wwPDB EM Validation Summary Report

Nov 2, 2026 – 03:28 PM JST

PDB ID	:	9XJ6 / pdb_00009xj6
EMDB ID	:	EMD-66929
Title	:	Portimine A-bound human translating ribosome - P/P-E/E State
Authors	:	Wang, Y.; Zhang, Y.; Gao, N.
Deposited on	:	2025-11-04
Resolution	:	2.78 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

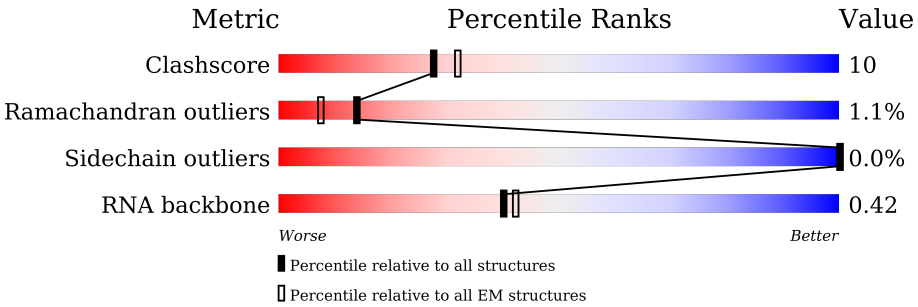
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

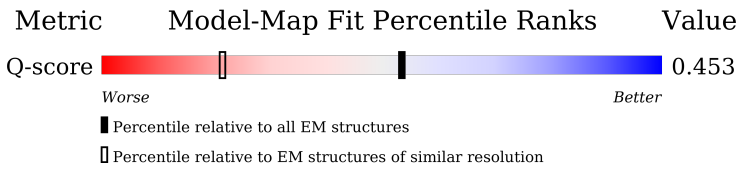
1 Overall quality at a glance

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

The reported resolution of this entry is 2.78 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	10754 (2.28 - 3.28)

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	L5	5070	19% 39% 27% 8% 26%
2	L7	121	75% 21%
3	L8	157	11% 61% 30% 8%

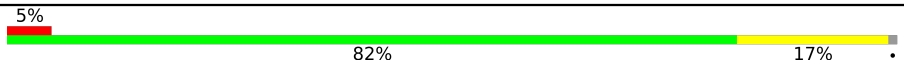
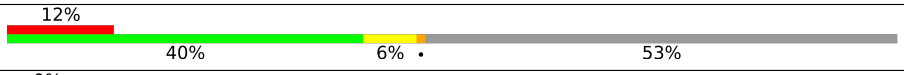
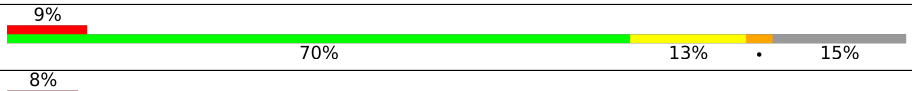
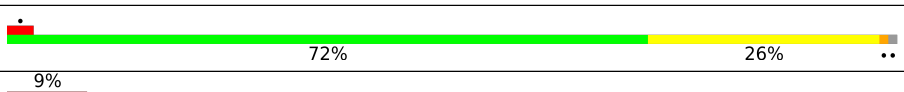
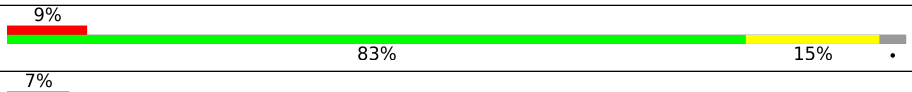
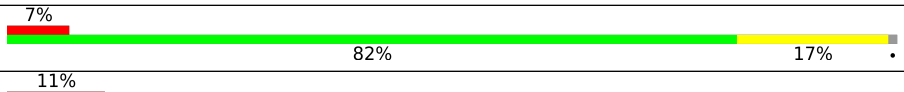
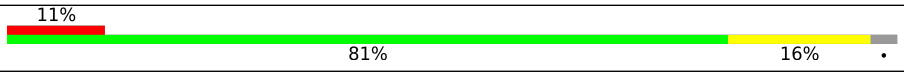
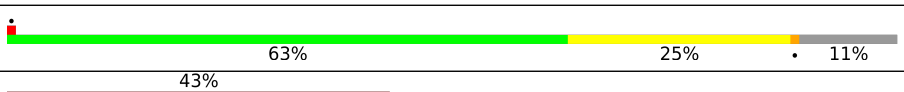
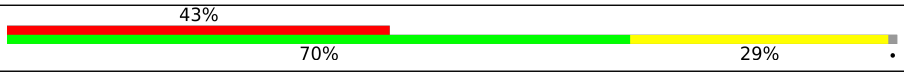
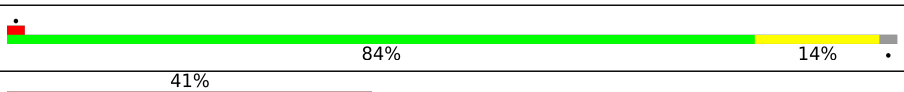
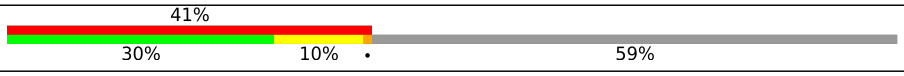
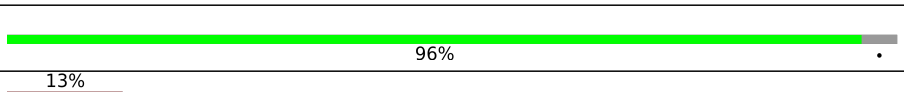
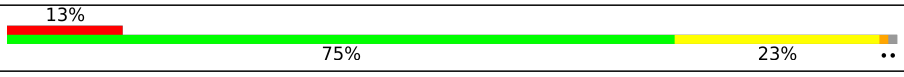
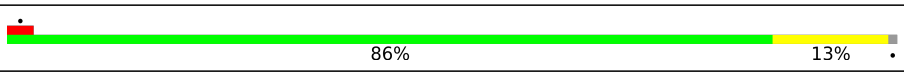
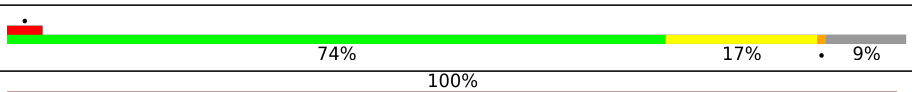
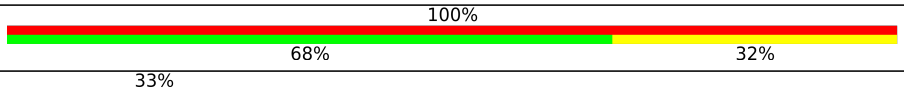
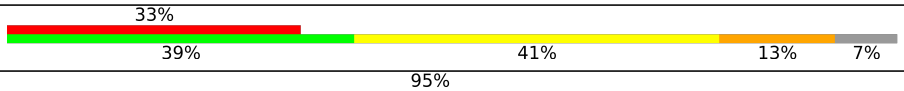
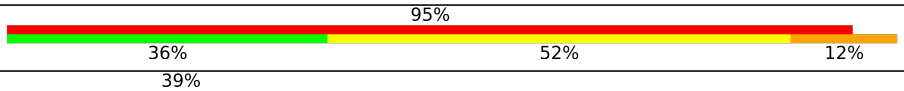
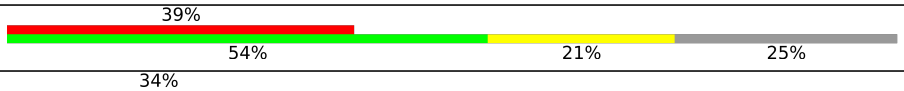
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Mol	Chain	Length	Quality of chain
4	LA	257	77% 19%
5	LB	403	5% 82% 17%
6	LC	427	5% 67% 19% 14%
7	LD	297	14% 75% 23%
8	LE	288	20% 61% 21% 16%
9	LF	248	6% 71% 19% 9%
10	LG	266	17% 75% 15% 9%
11	LH	192	14% 81% 18%
12	LI	214	18% 75% 24%
13	LJ	178	38% 72% 26%
14	LL	211	12% 80% 18%
15	LM	215	6% 49% 15% 35%
16	LN	204	82% 18%
17	LO	203	86% 13%
18	LP	184	72% 11% 17%
19	LQ	188	85% 14%
20	LR	196	16% 74% 21% 5%
21	LS	176	78% 21%
22	LT	160	12% 84% 16%
23	LU	128	42% 59% 20% 21%
24	LV	140	76% 17% 6%
25	LW	157	41% 56% 20% 21%
26	LX	156	5% 60% 16% 23%
27	LY	145	6% 74% 18% 8%
28	LZ	136	7% 77% 22%

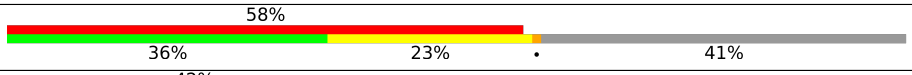
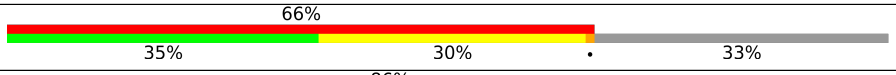
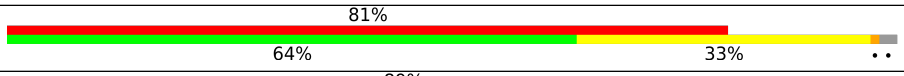
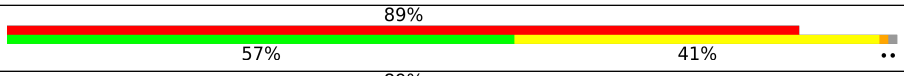
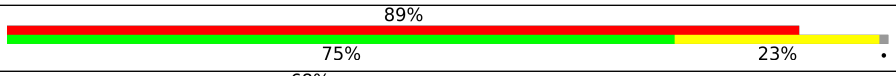
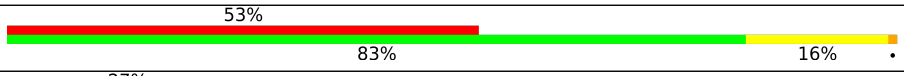
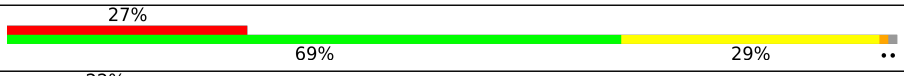
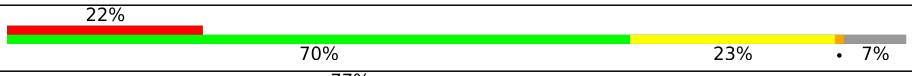
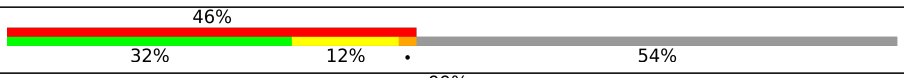
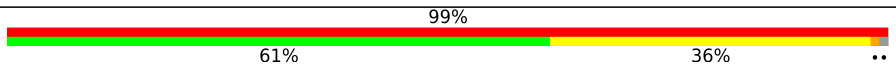
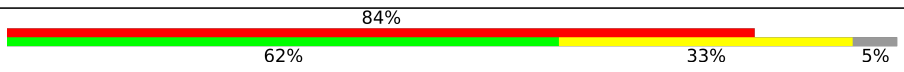
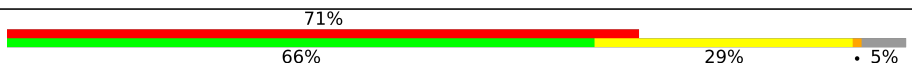
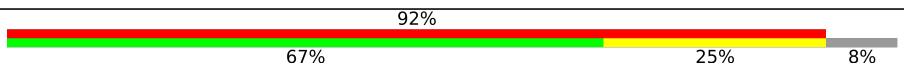
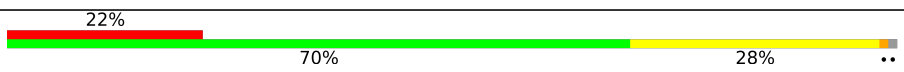
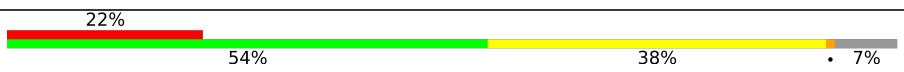
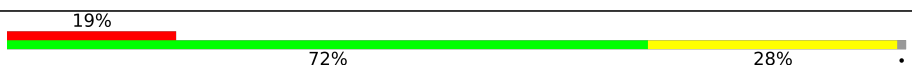
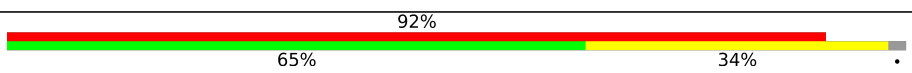
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Mol	Chain	Length	Quality of chain
29	La	148	
30	Lb	159	
31	Lc	115	
32	Ld	125	
33	Le	135	
34	Lf	110	
35	Lg	117	
36	Lh	123	
37	Li	105	
38	Lj	97	
39	Lk	70	
40	Ll	51	
41	Lm	128	
42	Ln	25	
43	Lo	106	
44	Lp	92	
45	Lr	137	
46	Lz	217	
47	S2	1869	
48	S6	75	
49	SA	295	
50	SB	264	
51	SD	243	
52	SE	263	
53	SF	204	

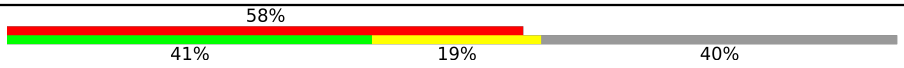
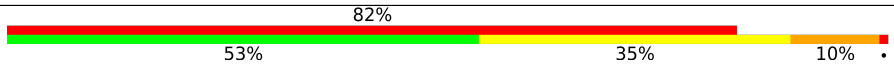
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Mol	Chain	Length	Quality of chain
54	SH	193	
55	SI	208	
56	SK	165	
57	SL	158	
58	SP	145	
59	SQ	146	
60	SR	135	
61	SS	152	
62	ST	145	
63	SU	119	
64	SV	83	
65	SX	143	
66	Sa	115	
67	Sc	69	
68	Sd	56	
69	Sf	156	
70	Sg	317	
71	SC	293	
72	SG	249	
73	SJ	194	
74	SM	132	
75	SN	151	
76	SO	151	
77	SW	130	
78	SY	133	

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Mol	Chain	Length	Quality of chain
79	SZ	125	
80	Sb	84	
81	Se	59	
82	Pt	77	

2 Entry composition (i)

There are 85 unique types of molecules in this entry. The entry contains 220451 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L5	3776	80184	35672	14597	26140	3775	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L7	120	2558	1141	456	842	119	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L8	156	3314	1480	585	1094	155	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	LA	248	1898	1189	389	314	6	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	LB	402	3238	2060	608	556	14	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LC	367	2919	1835	582	488	14	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 8 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	242	Total	C	N	O	S	0	0
			1958	1257	372	325	4		

- Molecule 9 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 10 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 12 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

- Molecule 13 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	176	Total	C	N	O	S	0	0
			1410	888	263	253	6		

- Molecule 14 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 15 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 16 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 17 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 19 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 20 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 21 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 22 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 23 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 25 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	124	Total	C	N	O	S	0	0
			1015	634	207	170	4		

- Molecule 26 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 27 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 28 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 29 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 30 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	75	Total	C	N	O	S	0	0
			610	378	130	99	3		

- Molecule 31 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 32 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 33 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 34 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 35 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 36 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 37 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 38 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 39 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 40 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 41 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 42 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 43 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 44 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 45 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 46 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lz	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

- Molecule 47 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S2	1742	Total	C	N	O	P	0	0
			36900	16458	6595	12106	1741		

- Molecule 48 is a RNA chain called HUMAN INITIATOR MET-TRNA-I.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S6	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 49 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SA	222	Total	C	N	O	S	0	0
			1747	1109	306	324	8		

- Molecule 50 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 51 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 52 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 53 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SF	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 54 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SH	189	Total	C	N	O	S	0	0
			1521	969	280	271	1		

- Molecule 55 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 56 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 57 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 58 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SP	97	Total	C	N	O	S	0	0
			804	505	155	138	6		

- Molecule 59 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SQ	146	Total	C	N	O	S	0	0
			1158	736	218	200	4		

- Molecule 60 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SR	132	Total	C	N	O	S	0	0
			1072	673	199	195	5		

- Molecule 61 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SS	150	Total	C	N	O	S	0	0
			1235	776	250	208	1		

- Molecule 62 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 63 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 64 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 65 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 66 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Sa	107	Total	C	N	O	S	0	0
			847	528	176	138	5		

- Molecule 67 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 68 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Sd	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 69 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Sf	71	Total	C	N	O	S	0	0
			581	367	109	98	7		

- Molecule 70 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 71 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 72 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 73 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 74 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SM	122	Total	C	N	O	S	0	0
			952	596	169	179	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	52	GLN	LEU	conflict	UNP P25398
SM	69	LEU	CYS	conflict	UNP P25398
SM	99	ASN	LYS	conflict	UNP P25398

- Molecule 75 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 76 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SO	140	Total	C	N	O	S	0	0
			1049	642	204	197	6		

- Molecule 77 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 78 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 79 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 80 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 81 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

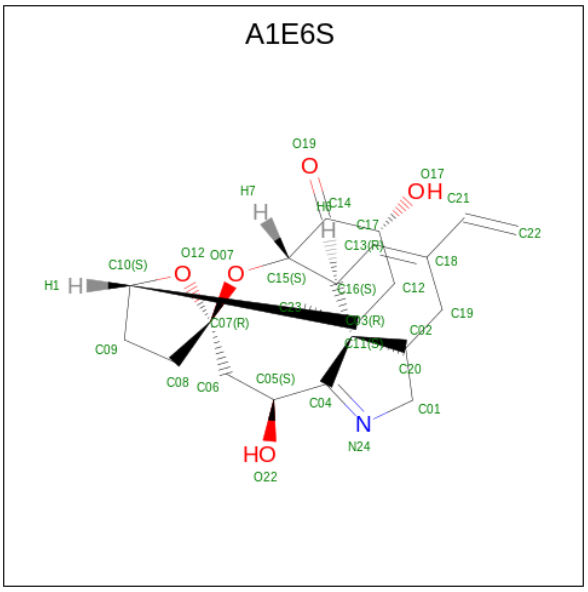
- Molecule 82 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	Pt	77	Total	C	N	O	P	S	0	0
			1646	734	298	536	77	1		

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
83	L5	146	Total Mg 146 146	0
83	L7	7	Total Mg 7 7	0
83	L8	5	Total Mg 5 5	0
83	LA	1	Total Mg 1 1	0
83	LH	1	Total Mg 1 1	0
83	LN	1	Total Mg 1 1	0
83	LP	1	Total Mg 1 1	0
83	LQ	1	Total Mg 1 1	0
83	LV	1	Total Mg 1 1	0
83	Le	1	Total Mg 1 1	0
83	Ll	1	Total Mg 1 1	0
83	S2	66	Total Mg 66 66	0
83	S6	7	Total Mg 7 7	0

- Molecule 84 is (1R,3S,8R,13S,14S,16R,18S,19S)-11-ethenyl-3,16-dihydroxy-18-methyl-22,23-dioxa-5-azapentacyclo[12.7.1.11,19.04,8.08,13]tricosa-4,11-dien-15-one (CCD ID: A1E6S) (formula: $C_{23}H_{31}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
84	L5	1	Total	C	N	O	0
			29	23	1	5	

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	Lg	1	Total	Zn	0
			1	1	
85	Lj	1	Total	Zn	0
			1	1	
85	Lm	1	Total	Zn	0
			1	1	
85	Lo	1	Total	Zn	0
			1	1	
85	Lp	1	Total	Zn	0
			1	1	
85	Sa	1	Total	Zn	0
			1	1	

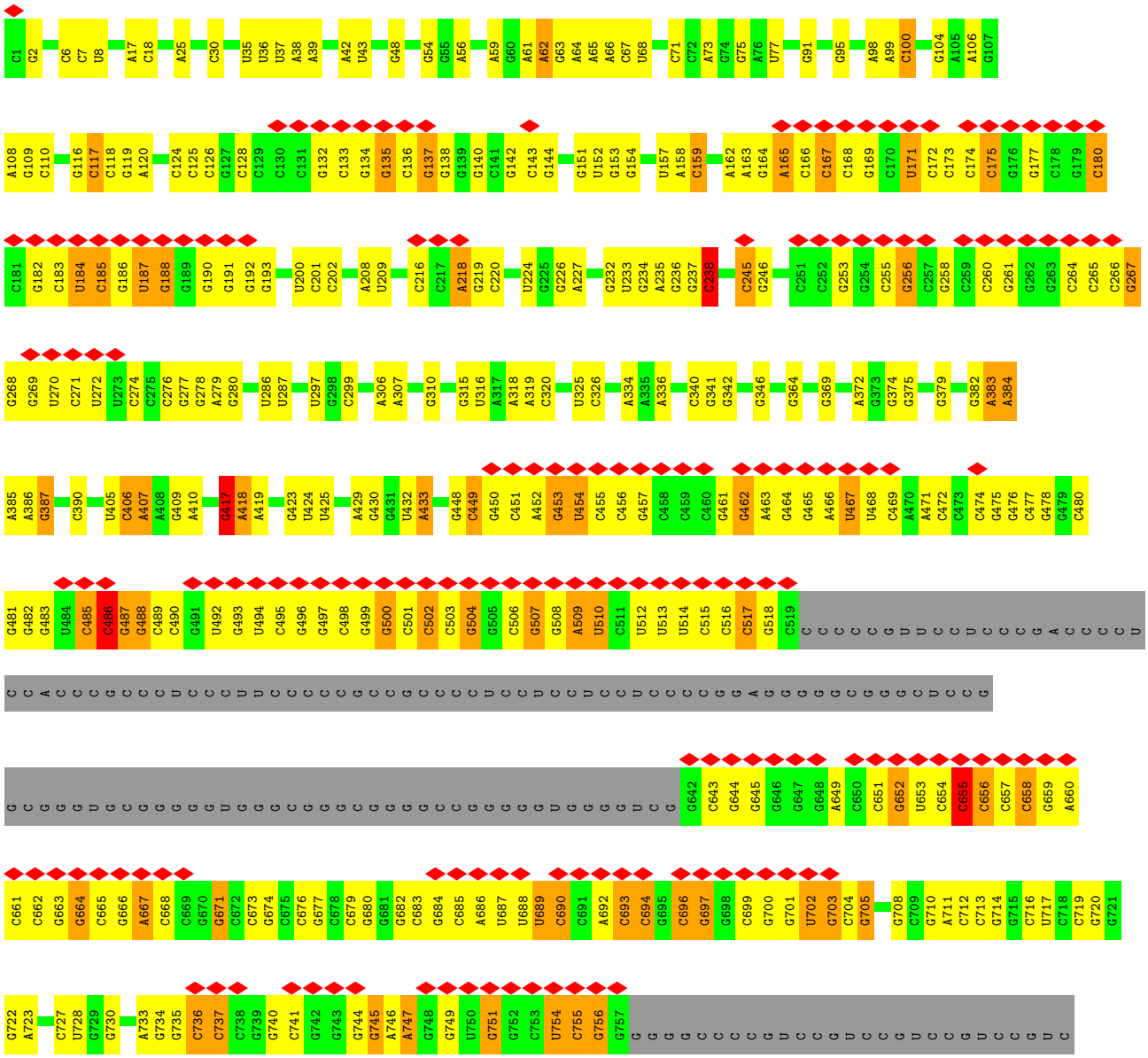
3 Residue-property plots (i)

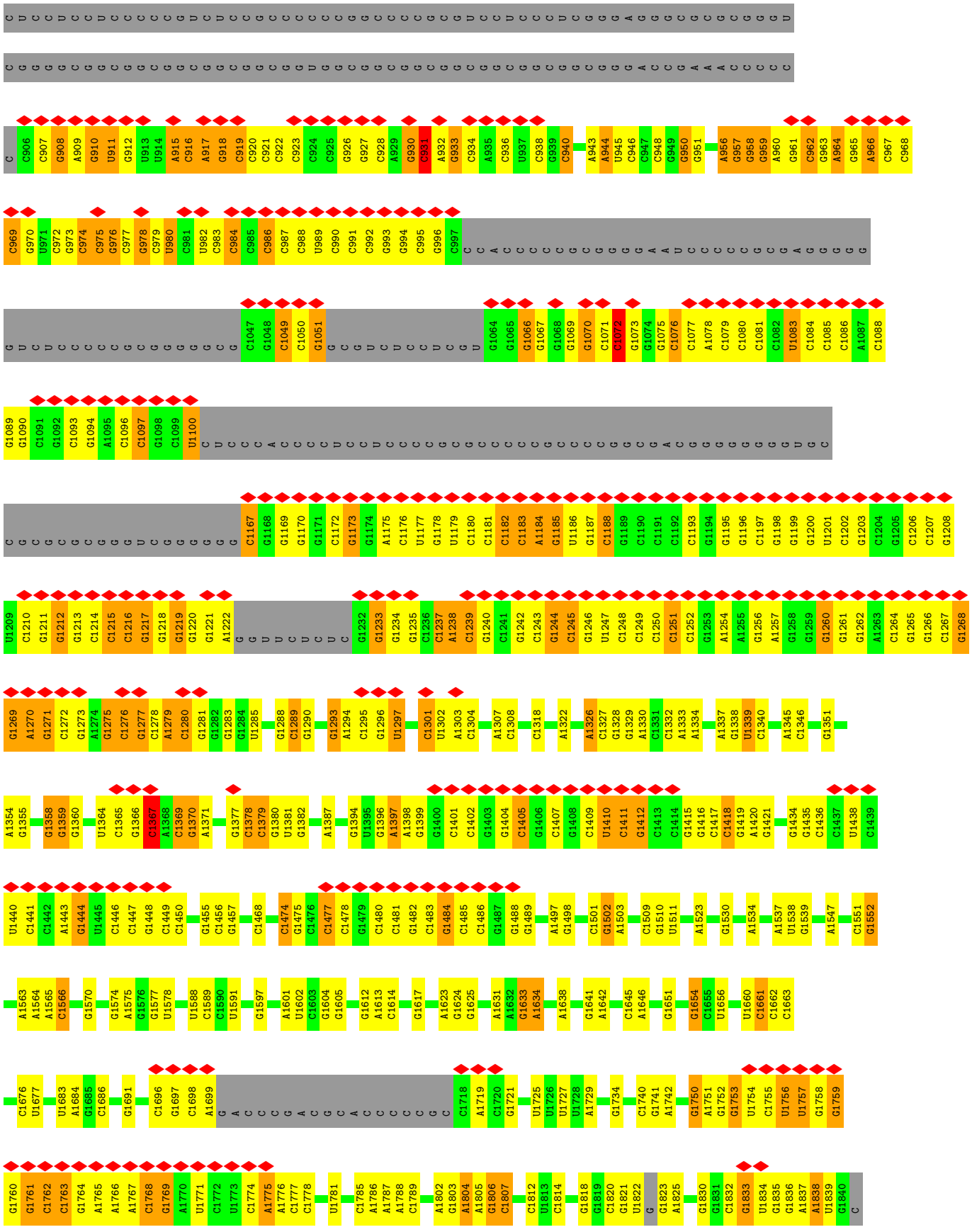
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

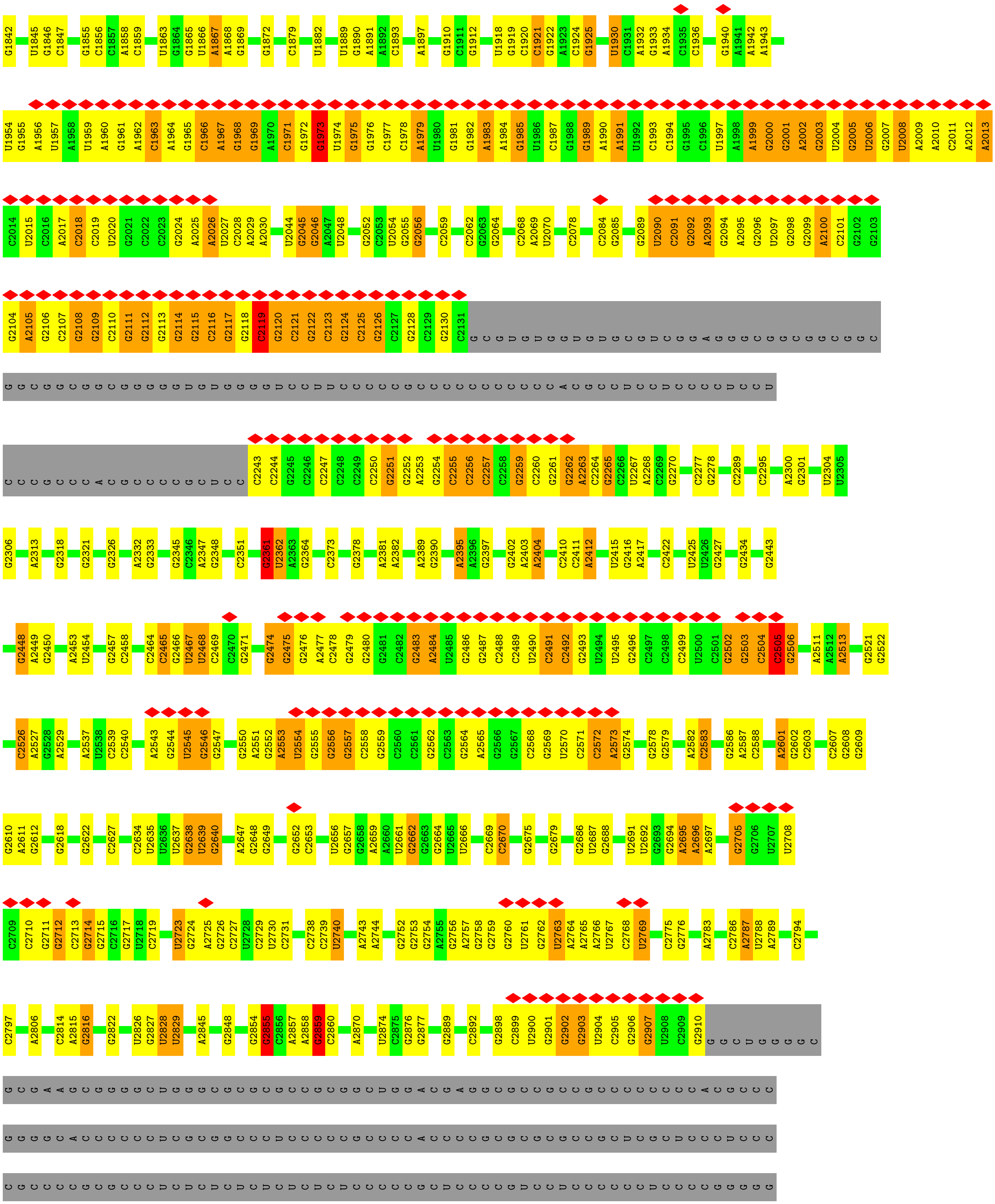
- Molecule 1: 28S ribosomal RNA

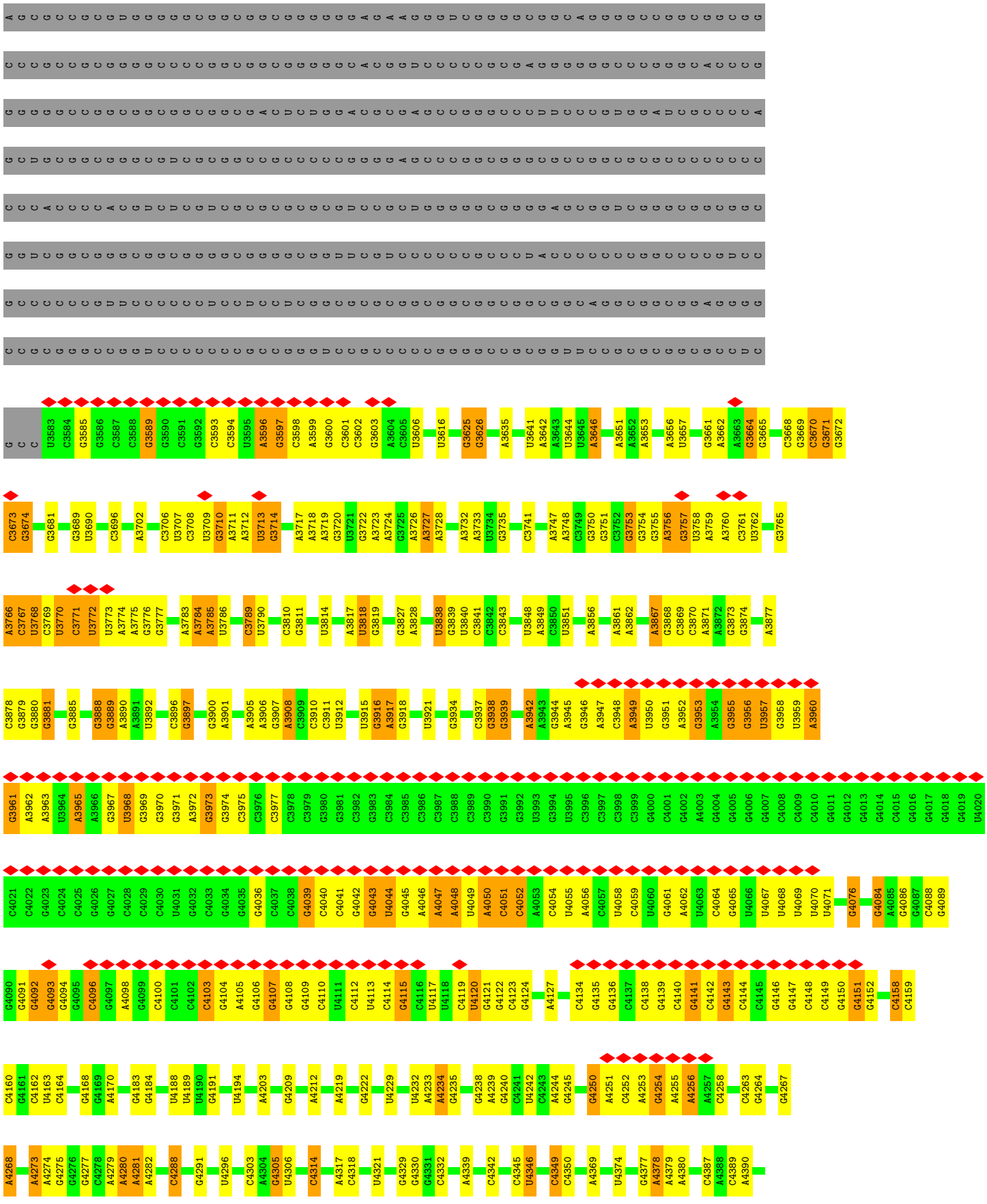
Chain L5:

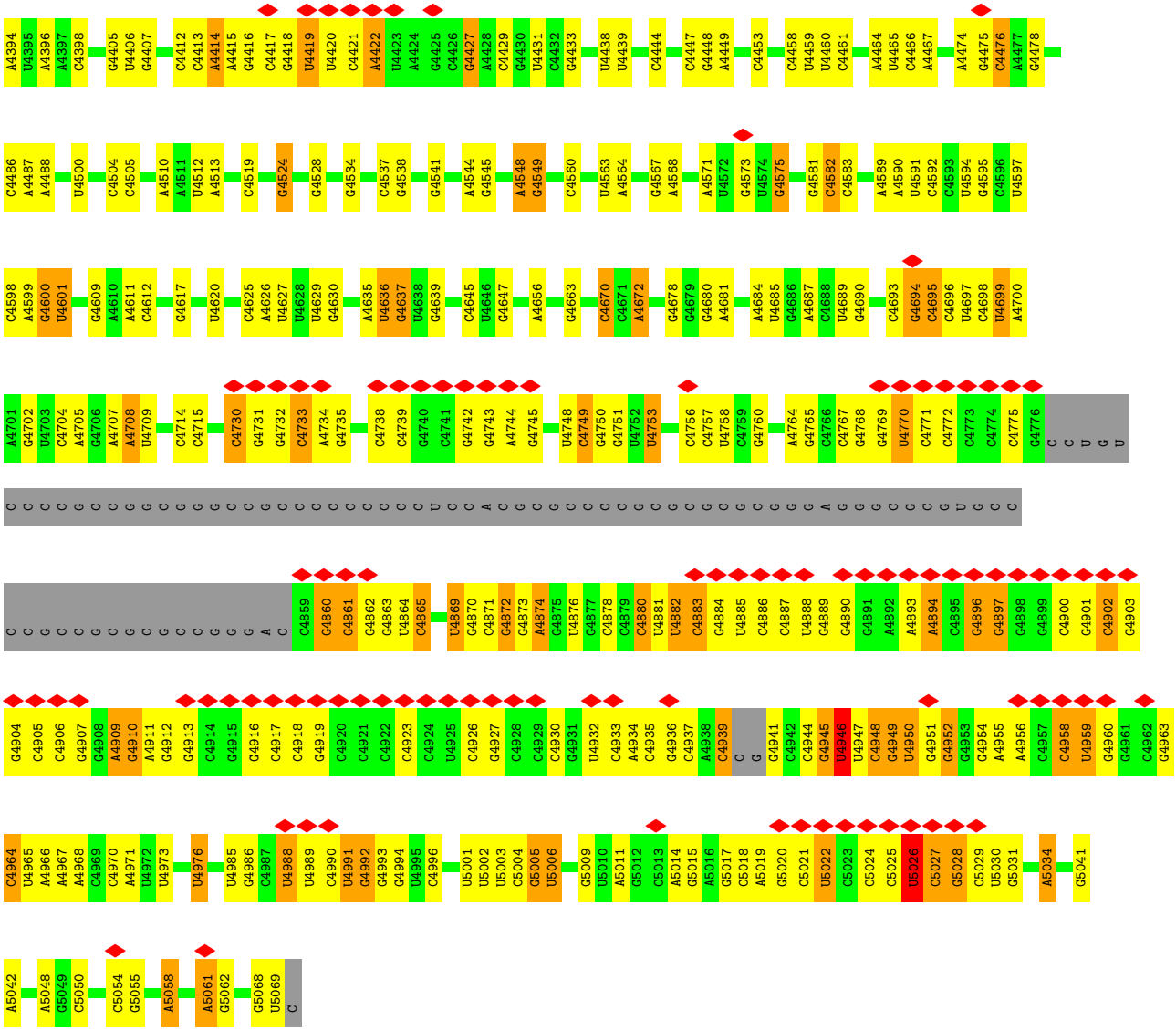







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C2797 A2806 C2814 A2815 G2816 G2822 U2826 G2827 U2828 U2829 A2845 G2848 G2854 G2855 C2856 A2857 A2858 G2859 C2860 A2870 U2874 C2875 G2876 C2877 G2889 C2892 G2898 C2899 U2900 G2901 G2902 G2903 U2904 C2905 C2906 G2907 U2908 C2909 G2910 G G C U G G G C
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G G C C C C G G C G C C C U C U C U C U U C U C U C U C U C U C C C C C G G U C C C C G G U C C C C U C C C C C C C U C C C C C G G G G G

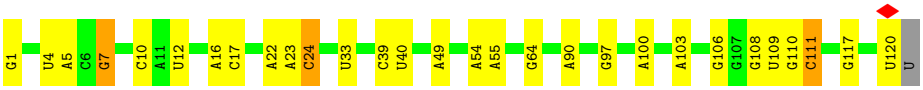




• Molecule 2: 5S ribosomal RNA

Chain L7:

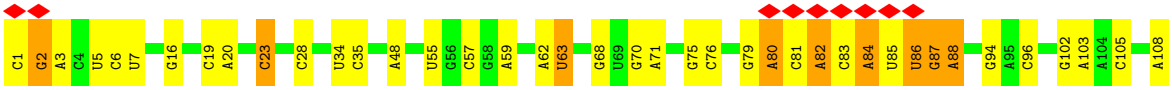


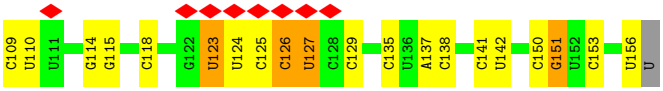


• Molecule 3: 5.8S ribosomal RNA

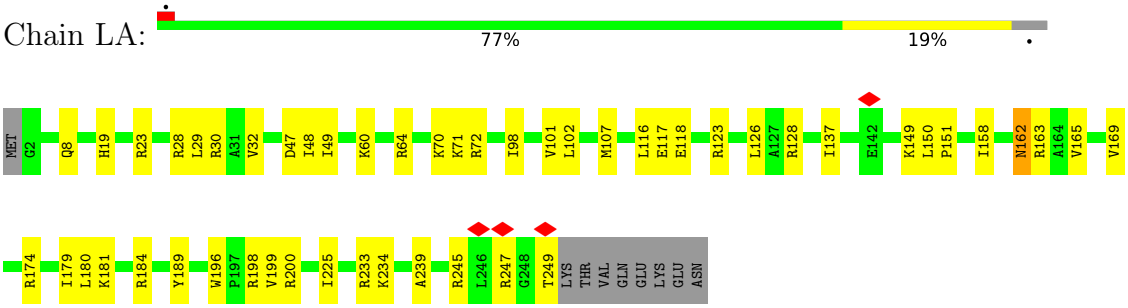
Chain L8:



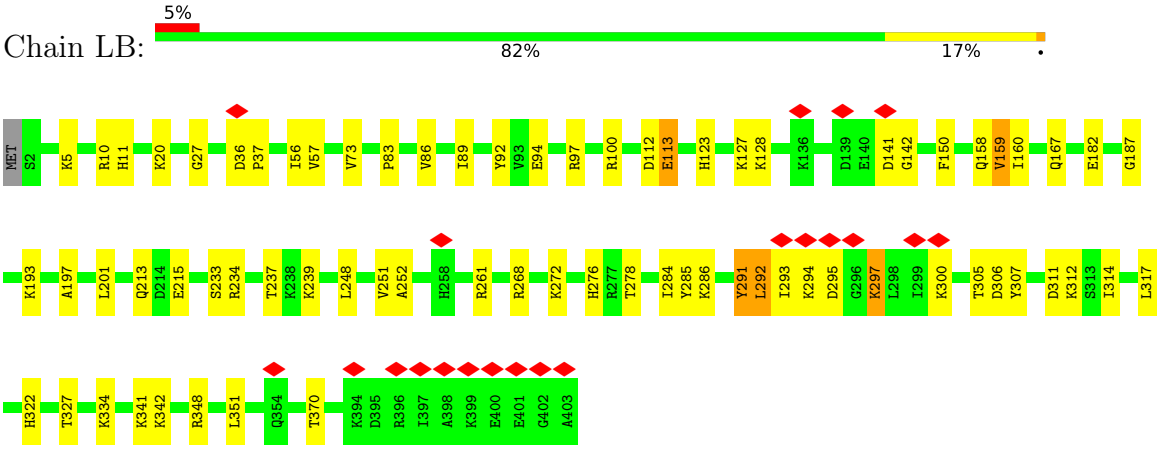




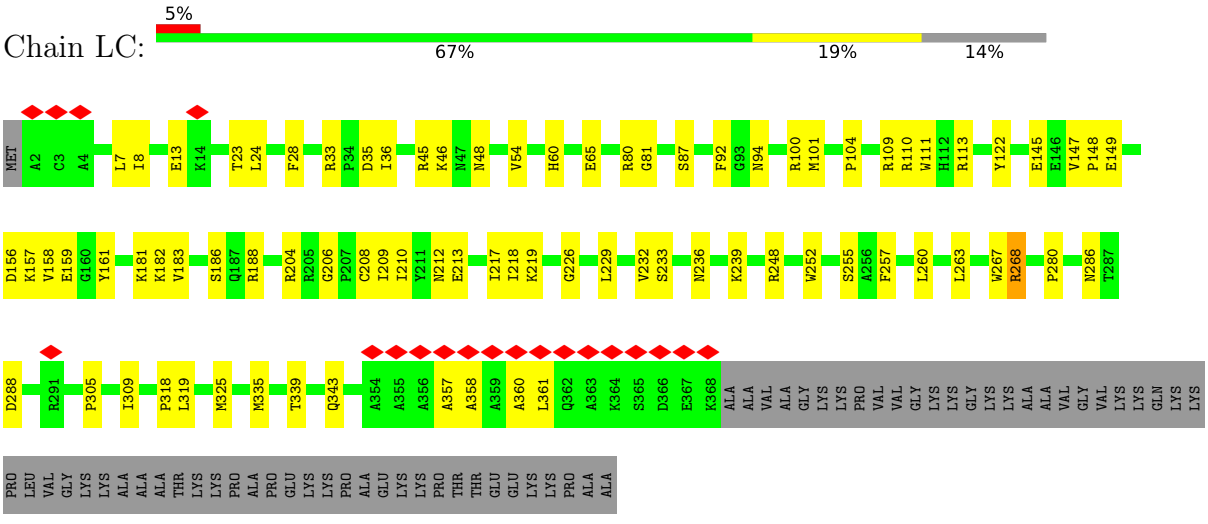
• Molecule 4: Large ribosomal subunit protein uL2



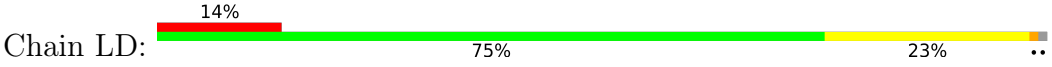
• Molecule 5: Large ribosomal subunit protein uL3

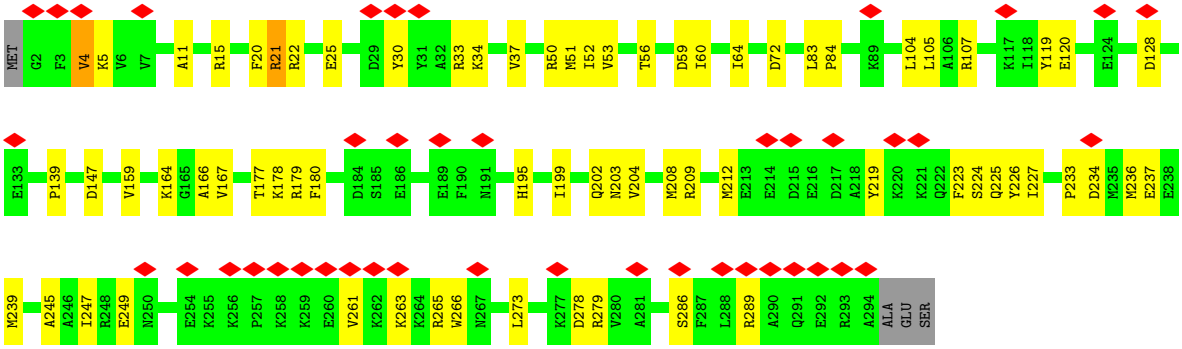


• Molecule 6: Large ribosomal subunit protein uL4



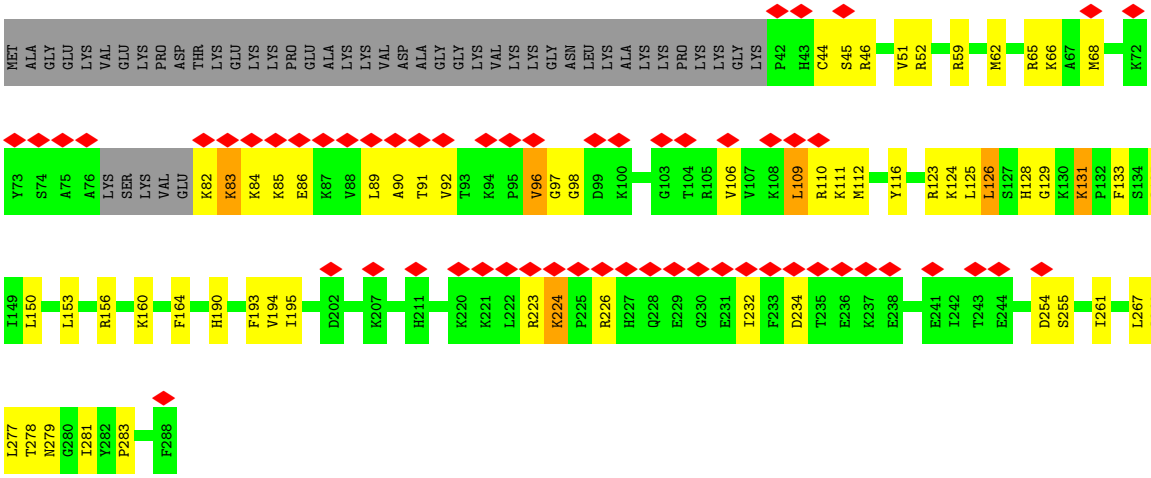
• Molecule 7: Large ribosomal subunit protein uL18





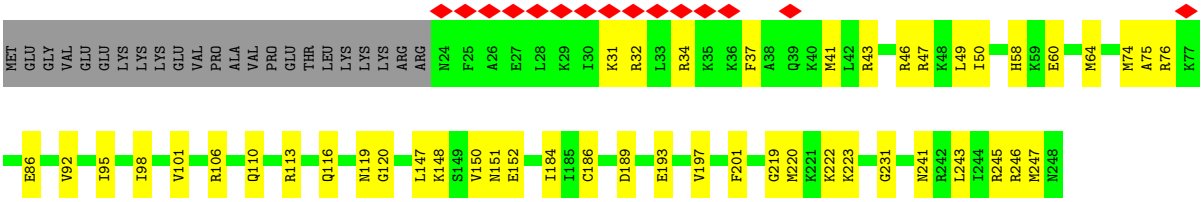
• Molecule 8: Large ribosomal subunit protein eL6



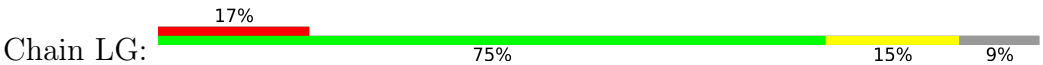


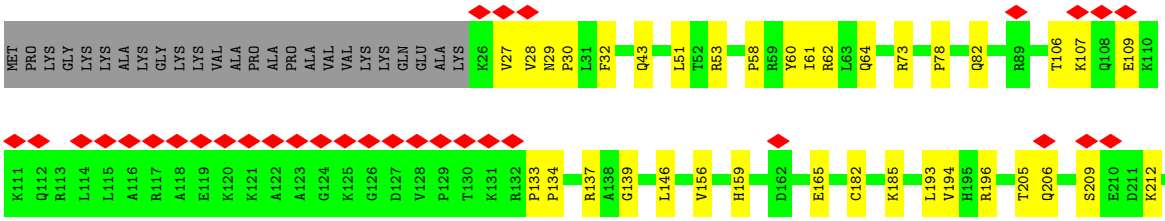
• Molecule 9: Large ribosomal subunit protein uL30

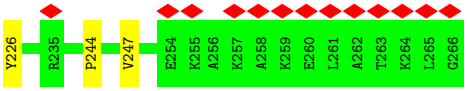




• Molecule 10: Large ribosomal subunit protein eL8



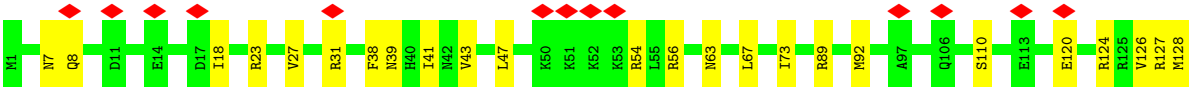


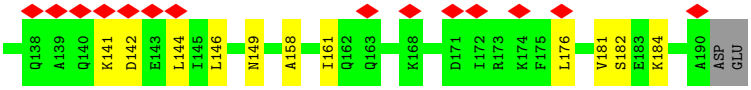


• Molecule 11: Large ribosomal subunit protein uL6

Chain LH:



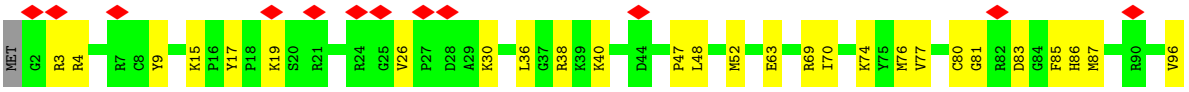


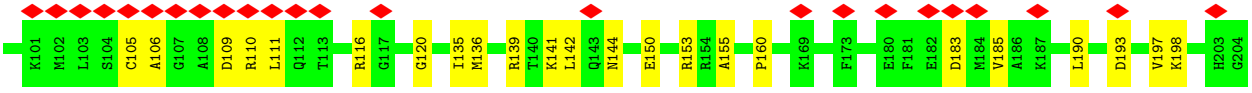


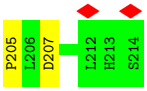
• Molecule 12: Ribosomal protein uL16-like

Chain LI:





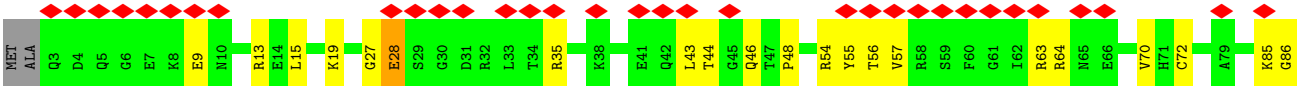


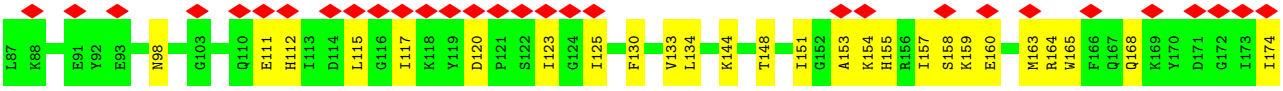


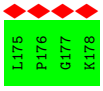
• Molecule 13: Large ribosomal subunit protein uL5

Chain LJ:





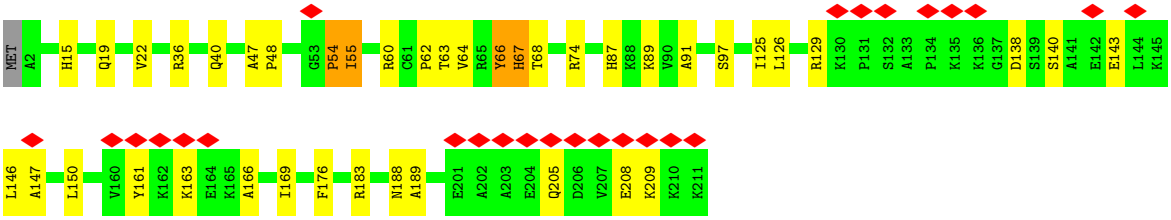




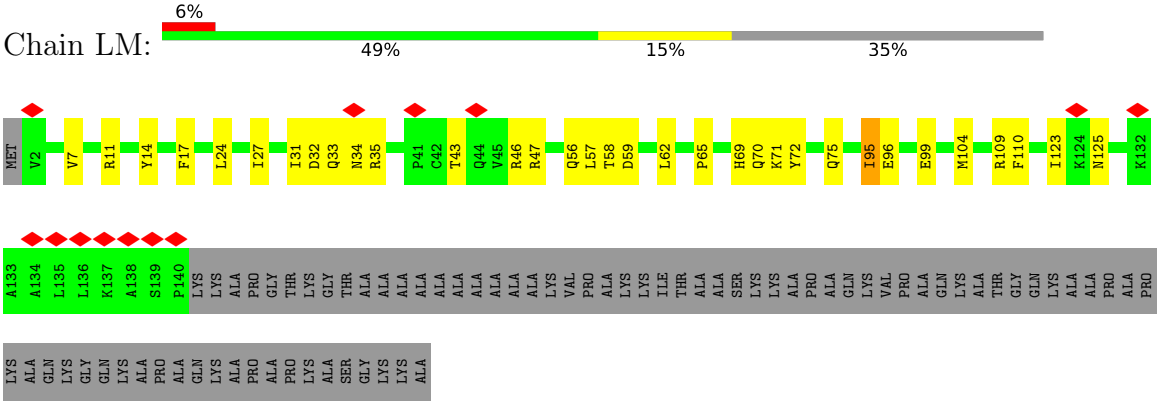
• Molecule 14: Large ribosomal subunit protein eL13

Chain LL:

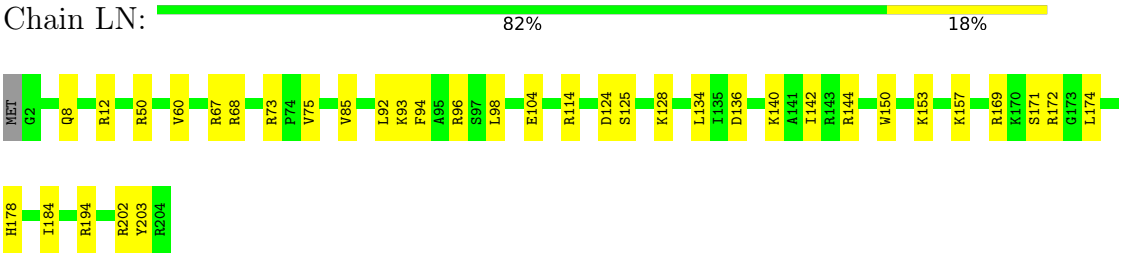




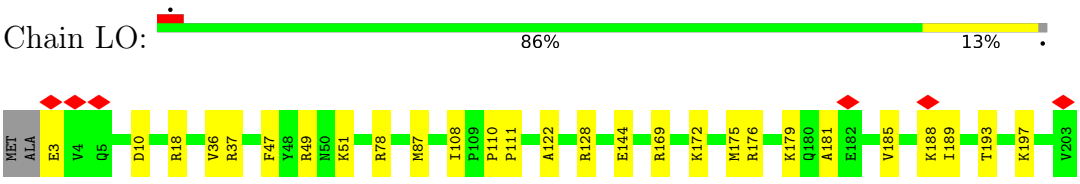
• Molecule 15: Large ribosomal subunit protein eL14



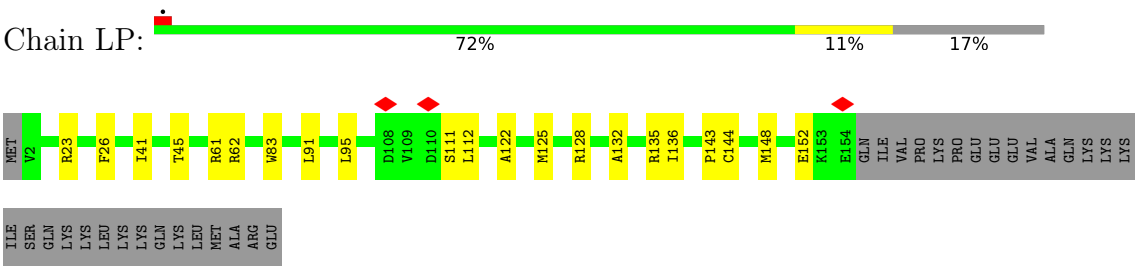
• Molecule 16: Large ribosomal subunit protein eL15



• Molecule 17: Large ribosomal subunit protein uL13

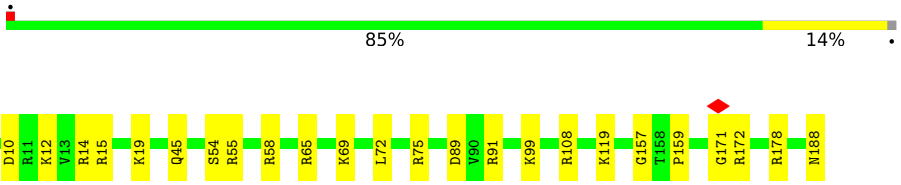


• Molecule 18: Large ribosomal subunit protein uL22



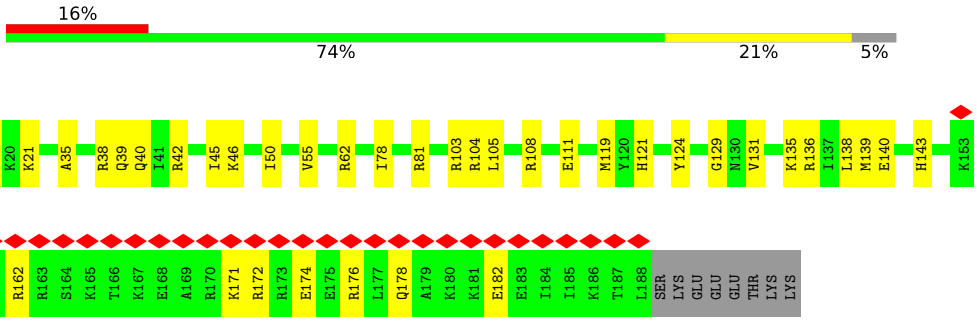
• Molecule 19: Large ribosomal subunit protein eL18

Chain LQ:



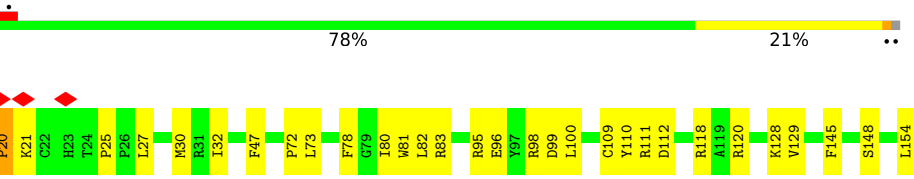
• Molecule 20: Large ribosomal subunit protein eL19

Chain LR:



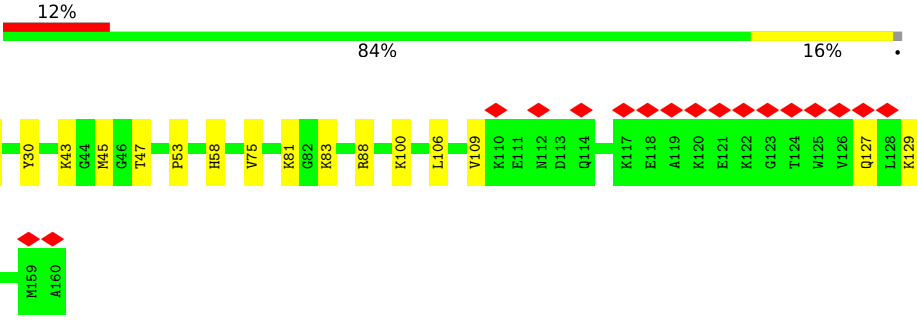
• Molecule 21: Large ribosomal subunit protein eL20

Chain LS:



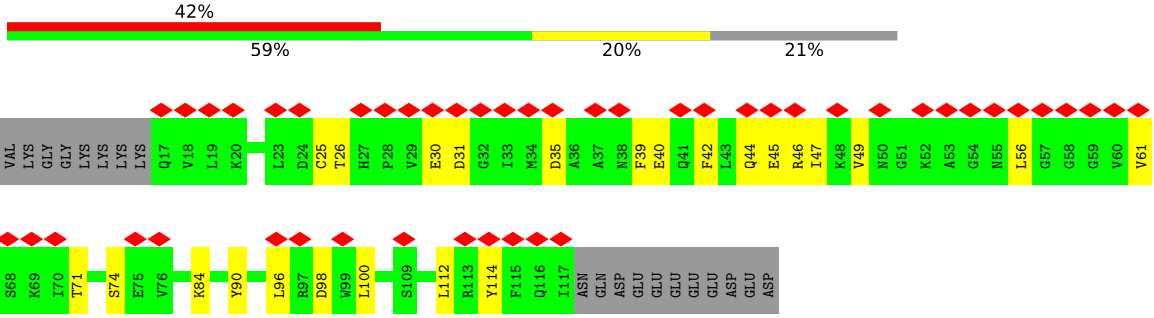
• Molecule 22: Large ribosomal subunit protein eL21

Chain LT:



• Molecule 23: Large ribosomal subunit protein eL22

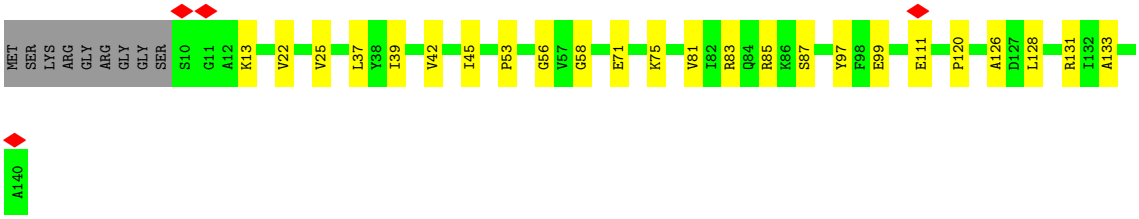
Chain LU:



• Molecule 24: Large ribosomal subunit protein uL14

Chain LV:

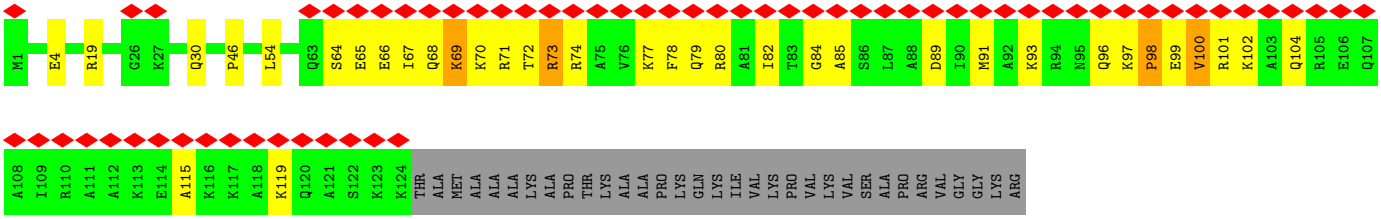




• Molecule 25: Large ribosomal subunit protein eL24

Chain LW:

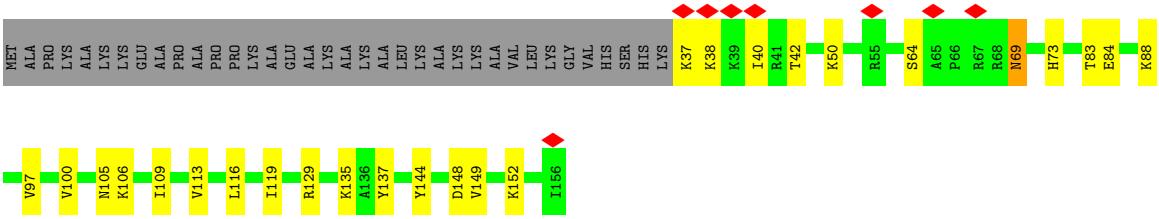




• Molecule 26: Large ribosomal subunit protein uL23

Chain LX:

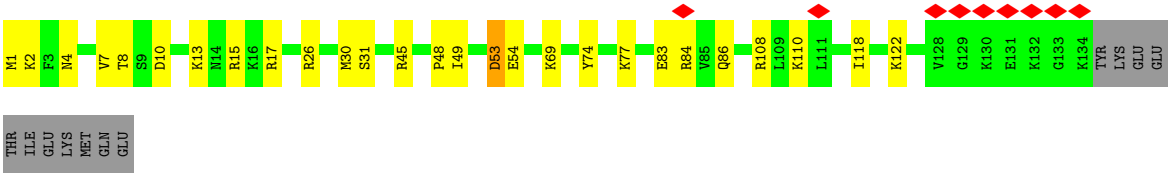




• Molecule 27: Large ribosomal subunit protein uL24

Chain LY:

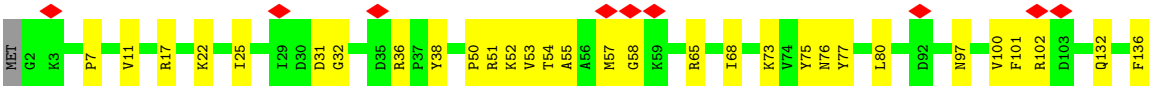




• Molecule 28: Large ribosomal subunit protein eL27

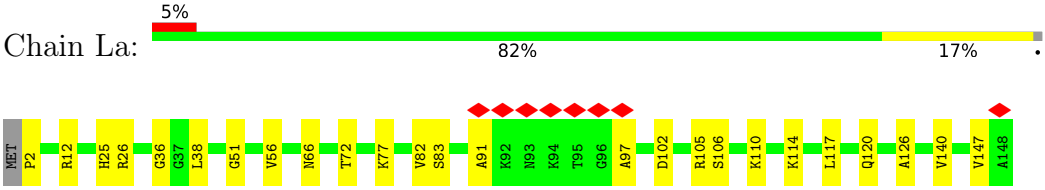
Chain LZ:





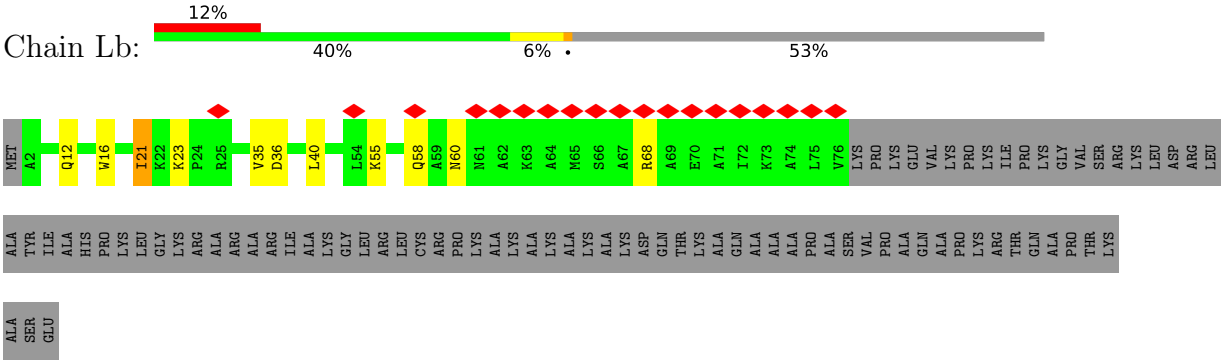
• Molecule 29: Large ribosomal subunit protein uL15

Chain La:



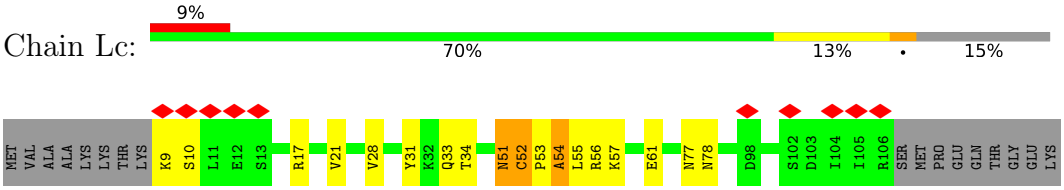
• Molecule 30: Large ribosomal subunit protein eL29

Chain Lb:



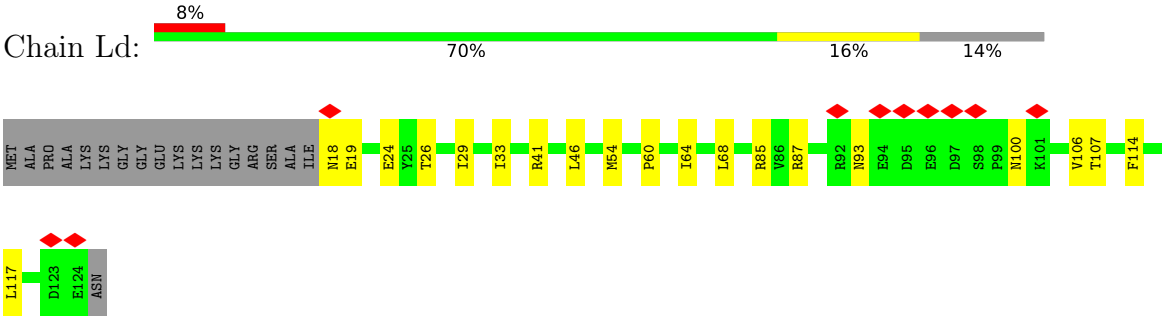
• Molecule 31: Large ribosomal subunit protein eL30

Chain Lc:



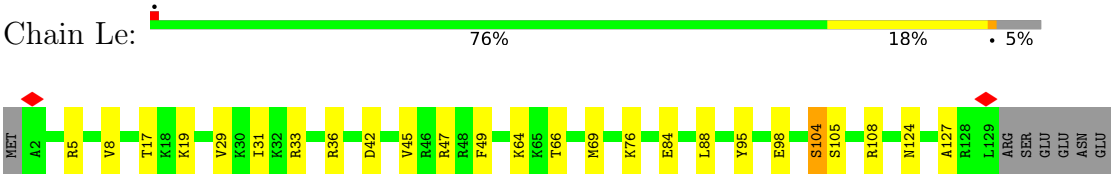
• Molecule 32: Large ribosomal subunit protein eL31

Chain Ld:



• Molecule 33: Large ribosomal subunit protein eL32

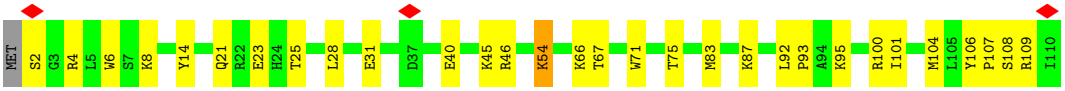
Chain Le:



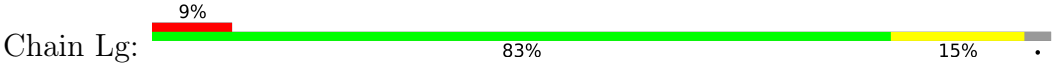
• Molecule 34: Large ribosomal subunit protein eL33

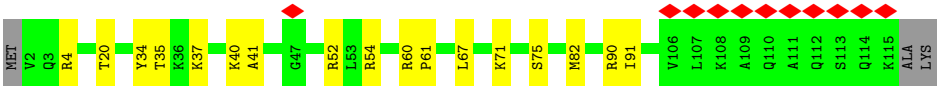
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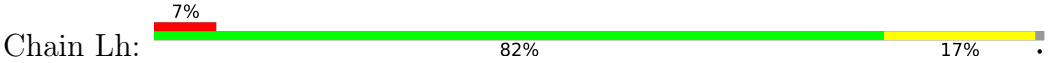


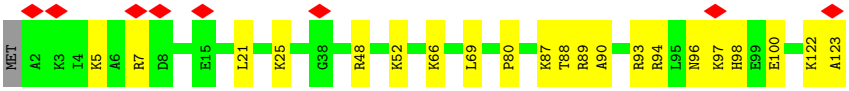
• Molecule 35: Large ribosomal subunit protein eL34



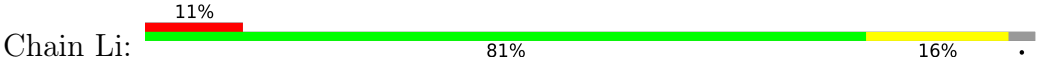


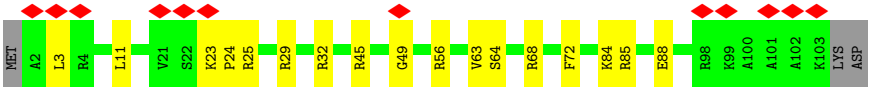
• Molecule 36: Large ribosomal subunit protein uL29





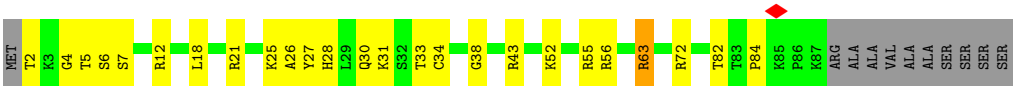
• Molecule 37: Large ribosomal subunit protein eL36





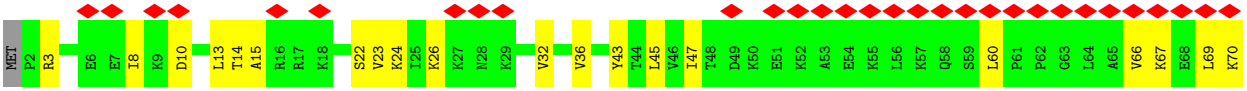
• Molecule 38: Large ribosomal subunit protein eL37



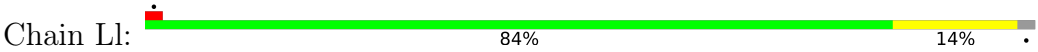


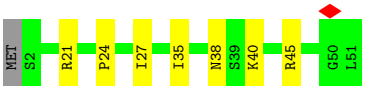
• Molecule 39: Large ribosomal subunit protein eL38





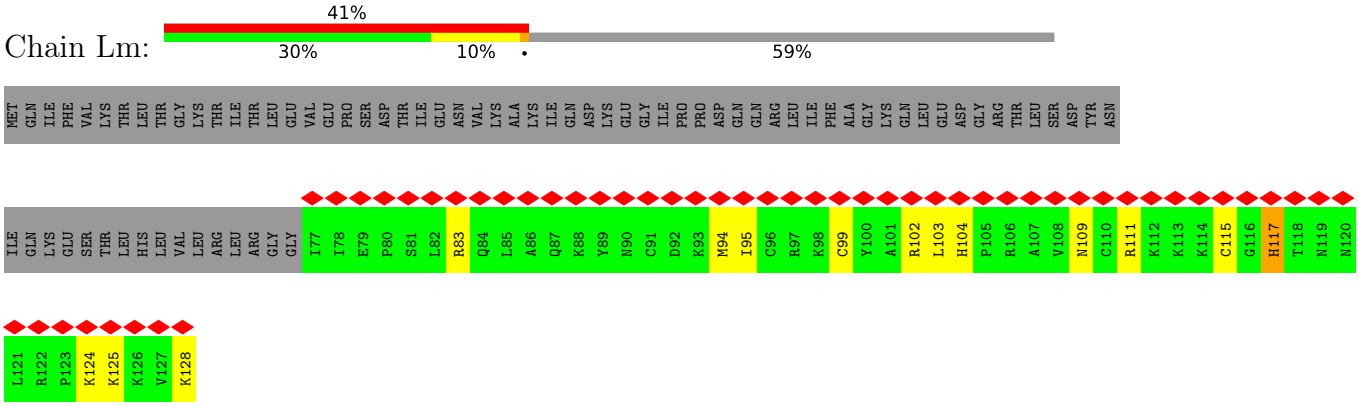
• Molecule 40: Large ribosomal subunit protein eL39





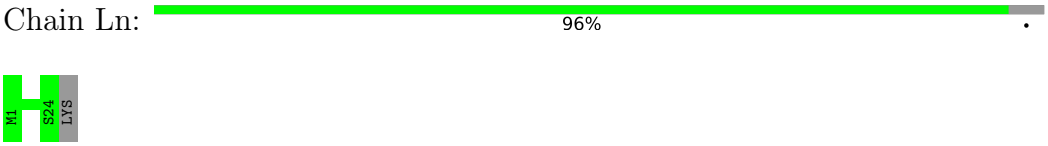
• Molecule 41: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm:



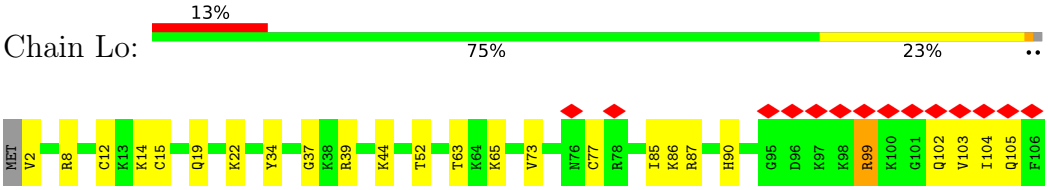
• Molecule 42: Small ribosomal subunit protein eS32

Chain Ln:



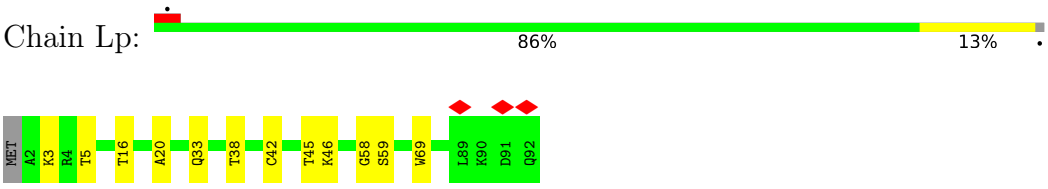
• Molecule 43: Large ribosomal subunit protein eL42

Chain Lo:



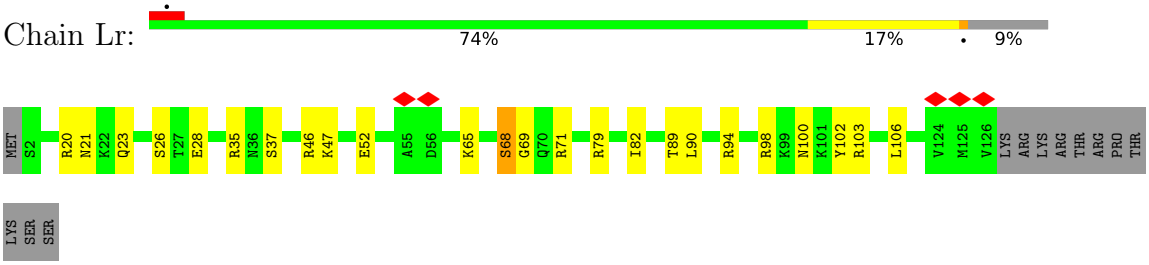
• Molecule 44: Large ribosomal subunit protein eL43

Chain Lp:



• Molecule 45: Large ribosomal subunit protein eL28

Chain Lr:



• Molecule 46: Large ribosomal subunit protein uL1

Chain Lz:

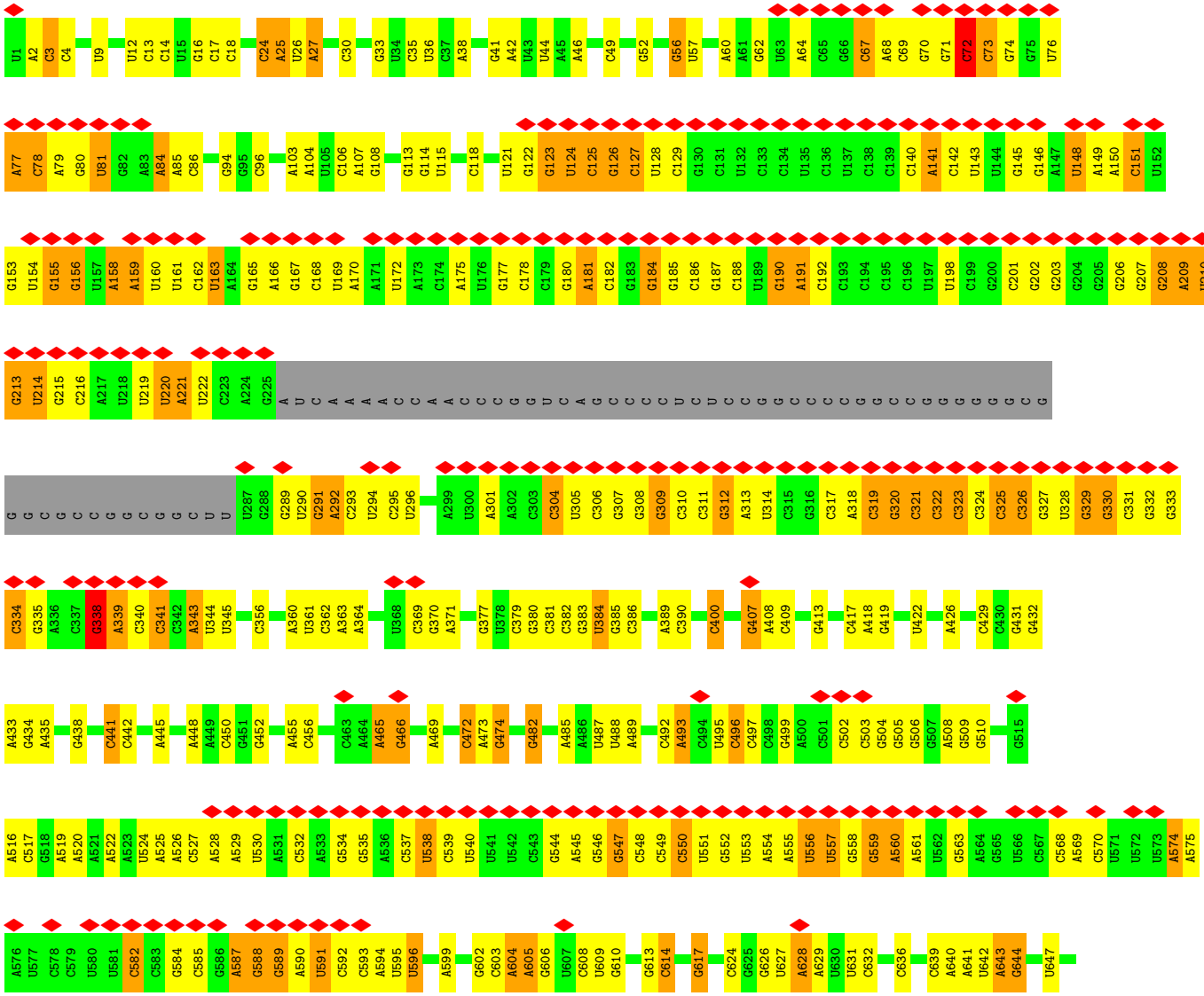


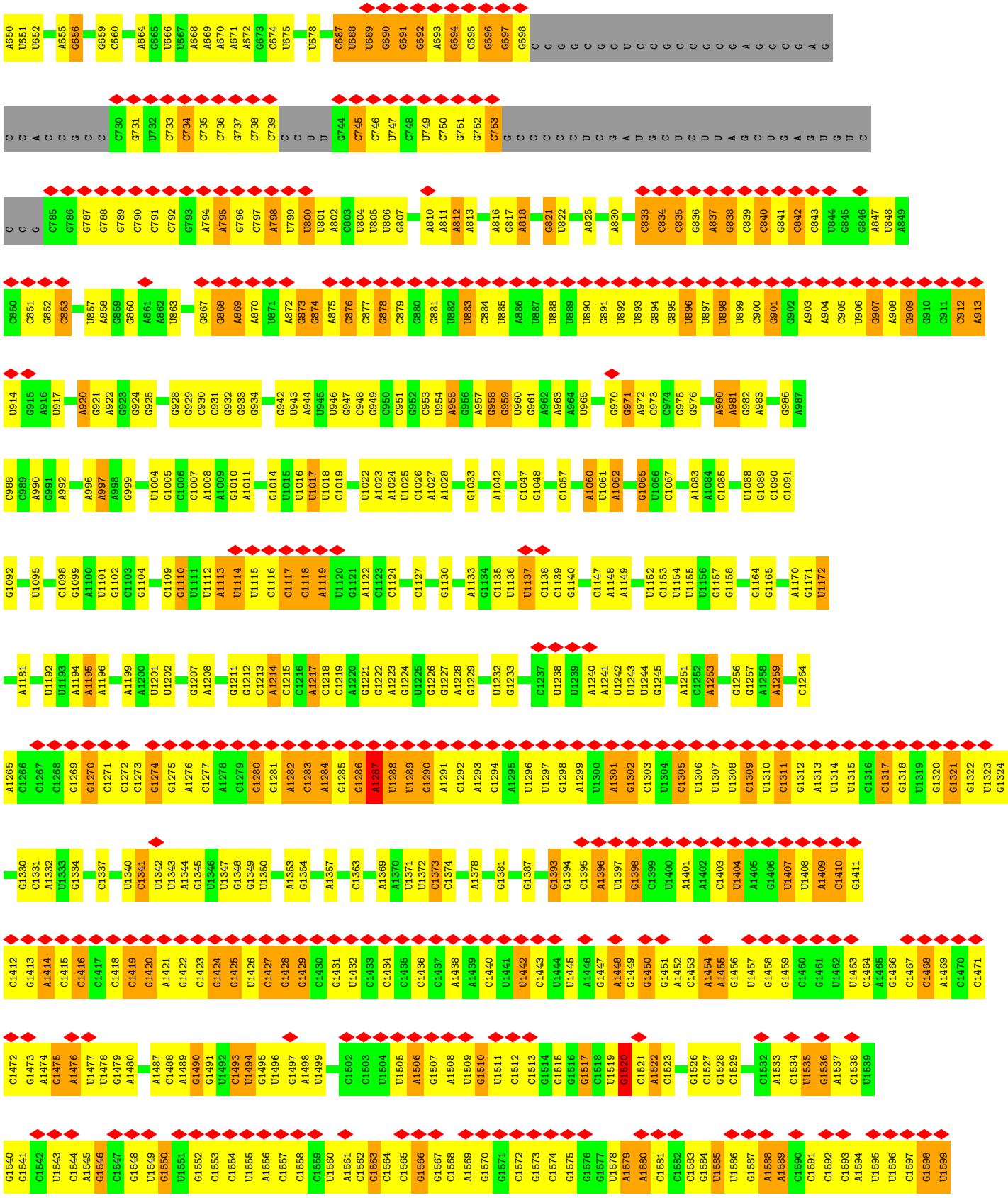


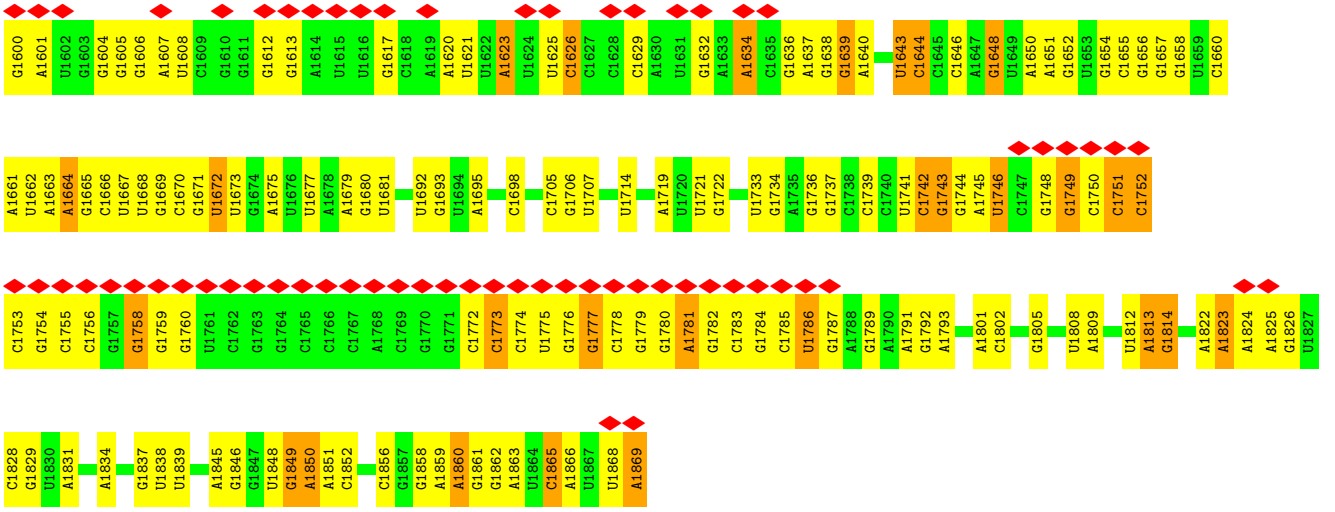
- Molecule 47: 18S ribosomal RNA

Chain S2:



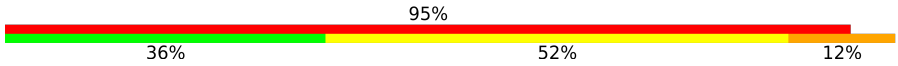


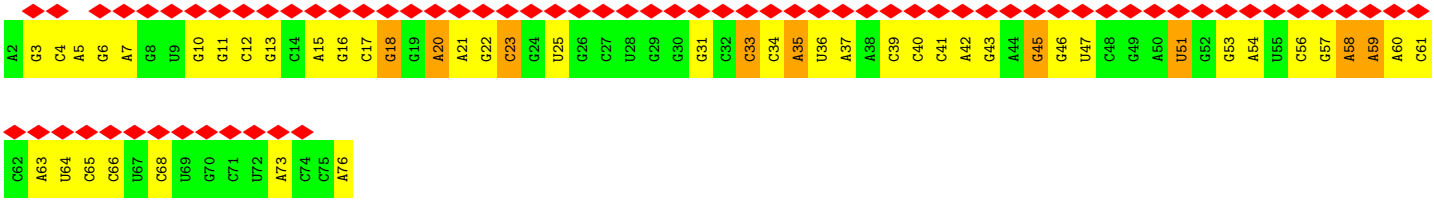

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C785 G786 G787 G788 G789 C790 C791 C792 G793 A794 A795 G796 C797 A798 U799 U800 U801 A802 C803 U804 U805 U806 G807 A810 A811 A812 A813 A816 G817 A818 G821 U822 A825 A830 C833 C834 C835 G836 A837 G838 C839 C840 G841 C842 C843 U844 G845 G846 A847 U848 A849
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G1092 U1095 C1098 G1099 A1100 U1101 C1102 C1103 G1104 C1109 G1110 U1111 U1112 A1113 U1114 U1115 C1116 C1117 C1118 A1119 U1120 C1121 A1122 C1123 C1124 C1127 G1130 A1133 G1134 C1135 U1136 U1137 C1138 C1139 G1140 C1147 A1148 A1149 U1152 C1153 U1154 U1155 U1156 G1157 G1158 G1164 G1165 A1170 G1171 U1172
A1181 U1192 U1193 A1194 A1195 A1196 A1199 A1200 U1201 U1202 G1207 A1208 G1211 G1212 C1213 A1214 C1215 C1216 A1217 C1218 C1219 A1220 G1221 G1222 A1223 G1224 U1225 G1226 G1227 A1228 G1229 U1232 G1233 C1237 U1238 U1239 A1240 A1241 U1242 U1243 U1244 G1245 A1251 C1252 A1253 G1256 G1257 A1258 A1259 C1264
A1265 C1266 C1267 C1268 G1269 G1270 C1271 C1272 C1273 G1274 G1275 A1276 C1277 A1278 C1279 G1280 G1281 A1282 C1283 A1284 G1285 G1286 A1287 U1288 U1289 G1290 A1291 C1292 A1293 G1294 A1295 U1296 U1297 G1298 A1299 U1300 A1301 G1302 C1303 U1304 C1305 U1306 U1307 U1308 C1309 U1310 C1311 G1312 A1313 U1314 U1315 C1316 C1317 G1318 U1319 G1320 G1321 G1322 U1323 G1324
G1330 C1331 A1332 U1333 G1334 C1337 U1340 C1341 U1342 U1343 A1344 G1345 U1346 U1347 G1348 G1349 U1350 A1353 G1354 A1357 C1363 A1369 A1370 U1371 U1372 C1373 C1374 A1378 G1381 G1387 G1393 G1394 C1395 A1396 U1397 G1398 C1399 U1400 A1401 A1402 C1403 U1404 A1405 G1406 U1407 U1408 A1409 C1410 G1411
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G1540 G1541 C1542 U1543 C1544 A1545 G1546 C1547 G1548 U1549 G1550 U1551 G1552 C1553 C1554 U1555 A1556 C1557 C1558 C1559 U1560 A1561 C1562 G1563 C1564 C1565 G1566 G1567 C1568 A1569 G1570 G1571 C1572 G1573 C1574 G1575 G1576 G1577 U1578 A1579 A1580 C1581 C1582 C1583 G1584 U1585 U1586 G1587 A1588 A1589 C1590 C1591 C1592 C1593 A1594 U1595 U1596 C1597 G1598 U1599



• Molecule 48: HUMAN INITIATOR MET-TRNA-I

Chain S6:

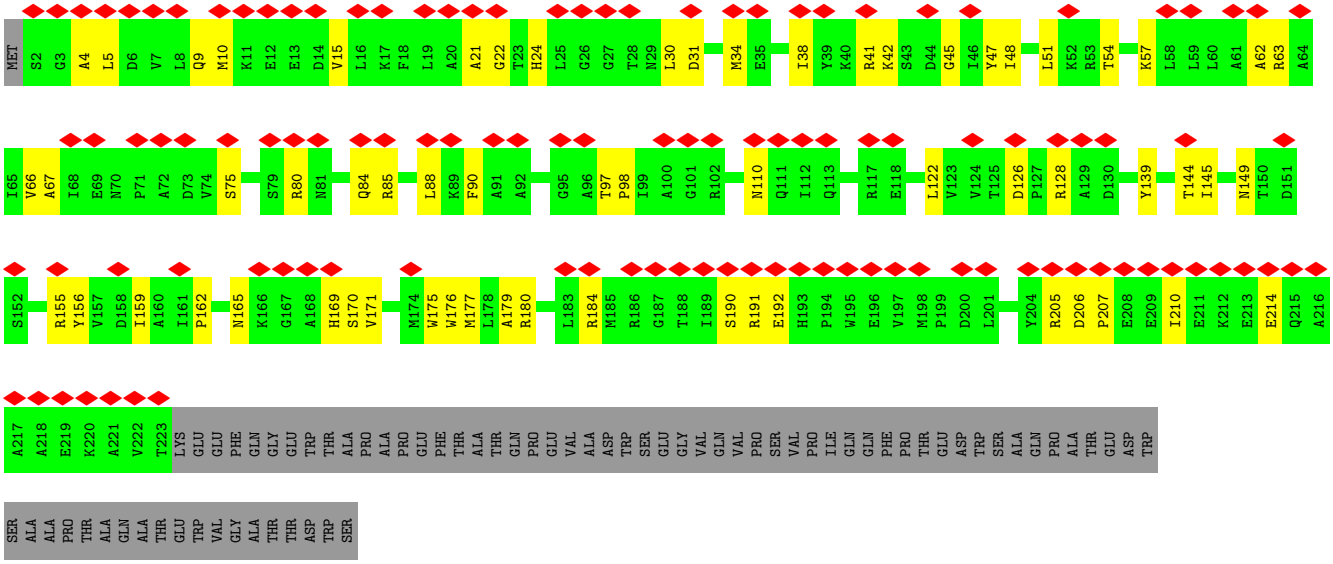




• Molecule 49: Small ribosomal subunit protein uS2

Chain SA:

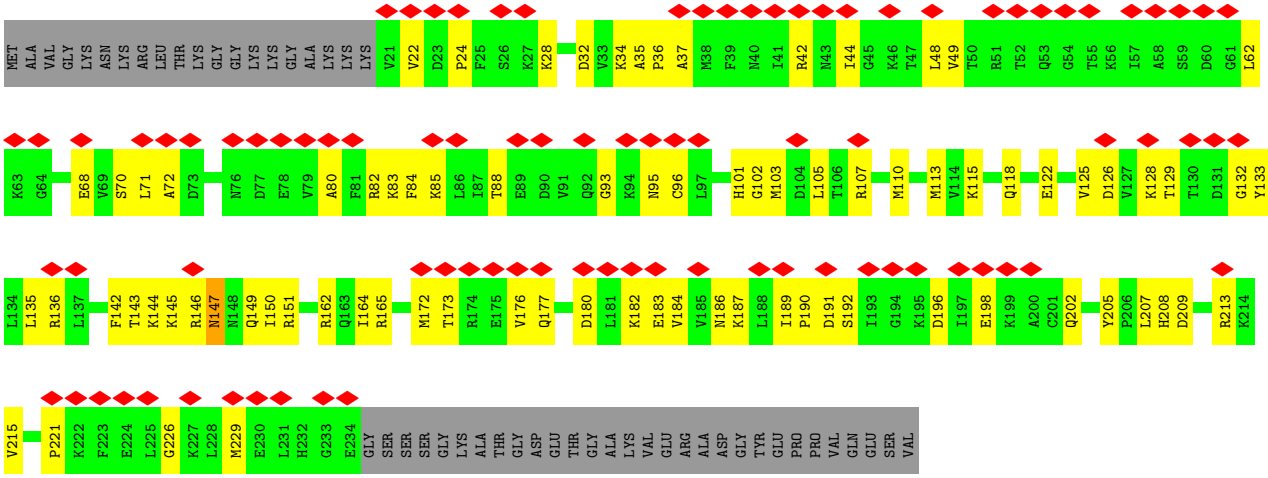




• Molecule 50: Small ribosomal subunit protein eS1

Chain SB:

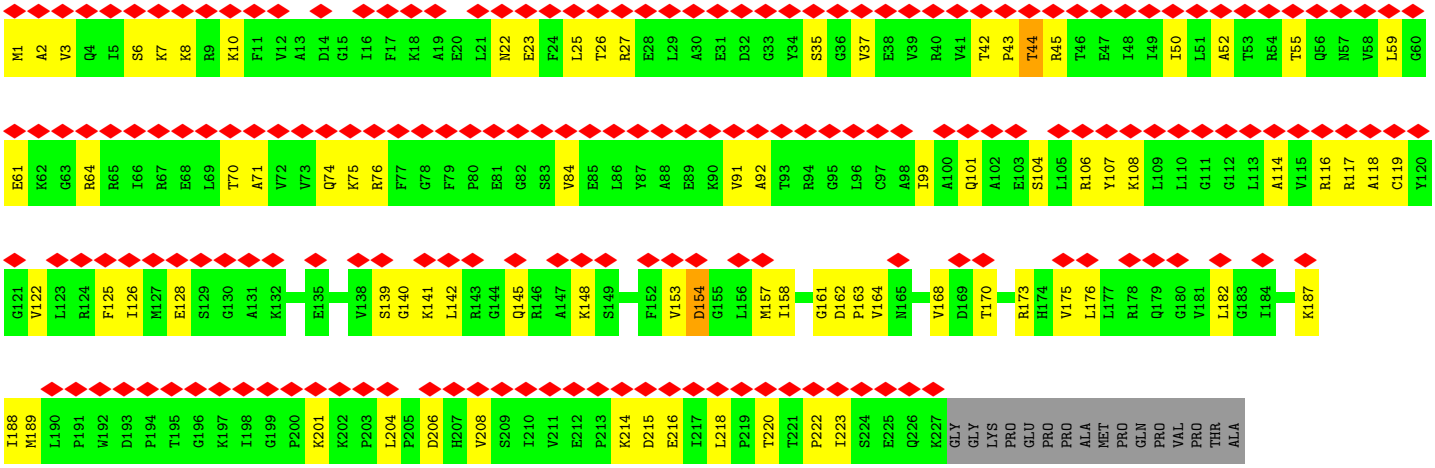




• Molecule 51: Small ribosomal subunit protein uS3

Chain SD:

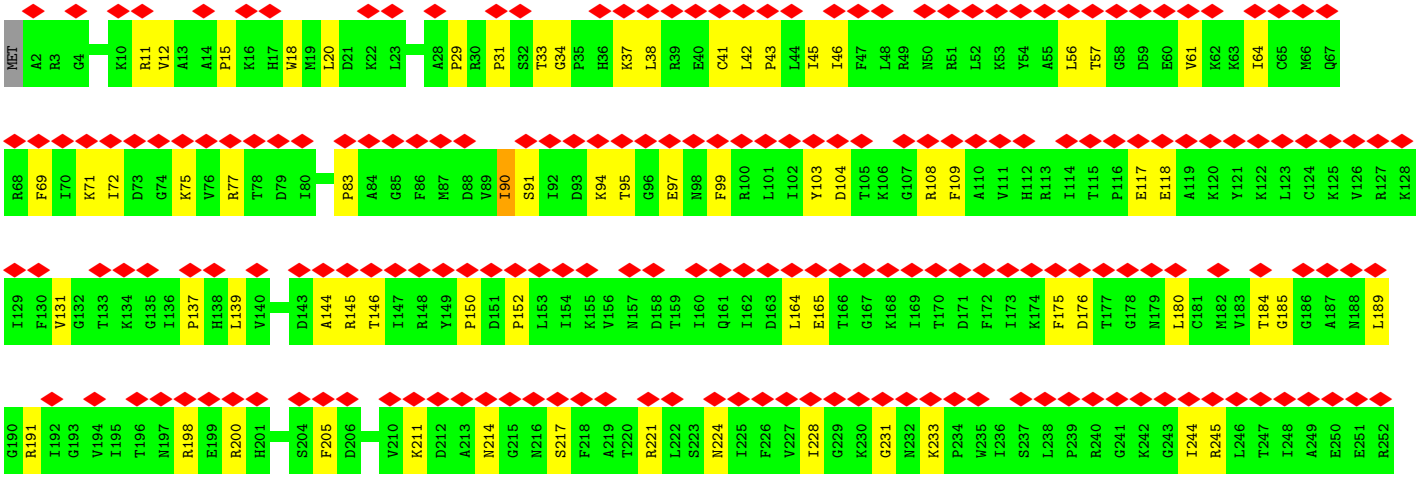


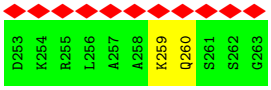


• Molecule 52: Small ribosomal subunit protein eS4, X isoform

Chain SE:



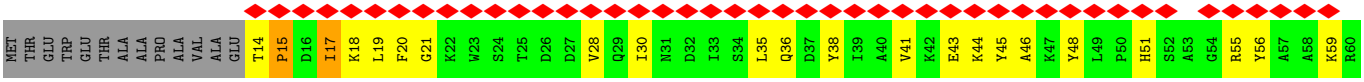


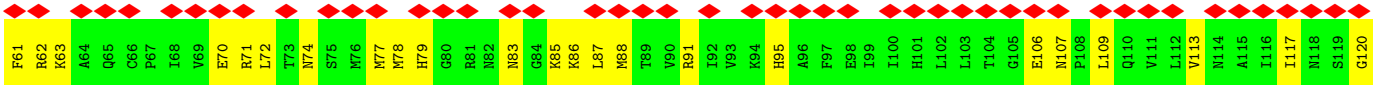


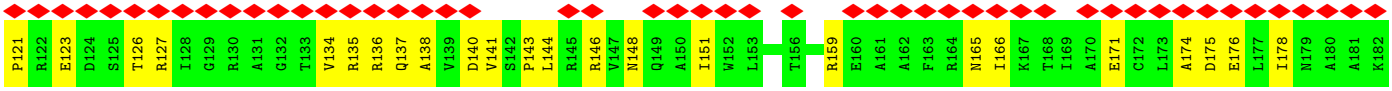
• Molecule 53: Small ribosomal subunit protein uS7

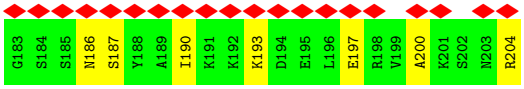
Chain SF:







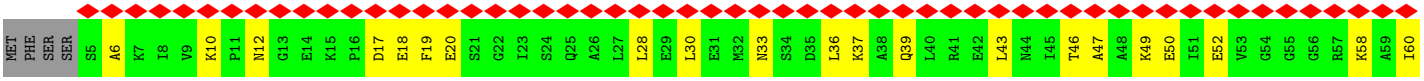


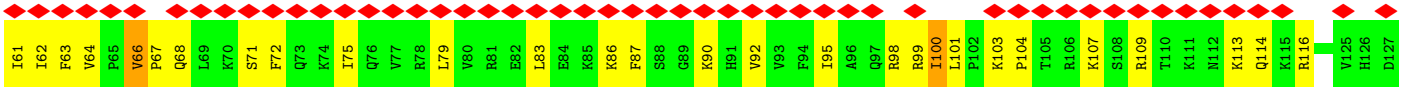


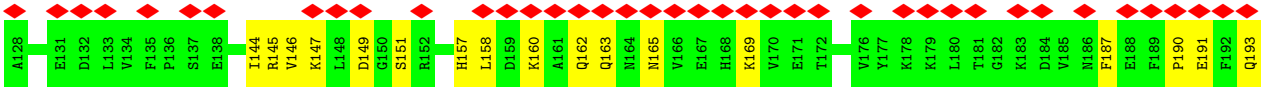
• Molecule 54: Small ribosomal subunit protein eS7

Chain SH:





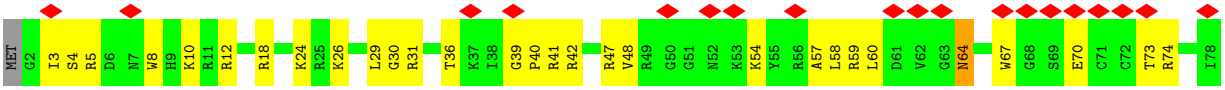


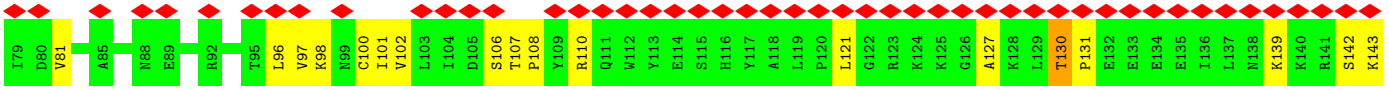


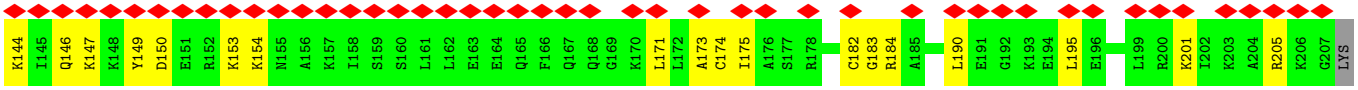
• Molecule 55: Small ribosomal subunit protein eS8

Chain SI:





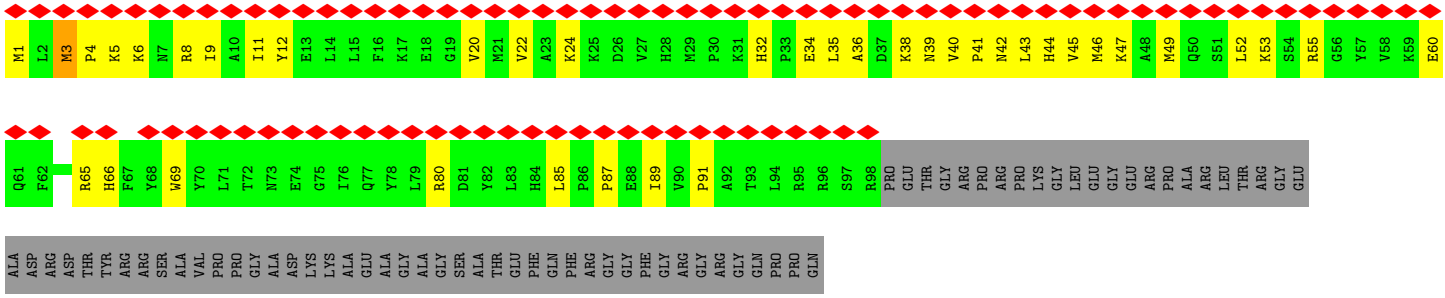




• Molecule 56: Small ribosomal subunit protein eS10

Chain SK:

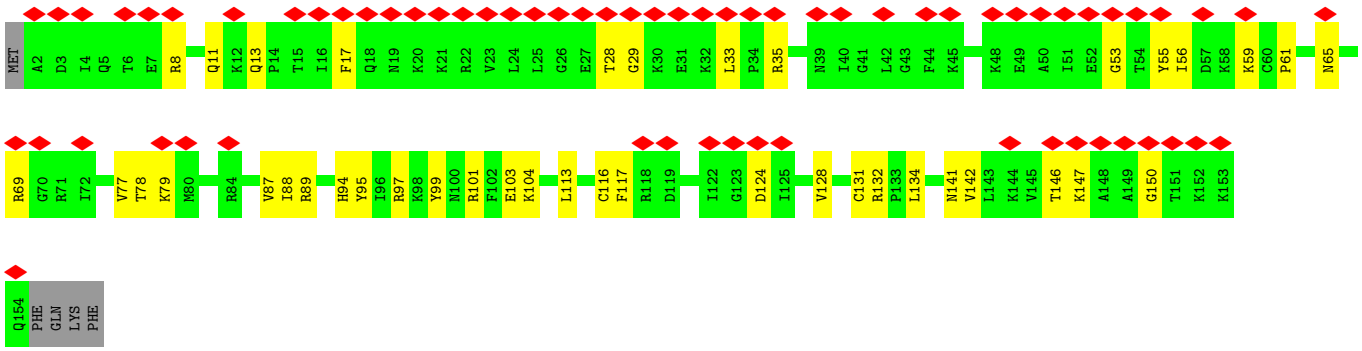




• Molecule 57: Small ribosomal subunit protein uS17

Chain SL:

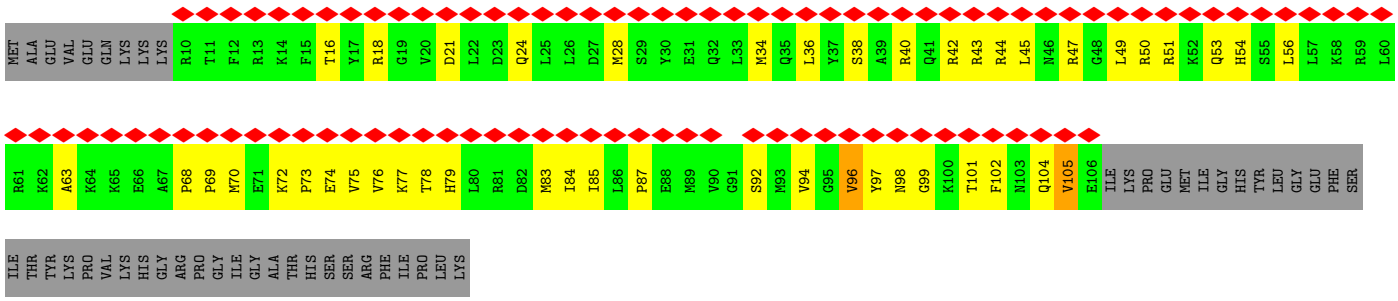




• Molecule 58: Small ribosomal subunit protein uS19

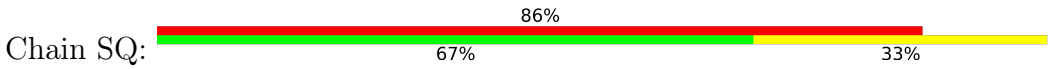
Chain SP:

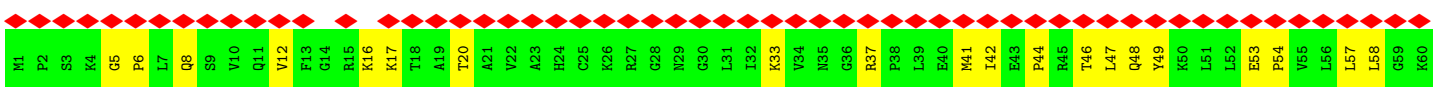


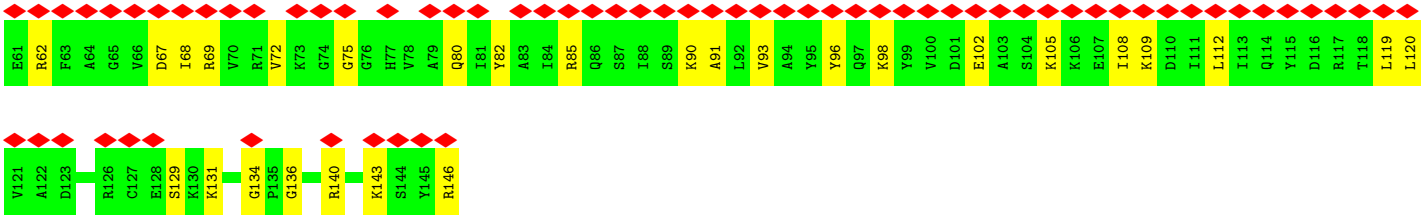


• Molecule 59: Small ribosomal subunit protein uS9

Chain SQ:



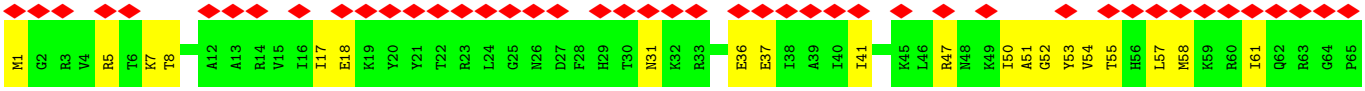


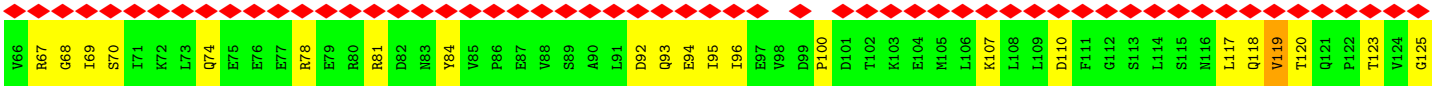


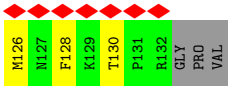
• Molecule 60: Small ribosomal subunit protein eS17

Chain SR:





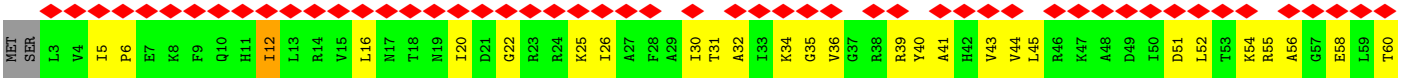


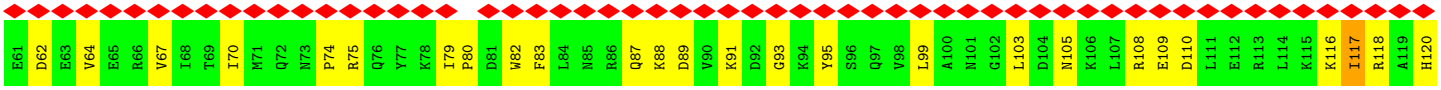


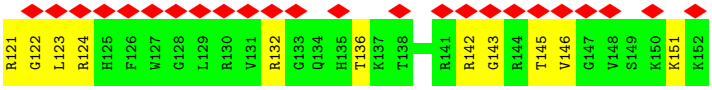
• Molecule 61: Small ribosomal subunit protein uS13

Chain SS:



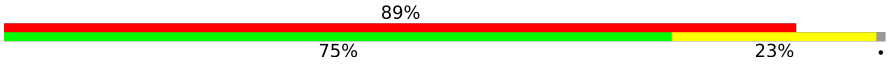


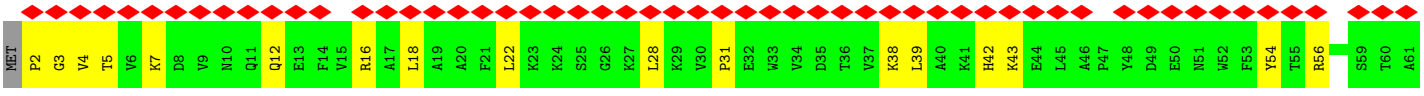


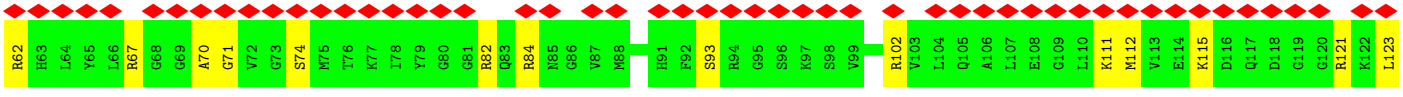


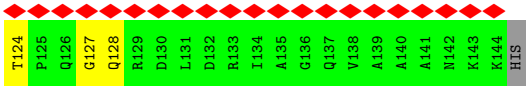
• Molecule 62: Small ribosomal subunit protein eS19

Chain ST:





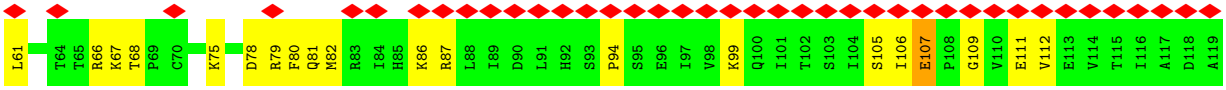




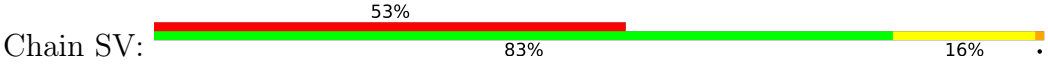
• Molecule 63: Small ribosomal subunit protein uS10

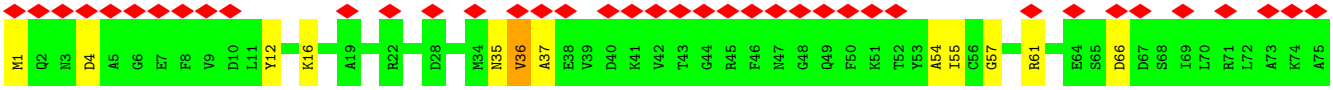


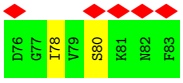




• Molecule 64: Small ribosomal subunit protein eS21

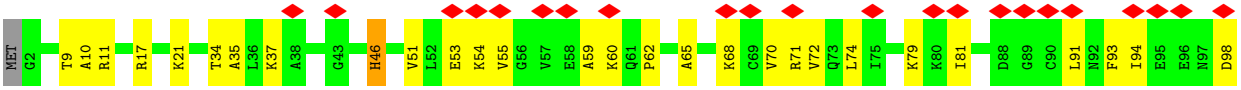


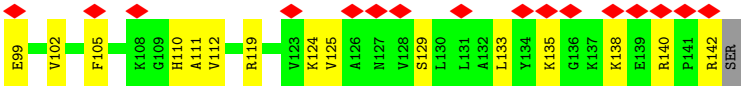




• Molecule 65: Small ribosomal subunit protein uS12

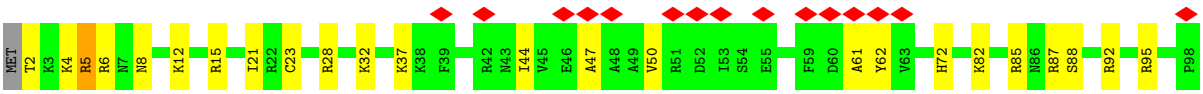


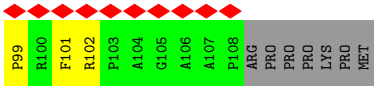




• Molecule 66: Small ribosomal subunit protein eS26

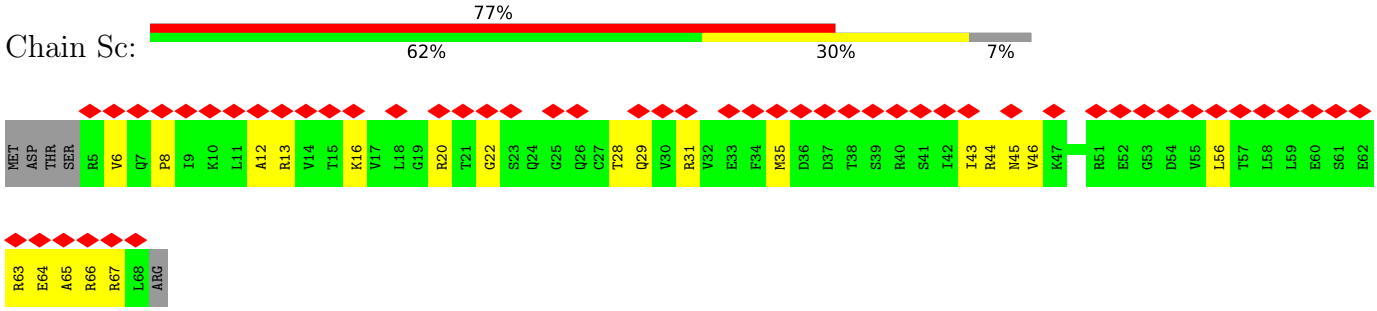






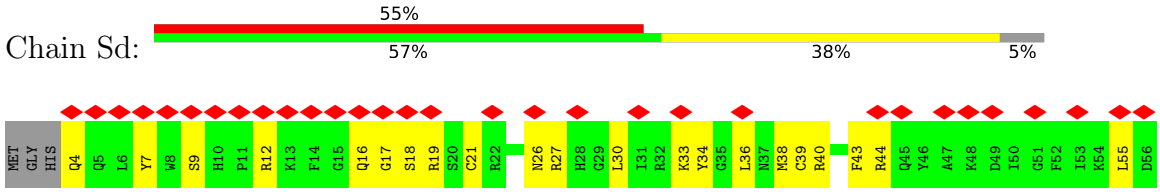
• Molecule 67: Small ribosomal subunit protein eS28

Chain Sc:



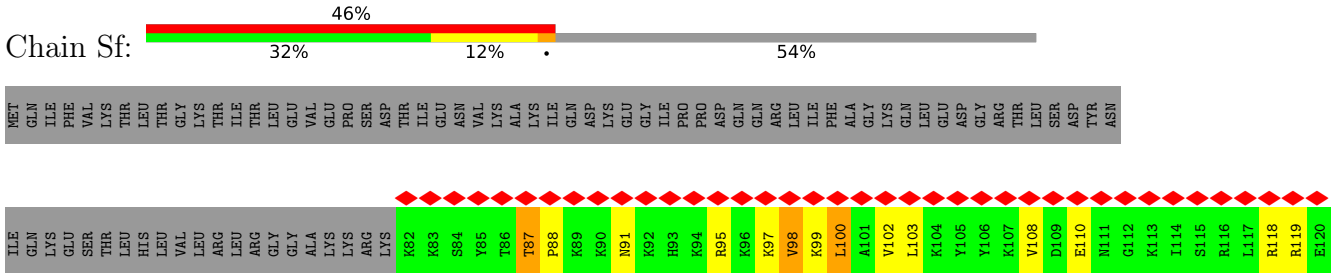
• Molecule 68: Small ribosomal subunit protein uS14

Chain Sd:



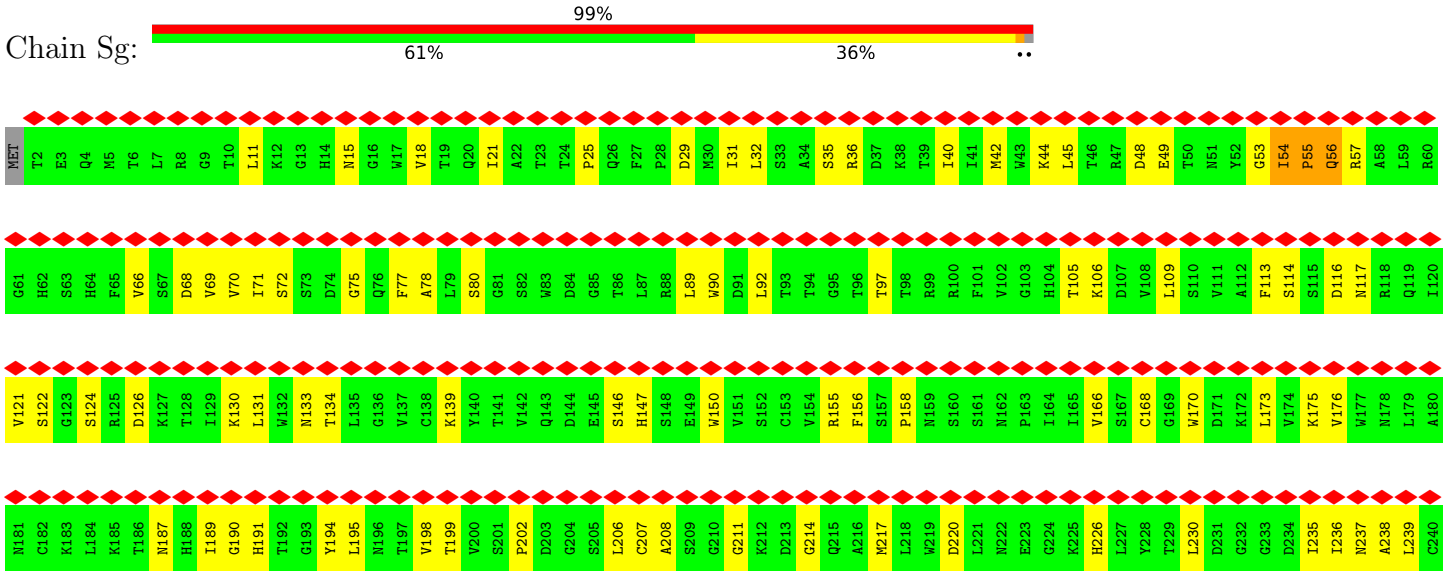
• Molecule 69: Ubiquitin

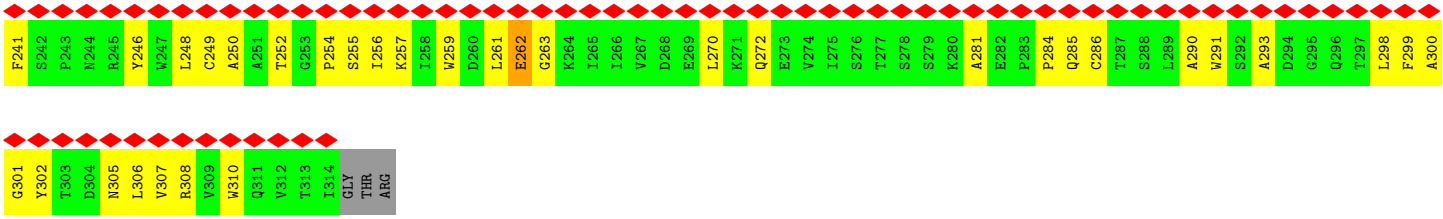
Chain Sf:



• Molecule 70: Small ribosomal subunit protein RACK1

Chain Sg:

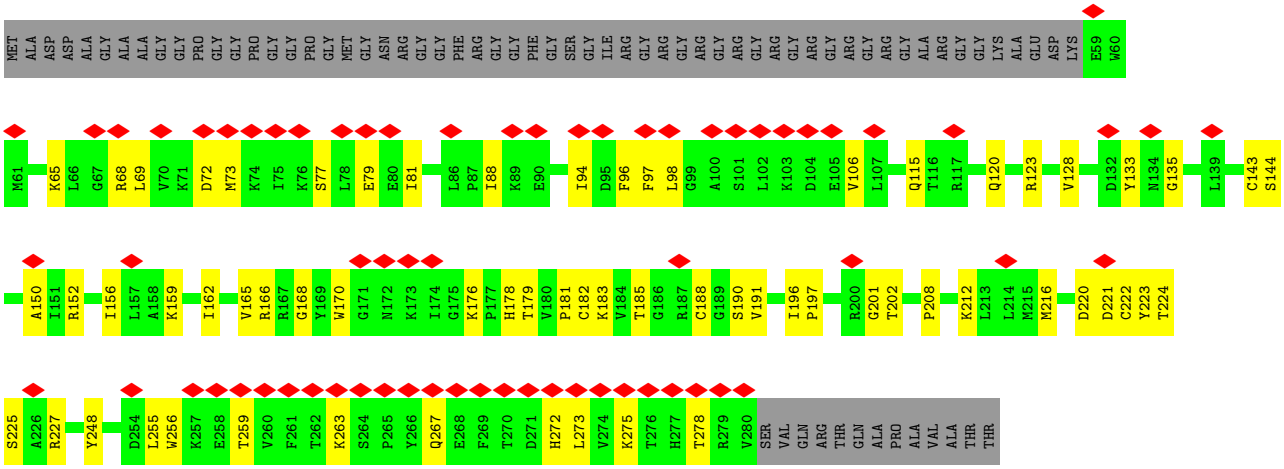




• Molecule 71: Small ribosomal subunit protein uS5

Chain SC:

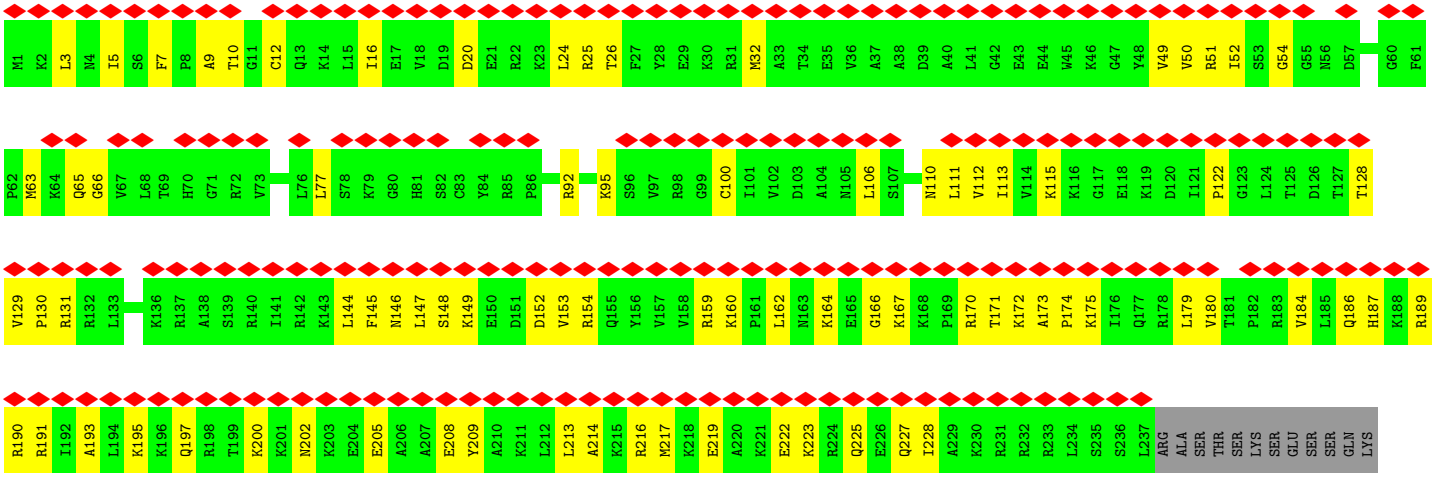




• Molecule 72: Small ribosomal subunit protein eS6

Chain SG:





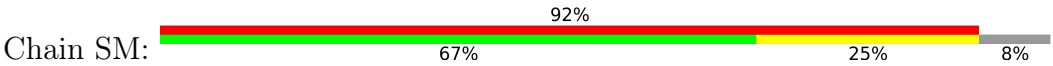
• Molecule 73: Small ribosomal subunit protein uS4

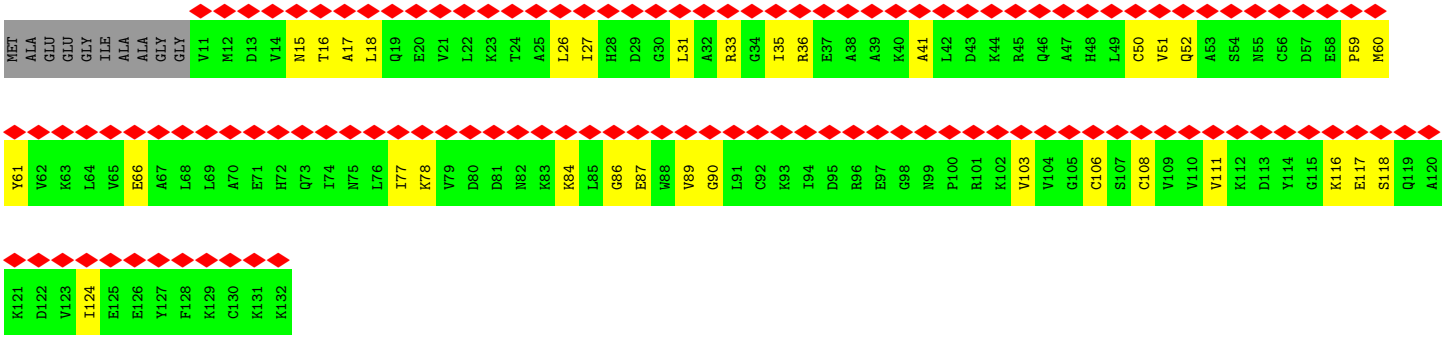
Chain SJ:





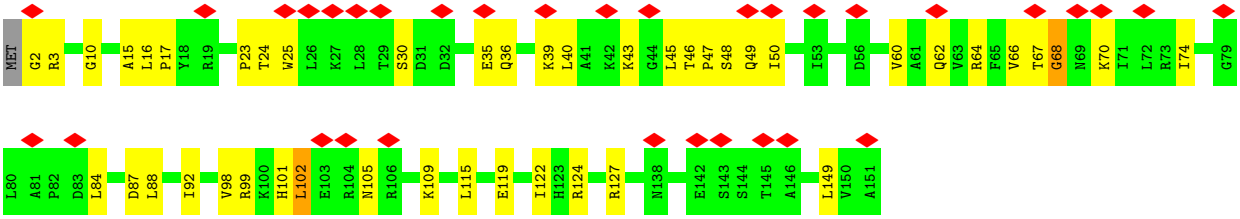
• Molecule 74: Small ribosomal subunit protein eS12





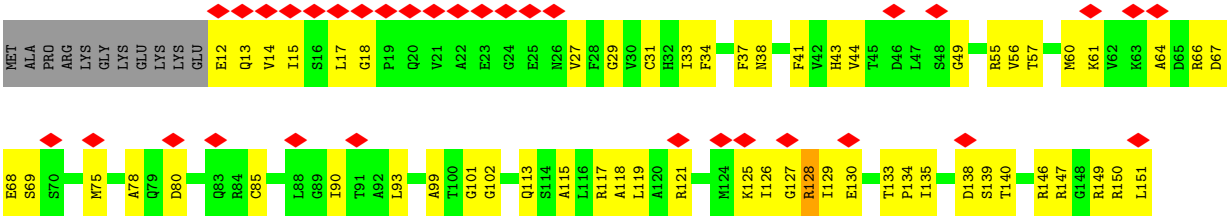
• Molecule 75: Small ribosomal subunit protein uS15





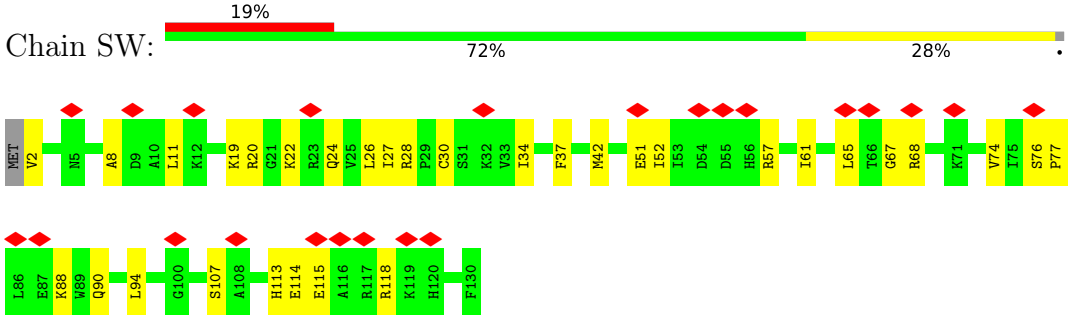
• Molecule 76: Small ribosomal subunit protein uS11





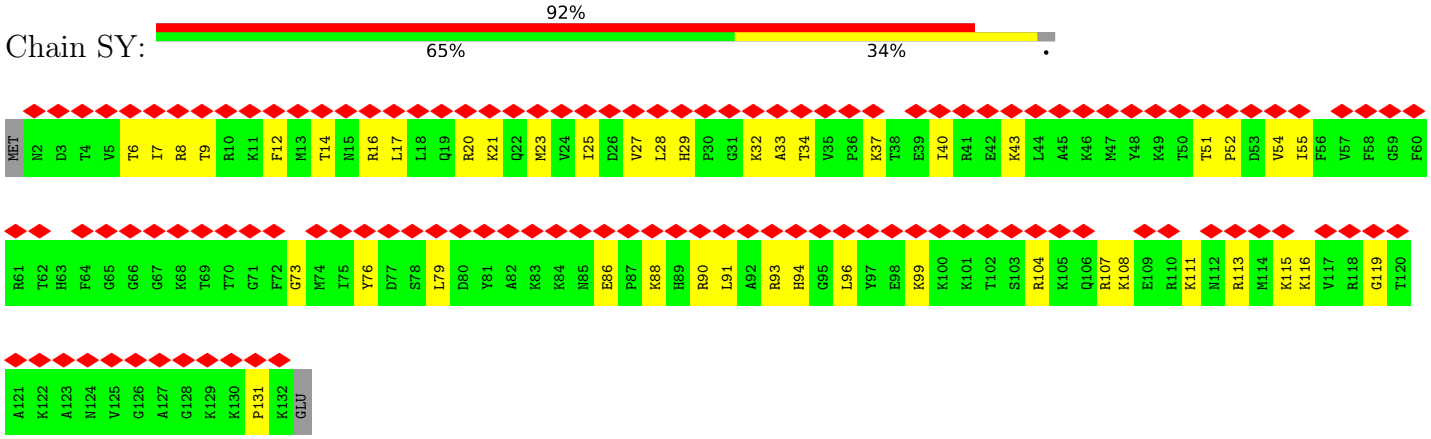
• Molecule 77: Small ribosomal subunit protein uS8

Chain SW:



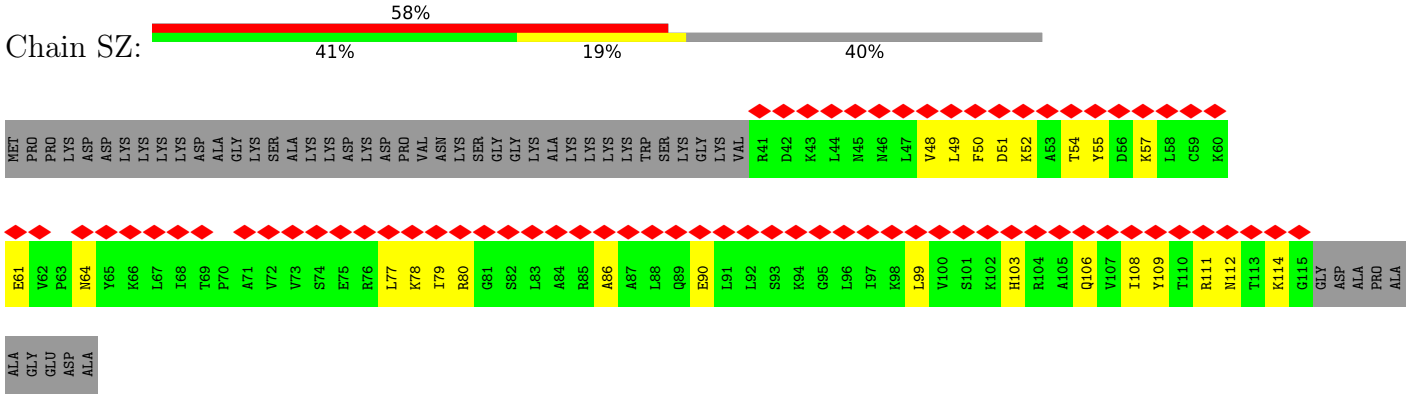
• Molecule 78: Small ribosomal subunit protein eS24

Chain SY:



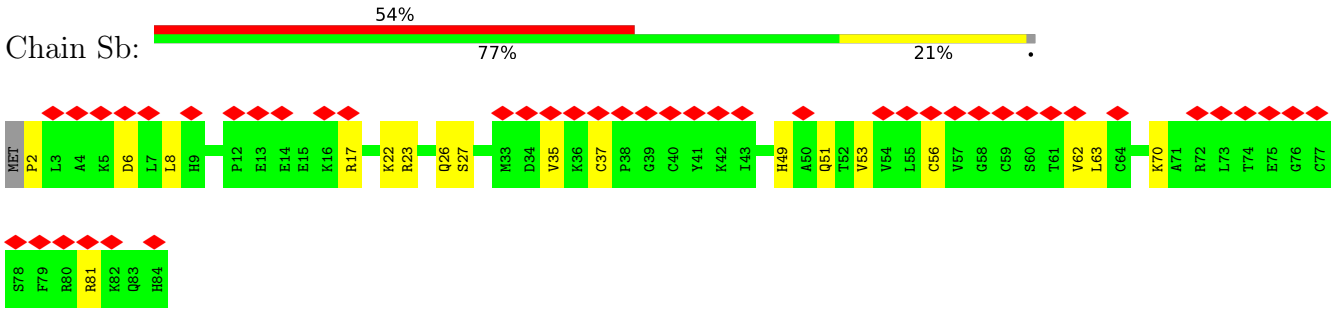
• Molecule 79: Small ribosomal subunit protein eS25

Chain SZ:



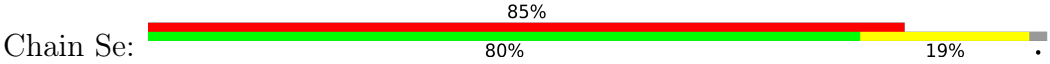
• Molecule 80: Small ribosomal subunit protein eS27

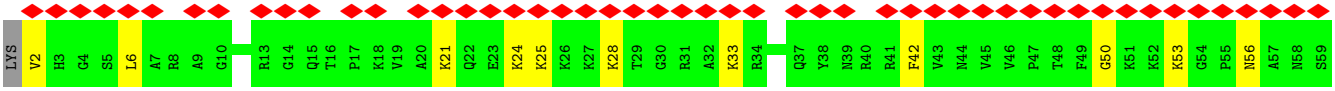
Chain Sb:



• Molecule 81: Small ribosomal subunit protein eS30

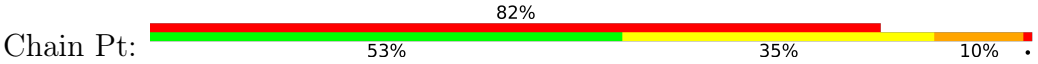
Chain Se:

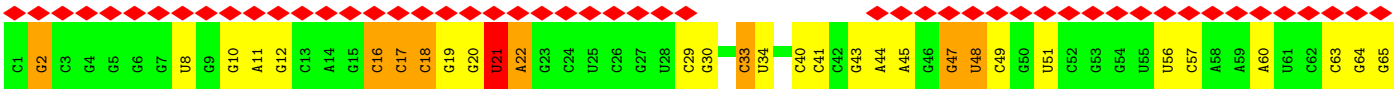


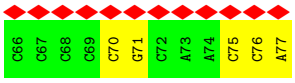


• Molecule 82: P-site tRNA

Chain Pt:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46205	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.895	Depositor
Minimum map value	-1.561	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.141	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	456.0, 456.0, 456.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, G7M, H2U, A1E6S, MG, ZN, 4SU, PSU

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	L5	0.33	0/89645	0.78	54/139764 (0.0%)
2	L7	0.29	0/2858	0.70	0/4455
3	L8	0.33	0/3701	0.75	0/5766
4	LA	0.22	0/1936	0.58	0/2596
5	LB	0.19	0/3306	0.53	0/4424
6	LC	0.21	0/2973	0.57	1/3992 (0.0%)
7	LD	0.18	0/2428	0.48	0/3252
8	LE	0.22	0/1996	0.67	4/2673 (0.1%)
9	LF	0.20	0/1905	0.47	0/2539
10	LG	0.18	0/1960	0.50	1/2637 (0.0%)
11	LH	0.20	0/1537	0.54	0/2066
12	LI	0.18	0/1751	0.49	0/2340
13	LJ	0.17	0/1433	0.48	0/1915
14	LL	0.20	0/1732	0.56	2/2315 (0.1%)
15	LM	0.20	0/1161	0.59	2/1554 (0.1%)
16	LN	0.22	0/1746	0.51	0/2338
17	LO	0.19	0/1682	0.46	0/2250
18	LP	0.22	0/1268	0.55	1/1701 (0.1%)
19	LQ	0.20	0/1537	0.50	0/2052
20	LR	0.17	0/1582	0.47	0/2091
21	LS	0.40	2/1493 (0.1%)	0.67	3/2003 (0.1%)
22	LT	0.21	0/1326	0.48	0/1770
23	LU	0.18	0/839	0.53	1/1126 (0.1%)
24	LV	0.21	0/993	0.56	0/1332
25	LW	0.22	0/1030	0.63	4/1364 (0.3%)
26	LX	0.20	0/1002	0.49	0/1345
27	LY	0.22	0/1132	0.52	0/1504
28	LZ	0.17	0/1130	0.45	0/1507
29	La	0.19	0/1191	0.52	0/1591
30	Lb	0.17	0/620	0.50	0/819
31	Lc	0.20	0/774	0.50	0/1038
32	Ld	0.21	0/903	0.51	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Le	0.22	0/1071	0.58	1/1429 (0.1%)
34	Lf	0.20	0/895	0.52	0/1198
35	Lg	0.20	0/916	0.52	0/1220
36	Lh	0.19	0/1023	0.52	0/1351
37	Li	0.17	0/843	0.50	0/1115
38	Lj	0.21	0/720	0.56	0/952
39	Lk	0.20	0/575	0.54	0/761
40	Ll	0.18	0/454	0.49	0/599
41	Lm	0.16	0/435	0.41	0/575
42	Ln	0.17	0/231	0.54	0/294
43	Lo	0.16	0/875	0.48	0/1153
44	Lp	0.18	0/718	0.52	0/953
45	Lr	0.19	0/1017	0.59	1/1364 (0.1%)
46	Lz	0.16	0/1769	0.52	0/2371
47	S2	0.24	0/41243	0.73	26/64257 (0.0%)
48	S6	0.18	0/1795	0.61	0/2798
49	SA	0.17	0/1784	0.52	1/2424 (0.0%)
50	SB	0.20	0/1765	0.54	1/2362 (0.0%)
51	SD	0.21	0/1793	0.56	1/2414 (0.0%)
52	SE	0.18	0/2118	0.47	0/2849
53	SF	0.19	0/1531	0.58	1/2059 (0.0%)
54	SH	0.22	0/1544	0.57	0/2068
55	SI	0.17	0/1715	0.48	0/2287
56	SK	0.26	0/851	0.56	0/1147
57	SL	0.17	0/1268	0.43	0/1696
58	SP	0.20	0/815	0.63	0/1087
59	SQ	0.18	0/1177	0.50	0/1575
60	SR	0.19	0/1086	0.60	0/1457
61	SS	0.15	0/1253	0.44	0/1676
62	ST	0.16	0/1131	0.51	0/1515
63	SU	0.19	0/831	0.53	0/1115
64	SV	0.15	0/643	0.41	0/860
65	SX	0.16	0/1116	0.50	0/1490
66	Sa	0.18	0/862	0.53	1/1156 (0.1%)
67	Sc	0.20	0/508	0.56	0/680
68	Sd	0.19	0/455	0.53	0/603
69	Sf	0.18	0/593	0.55	0/786
70	Sg	0.17	0/2493	0.50	0/3394
71	SC	0.18	0/1762	0.49	0/2381
72	SG	0.18	0/1946	0.50	0/2590
73	SJ	0.16	0/1550	0.52	0/2069
74	SM	0.16	0/962	0.53	0/1290
75	SN	0.18	0/1232	0.49	1/1656 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	SO	0.20	0/1062	0.56	0/1425
77	SW	0.18	0/1051	0.51	0/1406
78	SY	0.21	0/1083	0.54	0/1438
79	SZ	0.13	0/604	0.45	0/810
80	Sb	0.16	0/665	0.44	0/891
81	Se	0.20	0/465	0.56	0/612
82	Pt	0.28	0/1722	0.74	0/2682
All	All	0.26	2/236586 (0.0%)	0.68	107/347675 (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
8	LE	0	1
14	LL	0	1
49	SA	0	1
70	Sg	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	LS	20	PRO	CG-CD	-11.18	1.12	1.50
21	LS	20	PRO	N-CD	5.97	1.56	1.47

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	LS	20	PRO	N-CD-CG	-13.37	83.15	103.20
21	LS	20	PRO	CA-N-CD	-11.89	95.35	112.00
1	L5	654	C	C6-N1-C2	-9.16	116.64	120.30
1	L5	486	C	C2-N1-C1'	8.11	127.72	118.80
1	L5	486	C	N1-C2-O2	8.07	123.74	118.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	LE	224	LYS	Peptide

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Mol	Chain	Res	Type	Group
14	LL	66	TYR	Peptide
49	SA	31	ASP	Peptide
70	Sg	54	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L5	80184	0	40395	1068	0
2	L7	2558	0	1296	15	0
3	L8	3314	0	1683	37	0
4	LA	1898	0	1993	39	0
5	LB	3238	0	3376	52	0
6	LC	2919	0	3092	65	0
7	LD	2382	0	2410	51	0
8	LE	1958	0	2126	57	0
9	LF	1870	0	1996	43	0
10	LG	1927	0	2074	28	0
11	LH	1518	0	1601	26	0
12	LI	1711	0	1748	35	0
13	LJ	1410	0	1441	39	0
14	LL	1701	0	1818	32	0
15	LM	1138	0	1204	30	0
16	LN	1701	0	1749	29	0
17	LO	1650	0	1794	24	0
18	LP	1242	0	1269	12	0
19	LQ	1513	0	1628	19	0
20	LR	1566	0	1729	30	0
21	LS	1453	0	1490	31	0
22	LT	1298	0	1366	17	0
23	LU	825	0	850	17	0
24	LV	979	0	1039	16	0
25	LW	1015	0	1079	32	0
26	LX	985	0	1066	23	0
27	LY	1115	0	1205	20	0
28	LZ	1107	0	1182	19	0
29	La	1162	0	1213	24	0
30	Lb	610	0	650	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Lc	764	0	804	11	0
32	Ld	888	0	930	14	0
33	Le	1053	0	1147	23	0
34	Lf	876	0	912	23	0
35	Lg	906	0	1000	17	0
36	Lh	1015	0	1148	19	0
37	Li	832	0	917	13	0
38	Lj	705	0	738	23	0
39	Lk	569	0	637	14	0
40	Ll	444	0	483	6	0
41	Lm	429	0	466	13	0
42	Ln	230	0	276	0	0
43	Lo	862	0	931	17	0
44	Lp	708	0	756	9	0
45	Lr	1002	0	1068	19	0
46	Lz	1741	0	1854	52	0
47	S2	36900	0	18595	617	0
48	S6	1604	0	816	32	0
49	SA	1747	0	1751	45	0
50	SB	1738	0	1809	63	0
51	SD	1765	0	1865	60	0
52	SE	2076	0	2177	53	0
53	SF	1509	0	1563	72	0
54	SH	1521	0	1616	61	0
55	SI	1686	0	1772	51	0
56	SK	827	0	854	34	0
57	SL	1247	0	1323	28	0
58	SP	804	0	841	37	0
59	SQ	1158	0	1232	34	0
60	SR	1072	0	1130	39	0
61	SS	1235	0	1309	46	0
62	ST	1112	0	1146	26	0
63	SU	821	0	883	29	0
64	SV	636	0	637	14	0
65	SX	1098	0	1167	29	0
66	Sa	847	0	894	17	0
67	Sc	506	0	536	13	0
68	Sd	445	0	442	21	0
69	Sf	581	0	597	20	0
70	Sg	2436	0	2393	86	0
71	SC	1725	0	1813	46	0
72	SG	1923	0	2089	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
73	SJ	1525	0	1640	47	0
74	SM	952	0	983	21	0
75	SN	1208	0	1294	34	0
76	SO	1049	0	1073	48	0
77	SW	1034	0	1080	30	0
78	SY	1065	0	1142	36	0
79	SZ	598	0	656	19	0
80	Sb	651	0	672	16	0
81	Se	459	0	503	9	0
82	Pt	1646	0	842	20	0
83	L5	146	0	0	0	0
83	L7	7	0	0	0	0
83	L8	5	0	0	0	0
83	LA	1	0	0	0	0
83	LH	1	0	0	0	0
83	LN	1	0	0	0	0
83	LP	1	0	0	0	0
83	LQ	1	0	0	0	0
83	LV	1	0	0	0	0
83	Le	1	0	0	0	0
83	Ll	1	0	0	0	0
83	S2	66	0	0	0	0
83	S6	7	0	0	0	0
84	L5	29	0	0	0	0
85	Lg	1	0	0	0	0
85	Lj	1	0	0	0	0
85	Lm	1	0	0	0	0
85	Lo	1	0	0	0	0
85	Lp	1	0	0	0	0
85	Sa	1	0	0	0	0
All	All	220451	0	162764	3588	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 10.

The worst 5 of 3588 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)
1:L5:184:U:H3	1:L5:253:G:H1	1.04	1.02
25:LW:69:LYS:H	25:LW:70:LYS:HB2	1.23	0.99
1:L5:2552:G:H21	1:L5:2765:A:H62	1.01	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S6:11:G:H1	48:S6:25:U:H3	1.04	0.94
7:LD:104:LEU:HB2	7:LD:247:ILE:HD11	1.49	0.94

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	LA	246/257 (96%)	224 (91%)	20 (8%)	2 (1%)	16 40
5	LB	400/403 (99%)	366 (92%)	28 (7%)	6 (2%)	8 25
6	LC	365/427 (86%)	318 (87%)	45 (12%)	2 (0%)	24 52
7	LD	291/297 (98%)	270 (93%)	18 (6%)	3 (1%)	12 35
8	LE	238/288 (83%)	197 (83%)	35 (15%)	6 (2%)	4 14
9	LF	223/248 (90%)	210 (94%)	13 (6%)	0	100 100
10	LG	239/266 (90%)	215 (90%)	24 (10%)	0	100 100
11	LH	188/192 (98%)	171 (91%)	17 (9%)	0	100 100
12	LI	211/214 (99%)	196 (93%)	15 (7%)	0	100 100
13	LJ	174/178 (98%)	157 (90%)	15 (9%)	2 (1%)	11 32
14	LL	208/211 (99%)	188 (90%)	16 (8%)	4 (2%)	6 19
15	LM	137/215 (64%)	121 (88%)	15 (11%)	1 (1%)	18 44
16	LN	201/204 (98%)	190 (94%)	11 (6%)	0	100 100
17	LO	199/203 (98%)	188 (94%)	11 (6%)	0	100 100
18	LP	151/184 (82%)	138 (91%)	11 (7%)	2 (1%)	9 28
19	LQ	185/188 (98%)	176 (95%)	9 (5%)	0	100 100
20	LR	185/196 (94%)	180 (97%)	5 (3%)	0	100 100
21	LS	173/176 (98%)	153 (88%)	19 (11%)	1 (1%)	21 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
22	LT	157/160 (98%)	148 (94%)	7 (4%)	2 (1%)	9 28
23	LU	99/128 (77%)	91 (92%)	7 (7%)	1 (1%)	12 35
24	LV	129/140 (92%)	117 (91%)	12 (9%)	0	100 100
25	LW	122/157 (78%)	104 (85%)	16 (13%)	2 (2%)	7 23
26	LX	118/156 (76%)	112 (95%)	6 (5%)	0	100 100
27	LY	132/145 (91%)	124 (94%)	7 (5%)	1 (1%)	16 40
28	LZ	133/136 (98%)	117 (88%)	16 (12%)	0	100 100
29	La	145/148 (98%)	126 (87%)	19 (13%)	0	100 100
30	Lb	73/159 (46%)	66 (90%)	6 (8%)	1 (1%)	9 26
31	Lc	96/115 (84%)	88 (92%)	5 (5%)	3 (3%)	3 10
32	Ld	105/125 (84%)	97 (92%)	8 (8%)	0	100 100
33	Le	126/135 (93%)	113 (90%)	12 (10%)	1 (1%)	16 40
34	Lf	107/110 (97%)	98 (92%)	7 (6%)	2 (2%)	6 19
35	Lg	112/117 (96%)	108 (96%)	4 (4%)	0	100 100
36	Lh	120/123 (98%)	113 (94%)	6 (5%)	1 (1%)	16 40
37	Li	100/105 (95%)	93 (93%)	7 (7%)	0	100 100
38	Lj	84/97 (87%)	75 (89%)	8 (10%)	1 (1%)	10 30
39	Lk	67/70 (96%)	58 (87%)	8 (12%)	1 (2%)	8 25
40	Ll	48/51 (94%)	45 (94%)	3 (6%)	0	100 100
41	Lm	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	6 18
42	Ln	22/25 (88%)	20 (91%)	2 (9%)	0	100 100
43	Lo	102/106 (96%)	96 (94%)	5 (5%)	1 (1%)	12 35
44	Lp	89/92 (97%)	80 (90%)	8 (9%)	1 (1%)	11 32
45	Lr	123/137 (90%)	108 (88%)	14 (11%)	1 (1%)	16 40
46	Lz	215/217 (99%)	190 (88%)	25 (12%)	0	100 100
49	SA	220/295 (75%)	199 (90%)	21 (10%)	0	100 100
50	SB	212/264 (80%)	187 (88%)	23 (11%)	2 (1%)	14 37
51	SD	225/243 (93%)	195 (87%)	27 (12%)	3 (1%)	9 28
52	SE	260/263 (99%)	229 (88%)	29 (11%)	2 (1%)	16 40
53	SF	189/204 (93%)	158 (84%)	28 (15%)	3 (2%)	7 23
54	SH	187/193 (97%)	162 (87%)	23 (12%)	2 (1%)	11 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
55	SI	204/208 (98%)	175 (86%)	26 (13%)	3 (2%)	8 25
56	SK	96/165 (58%)	82 (85%)	13 (14%)	1 (1%)	12 35
57	SL	151/158 (96%)	138 (91%)	13 (9%)	0	100 100
58	SP	95/145 (66%)	61 (64%)	30 (32%)	4 (4%)	2 6
59	SQ	144/146 (99%)	124 (86%)	17 (12%)	3 (2%)	5 17
60	SR	130/135 (96%)	116 (89%)	13 (10%)	1 (1%)	16 40
61	SS	148/152 (97%)	126 (85%)	18 (12%)	4 (3%)	4 12
62	ST	141/145 (97%)	123 (87%)	16 (11%)	2 (1%)	9 26
63	SU	102/119 (86%)	90 (88%)	10 (10%)	2 (2%)	6 18
64	SV	81/83 (98%)	70 (86%)	9 (11%)	2 (2%)	4 14
65	SX	139/143 (97%)	124 (89%)	11 (8%)	4 (3%)	3 11
66	Sa	103/115 (90%)	85 (82%)	16 (16%)	2 (2%)	6 19
67	Sc	62/69 (90%)	47 (76%)	15 (24%)	0	100 100
68	Sd	51/56 (91%)	48 (94%)	3 (6%)	0	100 100
69	Sf	69/156 (44%)	53 (77%)	12 (17%)	4 (6%)	1 3
70	Sg	311/317 (98%)	272 (88%)	35 (11%)	4 (1%)	9 28
71	SC	220/293 (75%)	201 (91%)	16 (7%)	3 (1%)	9 26
72	SG	235/249 (94%)	205 (87%)	25 (11%)	5 (2%)	5 17
73	SJ	183/194 (94%)	165 (90%)	15 (8%)	3 (2%)	7 23
74	SM	120/132 (91%)	99 (82%)	18 (15%)	3 (2%)	4 14
75	SN	148/151 (98%)	139 (94%)	6 (4%)	3 (2%)	6 18
76	SO	138/151 (91%)	109 (79%)	24 (17%)	5 (4%)	2 8
77	SW	127/130 (98%)	119 (94%)	8 (6%)	0	100 100
78	SY	129/133 (97%)	117 (91%)	11 (8%)	1 (1%)	16 40
79	SZ	73/125 (58%)	61 (84%)	10 (14%)	2 (3%)	4 12
80	Sb	81/84 (96%)	70 (86%)	11 (14%)	0	100 100
81	Se	56/59 (95%)	49 (88%)	7 (12%)	0	100 100
All	All	11518/12904 (89%)	10291 (89%)	1105 (10%)	122 (1%)	14 32

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	LB	113	GLU

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Mol	Chain	Res	Type
7	LD	21	ARG
8	LE	131	LYS
14	LL	91	ALA
33	Le	104	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	LA	190/199 (96%)	189 (100%)	1 (0%)	81	92
5	LB	348/349 (100%)	348 (100%)	0	100	100
6	LC	305/348 (88%)	305 (100%)	0	100	100
7	LD	246/250 (98%)	246 (100%)	0	100	100
8	LE	215/252 (85%)	215 (100%)	0	100	100
9	LF	194/215 (90%)	194 (100%)	0	100	100
10	LG	203/223 (91%)	203 (100%)	0	100	100
11	LH	169/171 (99%)	169 (100%)	0	100	100
12	LI	180/181 (99%)	180 (100%)	0	100	100
13	LJ	148/149 (99%)	148 (100%)	0	100	100
14	LL	176/177 (99%)	176 (100%)	0	100	100
15	LM	118/161 (73%)	118 (100%)	0	100	100
16	LN	171/172 (99%)	171 (100%)	0	100	100
17	LO	173/174 (99%)	173 (100%)	0	100	100
18	LP	134/163 (82%)	134 (100%)	0	100	100
19	LQ	164/165 (99%)	163 (99%)	1 (1%)	78	91
20	LR	166/175 (95%)	166 (100%)	0	100	100
21	LS	156/157 (99%)	156 (100%)	0	100	100
22	LT	139/140 (99%)	139 (100%)	0	100	100
23	LU	91/115 (79%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	LV	101/107 (94%)	101 (100%)	0	100	100
25	LW	103/126 (82%)	103 (100%)	0	100	100
26	LX	108/133 (81%)	107 (99%)	1 (1%)	70	87
27	LY	124/135 (92%)	124 (100%)	0	100	100
28	LZ	117/118 (99%)	117 (100%)	0	100	100
29	La	120/121 (99%)	120 (100%)	0	100	100
30	Lb	63/126 (50%)	63 (100%)	0	100	100
31	Lc	83/97 (86%)	83 (100%)	0	100	100
32	Ld	98/110 (89%)	98 (100%)	0	100	100
33	Le	114/121 (94%)	114 (100%)	0	100	100
34	Lf	88/89 (99%)	88 (100%)	0	100	100
35	Lg	98/100 (98%)	98 (100%)	0	100	100
36	Lh	109/110 (99%)	109 (100%)	0	100	100
37	Li	86/89 (97%)	86 (100%)	0	100	100
38	Lj	73/80 (91%)	73 (100%)	0	100	100
39	Lk	64/65 (98%)	64 (100%)	0	100	100
40	Ll	47/48 (98%)	47 (100%)	0	100	100
41	Lm	48/116 (41%)	48 (100%)	0	100	100
42	Ln	23/24 (96%)	23 (100%)	0	100	100
43	Lo	93/94 (99%)	93 (100%)	0	100	100
44	Lp	74/75 (99%)	74 (100%)	0	100	100
45	Lr	109/121 (90%)	109 (100%)	0	100	100
46	Lz	195/196 (100%)	195 (100%)	0	100	100
49	SA	184/243 (76%)	184 (100%)	0	100	100
50	SB	195/231 (84%)	195 (100%)	0	100	100
51	SD	190/202 (94%)	190 (100%)	0	100	100
52	SE	224/225 (100%)	224 (100%)	0	100	100
53	SF	161/170 (95%)	161 (100%)	0	100	100
54	SH	169/173 (98%)	169 (100%)	0	100	100
55	SI	178/180 (99%)	177 (99%)	1 (1%)	78	91
56	SK	89/136 (65%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	SL	137/142 (96%)	137 (100%)	0	100	100
58	SP	87/130 (67%)	87 (100%)	0	100	100
59	SQ	121/121 (100%)	121 (100%)	0	100	100
60	SR	120/122 (98%)	120 (100%)	0	100	100
61	SS	130/132 (98%)	130 (100%)	0	100	100
62	ST	113/115 (98%)	113 (100%)	0	100	100
63	SU	94/107 (88%)	94 (100%)	0	100	100
64	SV	67/67 (100%)	67 (100%)	0	100	100
65	SX	113/115 (98%)	113 (100%)	0	100	100
66	Sa	90/98 (92%)	90 (100%)	0	100	100
67	Sc	57/62 (92%)	57 (100%)	0	100	100
68	Sd	47/49 (96%)	47 (100%)	0	100	100
69	Sf	64/140 (46%)	64 (100%)	0	100	100
70	Sg	272/275 (99%)	272 (100%)	0	100	100
71	SC	188/225 (84%)	188 (100%)	0	100	100
72	SG	207/218 (95%)	207 (100%)	0	100	100
73	SJ	161/168 (96%)	161 (100%)	0	100	100
74	SM	104/108 (96%)	104 (100%)	0	100	100
75	SN	130/131 (99%)	130 (100%)	0	100	100
76	SO	110/119 (92%)	110 (100%)	0	100	100
77	SW	112/113 (99%)	112 (100%)	0	100	100
78	SY	113/115 (98%)	113 (100%)	0	100	100
79	SZ	66/103 (64%)	66 (100%)	0	100	100
80	Sb	75/76 (99%)	75 (100%)	0	100	100
81	Se	47/48 (98%)	47 (100%)	0	100	100
All	All	10039/10996 (91%)	10035 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	LA	162	ASN
19	LQ	45	GLN
26	LX	69	ASN

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Mol	Chain	Res	Type
55	SI	64	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
50	SB	43	ASN
54	SH	25	GLN
77	SW	120	HIS
50	SB	101	HIS
52	SE	36	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3707/5070 (73%)	1041 (28%)	47 (1%)
2	L7	119/121 (98%)	15 (12%)	0
3	L8	155/157 (98%)	34 (21%)	1 (0%)
47	S2	1714/1869 (91%)	567 (33%)	22 (1%)
48	S6	74/75 (98%)	23 (31%)	2 (2%)
82	Pt	76/77 (98%)	14 (18%)	0
All	All	5845/7369 (79%)	1694 (28%)	72 (1%)

5 of 1694 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	2	G
1	L5	17	A
1	L5	25	A
1	L5	30	C
1	L5	39	A

5 of 72 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	S2	795	A
48	S6	34	C
47	S2	868	G
47	S2	1419	C
1	L5	2639	U

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

5 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
82	H2U	Pt	21	82	18,21,22	0.45	0	21,30,33	1.04	1 (4%)
82	4SU	Pt	8	82	18,21,22	4.29	8 (44%)	26,30,33	2.21	5 (19%)
82	OMC	Pt	33	47,82	19,22,23	0.54	0	26,31,34	0.78	1 (3%)
82	PSU	Pt	56	82	18,21,22	1.13	1 (5%)	22,30,33	1.73	4 (18%)
82	G7M	Pt	47	82	23,26,27	2.93	8 (34%)	35,39,42	2.18	10 (28%)

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
82	H2U	Pt	21	82	-	3/7/38/39	0/2/2/2
82	4SU	Pt	8	82	-	1/7/25/26	0/2/2/2
82	OMC	Pt	33	47,82	-	1/9/27/28	0/2/2/2
82	PSU	Pt	56	82	-	0/7/25/26	0/2/2/2
82	G7M	Pt	47	82	-	0/7/25/26	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	Pt	8	4SU	C2-N1	9.22	1.53	1.38
82	Pt	8	4SU	C4-N3	8.58	1.46	1.37
82	Pt	8	4SU	C2-N3	7.06	1.50	1.38
82	Pt	47	G7M	C2-N2	6.93	1.50	1.34
82	Pt	8	4SU	C5-C4	6.86	1.51	1.42

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
82	Pt	8	4SU	C4-N3-C2	-7.76	119.80	127.34
82	Pt	47	G7M	CN7-N7-C5	5.99	134.21	126.77
82	Pt	8	4SU	C5-C4-N3	5.33	119.64	114.69
82	Pt	47	G7M	CN7-N7-C8	-4.57	117.79	124.84
82	Pt	56	PSU	C4-N3-C2	-4.51	119.83	126.34

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	Pt	21	H2U	C3'-C4'-C5'-O5'
82	Pt	33	OMC	C1'-C2'-O2'-CM2
82	Pt	21	H2U	O4'-C4'-C5'-O5'
82	Pt	21	H2U	C4'-C5'-O5'-P
82	Pt	8	4SU	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	Pt	21	H2U	2	0
82	Pt	33	OMC	1	0
82	Pt	47	G7M	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 246 ligands modelled in this entry, 245 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
84	A1E6S	L5	5245	-	26,33,33	5.20	13 (50%)	12,52,52	2.11	4 (33%)

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
84	A1E6S	L5	5245	-	-	3/7/76/76	0/3/5/5

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	L5	5245	A1E6S	C17-C18	23.09	1.52	1.33
84	L5	5245	A1E6S	C11-C10	5.87	1.59	1.53
84	L5	5245	A1E6S	C12-C11	4.63	1.61	1.54
84	L5	5245	A1E6S	C03-C04	-4.27	1.46	1.50
84	L5	5245	A1E6S	C16-C17	3.79	1.56	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	L5	5245	A1E6S	C02-C03-C04	5.47	108.28	100.64
84	L5	5245	A1E6S	O12-C10-C09	-2.54	100.17	104.01
84	L5	5245	A1E6S	C19-C20-C03	2.46	116.03	112.02
84	L5	5245	A1E6S	C07-O12-C10	2.06	112.28	107.71

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
84	L5	5245	A1E6S	C17-C18-C21-C22
84	L5	5245	A1E6S	C19-C18-C21-C22
84	L5	5245	A1E6S	C10-C11-C12-C13

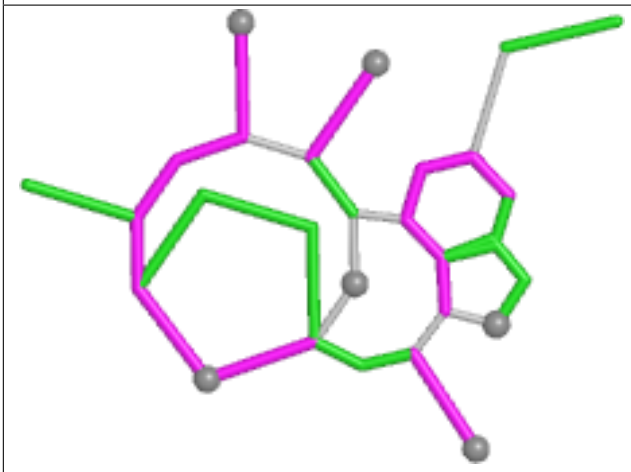
There are no ring outliers.

No monomer is involved in short contacts.

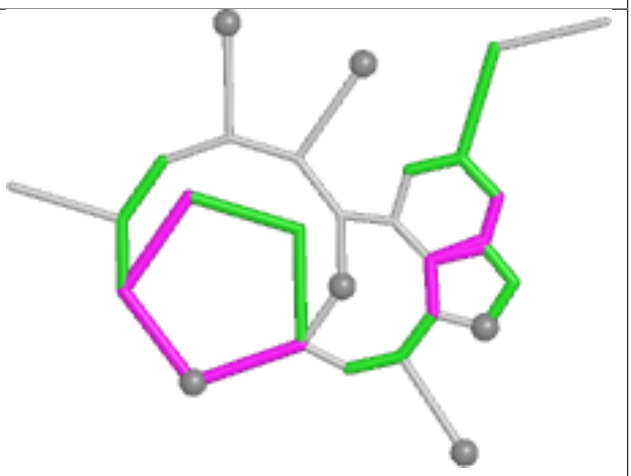
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

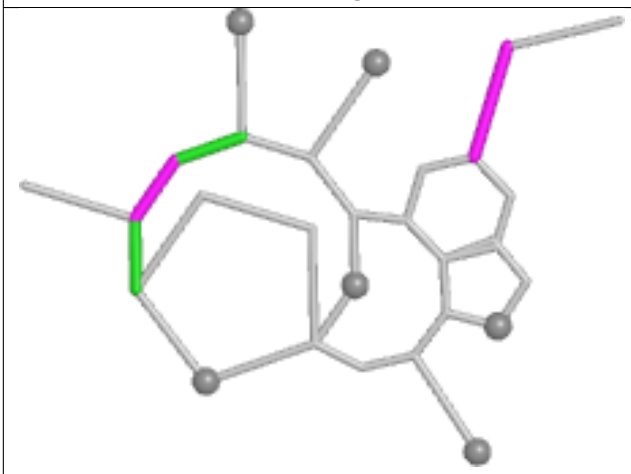
Ligand A1E6S L5 5245



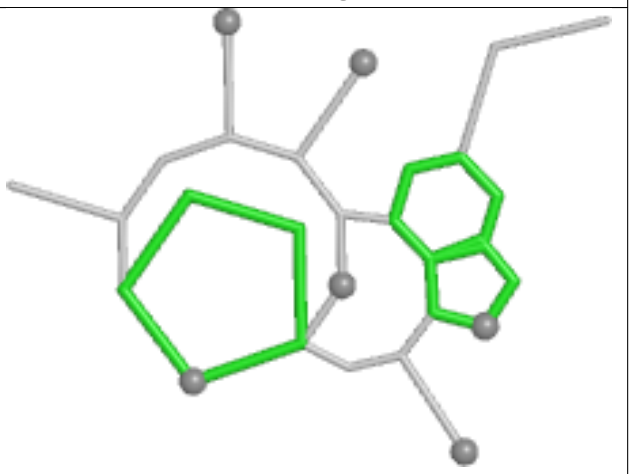
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
43	Lo	1
66	Sa	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lo	105:GLN	C	106:PHE	N	6.09
1	Sa	99:PRO	C	100:ARG	N	3.64

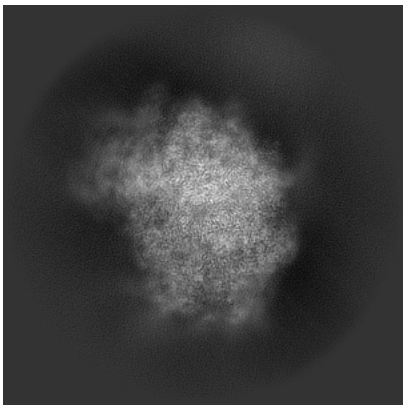
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66929. These allow visual inspection of the internal detail of the map and identification of artifacts.

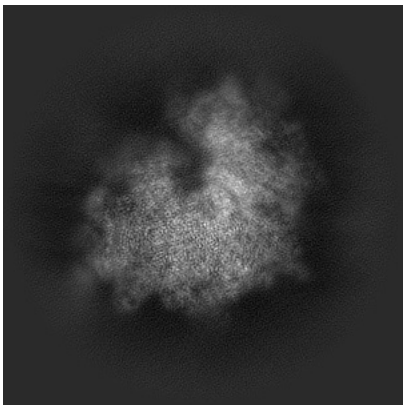
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

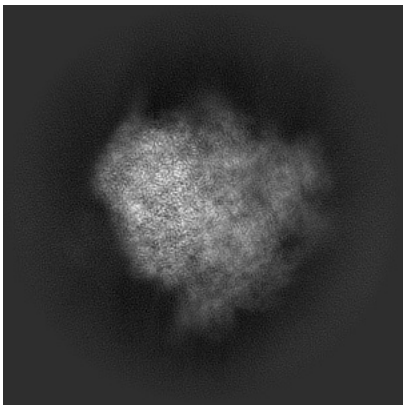
6.1.1 Primary map



X

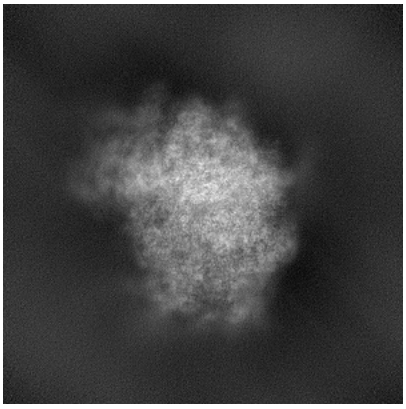


Y

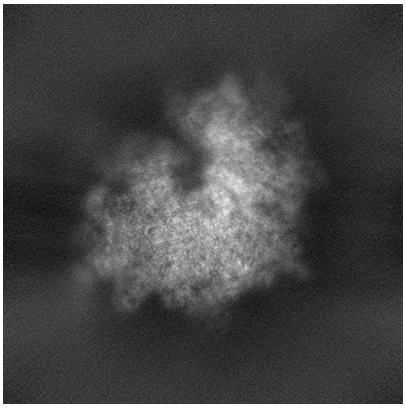


Z

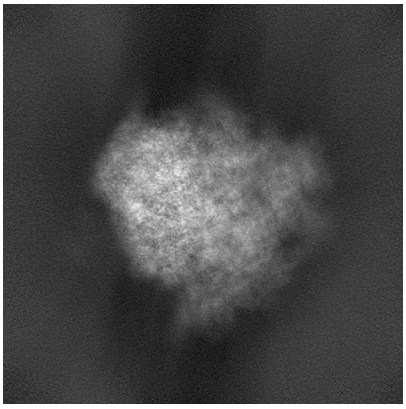
6.1.2 Raw map



X



Y

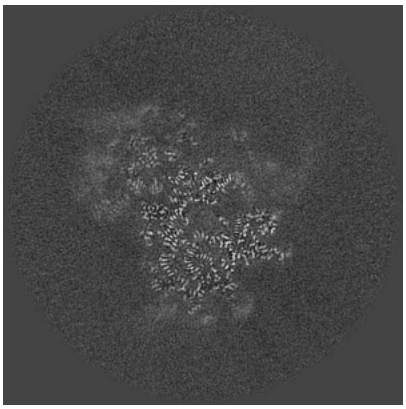


Z

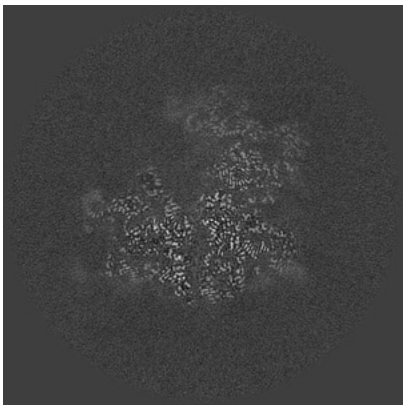
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

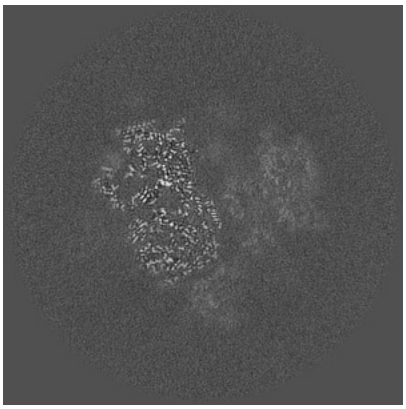
6.2.1 Primary map



X Index: 240

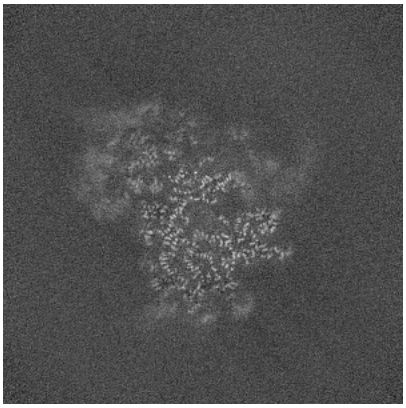


Y Index: 240

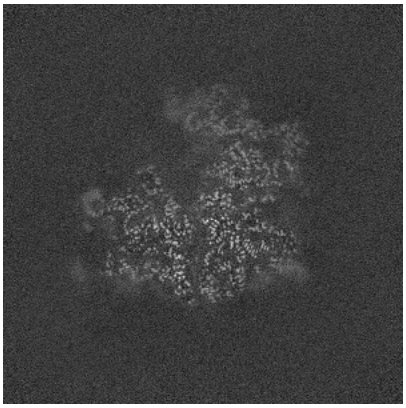


Z Index: 240

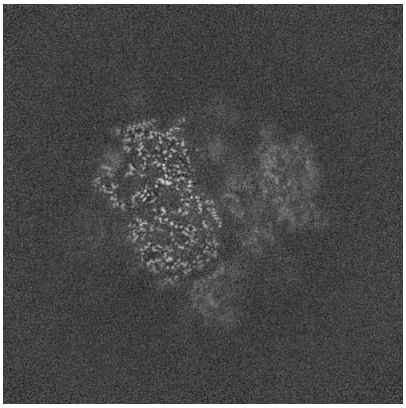
6.2.2 Raw map



X Index: 240



Y Index: 240

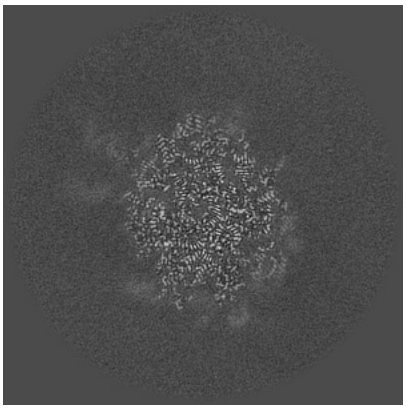


Z Index: 240

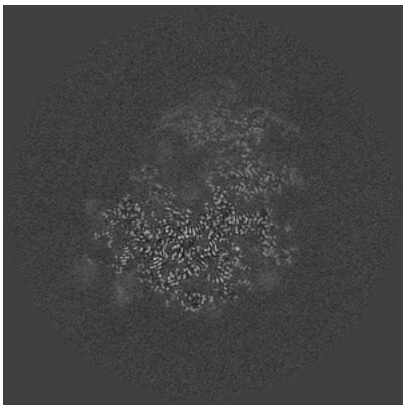
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

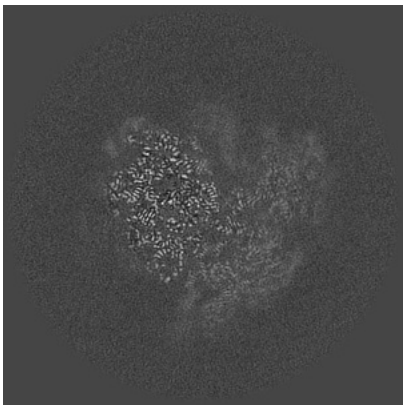
6.3.1 Primary map



X Index: 212

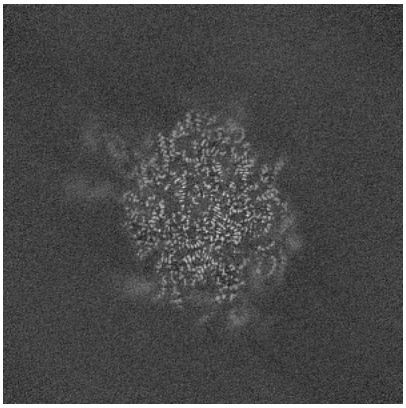


Y Index: 254

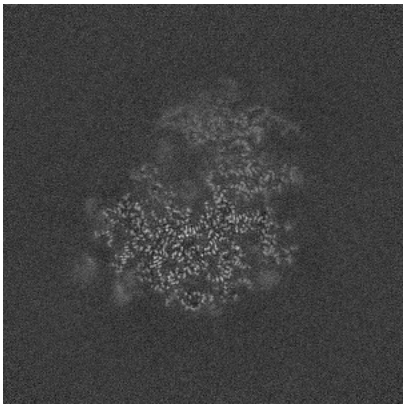


Z Index: 263

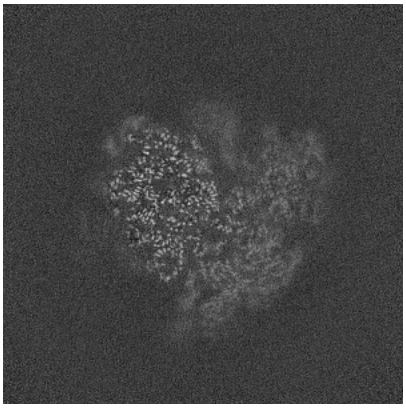
6.3.2 Raw map



X Index: 211



Y Index: 254

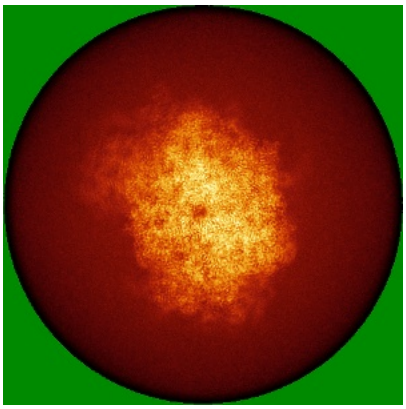


Z Index: 263

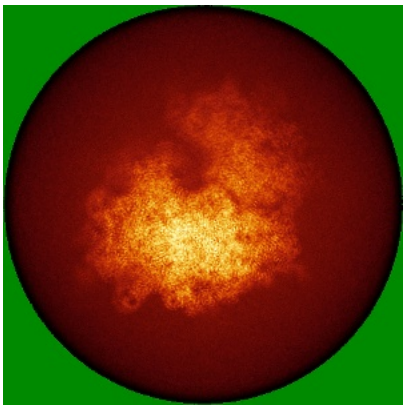
The images above show the largest variance slices of the map in three orthogonal directions.

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

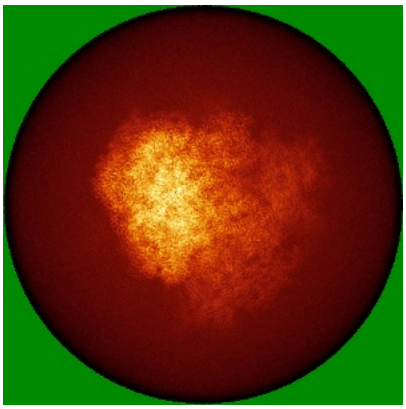
6.4.1 Primary map



X

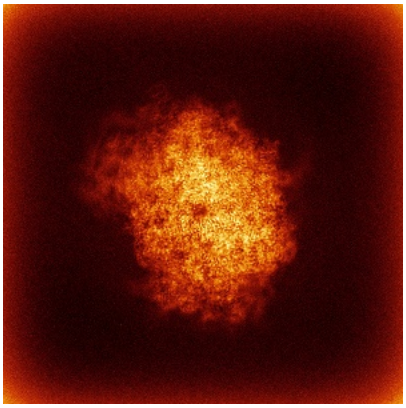


Y

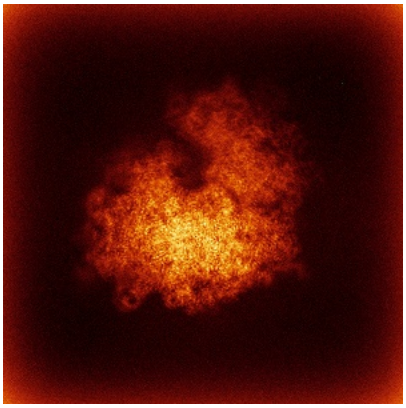


Z

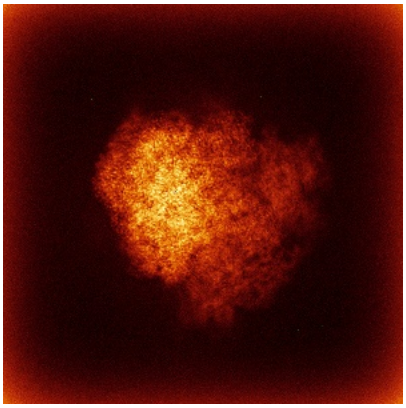
6.4.2 Raw map



X



Y

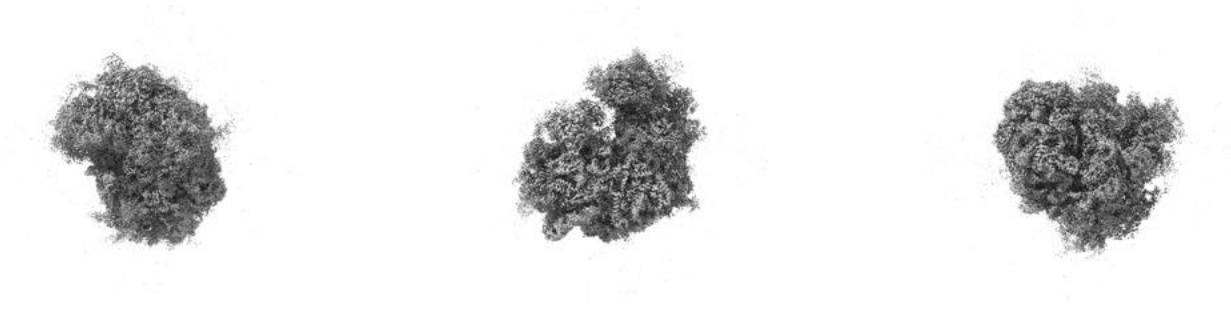


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

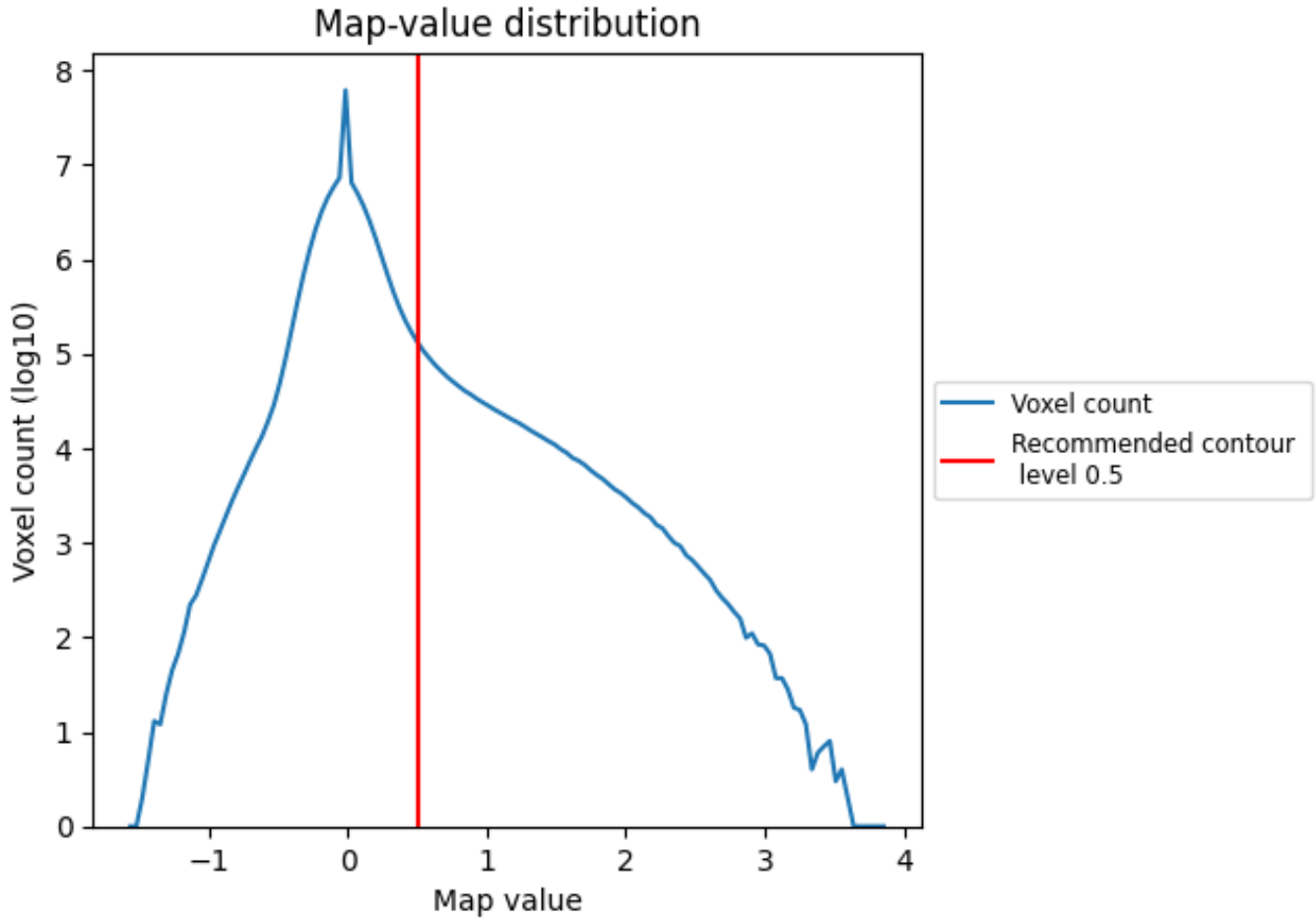
6.6 Mask visualisation (i)

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

7 Map analysis

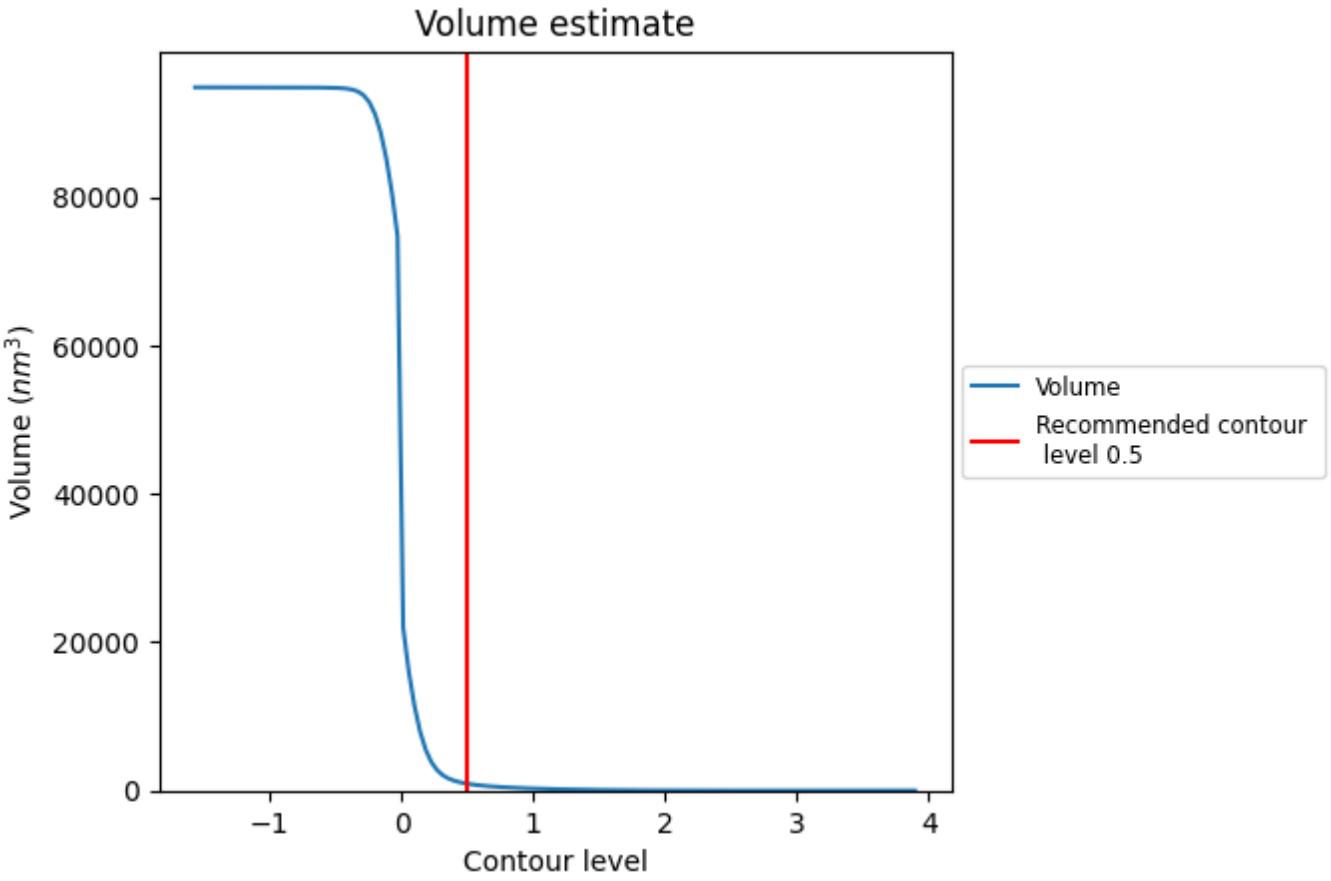
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

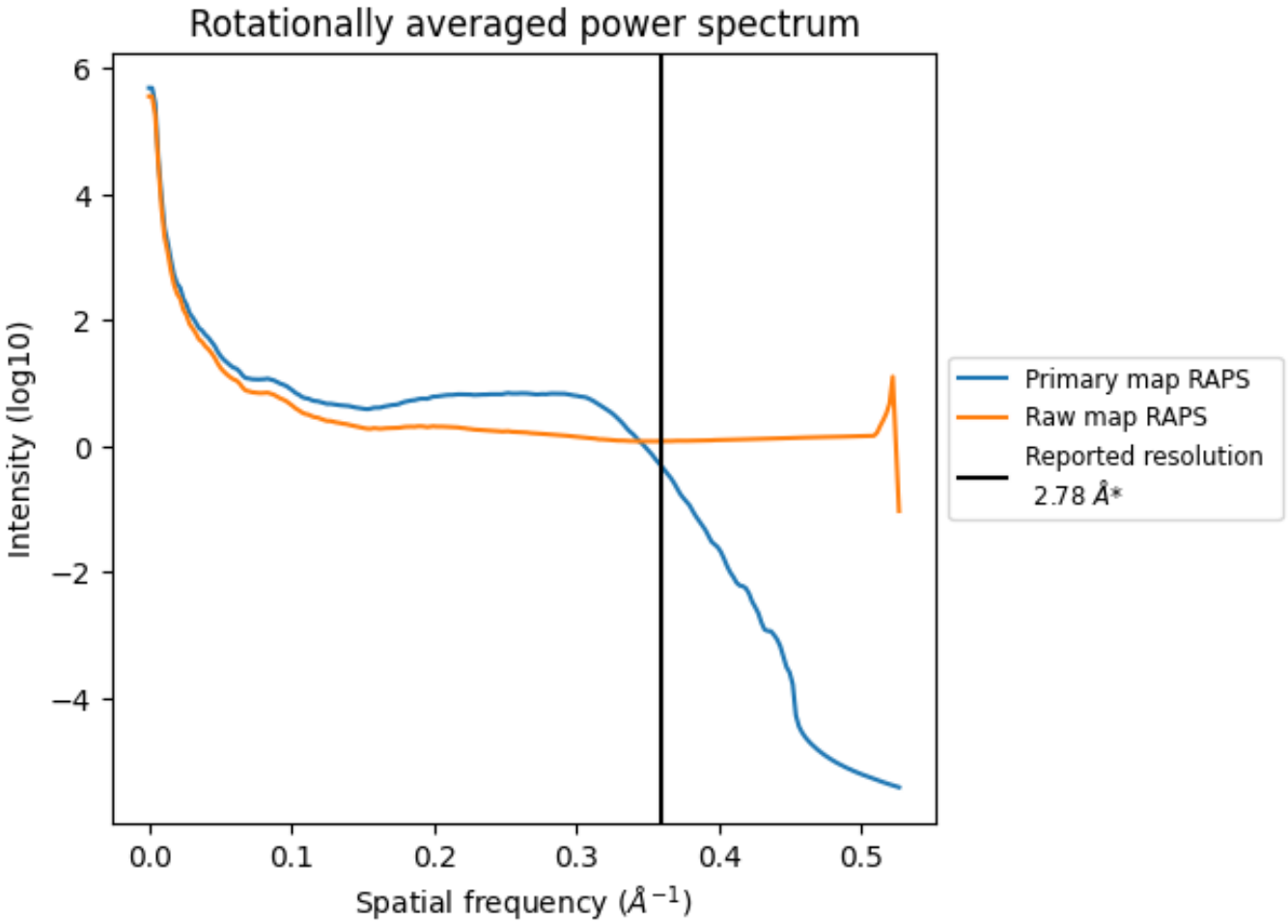
7.2 Volume estimate (i)



The volume at the recommended contour level is 930 nm^3; this corresponds to an approximate mass of 840 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)

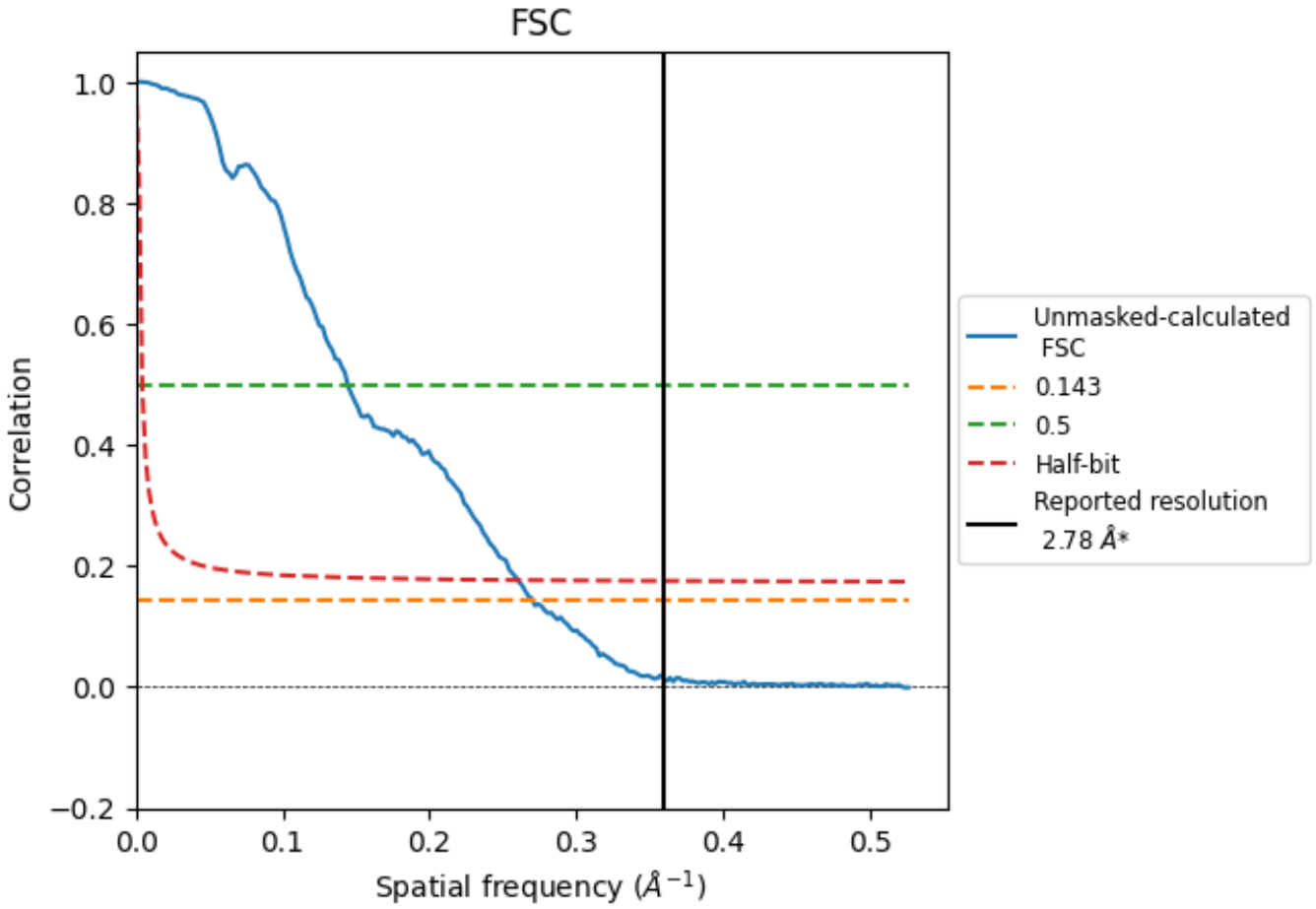


*Reported resolution corresponds to spatial frequency of 0.360 Å^{-1}

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 0.360 Å^{-1}

8.2 Resolution estimates (i)

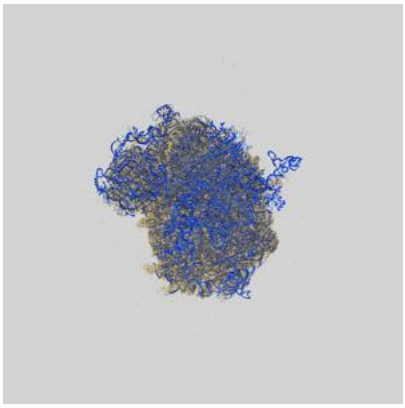
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.70	6.93	3.84

*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 3.70 differs from the reported value 2.78 by more than 10 %

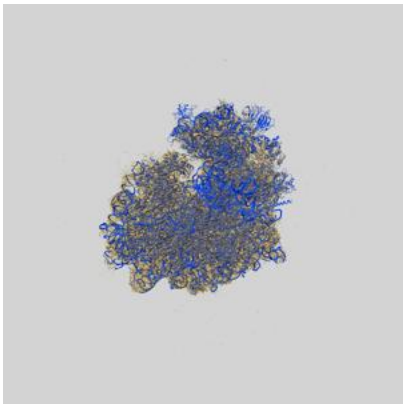
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66929 and PDB model 9XJ6. Per-residue inclusion information can be found in section 3 on page 21.

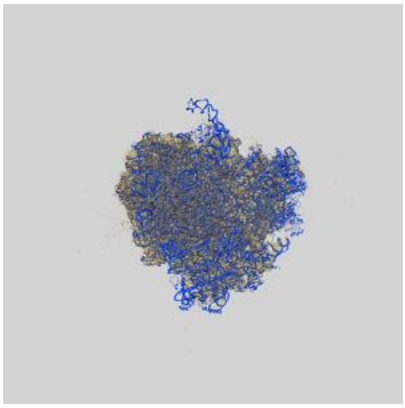
9.1 Map-model overlay



X



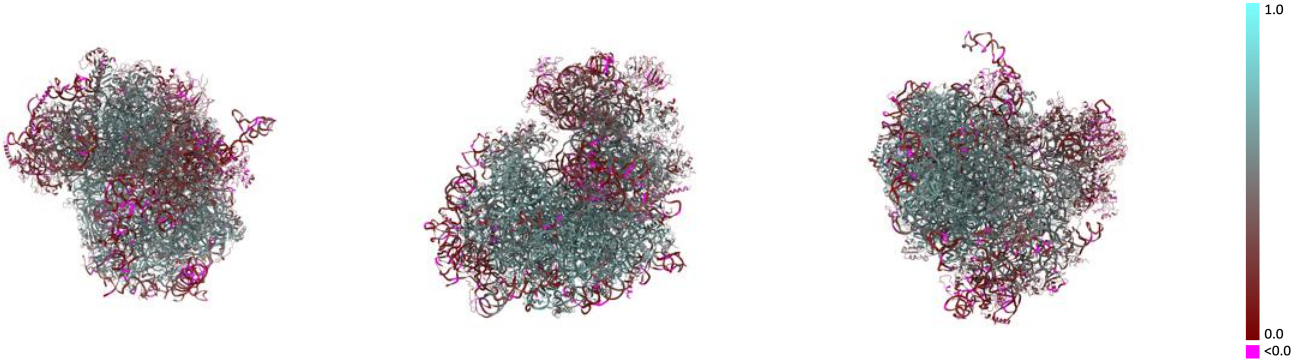
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

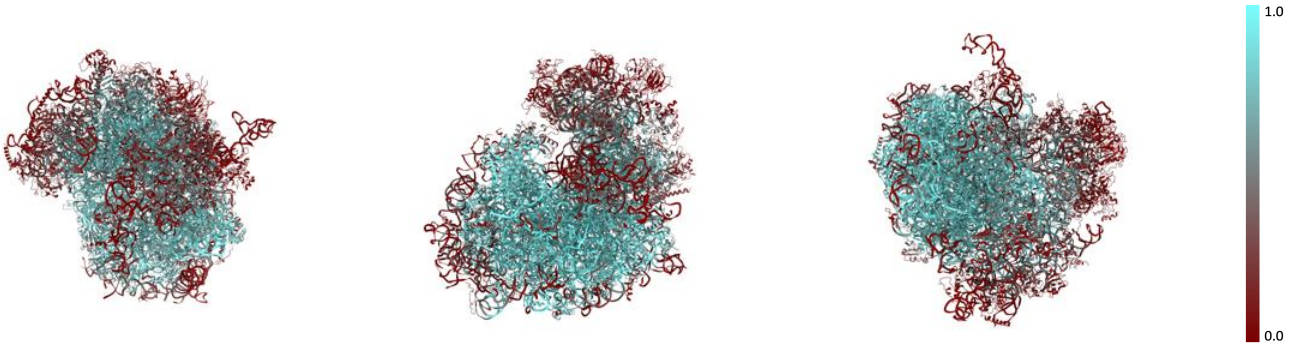
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

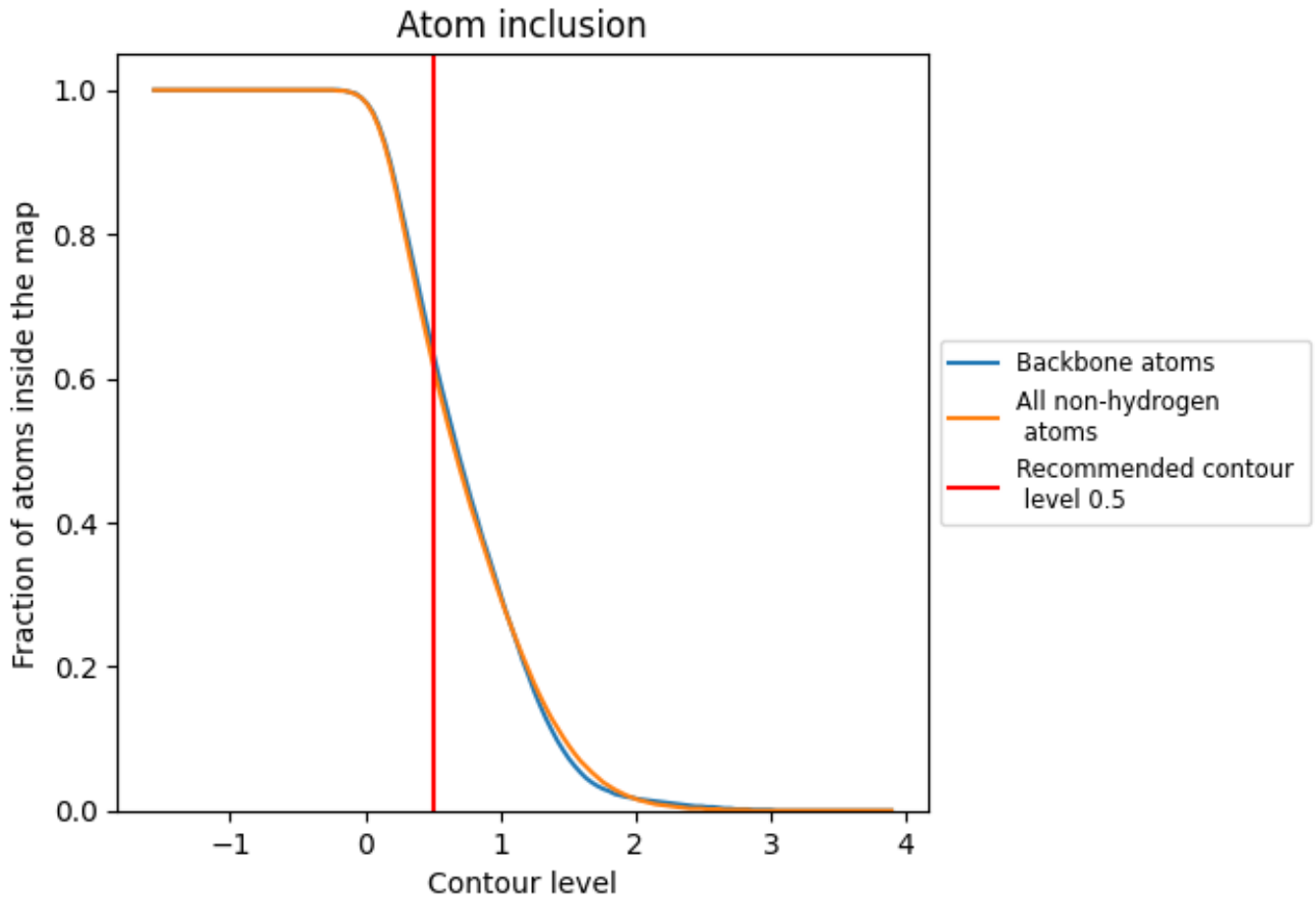
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6200	0.4530
L5	0.7290	0.4800
L7	0.9340	0.5950
L8	0.8810	0.5770
LA	0.9000	0.6010
LB	0.8180	0.5730
LC	0.8320	0.5710
LD	0.6960	0.5090
LE	0.6010	0.4510
LF	0.8390	0.5830
LG	0.6870	0.5070
LH	0.6520	0.5130
LI	0.6420	0.4920
LJ	0.4980	0.4290
LL	0.7570	0.5490
LM	0.7320	0.5300
LN	0.9230	0.6200
LO	0.8500	0.5960
LP	0.8670	0.5980
LQ	0.8900	0.6040
LR	0.6970	0.5060
LS	0.8340	0.5730
LT	0.7860	0.5630
LU	0.3990	0.4000
LV	0.8120	0.5870
LW	0.4290	0.3540
LX	0.7960	0.5600
LY	0.7780	0.5620
LZ	0.7240	0.5430
La	0.8770	0.6020
Lb	0.6890	0.5170
Lc	0.7300	0.5220
Ld	0.7790	0.5480
Le	0.8640	0.5990
Lf	0.8950	0.6050



Continued on next page...

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Chain	Atom inclusion	Q-score
Lg	0.7860	0.5610
Lh	0.7780	0.5650
Li	0.7180	0.5290
Lj	0.9140	0.6040
Lk	0.5100	0.4490
Ll	0.8440	0.5850
Lm	0.0020	0.0930
Ln	0.8710	0.6010
Lo	0.7560	0.5460
Lp	0.8140	0.5620
Lr	0.8450	0.5840
Lz	0.0040	0.0980
Pt	0.1910	0.2830
S2	0.5650	0.3940
S6	0.1070	0.1690
SA	0.3810	0.4470
SB	0.4600	0.4540
SC	0.5160	0.4730
SD	0.1890	0.3120
SE	0.2470	0.3670
SF	0.2120	0.3010
SG	0.1480	0.2550
SH	0.2080	0.3350
SI	0.3690	0.4000
SJ	0.3040	0.3910
SK	0.0680	0.1980
SL	0.4560	0.4570
SM	0.0010	0.0810
SN	0.6000	0.5110
SO	0.5660	0.4650
SP	0.0710	0.1620
SQ	0.1880	0.3120
SR	0.1900	0.3130
SS	0.1640	0.2820
ST	0.1440	0.2790
SU	0.2070	0.2980
SV	0.3910	0.4380
SW	0.6010	0.5230
SX	0.5600	0.4610
SY	0.1570	0.2950
SZ	0.1000	0.2200
Sa	0.6200	0.4810

Continued on next page...

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Chain	Atom inclusion	Q-score
Sb	0.3910	0.4260
Sc	0.2180	0.3190
Sd	0.3230	0.3440
Se	0.2090	0.2650
Sf	0.0020	0.1030
Sg	0.0240	0.2050