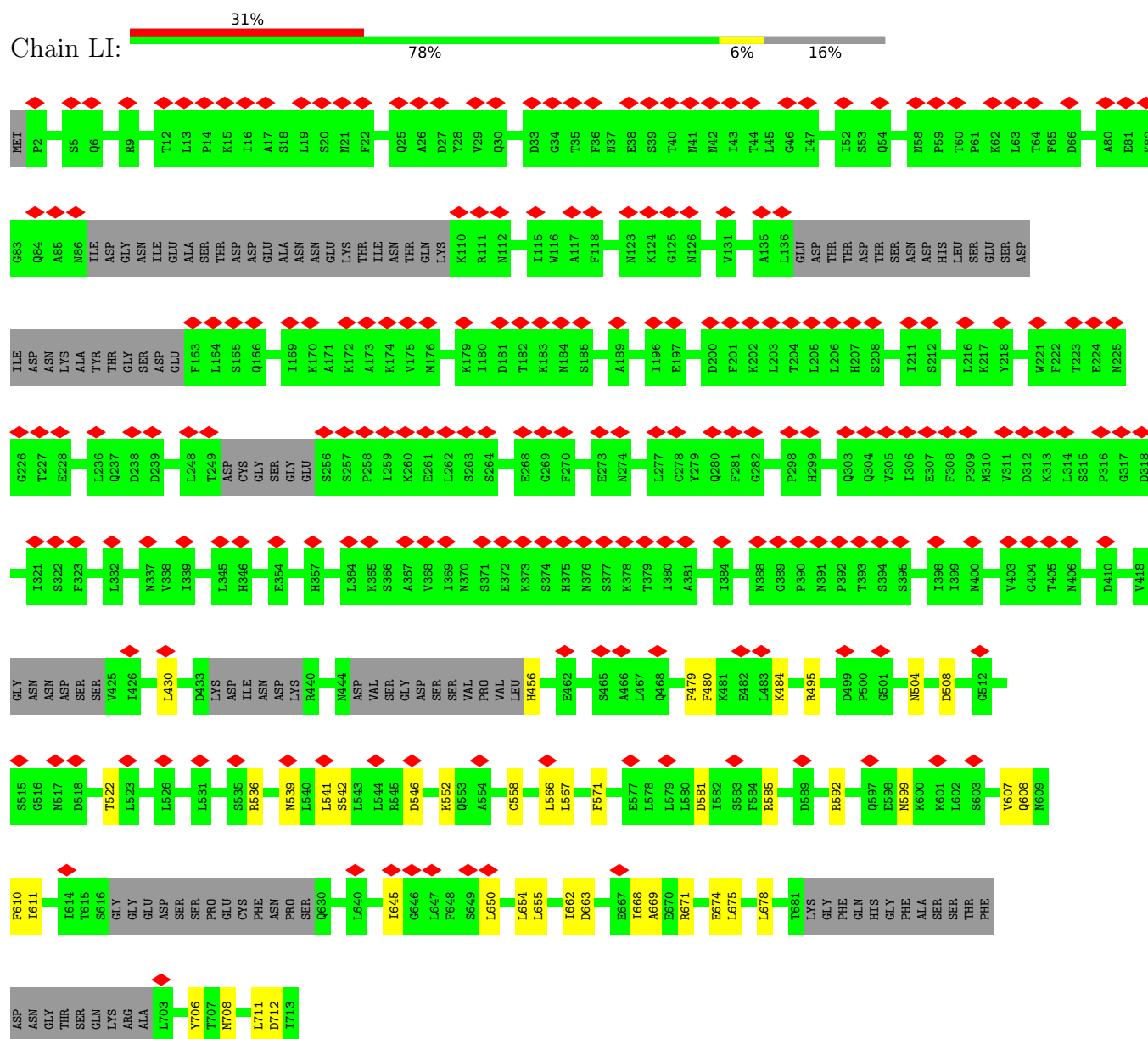


- Molecule 16: NET1-associated nuclear protein 1

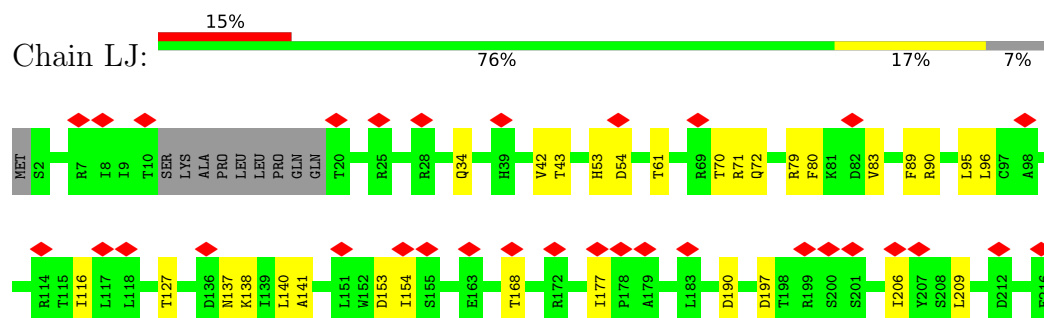
Chain LH:  9% 68% 22% 10%

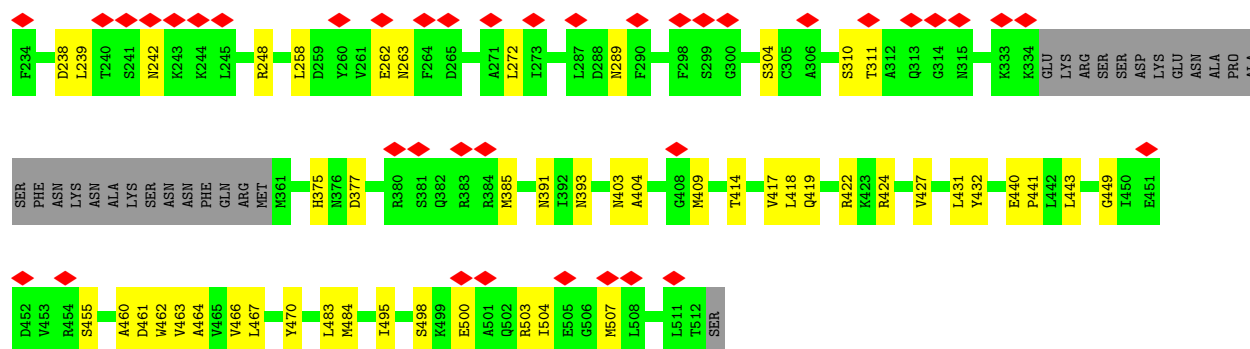


• Molecule 17: U3 small nucleolar RNA-associated protein 8



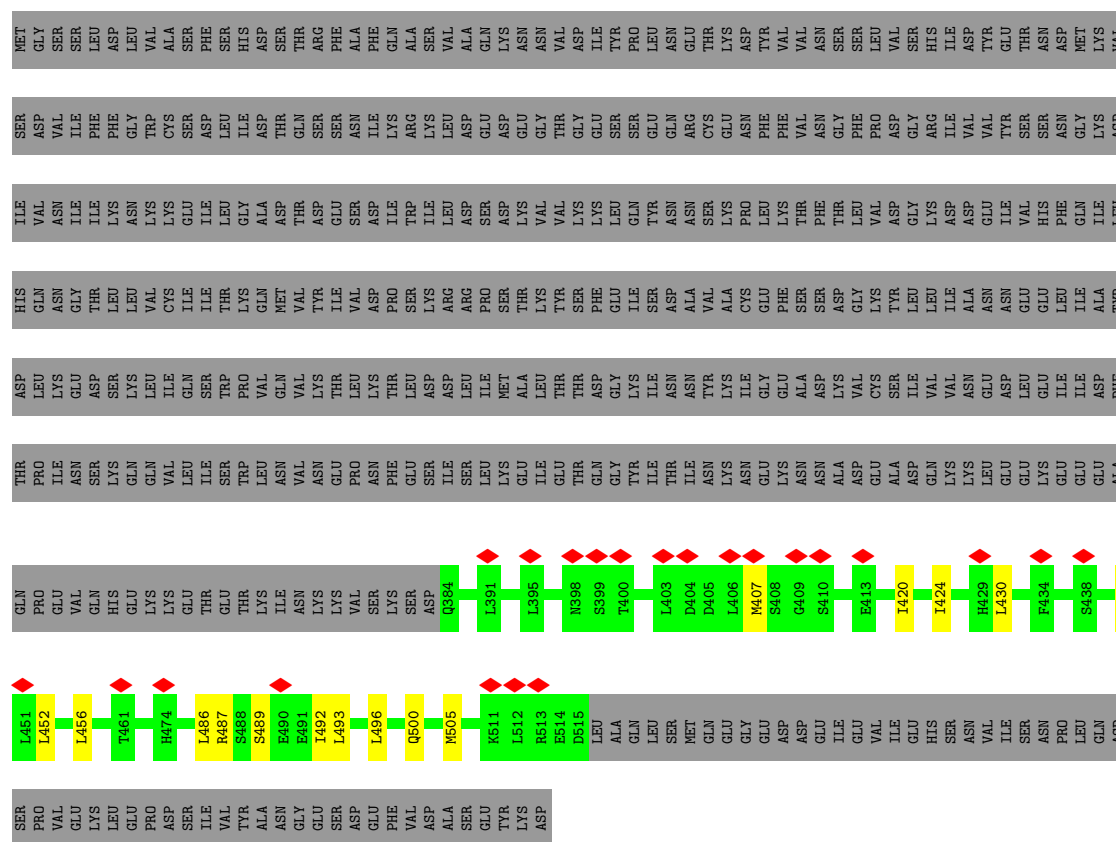
• Molecule 18: U3 small nucleolar RNA-associated protein 15





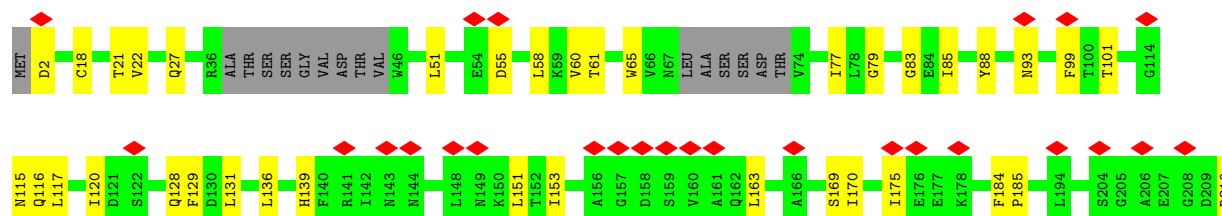
• Molecule 19: U3 small nucleolar RNA-associated protein 9

Chain LK: 20% 77%

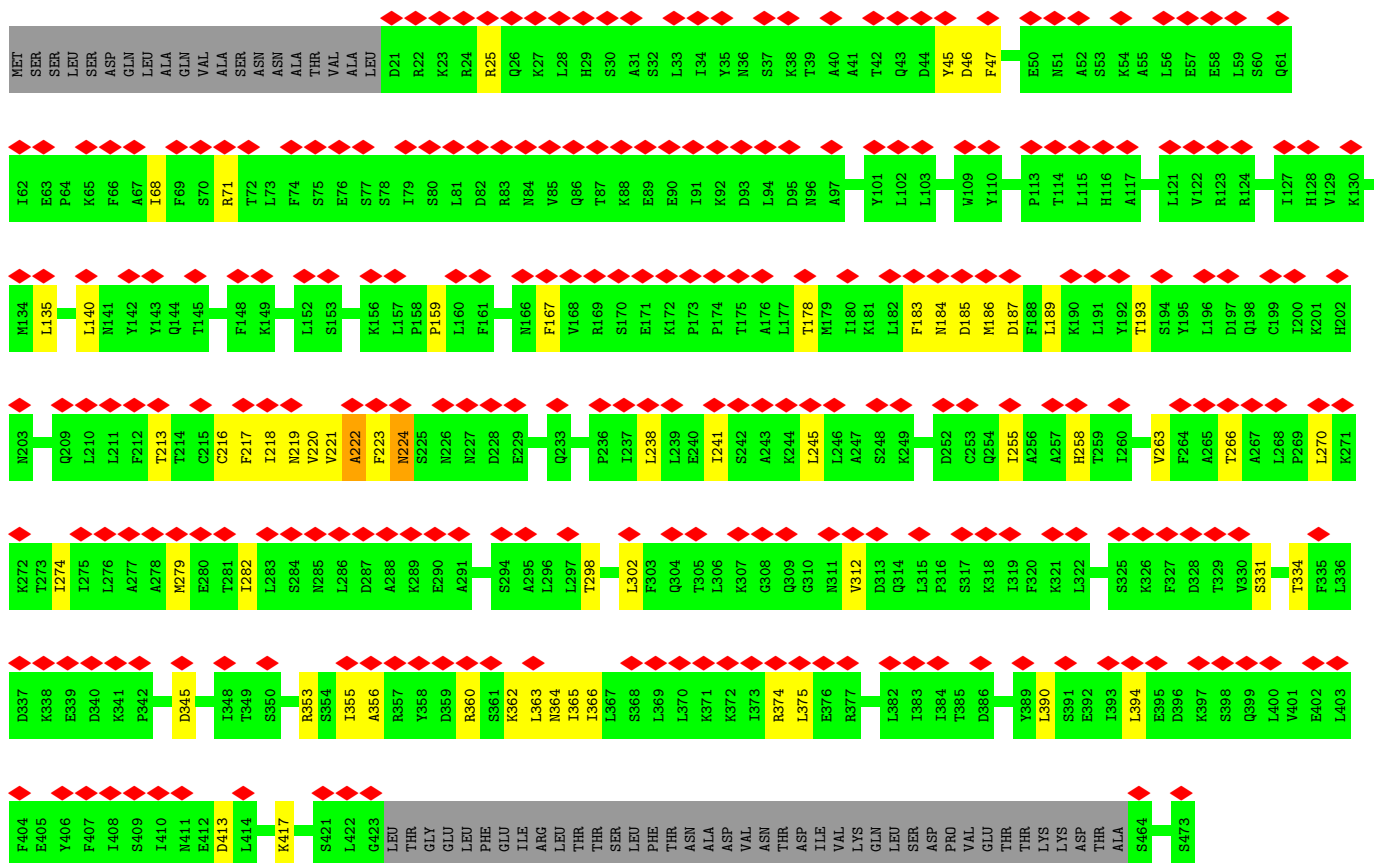
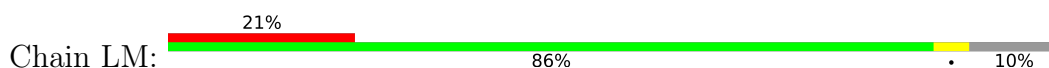


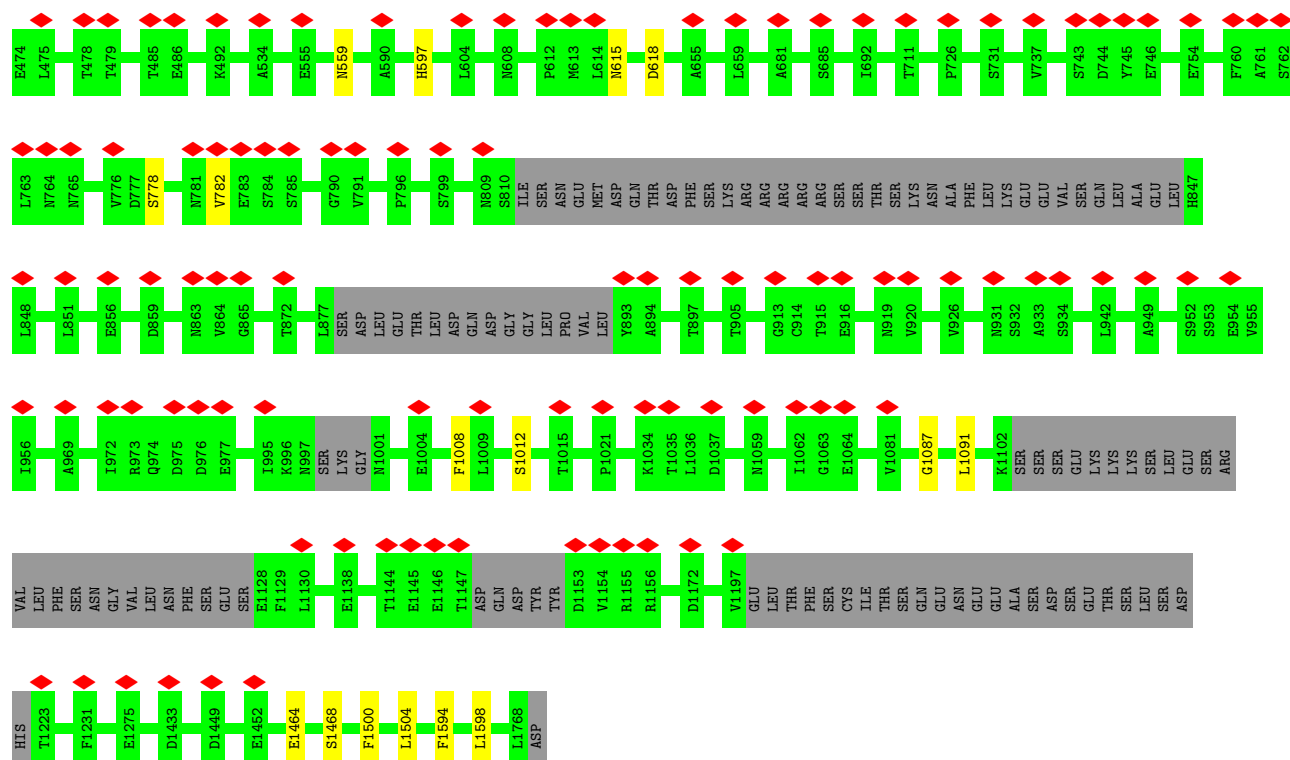
• Molecule 20: U3 small nucleolar RNA-associated protein 5

Chain LL: 14% 61% 14% 24%



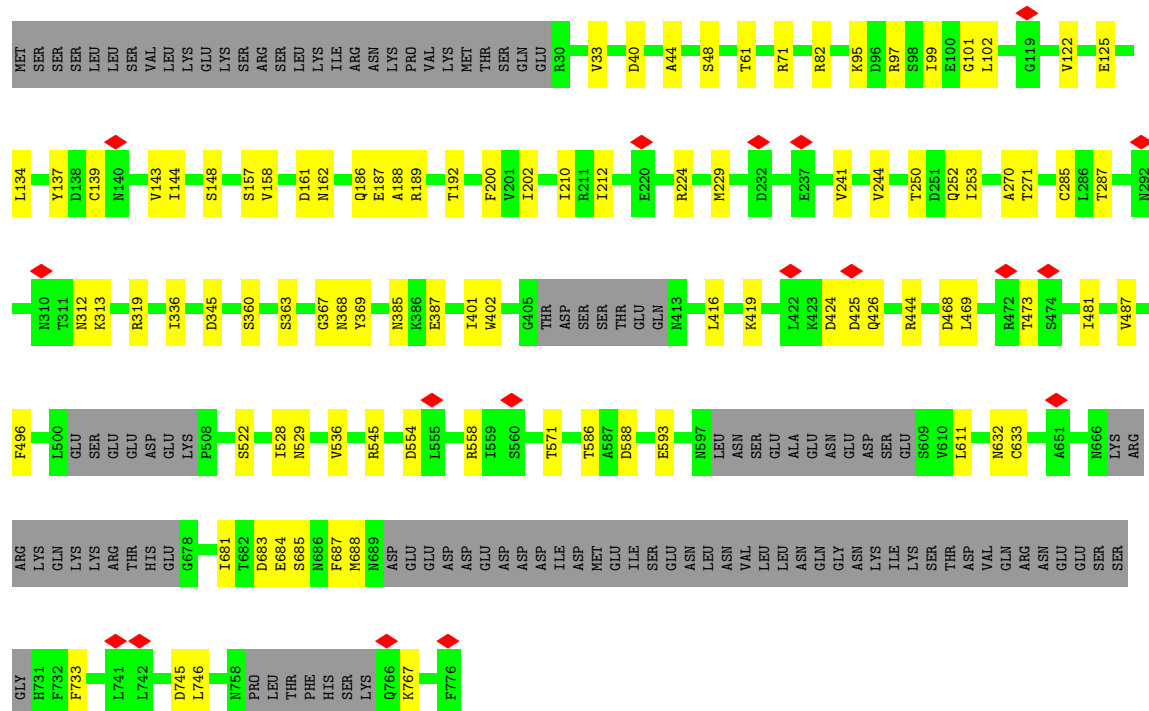
- Molecule 21: U3 small nucleolar RNA-associated protein 10



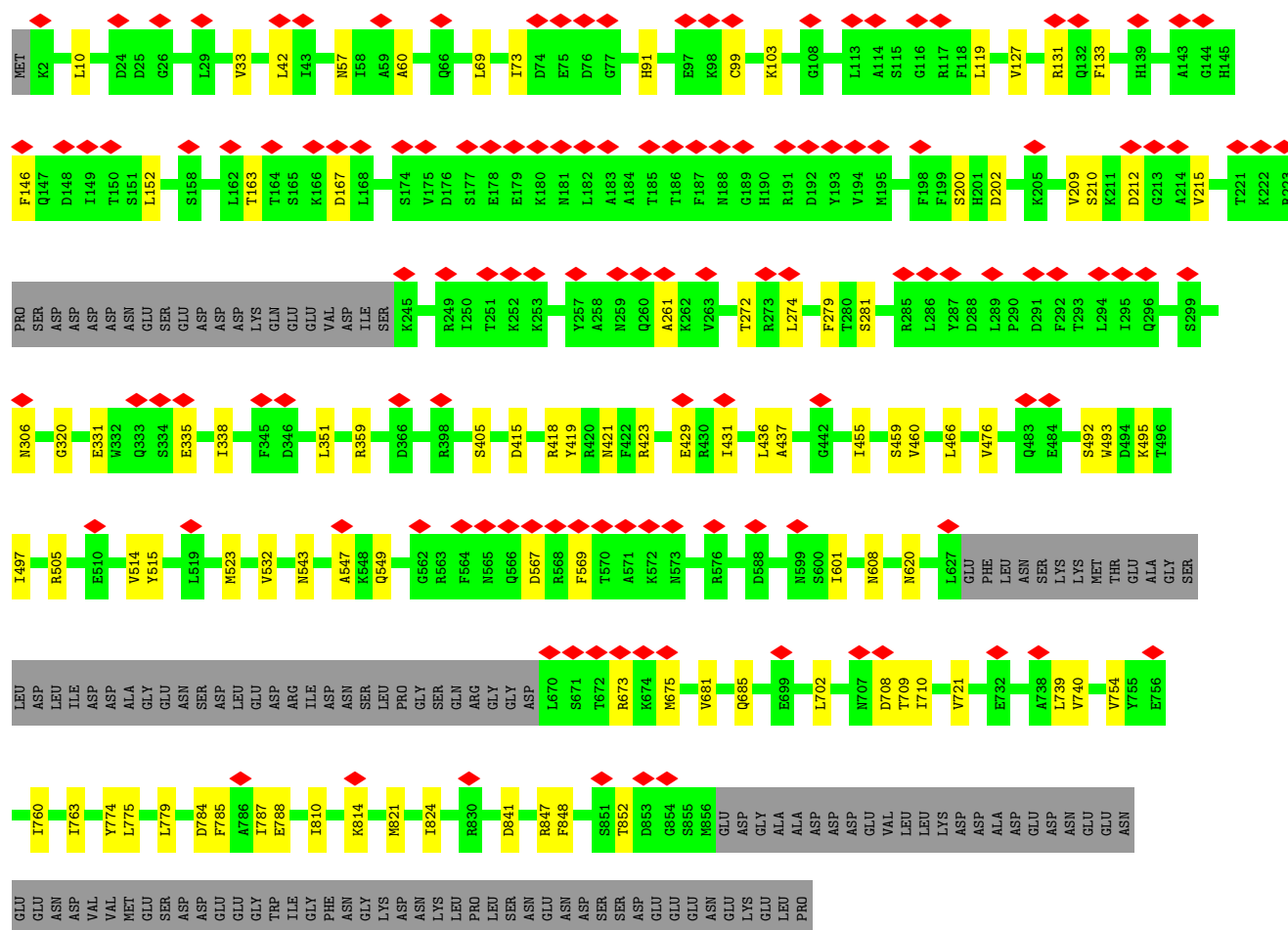
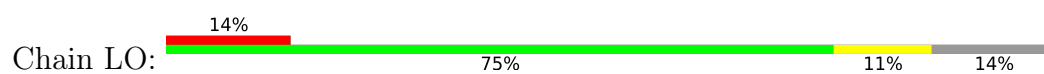


- Molecule 22: U3 small nucleolar RNA-associated protein 4

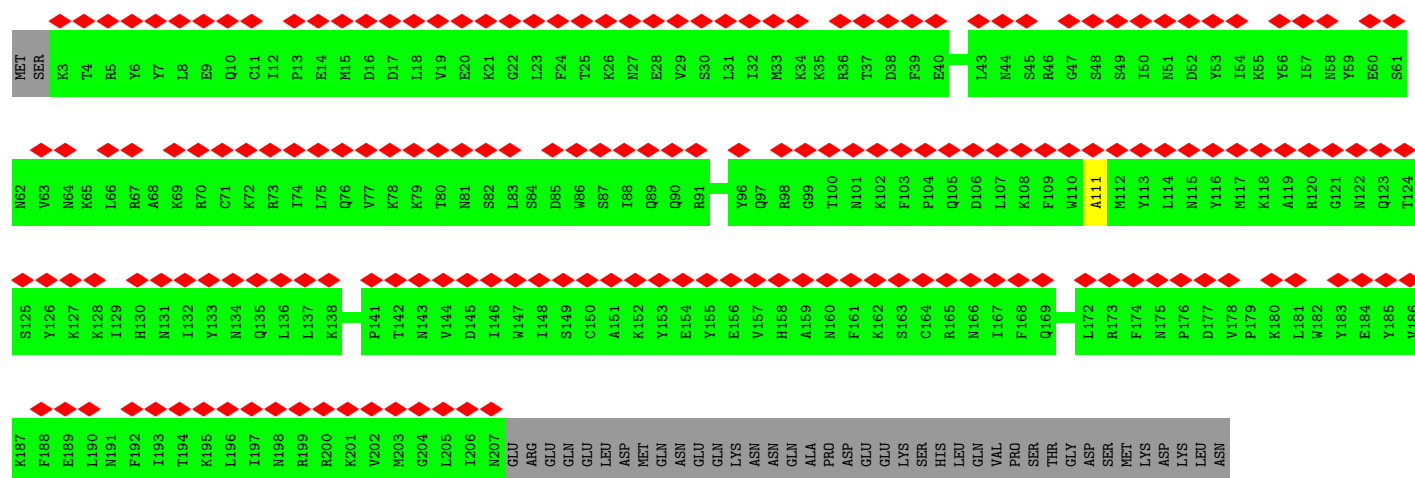
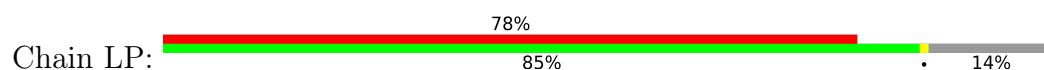
Chain LN: 73% 12% 15%

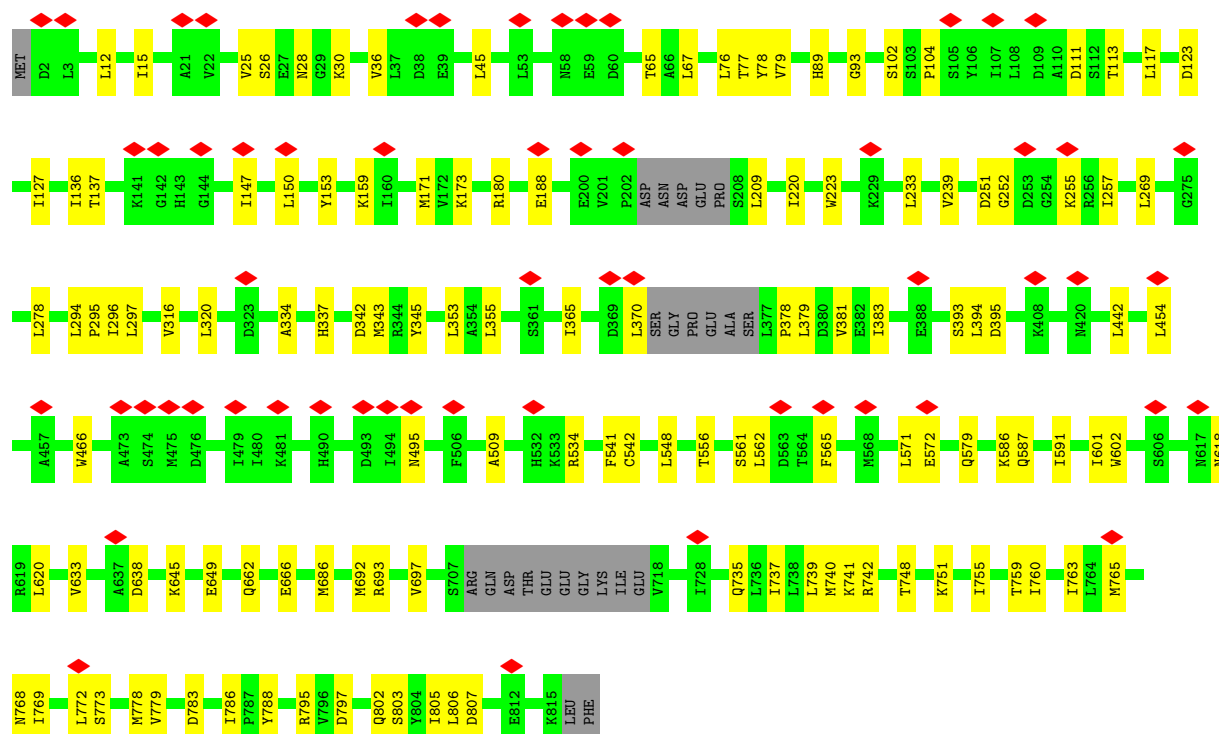


- Molecule 23: Periodic tryptophan protein 2

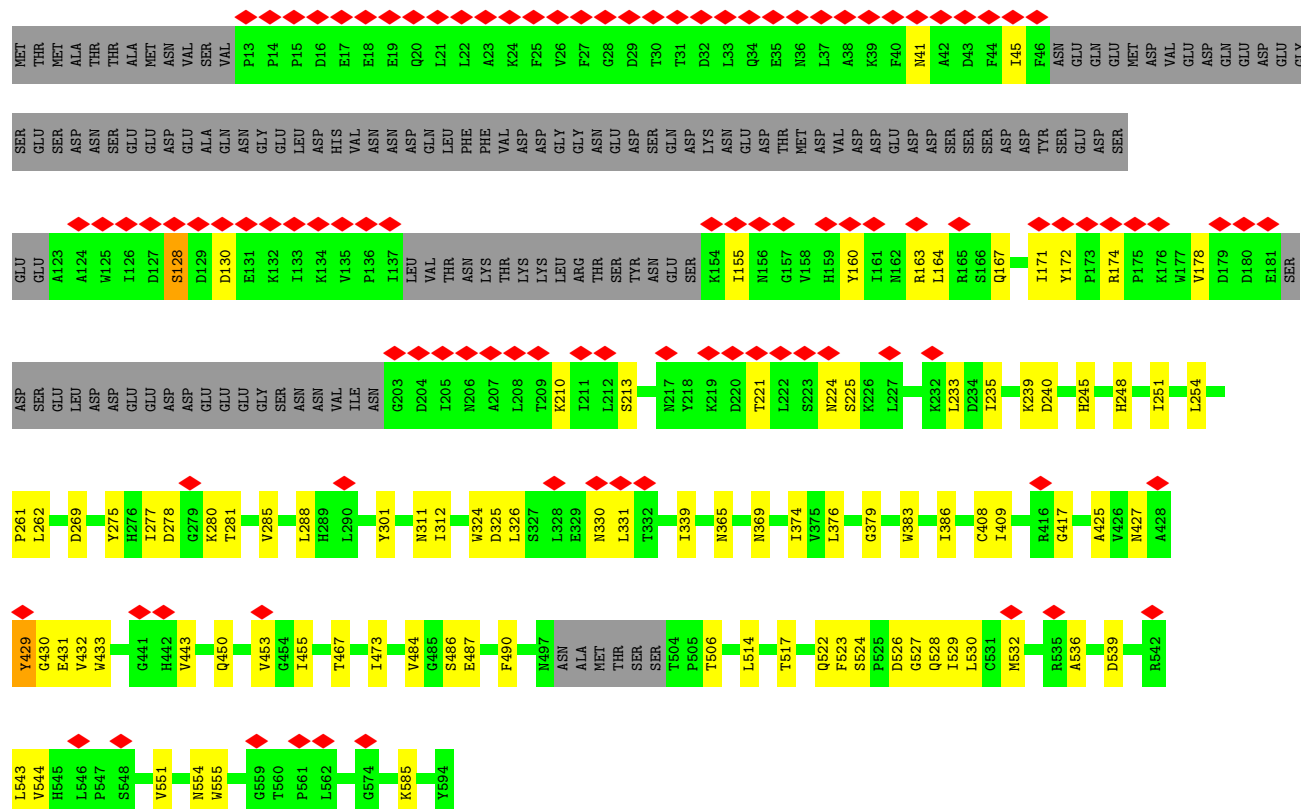


• Molecule 24: U3 small nucleolar RNA-associated protein 6

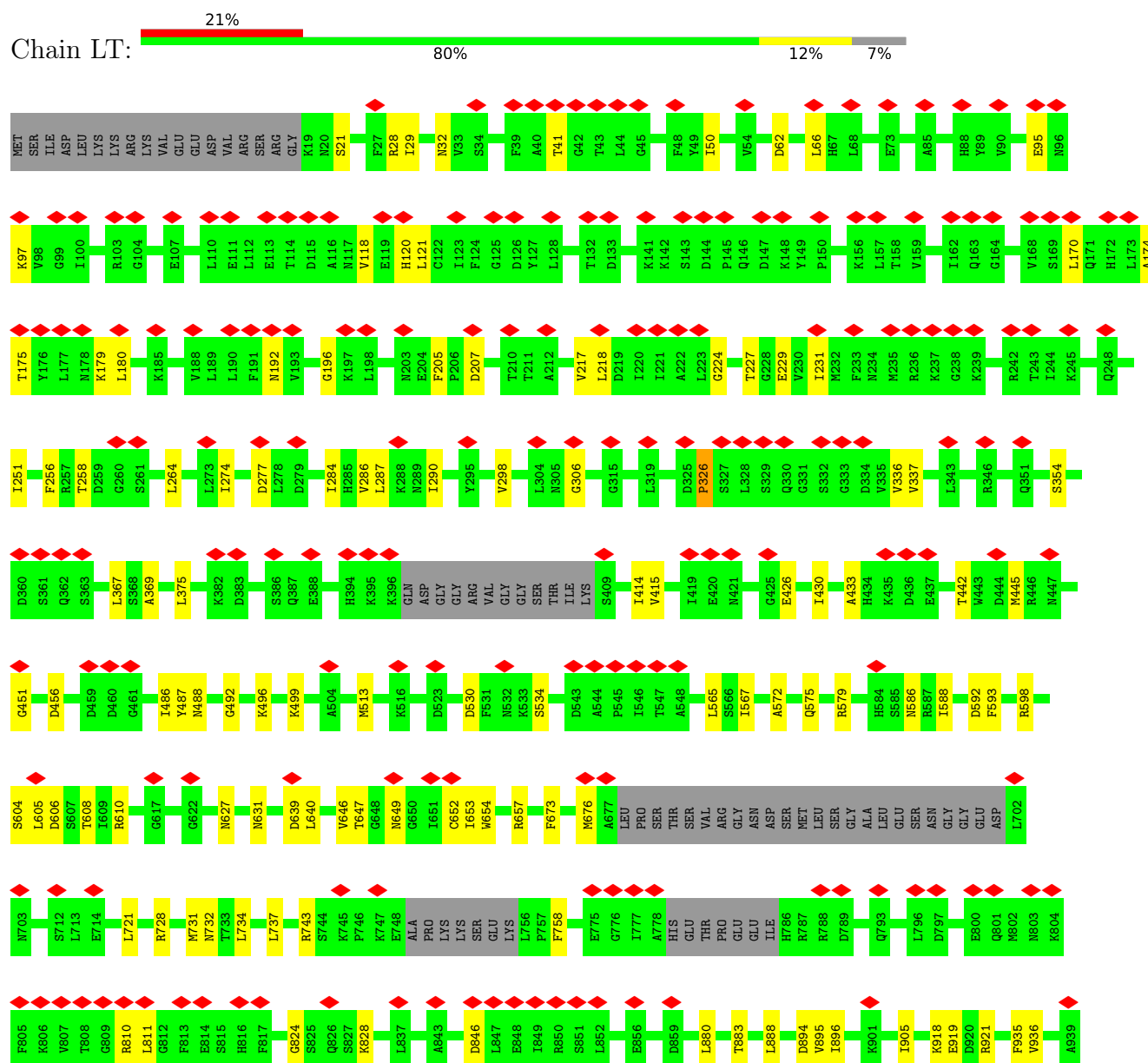




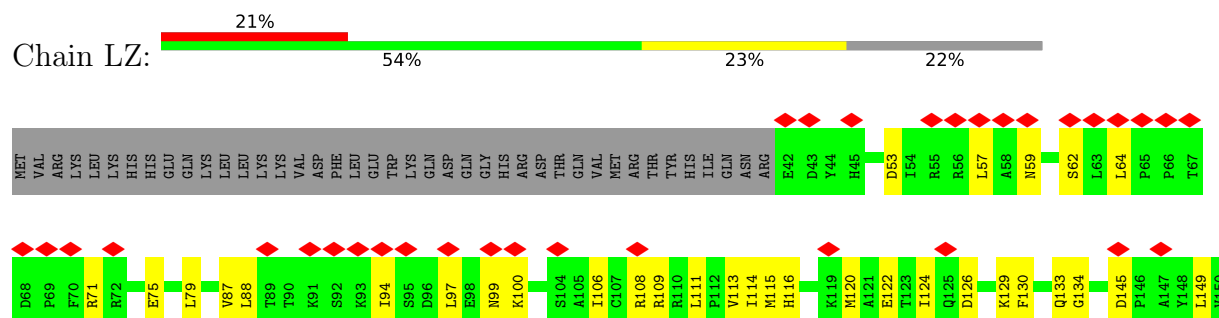
• Molecule 27: U3 small nucleolar RNA-associated protein 18

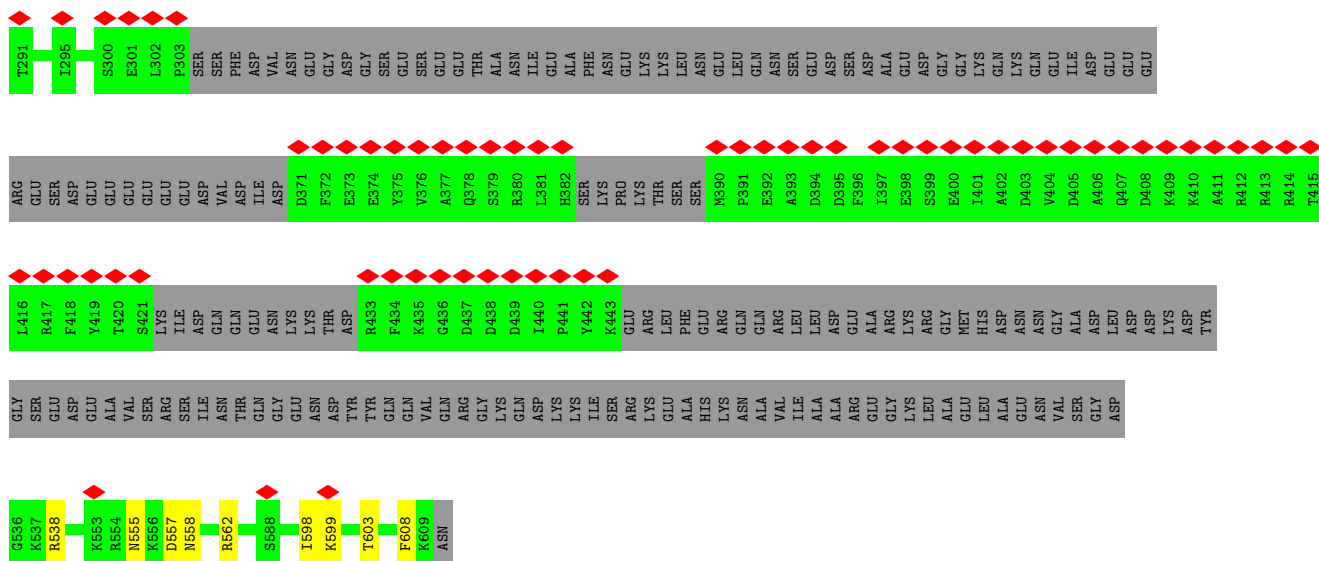


• Molecule 28: U3 small nucleolar RNA-associated protein 21

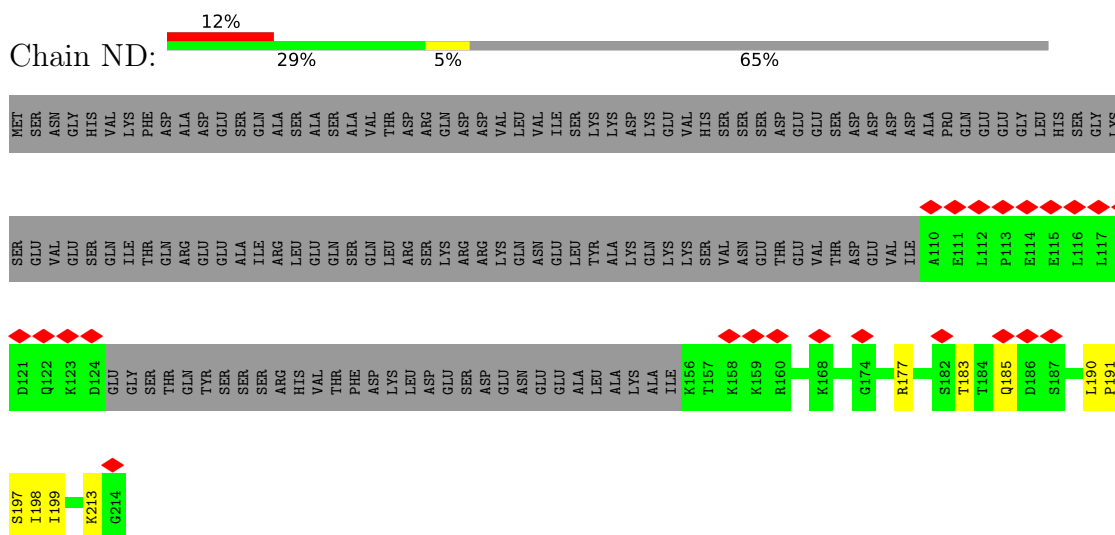


• Molecule 29: U3 small nucleolar ribonucleoprotein protein IMP3

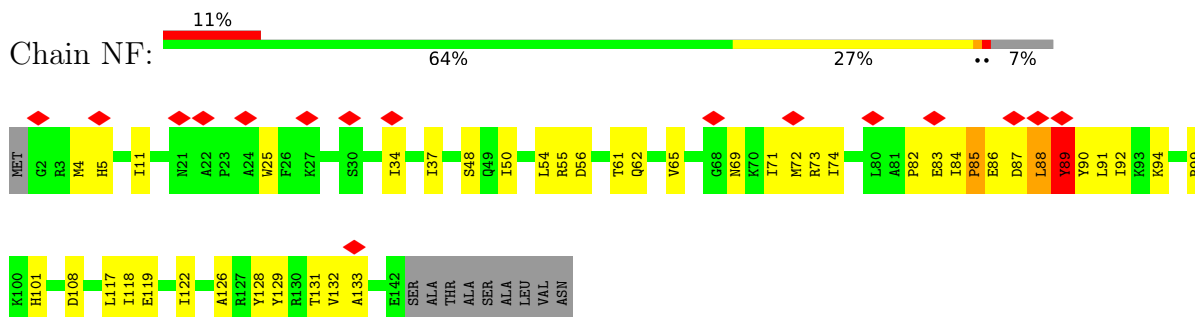




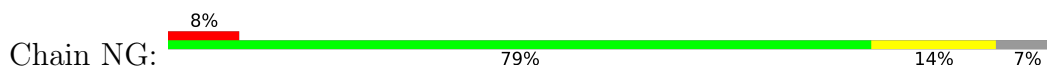
- Molecule 32: Bud site selection protein 21

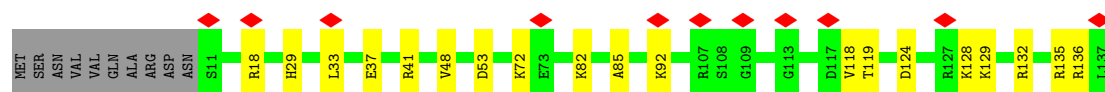


- Molecule 33: 40S ribosomal protein S13

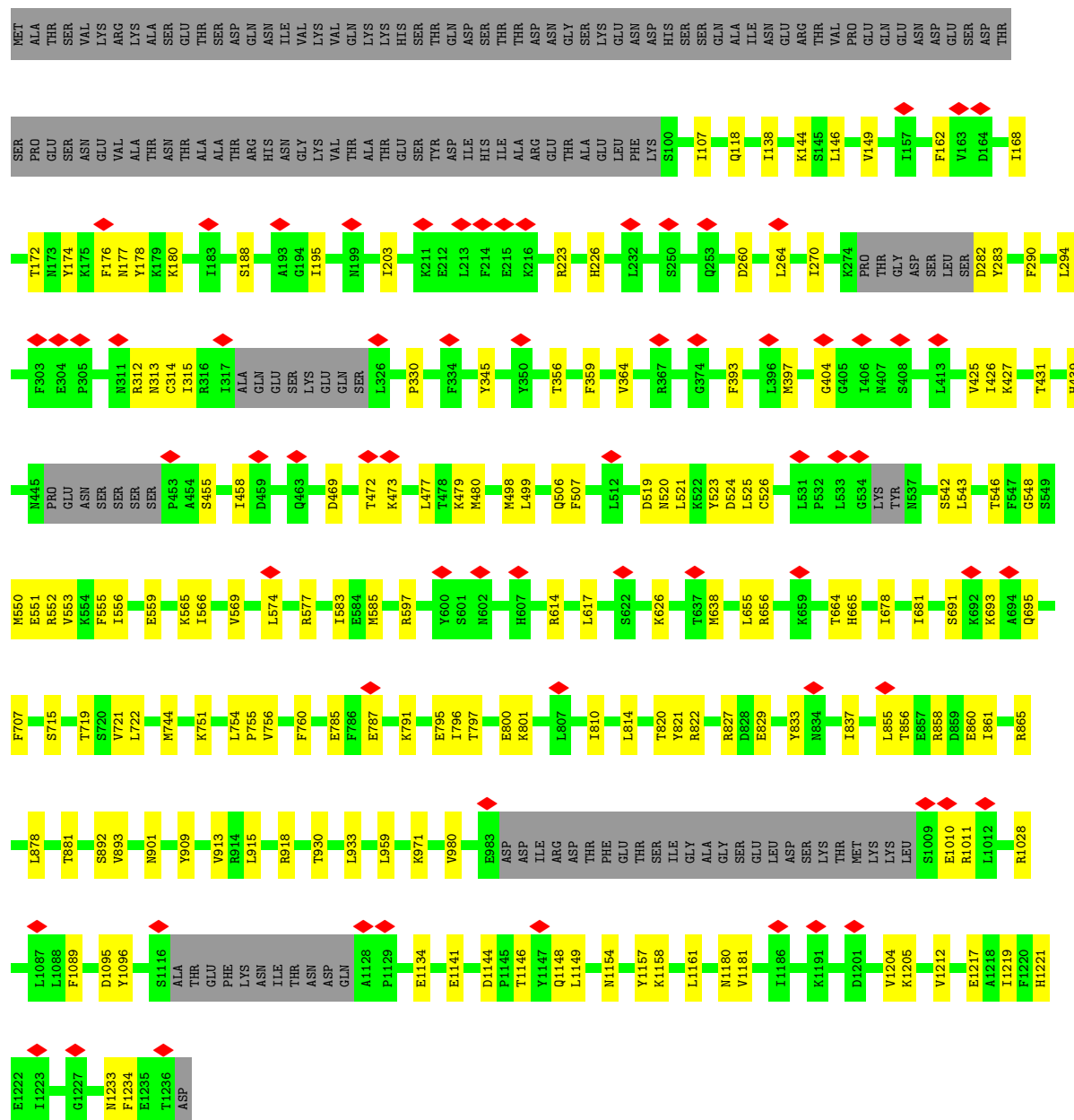
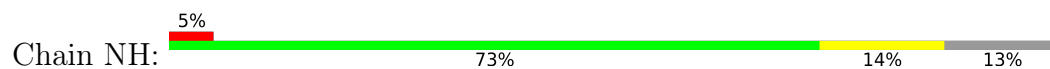


- Molecule 34: 40S ribosomal protein S14-A

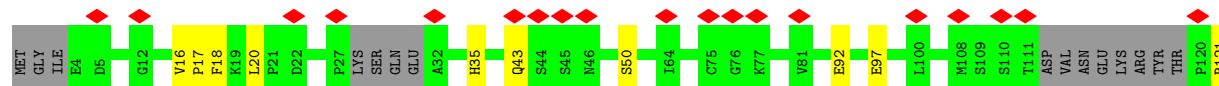


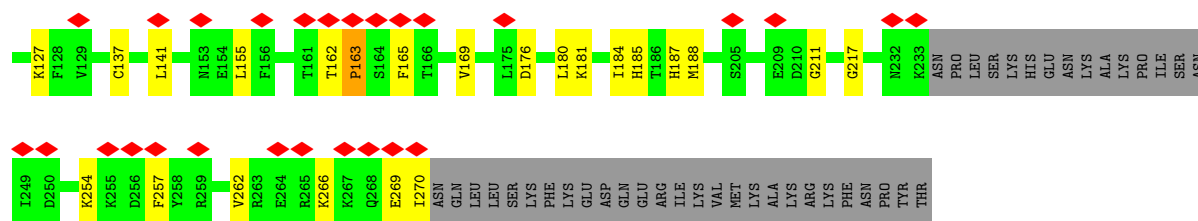


- Molecule 35: U3 small nucleolar RNA-associated protein 22

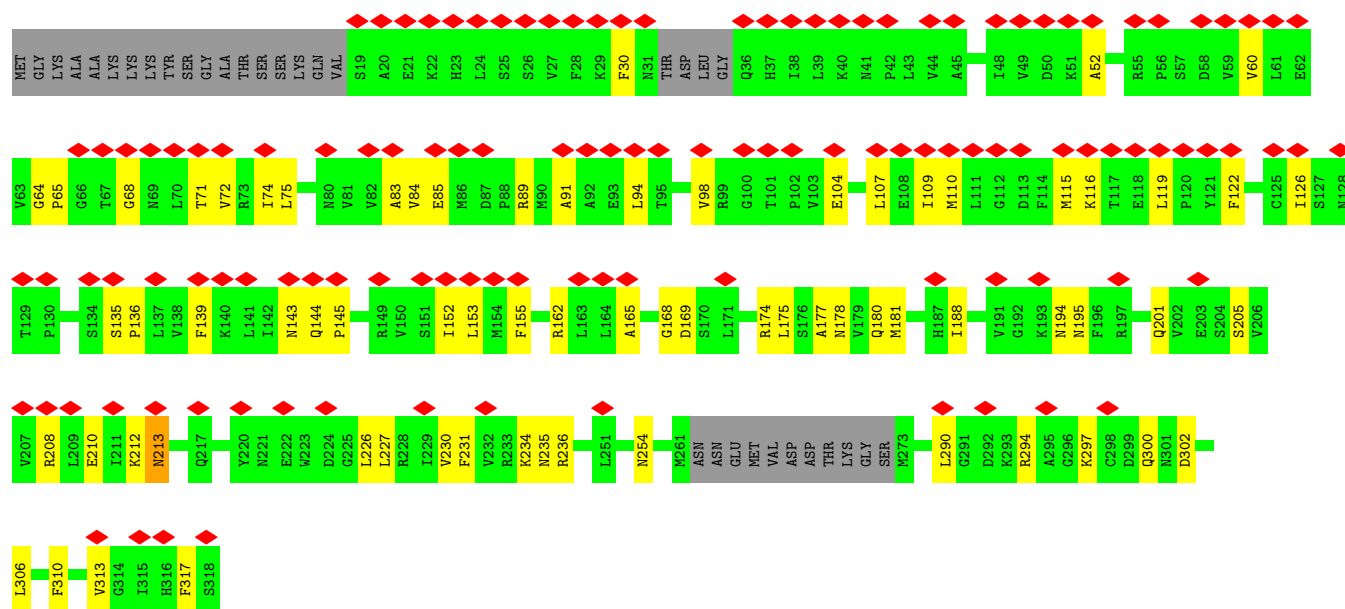
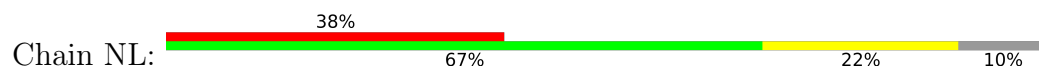


- Molecule 36: Ribosomal RNA-processing protein 7

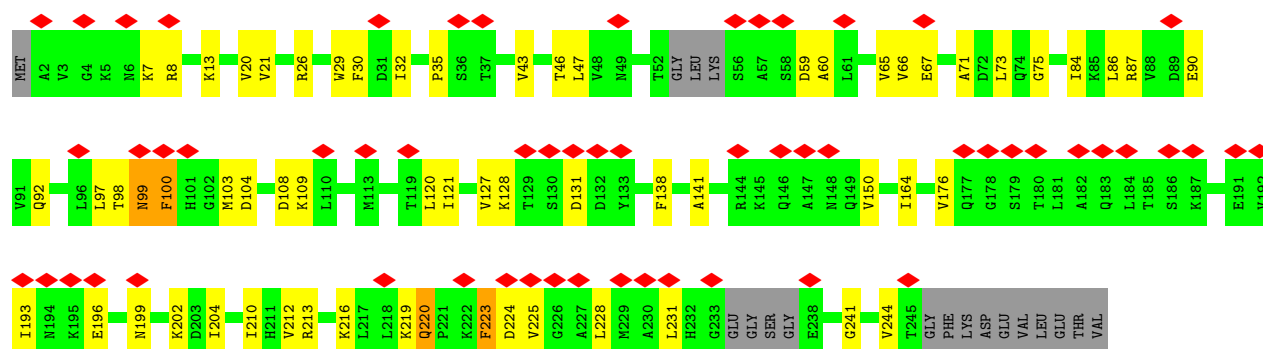




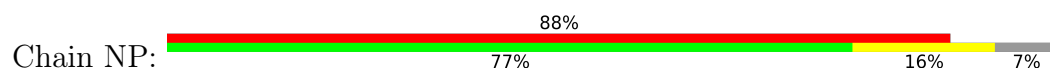
• Molecule 37: Dimethyladenosine transferase

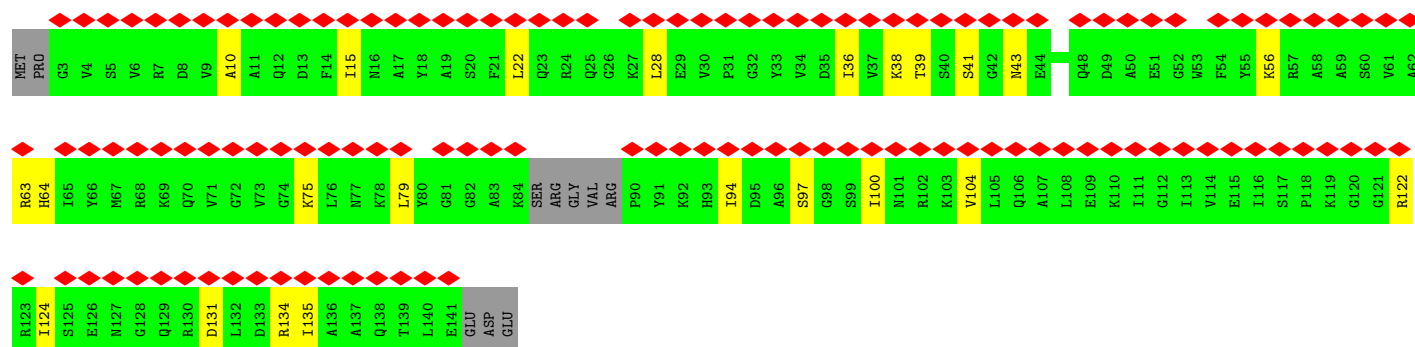


• Molecule 38: Small ribosomal subunit protein eS1A



• Molecule 39: 40S ribosomal protein S19-A

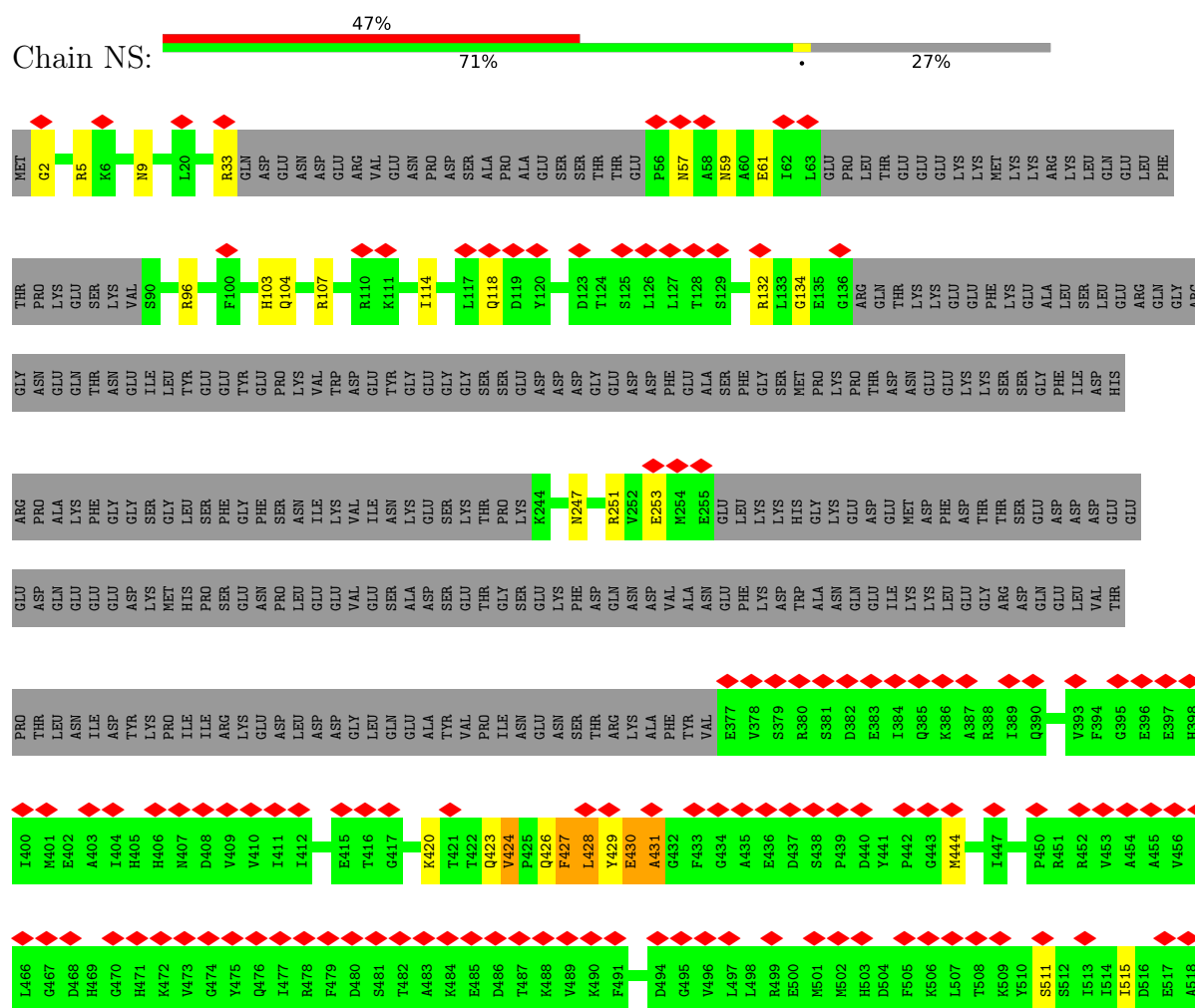




- Molecule 40: 40S ribosomal protein S27-A

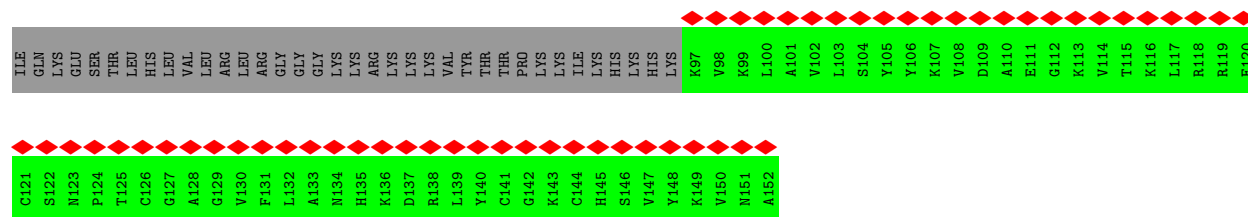


- Molecule 41: Probable ATP-dependent RNA helicase DHR1

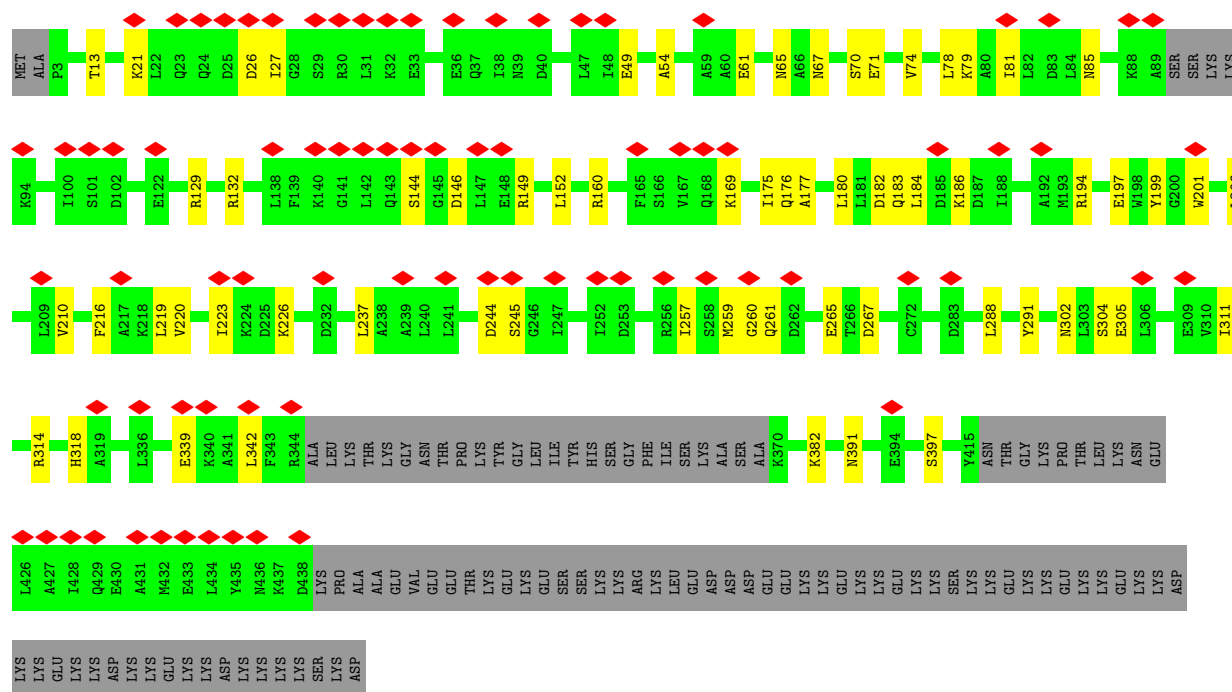




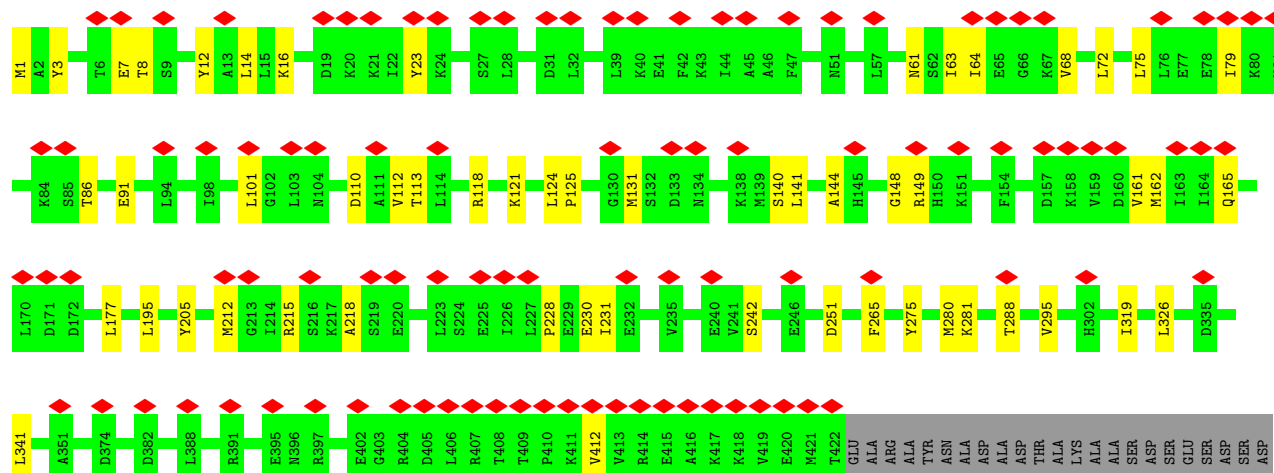
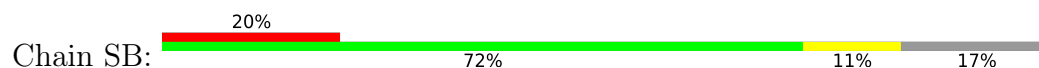


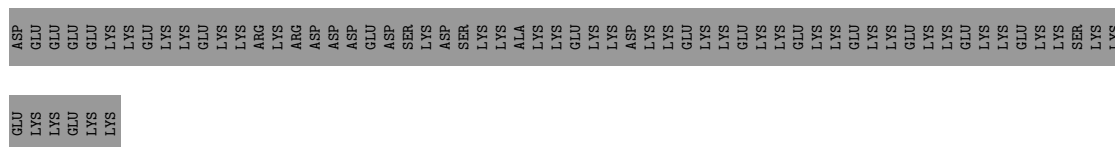


• Molecule 45: Nucleolar protein 56

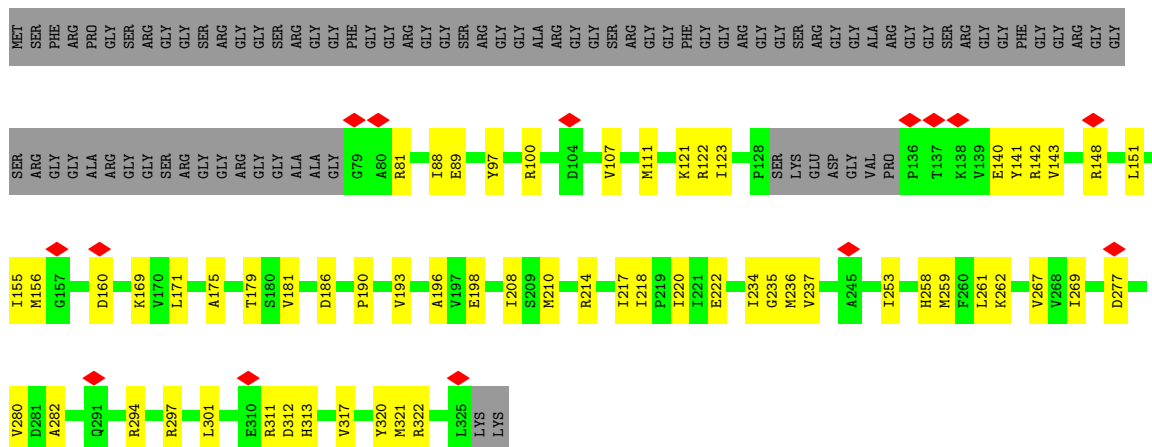


• Molecule 46: Nucleolar protein 58

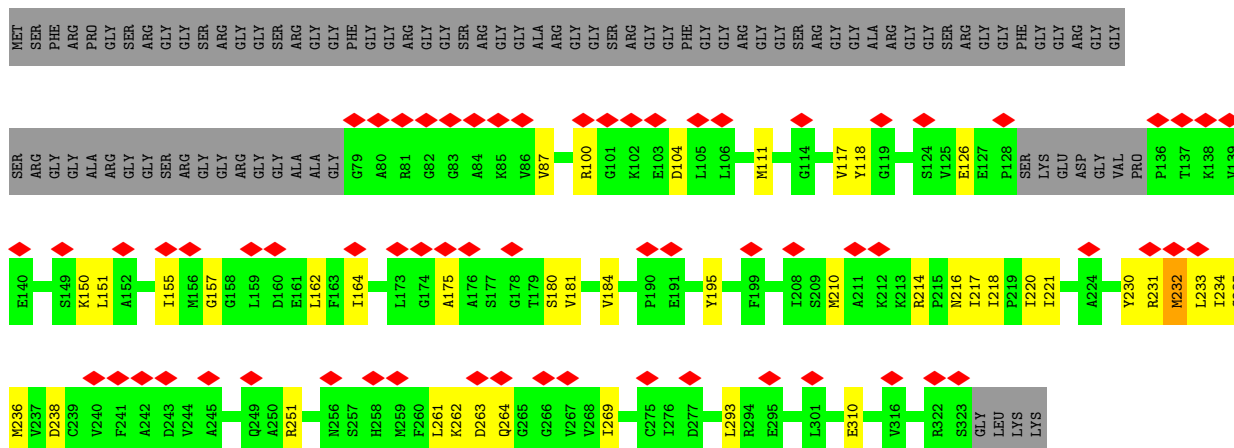




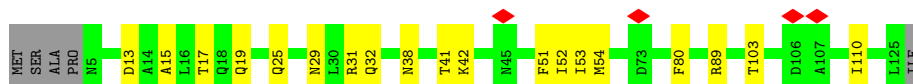
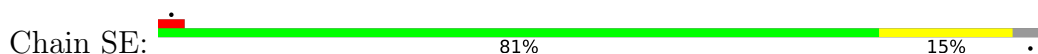
- Molecule 47: rRNA 2'-O-methyltransferase fibrillar



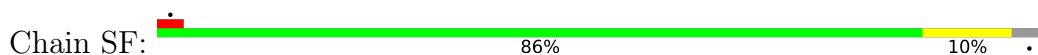
- Molecule 47: rRNA 2'-O-methyltransferase fibrillar

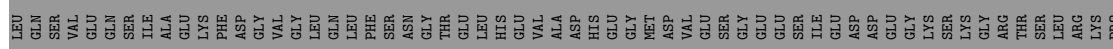


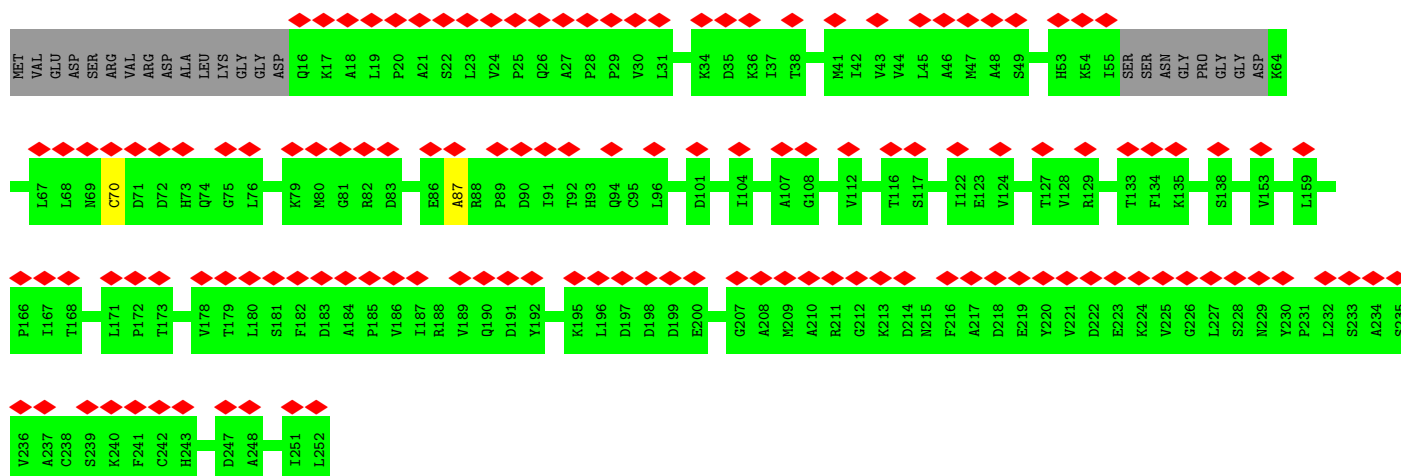
- Molecule 48: 13 kDa ribonucleoprotein-associated protein.



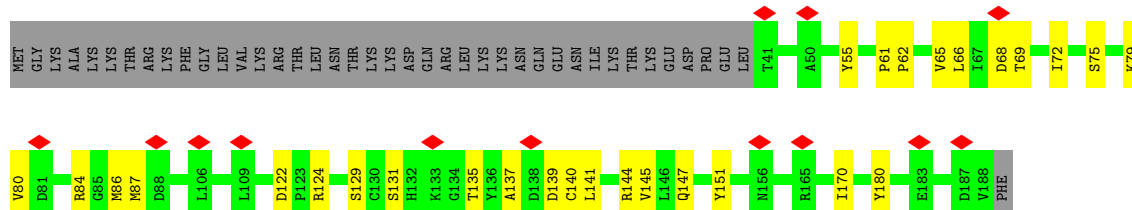
- Molecule 48: 13 kDa ribonucleoprotein-associated protein



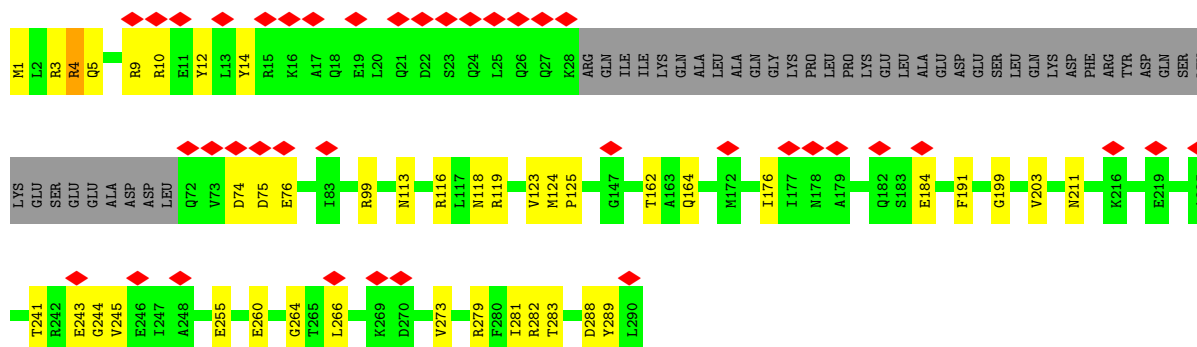
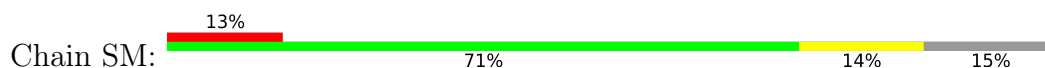




- Molecule 53: rRNA-processing protein FCF1

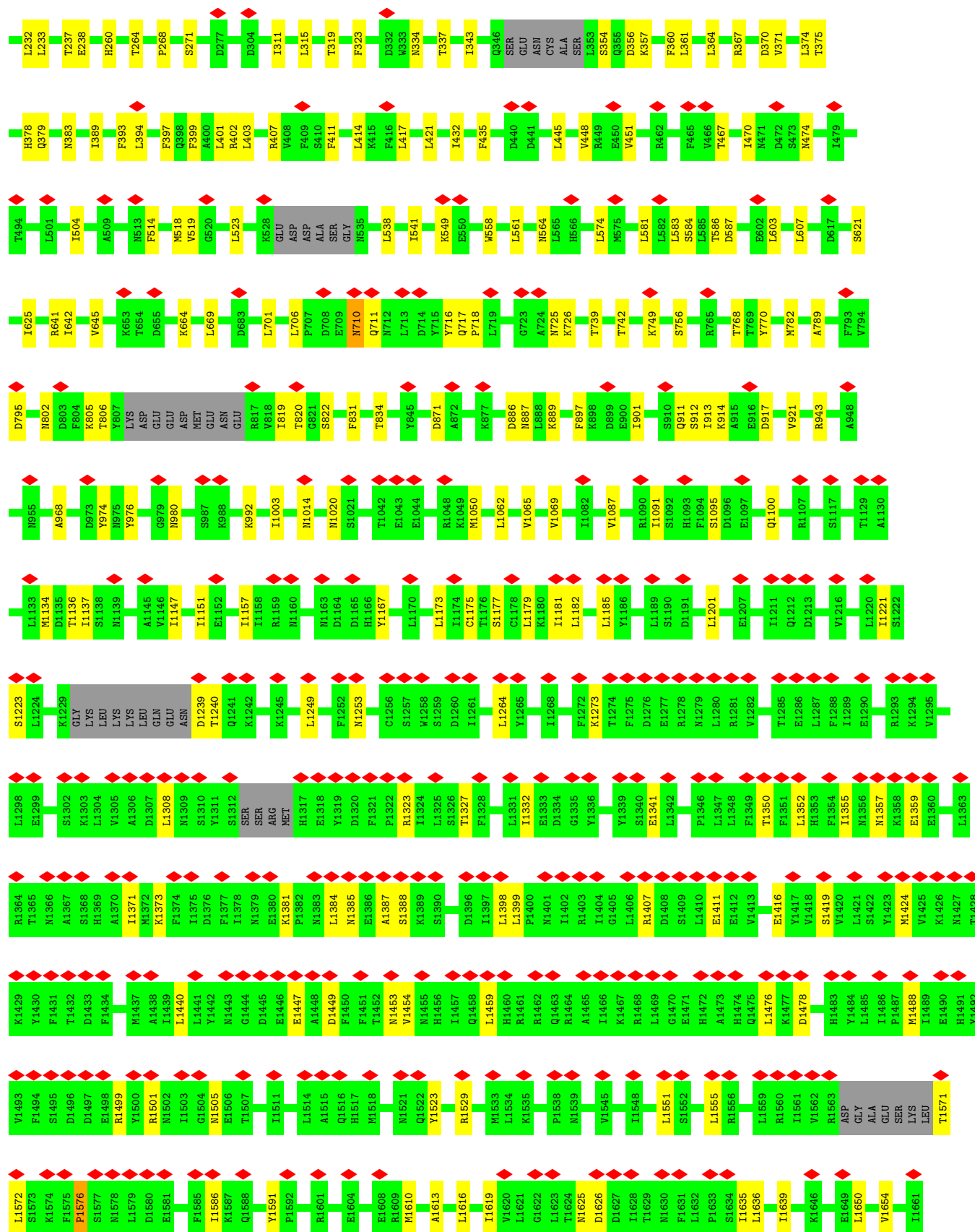


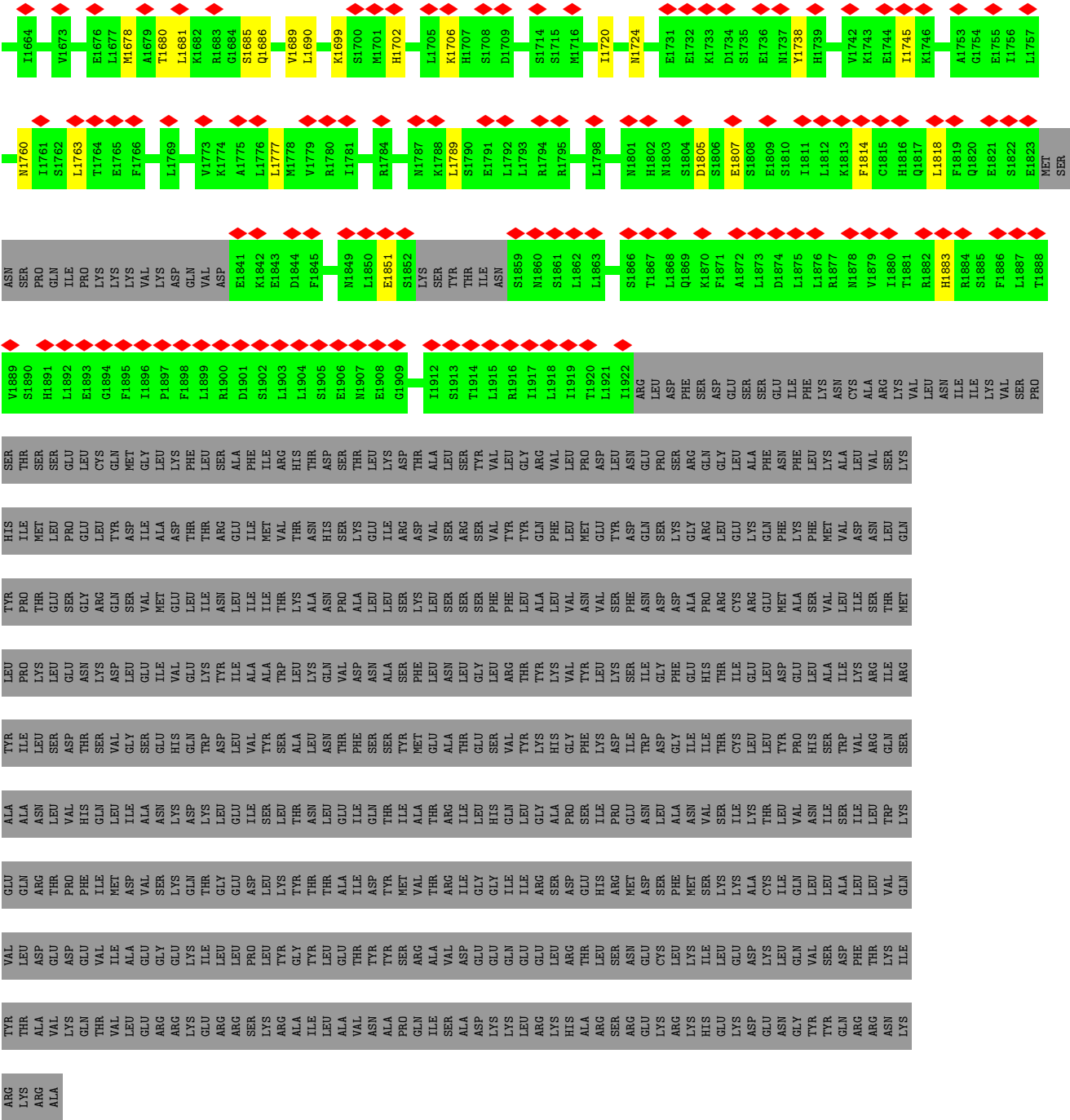
- Molecule 54: U3 small nucleolar ribonucleoprotein protein IMP4



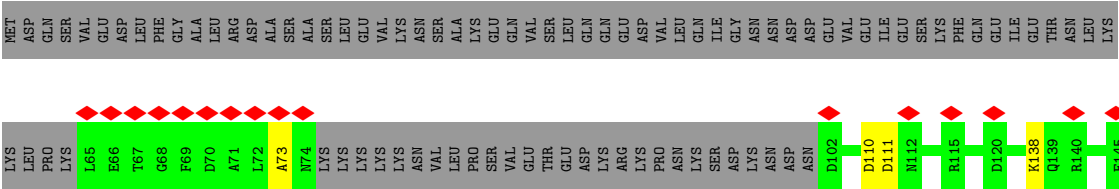
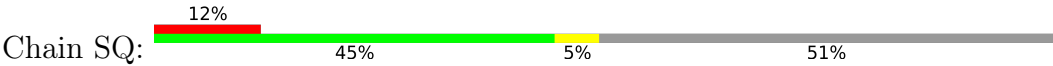
- Molecule 55: U3 small nucleolar RNA-associated protein 20





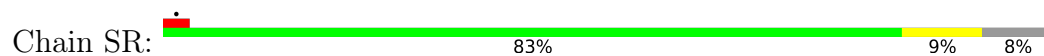


● Molecule 56: rRNA-processing protein FCF2

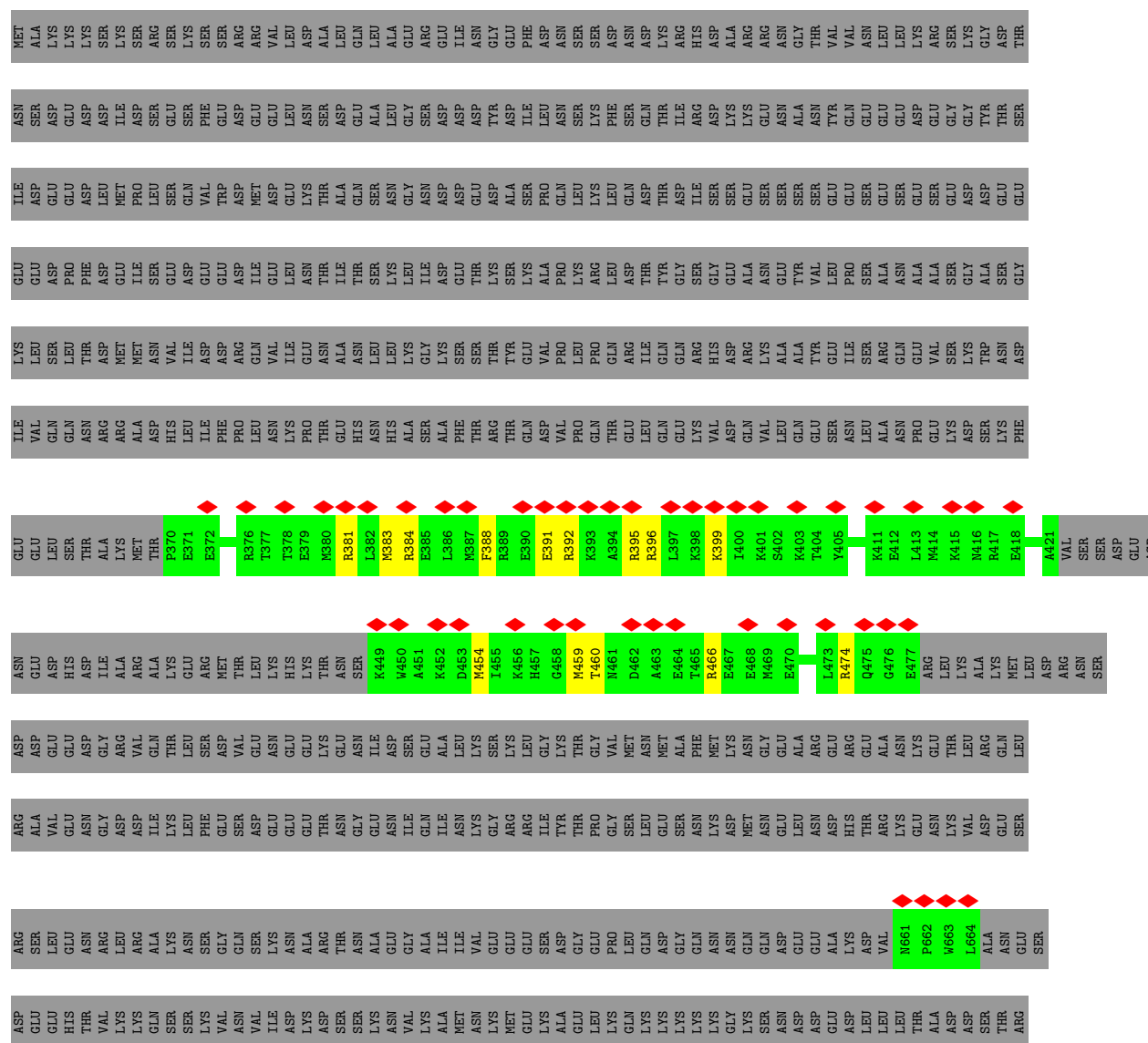


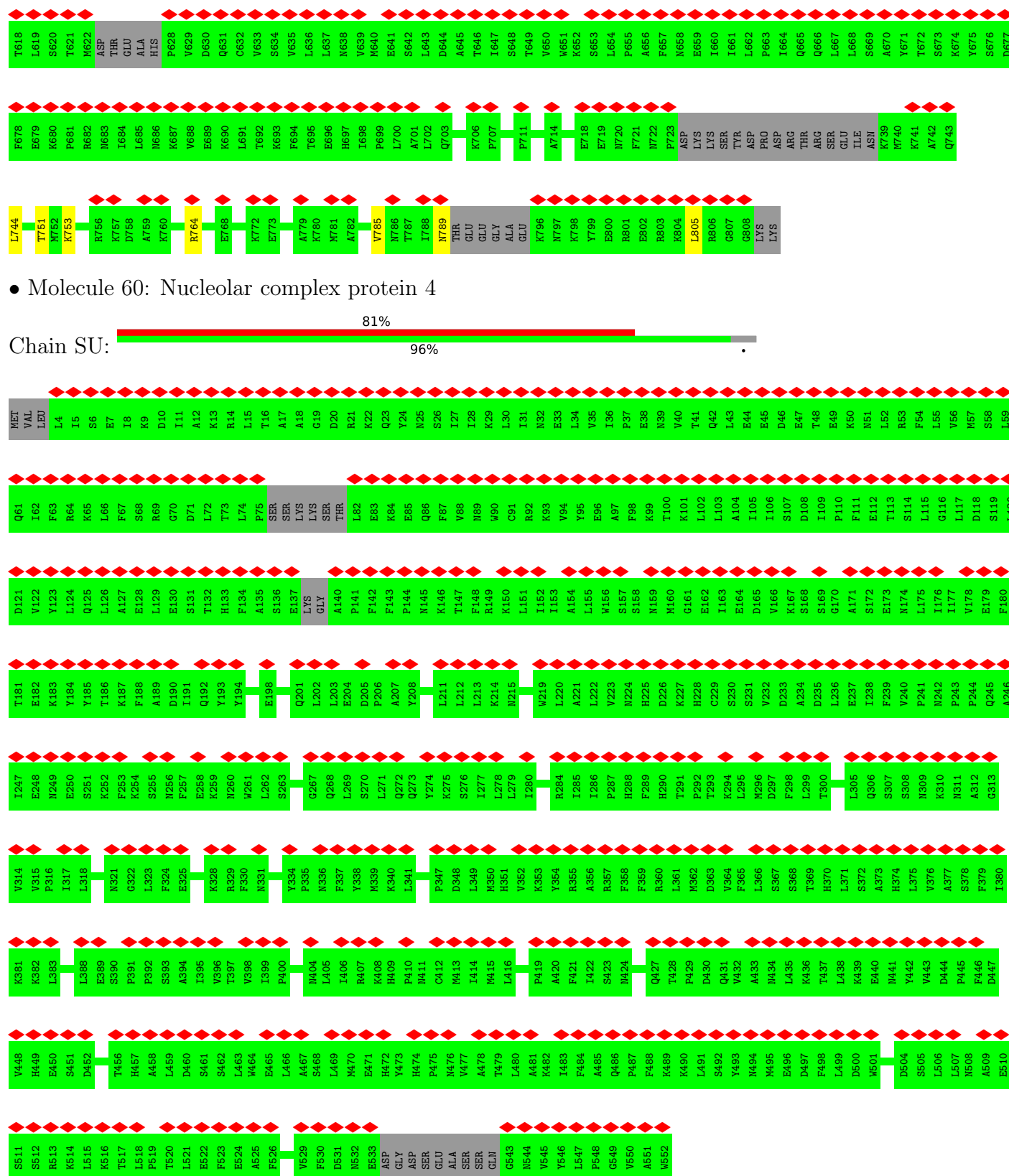


- Molecule 57: 40S ribosomal protein S23-A

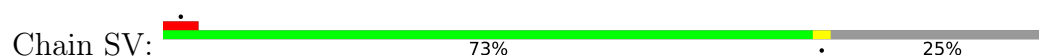


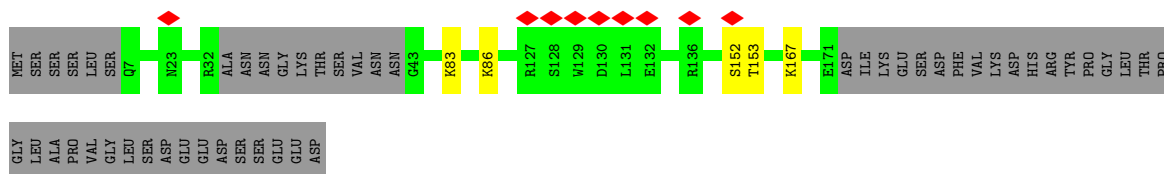
- Molecule 58: U3 small nucleolar RNA-associated protein 14



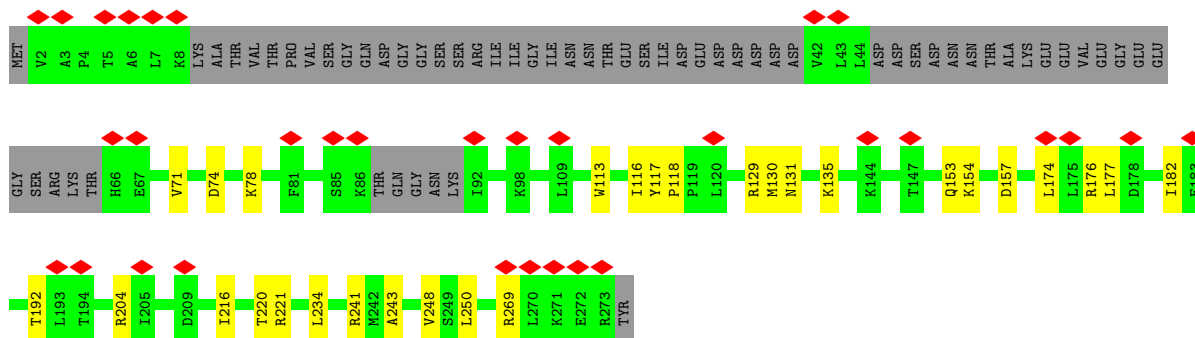


• Molecule 61: Regulator of rDNA transcription protein 14

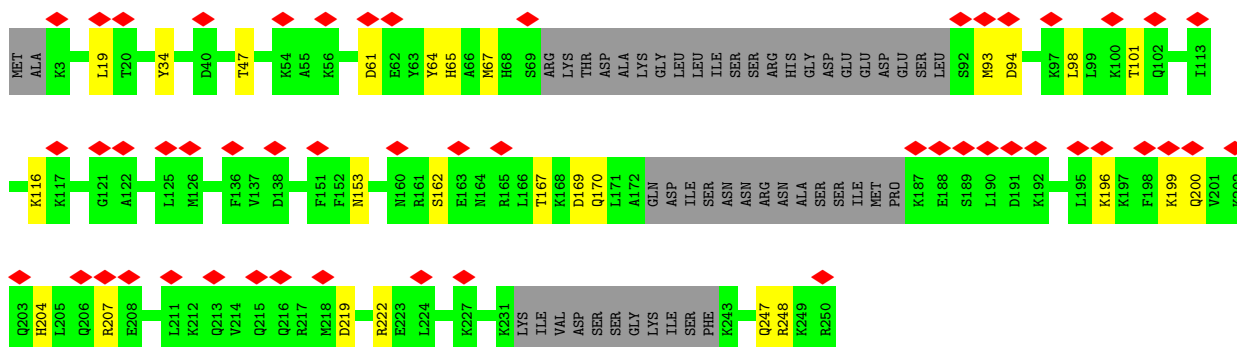




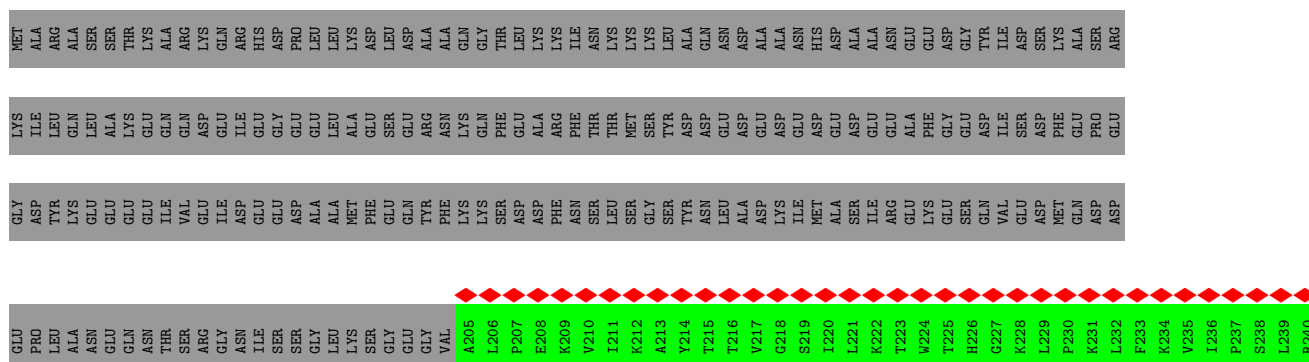
• Molecule 62: Pre-rRNA-processing protein PNO1



• Molecule 63: U3 small nucleolar RNA-associated protein 11



• Molecule 64: Essential nuclear protein 1



VAL ASN	L422		T423		F424		A425		Q426		R427		Y428		K429		N430		D431		I432		T433		Q434		D435		Q436		R437		D438		F439		L440		L441		E442		T443		V444		R445		Q446		R447		G448		H449		K450		D451		I452		G453		P454		E455		I456		R457		R458		E459		L460		L461		A462		G463		A464		S465		R466		GLU		PHE		VAL		ASP		PRO		GLN		GLU		ALA		ASN		ASP		LEU		MET		ILE		ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
	L362		P363		F364		S365		P366		P367		T368		T369		V370		F371		I372		K373		I374		L375		L376		D377		K378		K379		Y380		A381		L382		P383		Y384		Q385		T386		V387		D388		D389		C390		V391		Y392		Y393		F394		M395		R396		F397		R398		I399		L400		ASP		ASP		GLY		S404		N405		G406		E407		D408		A409		T410		R411		V412		L413		P414		V415		I416		W417		H418		K419		A420		F421																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
	H302		I303		Y304		R305		A306		V307		K308		K309		S310		L311		Y312		K313		P314		S315		A316		F317		F318		K319		G320		F321		L322		F323		P324		L325		V326		E327		T328		G329		C330		N331		V332		R333		E334		A335		T336		I337		A338		G339		S340		V341		L342		A343		K344		V345		S346		V347		P348		A349		L350		H351		S352		S353		A354		A355		L356		S357		Y358		L359		L360		R361																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
	N241		W242		Q243		D244		V245		I246		Y247		T248		T249		N250		P251		E252		E253		W254		S255		P256		H257		V258		V259		Y260		E261		A262		T263		K264		L265		F266		V267		S268		N269		L270		T271		A272		K273		E274		S275		Q276																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11394	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.863	Depositor
Minimum map value	0.000	Depositor
Average map value	0.094	Depositor
Map value standard deviation	0.169	Depositor
Recommended contour level	0.75	Depositor
Map size (Å)	535.75195, 535.75195, 535.75195	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.063, 1.063, 1.063	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, SEP, GTP, ATP, M7G, ADP, MG

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	0.09	0/1605	0.22	0/2494
2	L1	0.10	0/34578	0.27	0/53850
3	L2	0.09	0/4868	0.23	0/7561
4	L3	0.16	0/872	0.35	0/1173
5	L4	0.16	0/1977	0.42	1/2664 (0.0%)
6	L5	0.16	0/1655	0.39	0/2237
7	L6	0.16	0/1764	0.35	0/2359
8	L7	0.20	0/1451	0.49	0/1956
9	L8	0.13	0/1371	0.34	0/1833
10	L9	0.18	0/1495	0.40	1/2003 (0.0%)
11	LC	0.19	0/1015	0.45	0/1367
12	LD	0.16	0/1138	0.41	0/1533
13	LE	0.19	0/1039	0.45	0/1395
14	LF	0.17	0/1060	0.42	0/1412
15	LG	0.17	0/492	0.42	0/659
16	LH	0.17	0/6576	0.42	0/8902
17	LI	0.14	0/3835	0.35	0/5263
18	LJ	0.15	0/3851	0.37	0/5221
19	LK	0.14	0/1085	0.32	0/1463
20	LL	0.14	0/3939	0.36	0/5341
21	LM	0.13	0/9356	0.35	2/12933 (0.0%)
22	LN	0.13	0/5359	0.35	2/7255 (0.0%)
23	LO	0.12	0/6463	0.31	0/8748
24	LP	0.13	0/1907	0.34	0/2667
25	LQ	0.15	0/6620	0.39	0/8936
26	LR	0.13	0/6313	0.33	0/8551
27	LS	0.17	0/3735	0.41	2/5064 (0.0%)
28	LT	0.15	0/6921	0.34	1/9362 (0.0%)
29	LZ	0.22	0/1194	0.48	0/1610
30	NA	0.17	0/2442	0.38	0/3281
31	NB	0.12	0/1654	0.33	0/2243
32	ND	0.15	0/568	0.39	0/755

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	NF	0.36	0/1158	0.58	1/1559 (0.1%)
34	NG	0.15	0/952	0.36	0/1279
35	NH	0.14	0/8899	0.34	1/12035 (0.0%)
36	NI	0.17	0/1994	0.41	1/2684 (0.0%)
37	NL	0.18	0/2329	0.40	0/3144
38	NM	0.25	0/1915	0.51	0/2563
39	NP	0.13	0/1056	0.33	0/1416
40	NQ	0.17	0/605	0.43	0/817
41	NS	0.20	0/5100	0.44	1/7072 (0.0%)
42	NV	0.19	0/151	0.46	0/196
43	OH	0.09	0/595	0.27	0/827
44	OU	0.10	0/278	0.28	0/386
45	SA	0.13	0/3146	0.32	0/4240
46	SB	0.15	0/3293	0.34	0/4436
47	SC	0.17	0/1903	0.41	0/2567
47	SD	0.17	0/1885	0.37	0/2543
48	SE	0.17	0/928	0.38	0/1262
48	SF	0.17	0/928	0.43	0/1262
49	SG	0.12	0/3744	0.31	0/5040
50	SH	0.15	0/2832	0.38	0/3825
51	SI	0.15	0/6281	0.35	0/8457
52	SJ	0.12	0/1080	0.32	0/1508
52	SK	0.14	0/1170	0.37	0/1639
53	SL	0.16	0/1193	0.40	0/1611
54	SM	0.17	0/2046	0.36	0/2759
55	SP	0.13	0/15404	0.33	1/20833 (0.0%)
56	SQ	0.14	0/901	0.37	0/1204
57	SR	0.15	0/1069	0.38	0/1427
58	SS	0.15	0/799	0.37	0/1050
59	ST	0.13	0/3475	0.31	0/4761
60	SU	0.12	0/2726	0.31	0/3825
61	SV	0.13	0/854	0.37	0/1175
62	SW	0.16	0/1696	0.37	0/2282
63	SY	0.18	0/1736	0.43	0/2292
64	SZ	0.12	0/1326	0.31	0/1859
All	All	0.14	0/213645	0.35	14/297926 (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
21	LM	0	2
33	NF	0	2
38	NM	0	4
41	NS	0	4
47	SD	0	1
48	SF	0	1
54	SM	0	1
All	All	0	15

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	NF	89	TYR	CA-CB-CG	8.98	130.07	113.90
21	LM	222	ALA	CA-C-N	8.80	136.08	122.08
21	LM	222	ALA	C-N-CA	8.80	136.08	122.08
36	NI	163	PRO	CA-N-CD	-8.79	99.69	112.00
28	LT	326	PRO	CA-N-CD	-8.35	100.31	112.00

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	LM	222	ALA	Peptide
21	LM	224	ASN	Peptide
33	NF	88	LEU	Peptide
33	NF	89	TYR	Sidechain
38	NM	99	ASN	Peptide

5.2 Too-close contacts

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	1437	0	722	7	0
2	L1	30918	0	15571	213	0
3	L2	4394	0	2229	19	0
4	L3	862	0	900	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L4	1936	0	2019	30	0
6	L5	1635	0	1697	29	0
7	L6	1740	0	1835	36	0
8	L7	1427	0	1499	35	0
9	L8	1348	0	1366	17	0
10	L9	1470	0	1554	15	0
11	LC	997	0	1054	19	0
12	LD	1112	0	1179	15	0
13	LE	1022	0	1060	25	0
14	LF	1046	0	1114	18	0
15	LG	490	0	529	8	0
16	LH	6449	0	6398	141	0
17	LI	3792	0	2859	37	0
18	LJ	3773	0	3761	66	0
19	LK	1068	0	1120	18	0
20	LL	3871	0	3876	77	0
21	LM	9274	0	6159	53	0
22	LN	5263	0	5270	67	0
23	LO	6321	0	6235	68	0
24	LP	1901	0	836	3	0
25	LQ	6494	0	6544	127	0
26	LR	6207	0	6247	87	0
27	LS	3662	0	3639	67	0
28	LT	6787	0	6685	84	0
29	LZ	1173	0	1208	33	0
30	NA	2426	0	2263	56	0
31	NB	1645	0	1277	21	0
32	ND	564	0	587	13	0
33	NF	1135	0	1197	47	0
34	NG	941	0	979	15	0
35	NH	8693	0	8806	112	0
36	NI	1953	0	1933	25	0
37	NL	2285	0	2359	48	0
38	NM	1891	0	1995	56	0
39	NP	1040	0	1057	17	0
40	NQ	595	0	610	19	0
41	NS	5051	0	2958	30	0
42	NV	149	0	172	2	0
43	OH	594	0	298	1	0
44	OU	278	0	135	0	0
45	SA	3100	0	3084	43	0
46	SB	3255	0	3379	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	SC	1865	0	1908	48	0
47	SD	1850	0	1889	37	0
48	SE	916	0	964	14	0
48	SF	916	0	964	10	0
49	SG	3672	0	3690	32	0
50	SH	2781	0	2878	34	0
51	SI	6144	0	6331	91	0
52	SJ	1074	0	514	0	0
52	SK	1160	0	570	1	0
53	SL	1171	0	1229	20	0
54	SM	2009	0	2027	34	0
55	SP	15102	0	15321	176	0
56	SQ	885	0	866	12	0
57	SR	1052	0	1120	13	0
58	SS	791	0	815	14	0
59	ST	3455	0	2276	22	0
60	SU	2703	0	1302	0	0
61	SV	852	0	476	3	0
62	SW	1669	0	1747	24	0
63	SY	1715	0	1789	21	0
64	SZ	1314	0	649	1	0
65	L1	35	0	0	0	0
65	NH	1	0	0	0	0
65	NS	1	0	0	0	0
65	SI	1	0	0	0	0
66	NH	31	0	12	1	0
67	NQ	1	0	0	0	0
67	SL	1	0	0	0	0
68	NS	27	0	12	0	0
69	SI	32	0	12	0	0
All	All	206690	0	177615	2188	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 2188 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)
8:L7:67:LEU:HD22	8:L7:94:ALA:HB2	1.45	0.98
2:L1:446:A:OP1	5:L4:59:ARG:NH1	2.04	0.90
37:NL:98:VAL:HG11	37:NL:107:LEU:HD23	1.52	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:NH:787:GLU:OE2	38:NM:199:ASN:ND2	2.05	0.89
23:LO:841:ASP:OD1	25:LQ:903:GLN:NE2	2.08	0.86

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	102/146 (70%)	100 (98%)	2 (2%)	0	100	100
5	L4	242/261 (93%)	235 (97%)	7 (3%)	0	100	100
6	L5	202/225 (90%)	198 (98%)	4 (2%)	0	100	100
7	L6	214/236 (91%)	208 (97%)	6 (3%)	0	100	100
8	L7	174/190 (92%)	171 (98%)	3 (2%)	0	100	100
9	L8	166/200 (83%)	165 (99%)	1 (1%)	0	100	100
10	L9	179/197 (91%)	176 (98%)	3 (2%)	0	100	100
11	LC	126/143 (88%)	123 (98%)	3 (2%)	0	100	100
12	LD	135/156 (86%)	130 (96%)	5 (4%)	0	100	100
13	LE	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
14	LF	128/135 (95%)	126 (98%)	2 (2%)	0	100	100
15	LG	60/67 (90%)	60 (100%)	0	0	100	100
16	LH	788/896 (88%)	769 (98%)	19 (2%)	0	100	100
17	LI	582/713 (82%)	570 (98%)	12 (2%)	0	100	100
18	LJ	470/513 (92%)	460 (98%)	10 (2%)	0	100	100
19	LK	130/575 (23%)	129 (99%)	1 (1%)	0	100	100
20	LL	475/643 (74%)	461 (97%)	14 (3%)	0	100	100
21	LM	1583/1769 (90%)	1552 (98%)	31 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	LN	649/776 (84%)	639 (98%)	10 (2%)	0	100	100
23	LO	786/923 (85%)	776 (99%)	10 (1%)	0	100	100
24	LP	375/440 (85%)	373 (100%)	2 (0%)	0	100	100
25	LQ	806/943 (86%)	795 (99%)	11 (1%)	0	100	100
26	LR	785/817 (96%)	767 (98%)	18 (2%)	0	100	100
27	LS	452/594 (76%)	437 (97%)	15 (3%)	0	100	100
28	LT	861/939 (92%)	845 (98%)	16 (2%)	0	100	100
29	LZ	140/183 (76%)	140 (100%)	0	0	100	100
30	NA	312/593 (53%)	312 (100%)	0	0	100	100
31	NB	248/610 (41%)	247 (100%)	1 (0%)	0	100	100
32	ND	70/214 (33%)	69 (99%)	1 (1%)	0	100	100
33	NF	139/151 (92%)	131 (94%)	6 (4%)	2 (1%)	9	39
34	NG	125/137 (91%)	121 (97%)	4 (3%)	0	100	100
35	NH	1063/1237 (86%)	1047 (98%)	16 (2%)	0	100	100
36	NI	232/297 (78%)	227 (98%)	5 (2%)	0	100	100
37	NL	279/318 (88%)	278 (100%)	1 (0%)	0	100	100
38	NM	231/255 (91%)	221 (96%)	9 (4%)	1 (0%)	30	66
39	NP	130/144 (90%)	125 (96%)	5 (4%)	0	100	100
40	NQ	77/82 (94%)	75 (97%)	2 (3%)	0	100	100
41	NS	917/1267 (72%)	894 (98%)	22 (2%)	1 (0%)	48	82
42	NV	17/733 (2%)	17 (100%)	0	0	100	100
43	OH	118/143 (82%)	117 (99%)	1 (1%)	0	100	100
44	OU	54/152 (36%)	54 (100%)	0	0	100	100
45	SA	390/504 (77%)	386 (99%)	4 (1%)	0	100	100
46	SB	420/511 (82%)	409 (97%)	11 (3%)	0	100	100
47	SC	237/327 (72%)	233 (98%)	4 (2%)	0	100	100
47	SD	234/327 (72%)	233 (100%)	1 (0%)	0	100	100
48	SE	119/126 (94%)	118 (99%)	1 (1%)	0	100	100
48	SF	119/126 (94%)	117 (98%)	2 (2%)	0	100	100
49	SG	453/573 (79%)	448 (99%)	5 (1%)	0	100	100
50	SH	358/367 (98%)	351 (98%)	7 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	SI	744/1183 (63%)	732 (98%)	12 (2%)	0	100	100
52	SJ	207/252 (82%)	204 (99%)	3 (1%)	0	100	100
52	SK	225/252 (89%)	223 (99%)	2 (1%)	0	100	100
53	SL	146/189 (77%)	142 (97%)	4 (3%)	0	100	100
54	SM	243/290 (84%)	238 (98%)	5 (2%)	0	100	100
55	SP	1832/2493 (74%)	1809 (99%)	23 (1%)	0	100	100
56	SQ	103/217 (48%)	102 (99%)	1 (1%)	0	100	100
57	SR	130/145 (90%)	130 (100%)	0	0	100	100
58	SS	86/899 (10%)	86 (100%)	0	0	100	100
59	ST	573/810 (71%)	568 (99%)	5 (1%)	0	100	100
60	SU	524/552 (95%)	521 (99%)	3 (1%)	0	100	100
61	SV	151/206 (73%)	149 (99%)	2 (1%)	0	100	100
62	SW	205/274 (75%)	202 (98%)	3 (2%)	0	100	100
63	SY	193/250 (77%)	189 (98%)	4 (2%)	0	100	100
64	SZ	255/483 (53%)	252 (99%)	3 (1%)	0	100	100
All	All	22696/30499 (74%)	22306 (98%)	386 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	NF	89	TYR
41	NS	431	ALA
38	NM	100	PHE
33	NF	85	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L3	96/129 (74%)	96 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	L4	208/222 (94%)	208 (100%)	0	100	100
6	L5	179/191 (94%)	179 (100%)	0	100	100
7	L6	185/201 (92%)	185 (100%)	0	100	100
8	L7	158/170 (93%)	158 (100%)	0	100	100
9	L8	137/161 (85%)	137 (100%)	0	100	100
10	L9	156/166 (94%)	156 (100%)	0	100	100
11	LC	107/119 (90%)	107 (100%)	0	100	100
12	LD	124/137 (90%)	123 (99%)	1 (1%)	73	77
13	LE	110/111 (99%)	110 (100%)	0	100	100
14	LF	109/113 (96%)	108 (99%)	1 (1%)	70	75
15	LG	55/60 (92%)	55 (100%)	0	100	100
16	LH	743/826 (90%)	743 (100%)	0	100	100
17	LI	244/657 (37%)	244 (100%)	0	100	100
18	LJ	421/454 (93%)	421 (100%)	0	100	100
19	LK	124/533 (23%)	124 (100%)	0	100	100
20	LL	438/574 (76%)	438 (100%)	0	100	100
21	LM	406/1633 (25%)	406 (100%)	0	100	100
22	LN	603/713 (85%)	603 (100%)	0	100	100
23	LO	695/812 (86%)	695 (100%)	0	100	100
24	LP	8/414 (2%)	8 (100%)	0	100	100
25	LQ	723/832 (87%)	723 (100%)	0	100	100
26	LR	698/719 (97%)	697 (100%)	1 (0%)	88	88
27	LS	406/528 (77%)	406 (100%)	0	100	100
28	LT	740/819 (90%)	740 (100%)	0	100	100
29	LZ	132/172 (77%)	132 (100%)	0	100	100
30	NA	235/535 (44%)	235 (100%)	0	100	100
31	NB	99/538 (18%)	99 (100%)	0	100	100
32	ND	57/196 (29%)	57 (100%)	0	100	100
33	NF	121/128 (94%)	121 (100%)	0	100	100
34	NG	96/105 (91%)	96 (100%)	0	100	100
35	NH	982/1125 (87%)	982 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	NI	220/274 (80%)	220 (100%)	0	100	100
37	NL	257/283 (91%)	256 (100%)	1 (0%)	84	82
38	NM	210/224 (94%)	210 (100%)	0	100	100
39	NP	107/116 (92%)	107 (100%)	0	100	100
40	NQ	68/71 (96%)	68 (100%)	0	100	100
41	NS	135/1140 (12%)	135 (100%)	0	100	100
42	NV	14/671 (2%)	14 (100%)	0	100	100
43	OH	2/119 (2%)	2 (100%)	0	100	100
44	OU	1/135 (1%)	1 (100%)	0	100	100
45	SA	328/435 (75%)	328 (100%)	0	100	100
46	SB	352/433 (81%)	352 (100%)	0	100	100
47	SC	200/240 (83%)	200 (100%)	0	100	100
47	SD	198/240 (82%)	198 (100%)	0	100	100
48	SE	100/104 (96%)	100 (100%)	0	100	100
48	SF	100/104 (96%)	100 (100%)	0	100	100
49	SG	399/503 (79%)	399 (100%)	0	100	100
50	SH	307/312 (98%)	307 (100%)	0	100	100
51	SI	668/1039 (64%)	667 (100%)	1 (0%)	88	88
52	SJ	9/222 (4%)	9 (100%)	0	100	100
52	SK	12/222 (5%)	12 (100%)	0	100	100
53	SL	131/169 (78%)	131 (100%)	0	100	100
54	SM	220/258 (85%)	220 (100%)	0	100	100
55	SP	1725/2307 (75%)	1723 (100%)	2 (0%)	88	88
56	SQ	91/200 (46%)	91 (100%)	0	100	100
57	SR	113/120 (94%)	113 (100%)	0	100	100
58	SS	81/808 (10%)	81 (100%)	0	100	100
59	ST	136/732 (19%)	136 (100%)	0	100	100
60	SU	27/506 (5%)	27 (100%)	0	100	100
61	SV	20/192 (10%)	20 (100%)	0	100	100
62	SW	183/238 (77%)	183 (100%)	0	100	100
63	SY	191/234 (82%)	191 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	SZ	14/424 (3%)	14 (100%)	0	100	100
All	All	16214/27168 (60%)	16207 (100%)	7 (0%)	100	100

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	NL	213	ASN
51	SI	5	ASN
55	SP	1014	ASN
55	SP	710	ASN
26	LR	802	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 144 such sidechains are listed below:

Mol	Chain	Res	Type
51	SI	882	ASN
62	SW	197	HIS
54	SM	113	ASN
55	SP	446	GLN
26	LR	83	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L0	63/700 (9%)	10 (15%)	0
2	L1	1431/1803 (79%)	292 (20%)	10 (0%)
3	L2	198/334 (59%)	25 (12%)	1 (0%)
All	All	1692/2837 (59%)	327 (19%)	11 (0%)

5 of 327 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L0	7	A
1	L0	63	G
1	L0	64	U
1	L0	83	U
1	L0	85	G

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L1	1082	C
2	L1	1555	A
3	L2	156	U
2	L1	1568	C
2	L1	585	A

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
27	SEP	LS	128	27	8,9,10	1.61	1 (12%)	7,12,14	1.33	1 (14%)

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
27	SEP	LS	128	27	-	6/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	LS	128	SEP	P-O1P	3.54	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	LS	128	SEP	OG-CB-CA	2.67	110.74	108.14

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	LS	128	SEP	C-CA-CB-OG
27	LS	128	SEP	CA-CB-OG-P
27	LS	128	SEP	CB-OG-P-O2P
27	LS	128	SEP	CB-OG-P-O3P
27	LS	128	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	LS	128	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 40 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
69	GTP	SI	2001	65	33,34,34	1.82	4 (12%)	50,54,54	1.47	6 (12%)
66	ATP	NH	1300	65	32,33,33	0.26	0	48,52,52	0.65	0
68	ADP	NS	1301	65	28,29,29	1.41	4 (14%)	43,45,45	1.91	9 (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
69	GTP	SI	2001	65	-	0/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	ATP	NH	1300	65	-	2/22/38/38	0/3/3/3
68	ADP	NS	1301	65	-	4/16/32/32	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)
69	SI	2001	GTP	C5-N7	6.72	1.52	1.39
68	NS	1301	ADP	C5-C4	4.59	1.47	1.39
69	SI	2001	GTP	C8-N9	-4.21	1.28	1.37
69	SI	2001	GTP	C4-N9	-3.74	1.28	1.38
68	NS	1301	ADP	C5-C6	2.75	1.48	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	SI	2001	GTP	C8-N9-C4	7.13	119.39	106.03
68	NS	1301	ADP	C5-C4-N3	-6.39	117.92	126.72
68	NS	1301	ADP	N3-C4-N9	4.94	135.57	127.17
68	NS	1301	ADP	C2-N3-C4	4.17	122.02	111.83
68	NS	1301	ADP	N3-C2-N1	-3.75	122.90	128.58

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
68	NS	1301	ADP	PA-O3A-PB-O3B
68	NS	1301	ADP	C5'-O5'-PA-O2A
68	NS	1301	ADP	C5'-O5'-PA-O3A
68	NS	1301	ADP	PA-O3A-PB-O1B
66	NH	1300	ATP	PA-O3A-PB-O2B

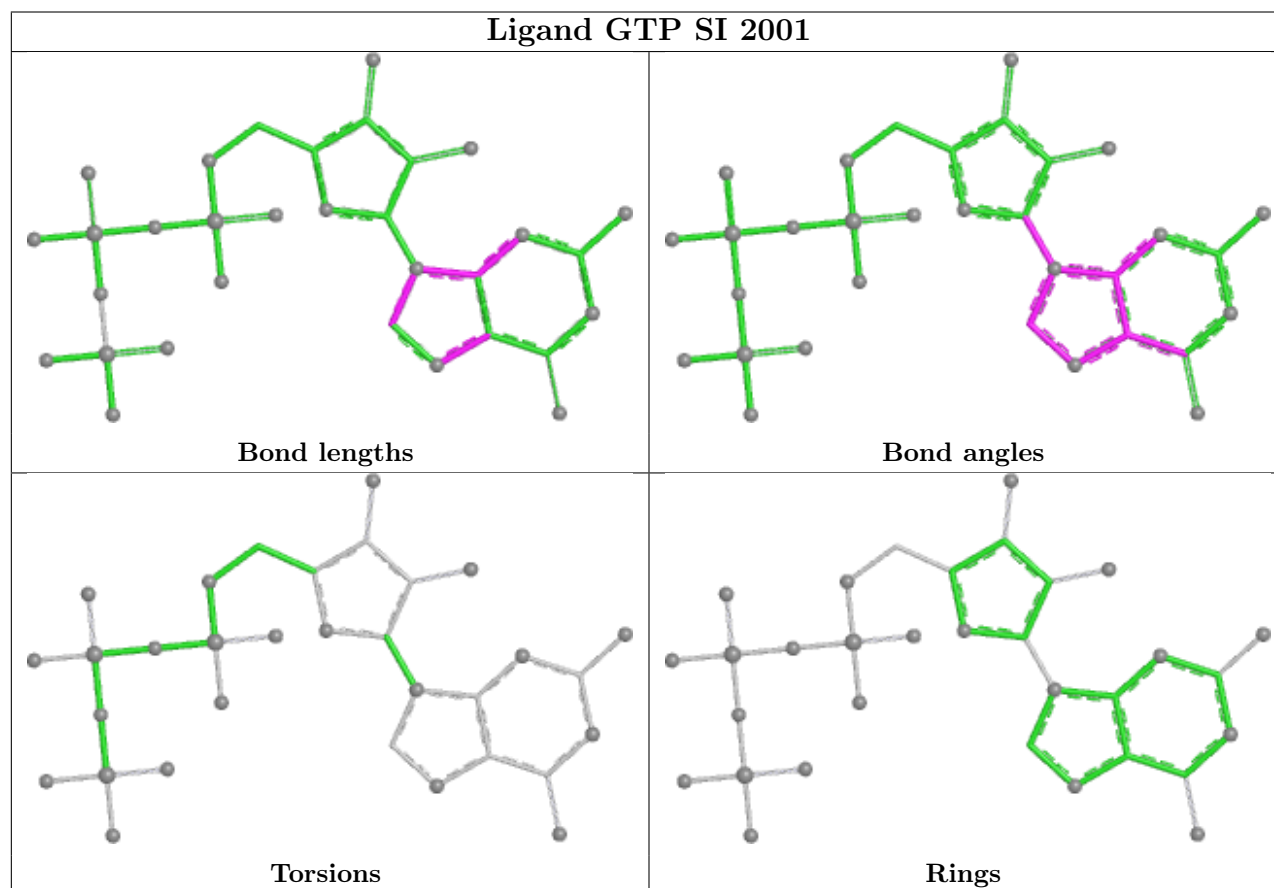
There are no ring outliers.

1 monomer is involved in 1 short contact:

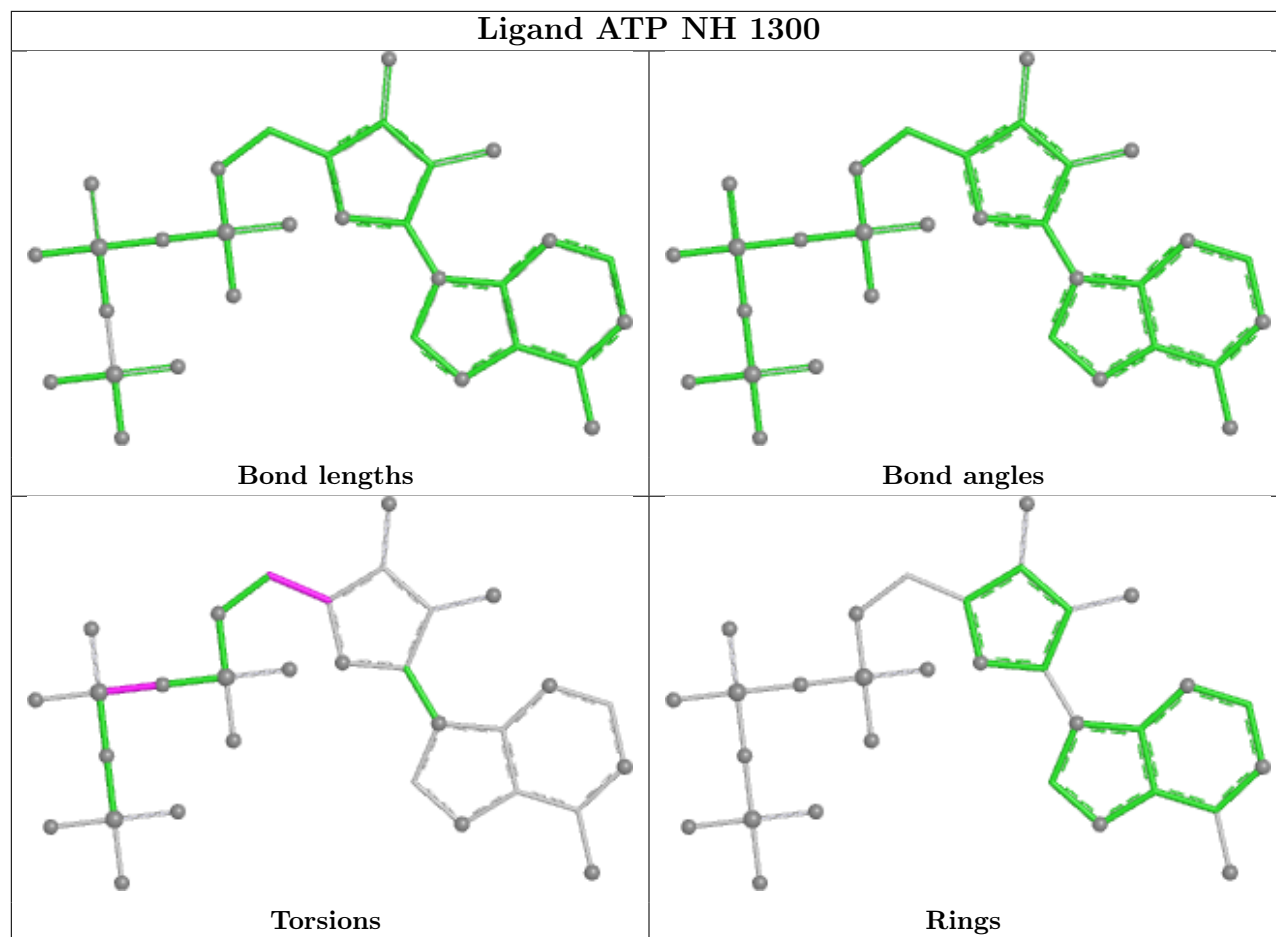
Mol	Chain	Res	Type	Clashes	Symm-Clashes
66	NH	1300	ATP	1	0

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 than 5% of the Mogul distribution of torsion angles is

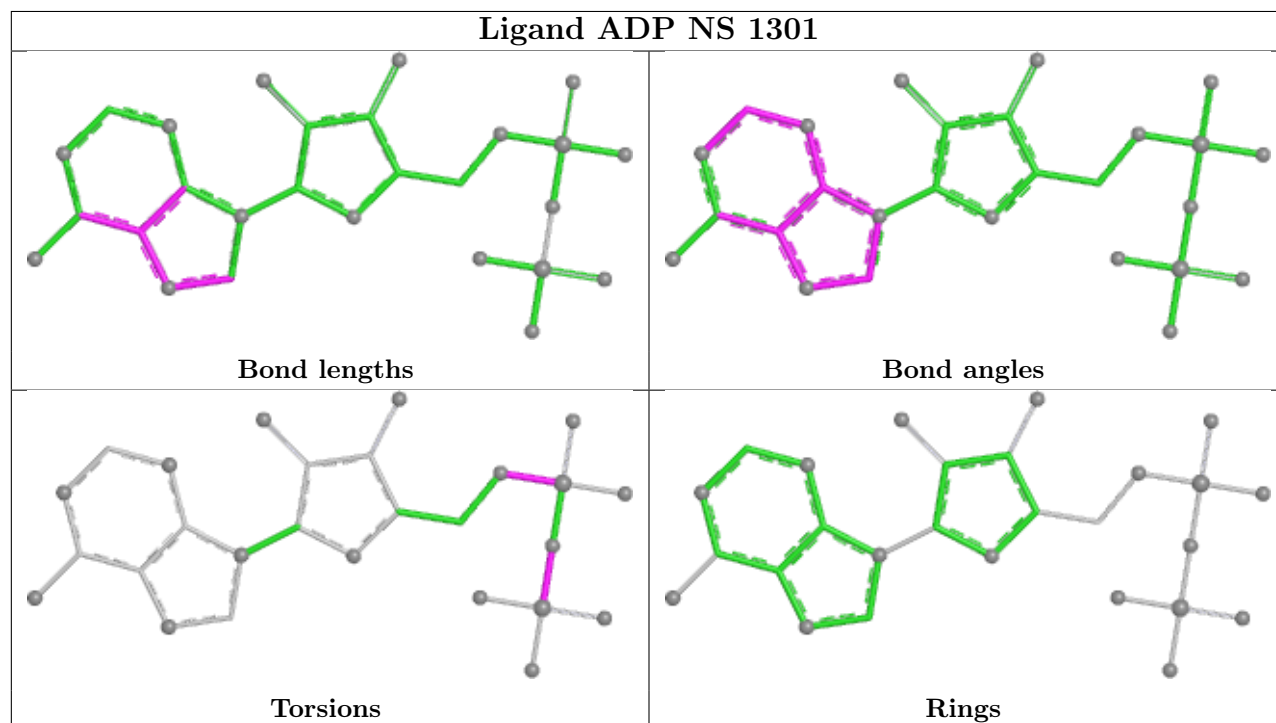
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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 ATP NH 1300



Ligand ADP NS 1301



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

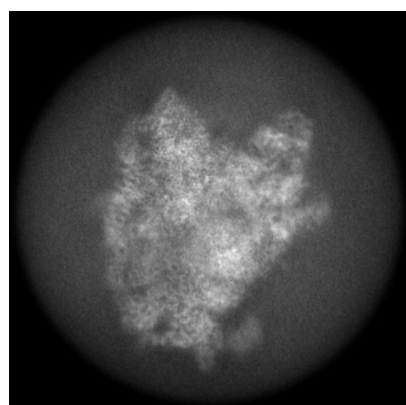
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49086. These allow visual inspection of the internal detail of the map and identification of artifacts.

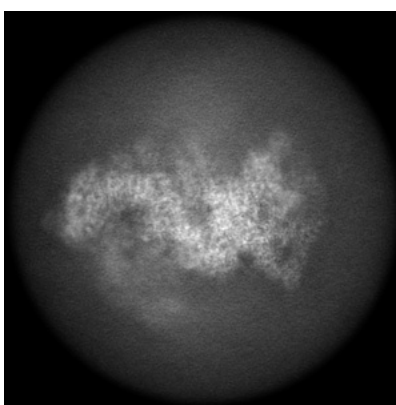
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

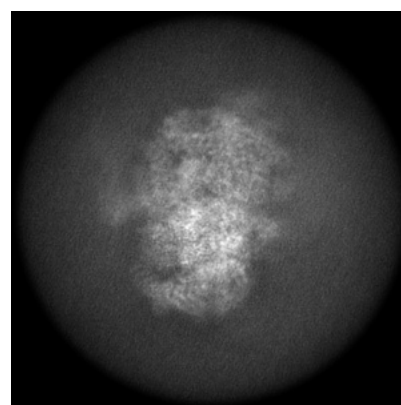
6.1.1 Primary map



X



Y

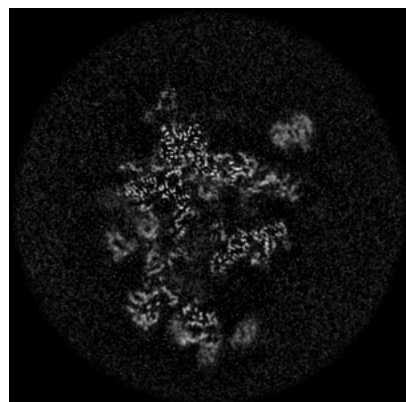


Z

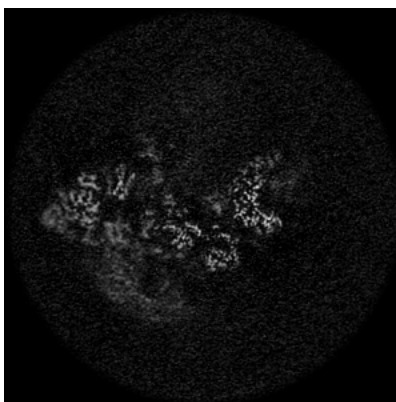
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

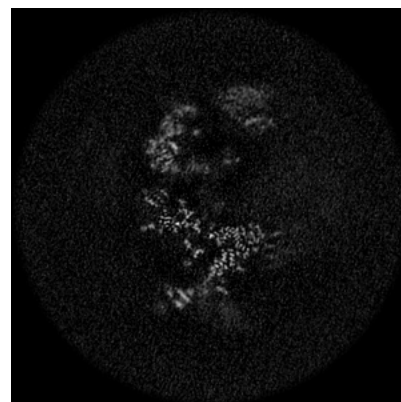
6.2.1 Primary map



X Index: 252



Y Index: 252

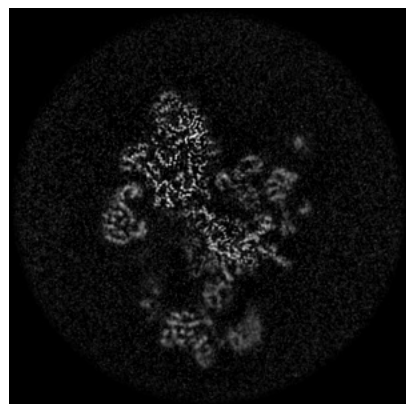


Z Index: 252

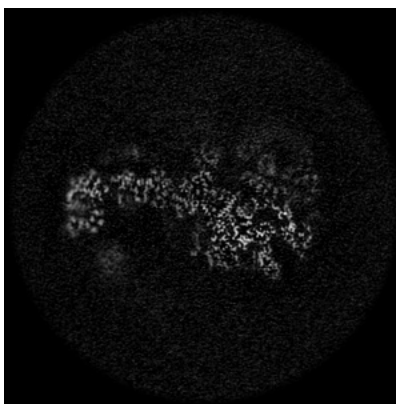
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

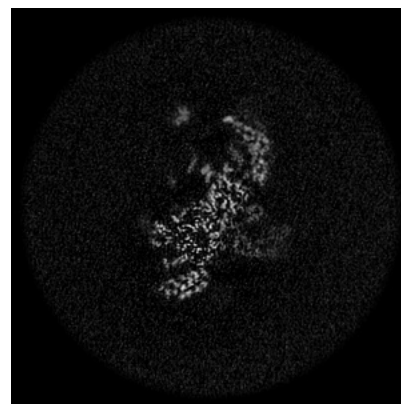
6.3.1 Primary map



X Index: 227



Y Index: 216

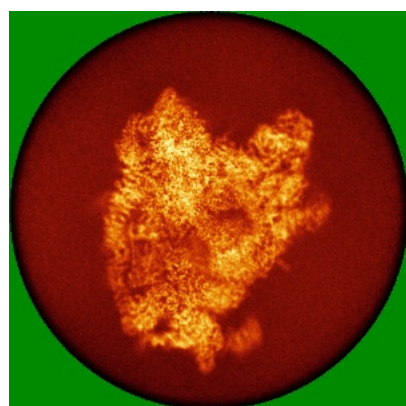


Z Index: 317

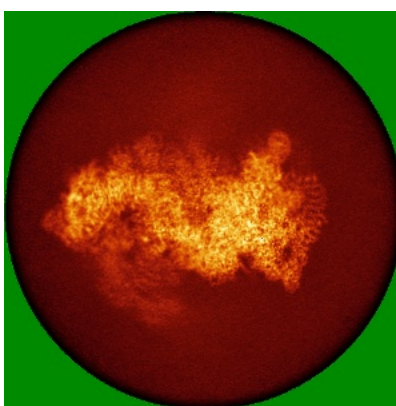
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

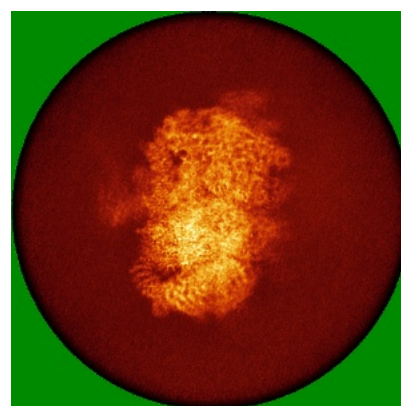
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

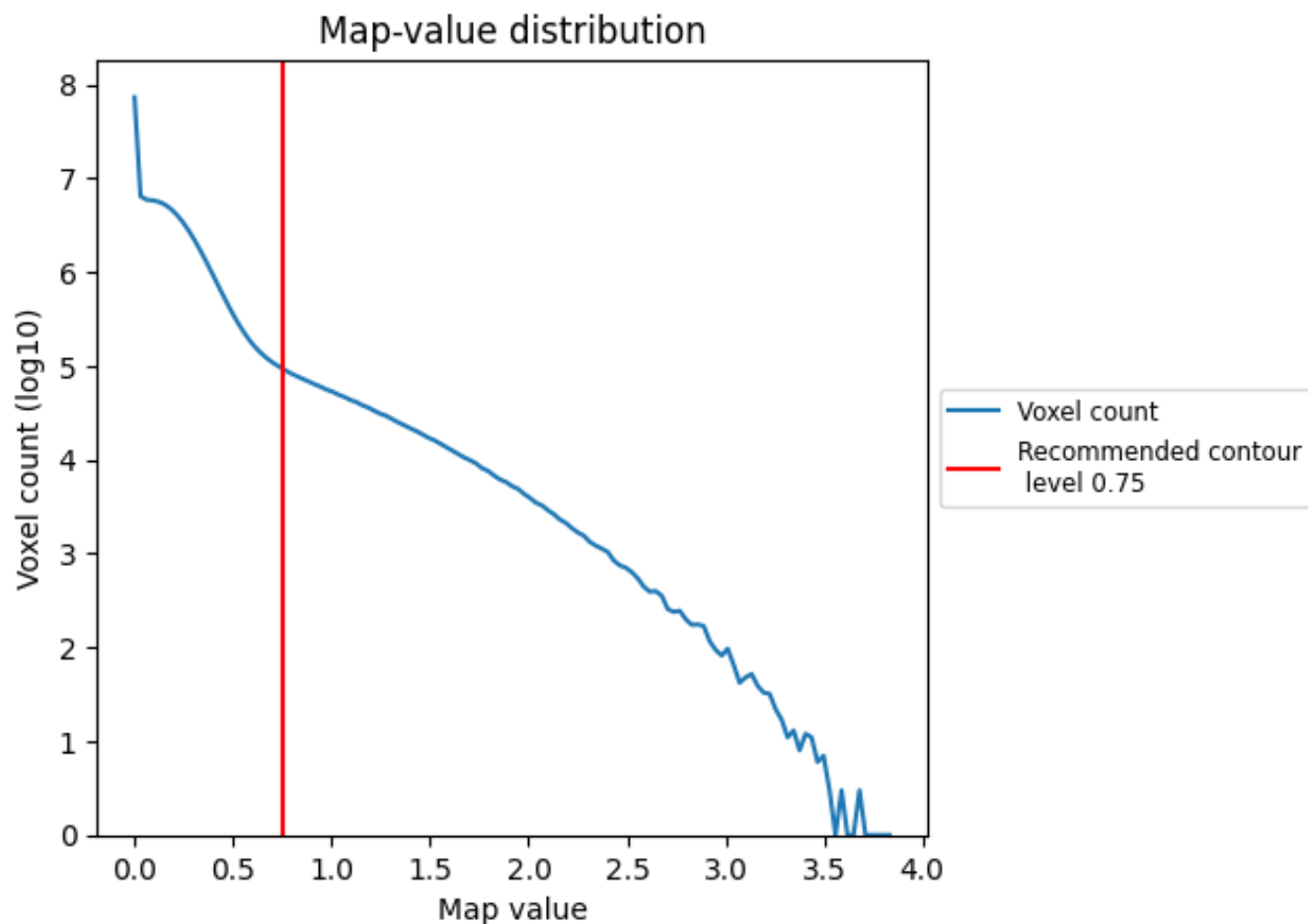
6.6 Mask visualisation

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

7 Map analysis [i](#)

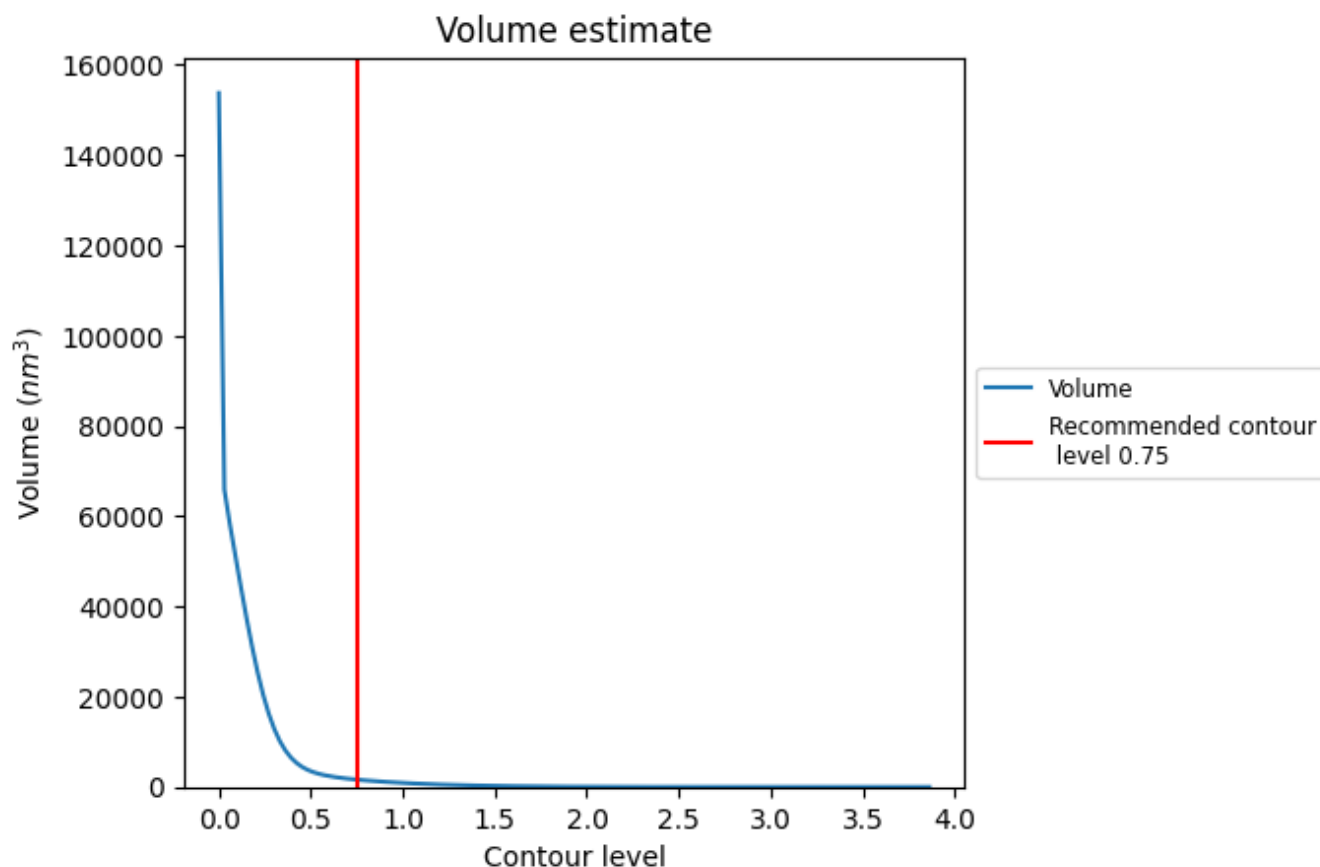
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

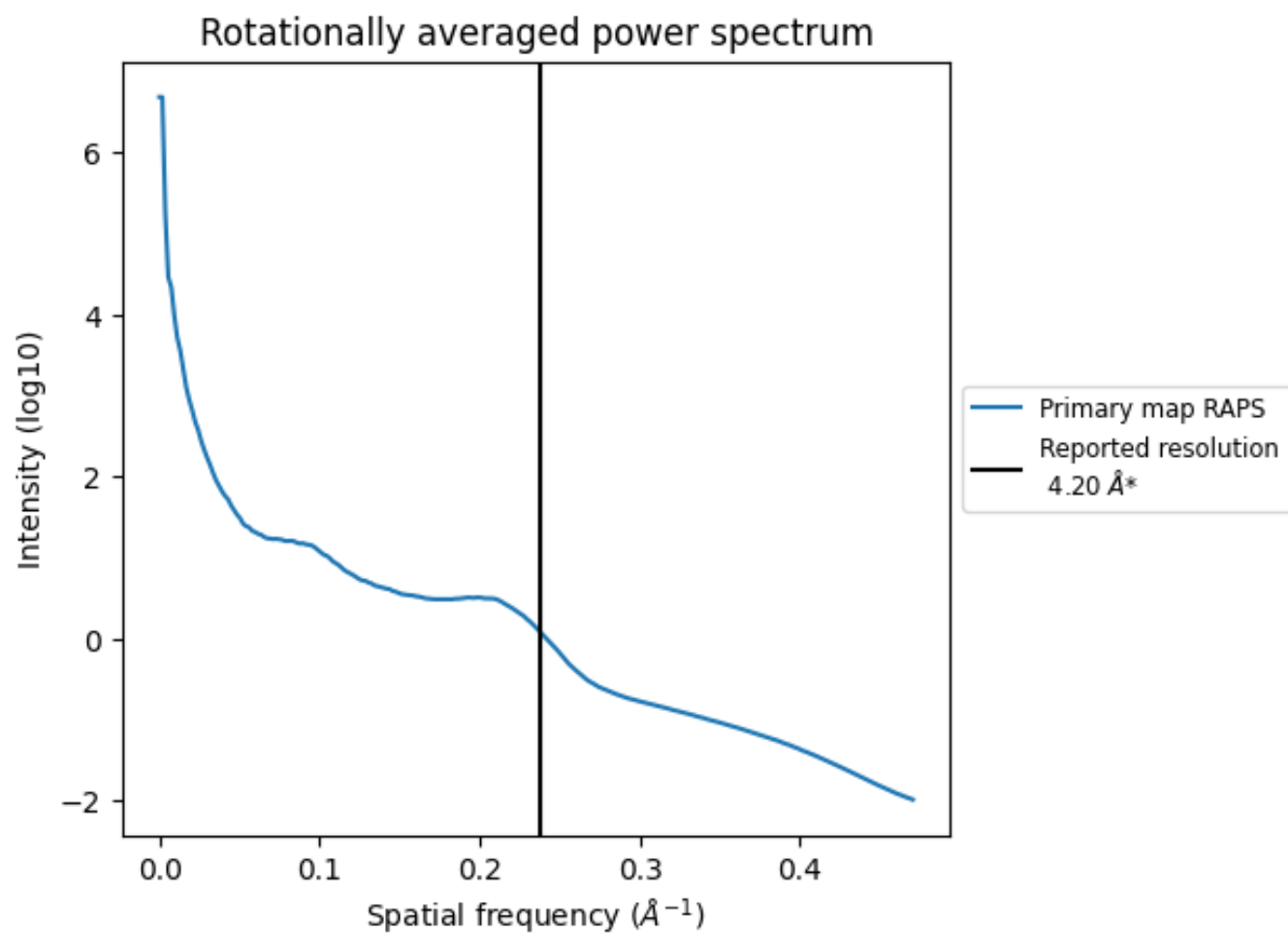
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1623 nm³; this corresponds to an approximate mass of 1466 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation

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

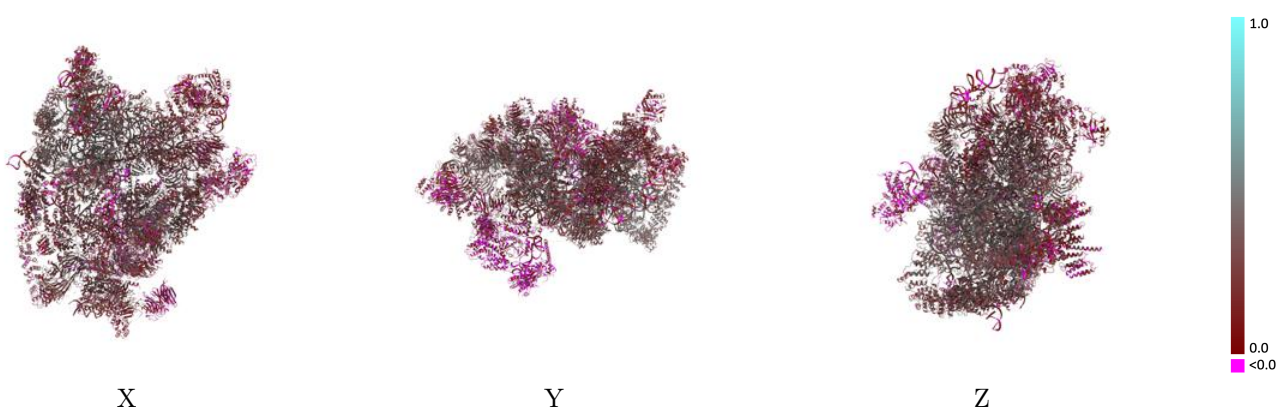
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49086 and PDB model 9N76. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)

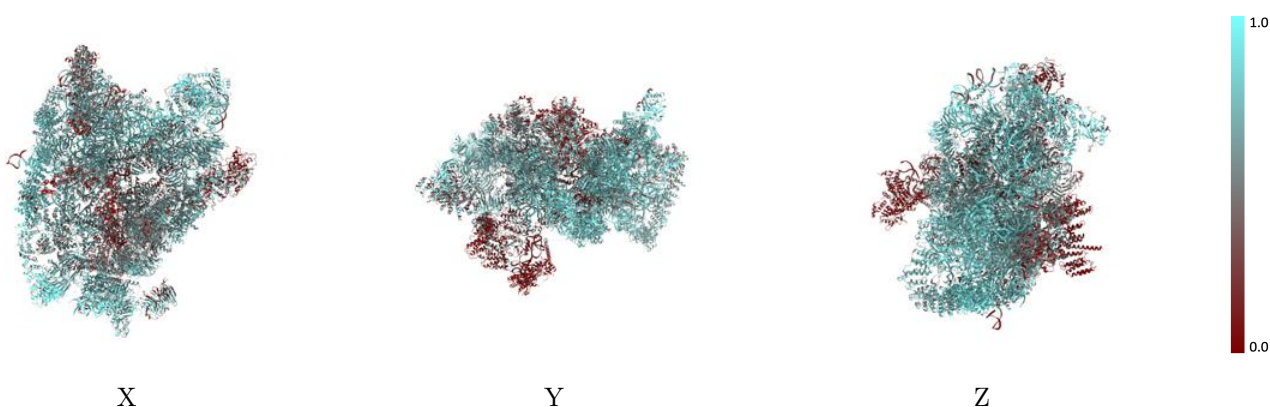
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



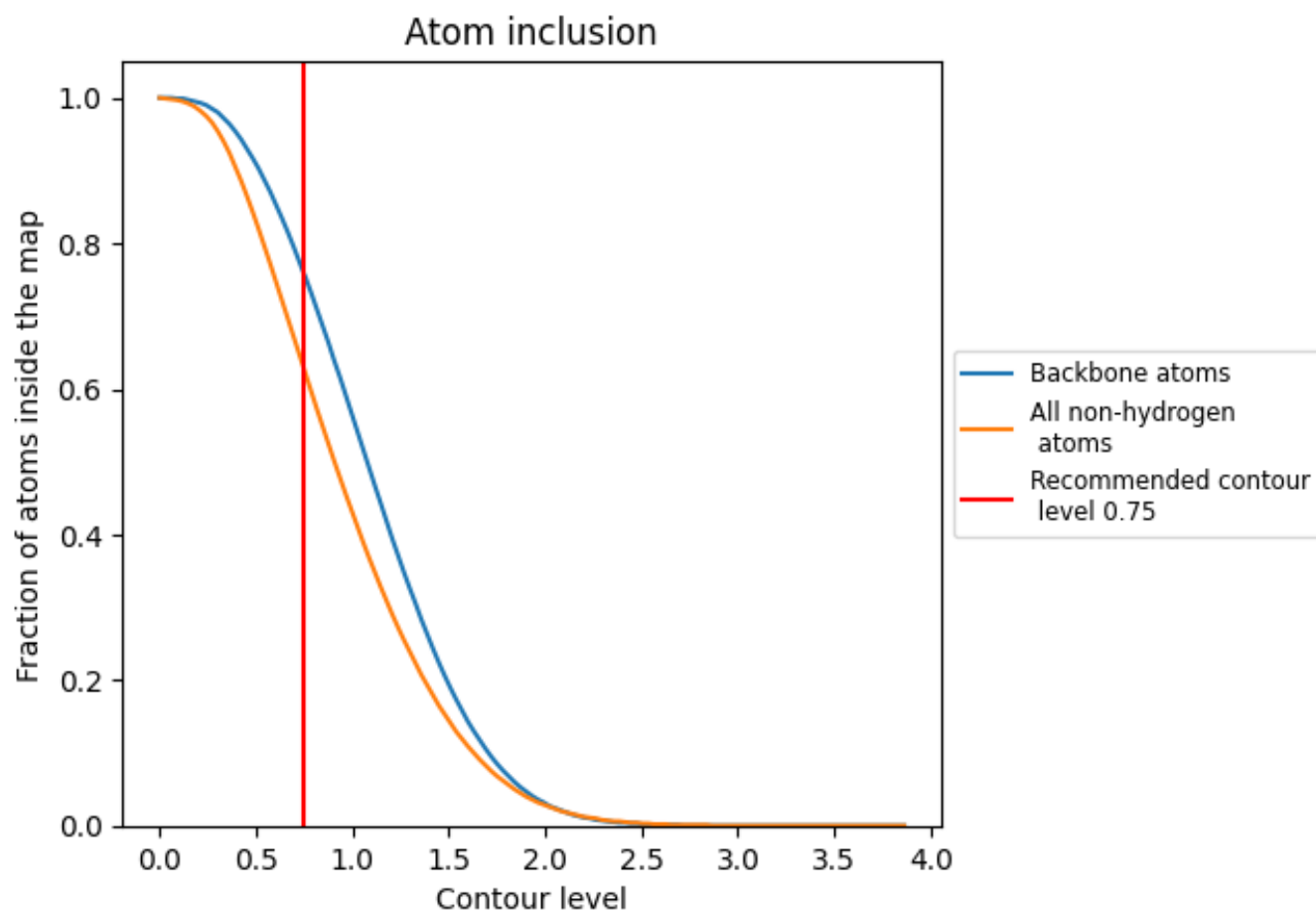
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.75).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6260	 0.2730
L0	 0.7610	 0.2410
L1	 0.7540	 0.2990
L2	 0.7320	 0.2630
L3	 0.1260	 0.1370
L4	 0.7400	 0.4150
L5	 0.6590	 0.2880
L6	 0.7440	 0.3900
L7	 0.4150	 0.1970
L8	 0.7670	 0.4040
L9	 0.7460	 0.4050
LC	 0.6470	 0.3570
LD	 0.7550	 0.4030
LE	 0.6750	 0.3930
LF	 0.7530	 0.3680
LG	 0.6660	 0.3920
LH	 0.7000	 0.2670
LI	 0.5720	 0.1340
LJ	 0.6390	 0.1870
LK	 0.6340	 0.1670
LL	 0.6380	 0.2270
LM	 0.6610	 0.2400
LN	 0.7540	 0.3010
LO	 0.6010	 0.3320
LP	 0.1570	 0.1780
LQ	 0.7580	 0.2910
LR	 0.7060	 0.2360
LS	 0.5870	 0.2800
LT	 0.5580	 0.2910
LZ	 0.5220	 0.2850
NA	 0.5620	 0.2810
NB	 0.5220	 0.2560
ND	 0.5120	 0.2250
NF	 0.6470	 0.3350
NG	 0.6950	 0.2930



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
NH	 0.7350	 0.2010
NI	 0.6540	 0.1920
NL	 0.4630	 0.2150
NM	 0.5590	 0.2620
NP	 0.1180	 0.2200
NQ	 0.6290	 0.3320
NS	 0.3680	 0.1770
NV	 0.3500	 0.2930
OH	 0.0100	 -0.0030
OU	 0.0070	 0.0040
SA	 0.5870	 0.2830
SB	 0.5540	 0.2600
SC	 0.6650	 0.3790
SD	 0.5380	 0.2640
SE	 0.7010	 0.2880
SF	 0.7000	 0.3920
SG	 0.7210	 0.3690
SH	 0.7270	 0.3700
SI	 0.7240	 0.3880
SJ	 0.2800	 0.1200
SK	 0.4200	 0.1460
SL	 0.6850	 0.4040
SM	 0.6270	 0.3610
SP	 0.5730	 0.2910
SQ	 0.5760	 0.3640
SR	 0.7140	 0.4110
SS	 0.3750	 0.2110
ST	 0.2210	 0.1300
SU	 0.2030	 0.0830
SV	 0.7920	 0.2830
SW	 0.6420	 0.2580
SY	 0.5530	 0.2880
SZ	 0.0560	 0.0190