wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2023 – 05:55 AM EDT

PDB ID	:	6O3M
Title	:	Unmodified tRNA(Pro) bound to Thermus thermophilus 70S (cognate)
Authors	:	Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.
Deposited on	:	2019-02-26
Resolution	:	3.97 Å(reported)

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

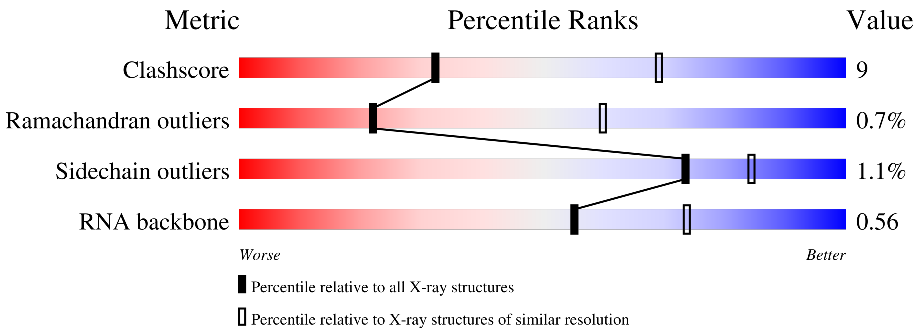
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.97 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1099 (4.26-3.70)
Ramachandran outliers	138981	1061 (4.26-3.70)
Sidechain outliers	138945	1053 (4.26-3.70)
RNA backbone	3102	1041 (4.84-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1521	 49% 40% 9% ••
1	XA	1521	 48% 40% 9% ••
2	QB	256	 73% 18% • 8%
2	XB	256	 73% 19% • 8%
3	QC	239	 59% 26% • 14%
3	XC	239	 65% 21% 14%

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Mol	Chain	Length	Quality of chain
4	QD	209	72% 27% •
4	XD	209	67% 30% •
5	QE	162	74% 18% • 7%
5	XE	162	71% 22% 7%
6	QF	101	77% 23%
6	XF	101	88% 12%
7	QG	156	72% 24% • •
7	XG	156	78% 21% ••
8	QH	138	69% 29% ••
8	XH	138	67% 30% ••
9	QI	128	67% 28% • •
9	XI	128	68% 30% • •
10	QJ	105	62% 32% 6%
10	XJ	105	61% 29% • 9%
11	QK	129	69% 23% 8%
11	XK	129	71% 19% 10%
12	QL	132	68% 25% • 5%
12	XL	132	72% 20% • 8%
13	QM	126	60% 33% • 5%
13	XM	126	67% 25% • 6%
14	QN	61	70% 25% • •
14	XN	61	59% 38% • •
15	QO	89	75% 24% •
15	XO	89	80% 18% •
16	QP	88	78% 17% 5%

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Mol	Chain	Length	Quality of chain
16	XP	88	84% 11% 5%
17	QQ	105	81% 13% • 5%
17	XQ	105	74% 20% • 5%
18	QR	88	63% 17% 20%
18	XR	88	63% 17% 20%
19	QS	93	65% 25% 11%
19	XS	93	73% 17% 10%
20	QT	106	75% 19% 7%
20	XT	106	72% 22% 7%
21	QU	27	74% 19% 7%
21	XU	27	56% 37% 7%
22	QV	77	52% 35% 13%
22	XV	77	58% 26% 16%
23	QX	19	32% 53% 11% 5%
23	XX	19	37% 58% 5%
24	RA	2915	49% 39% 10% ••
24	YA	2915	48% 40% 10% ••
25	RB	122	60% 27% 10% • •
25	YB	122	61% 25% 12% •
26	RD	276	72% 26% •
26	YD	276	74% 24% •
27	RE	206	68% 30% •
27	YE	206	71% 27% •
28	RF	210	81% 15% •
28	YF	210	82% 14% •

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Mol	Chain	Length	Quality of chain
29	RG	182	74% 24% •••
29	YG	182	68% 29% ••
30	RH	180	69% 26% ••
30	YH	180	78% 17% ••
31	RI	148	82% 16% ••
31	YI	148	85% 12% ••
32	RN	140	80% 19% •
32	YN	140	80% 18% ••
33	RO	122	74% 26%
33	YO	122	80% 20%
34	RP	150	70% 30%
34	YP	150	75% 23% •
35	RQ	141	73% 26% •
35	YQ	141	72% 26% •
36	RR	118	75% 24% ••
36	YR	118	84% 15% •
37	RS	112	71% 29% •
37	YS	112	76% 23% •
38	RT	146	70% 22% • 6%
38	YT	146	69% 23% • 6%
39	RU	118	85% 13% ••
39	YU	118	81% 17% ••
40	RV	101	74% 24% •
40	YV	101	74% 25% •
41	RW	113	79% 21%

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Mol	Chain	Length	Quality of chain
41	YW	113	
42	RX	96	
42	YX	96	
43	RY	110	
43	YY	110	
44	RZ	206	
44	YZ	206	
45	R0	85	
45	Y0	85	
46	R1	98	
46	Y1	98	
47	R2	72	
47	Y2	72	
48	R3	60	
48	Y3	60	
49	R4	71	
49	Y4	71	
50	R5	60	
50	Y5	60	
51	R6	54	
51	Y6	54	
52	R7	49	
52	Y7	49	
53	R8	65	
53	Y8	65	

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Mol	Chain	Length	Quality of chain
54	R9	37	
54	Y9	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	SF4	XD	301	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 291782 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	QA	1500	32247	14353	5981	10414	1499	0	0	0
1	XA	1500	32249	14354	5984	10412	1499	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	QB	235	1907	1217	342	343	5	0	0	0
2	XB	236	1915	1223	343	344	5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	QC	205	1605	1011	313	280	1	0	0	0
3	XC	205	1605	1011	313	280	1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	QD	208	1703	1066	339	291	7	0	0	0
4	XD	208	1703	1066	339	291	7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	QI	125	Total	C	N	O	0	0	0
			989	627	191	171			
9	XI	126	Total	C	N	O	0	0	0
			998	633	193	172			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	XL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
13	XM	119	Total	C	N	O	S	0	0	0
			946	585	195	164	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	QN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	XN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	84	Total 705	C 446	N 140	O 118	S 1	0	0	0
16	XP	84	Total 705	C 446	N 140	O 118	S 1	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	100	Total 834	C 534	N 155	O 143	S 2	0	0	0
17	XQ	100	Total 834	C 534	N 155	O 143	S 2	0	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total 574	C 367	N 112	O 95	0	0	0
18	XR	70	Total 574	C 367	N 112	O 95	0	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total 665	C 424	N 124	O 115	S 2	0	0	0
19	XS	84	Total 674	C 430	N 126	O 116	S 2	0	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total 763	C 470	N 162	O 129	S 2	0	0	0
20	XT	99	Total 763	C 470	N 162	O 129	S 2	0	0	0

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	QU	25	217	134	52	31	0	0	0
21	XU	25	217	134	52	31	0	0	0

- Molecule 22 is a RNA chain called P-site ASLPro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	QV	77	1647	733	295	542	77	0	0	0
22	XV	77	1647	733	295	542	77	0	0	0

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	QX	19	418	186	86	127	19	0	0	0
23	XX	19	418	186	86	127	19	0	0	0

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	RA	2882	62071	27627	11611	19952	2881	0	0	0
24	YA	2883	62091	27636	11613	19960	2882	0	0	0

- Molecule 25 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
25	RB	120	2573	1146	476	832	119	0	0	0
25	YB	120	2573	1146	476	832	119	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	RD	272	2115	1335	420	357	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	YD	272	2115	1335	420	357	3	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	RE	205	1568	991	300	271	6	0	0	0
27	YE	205	1568	991	300	271	6	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	RF	202	1585	1011	297	275	2	0	0	0
28	YF	202	1585	1011	297	275	2	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	RG	181	1474	942	268	260	4	0	0	0
29	YG	181	1474	942	268	260	4	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	RH	174	1336	848	251	236	1	0	0	0
30	YH	174	1336	848	251	236	1	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	RI	146	1136	726	201	208	1	0	0	0
31	YI	146	1136	726	201	208	1	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
32	RN	138	Total C N O S 1104 712 206 182 4	0	0	0
32	YN	138	Total C N O S 1104 712 206 182 4	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
33	RO	122	Total C N O S 933 588 171 170 4	0	0	0
33	YO	122	Total C N O S 933 588 171 170 4	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
34	RP	150	Total C N O S 1145 712 232 198 3	0	0	0
34	YP	147	Total C N O S 1122 698 229 192 3	0	0	0

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
35	RQ	141	Total C N O S 1122 715 212 188 7	0	0	0
35	YQ	141	Total C N O S 1122 715 212 188 7	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
36	RR	117	Total C N O 960 599 202 159	0	0	0
36	YR	117	Total C N O 960 599 202 159	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	RS	111	Total	C	N	O	0	0	0
			882	556	176	150			
37	YS	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
38	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
39	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
40	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
41	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	RX	92	Total	C	N	O	0	0	0
			725	471	131	123			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	YX	92	Total 725	C 471	N 131	O 123	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RY	107	Total 818	C 525	N 155	O 132	S 6	0	0	0
43	YY	107	Total 818	C 525	N 155	O 132	S 6	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RZ	183	Total 1461	C 933	N 260	O 265	S 3	0	0	0
44	YZ	183	Total 1461	C 933	N 260	O 265	S 3	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	R0	81	Total 643	C 398	N 137	O 107	S 1	0	0	0
45	Y0	74	Total 593	C 367	N 126	O 99	S 1	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R1	97	Total 763	C 481	N 150	O 131	S 1	0	0	0
46	Y1	93	Total 729	C 457	N 145	O 126	S 1	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R2	69	Total 581	C 358	N 118	O 104	S 1	0	0	0
47	Y2	69	Total 581	C 358	N 118	O 104	S 1	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
48	R3	59	Total C N O 469 298 90 81	0	0	0
48	Y3	59	Total C N O 469 298 90 81	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
49	R4	69	Total C N O S 565 356 103 101 5	0	0	0
49	Y4	69	Total C N O S 565 356 103 101 5	0	0	0

- Molecule 50 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
50	R5	59	Total C N O S 459 288 90 76 5	0	0	0
50	Y5	59	Total C N O S 459 288 90 76 5	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
51	R6	53	Total C N O S 453 281 91 77 4	0	0	0
51	Y6	53	Total C N O S 453 281 91 77 4	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
52	R7	47	Total C N O S 409 251 102 54 2	0	0	0
52	Y7	48	Total C N O S 418 257 104 55 2	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
53	R8	64	Total C N O S 517 331 102 82 2	0	0	0
53	Y8	64	Total C N O S 517 331 102 82 2	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
54	R9	37	Total C N O S 307 188 68 47 4	0	0	0
54	Y9	37	Total C N O S 307 188 68 47 4	0	0	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

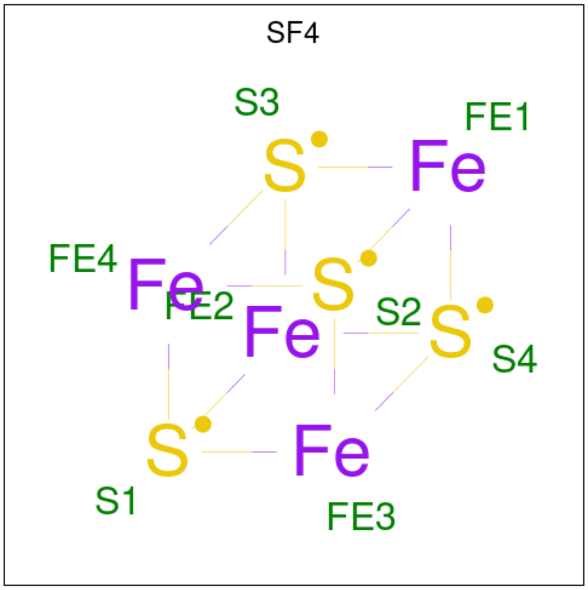
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	QA	69	Total Mg 69 69	0	0
55	QE	1	Total Mg 1 1	0	0
55	QH	1	Total Mg 1 1	0	0
55	QV	1	Total Mg 1 1	0	0
55	RA	381	Total Mg 381 381	0	0
55	RB	9	Total Mg 9 9	0	0
55	RD	1	Total Mg 1 1	0	0
55	RE	1	Total Mg 1 1	0	0
55	RQ	1	Total Mg 1 1	0	0
55	R1	1	Total Mg 1 1	0	0
55	XA	67	Total Mg 67 67	0	0
55	XE	1	Total Mg 1 1	0	0
55	YA	454	Total Mg 454 454	0	0
55	YB	8	Total Mg 8 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	YD	2	Total Mg 2 2	0	0
55	YE	1	Total Mg 1 1	0	0
55	YP	1	Total Mg 1 1	0	0
55	YQ	2	Total Mg 2 2	0	0
55	YR	2	Total Mg 2 2	0	0
55	Y0	1	Total Mg 1 1	0	0
55	Y5	1	Total Mg 1 1	0	0
55	Y7	2	Total Mg 2 2	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	QD	1	Total Fe S 8 4 4	0	0
56	XD	1	Total Fe S 8 4 4	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	QN	1	Total Zn 1 1	0	0
57	RY	1	Total Zn 1 1	0	0
57	R4	1	Total Zn 1 1	0	0
57	R5	1	Total Zn 1 1	0	0
57	R6	1	Total Zn 1 1	0	0
57	R9	1	Total Zn 1 1	0	0
57	XN	1	Total Zn 1 1	0	0
57	YY	1	Total Zn 1 1	0	0
57	Y4	1	Total Zn 1 1	0	0
57	Y5	1	Total Zn 1 1	0	0
57	Y6	1	Total Zn 1 1	0	0
57	Y9	1	Total Zn 1 1	0	0

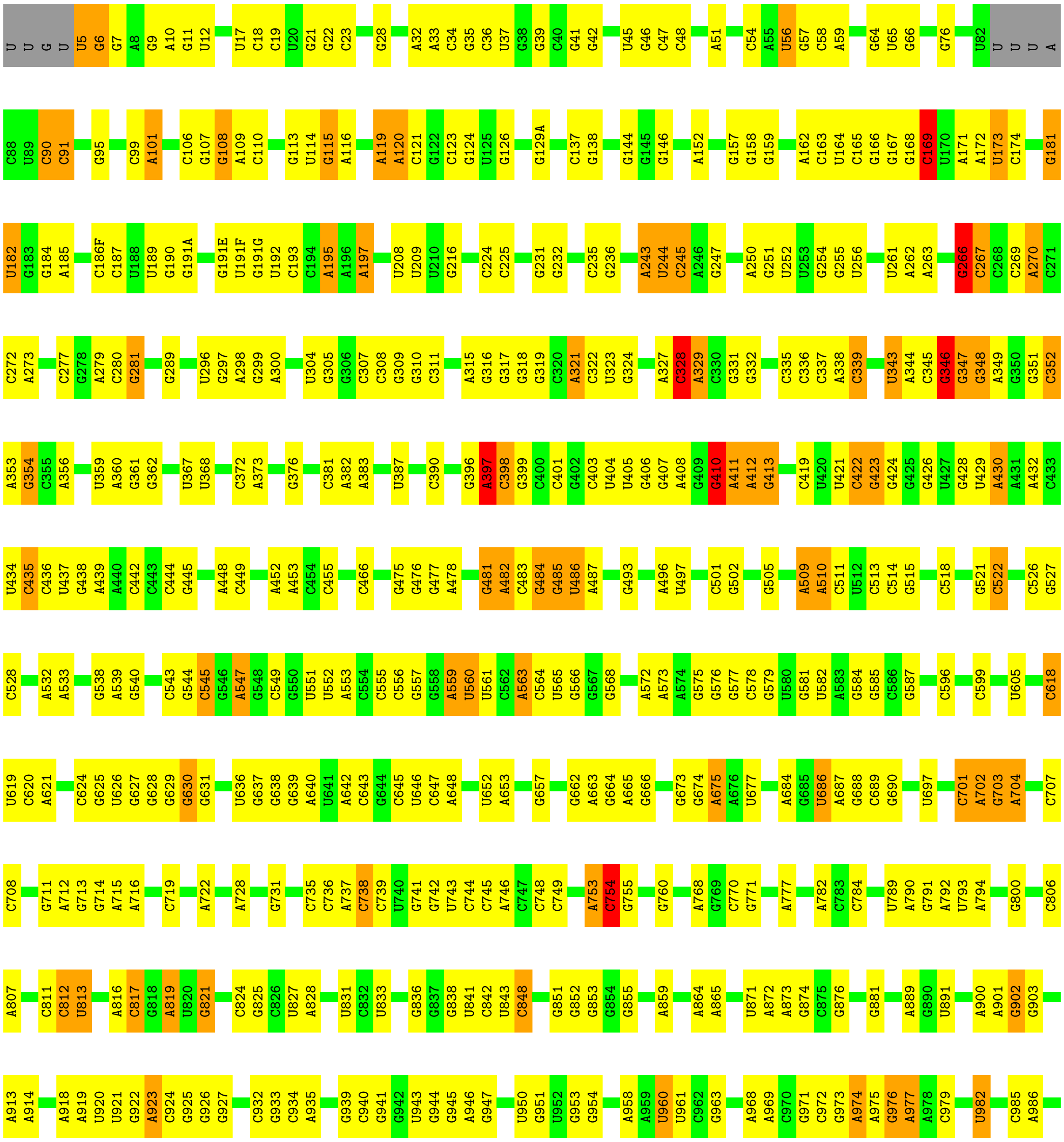
3 Residue-property plots ⓘ

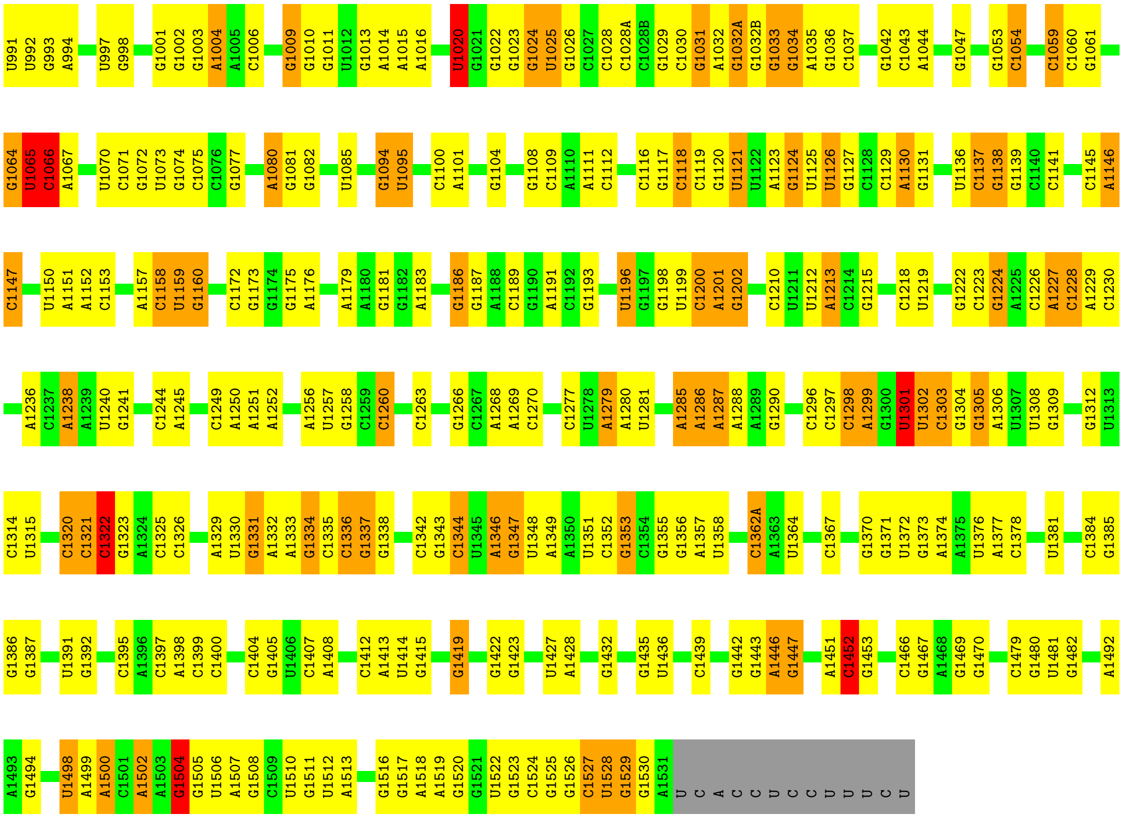
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

- Molecule 1: 16S rRNA

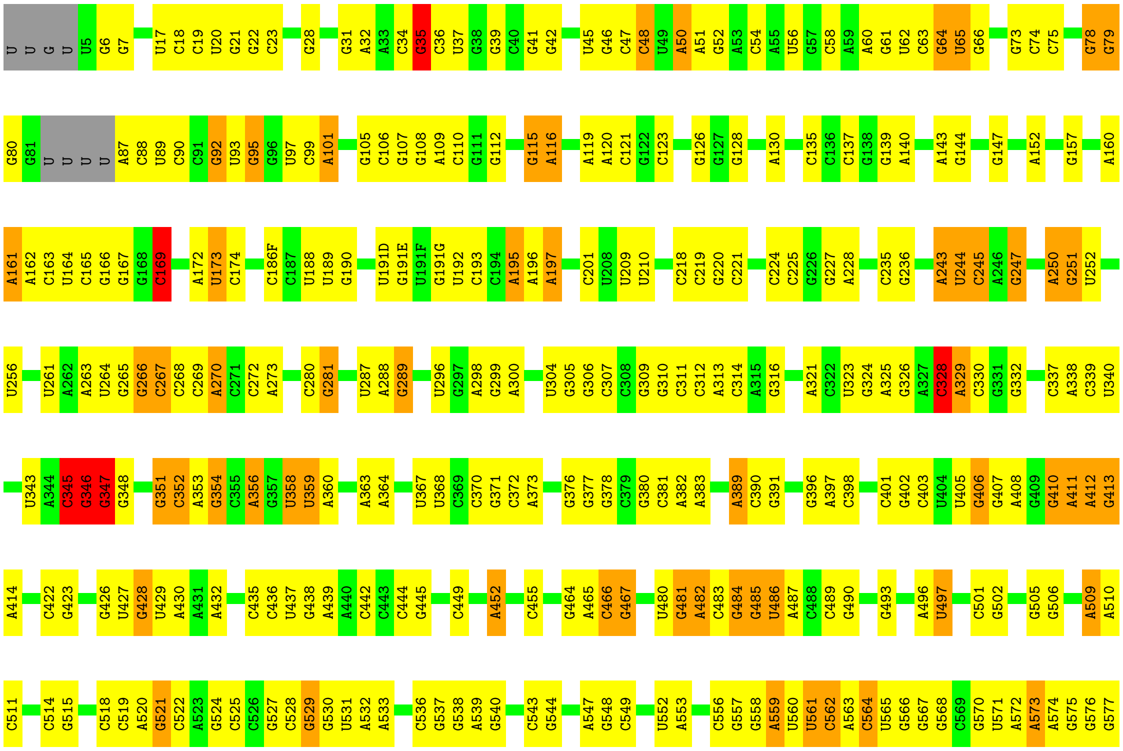
Chain QA:

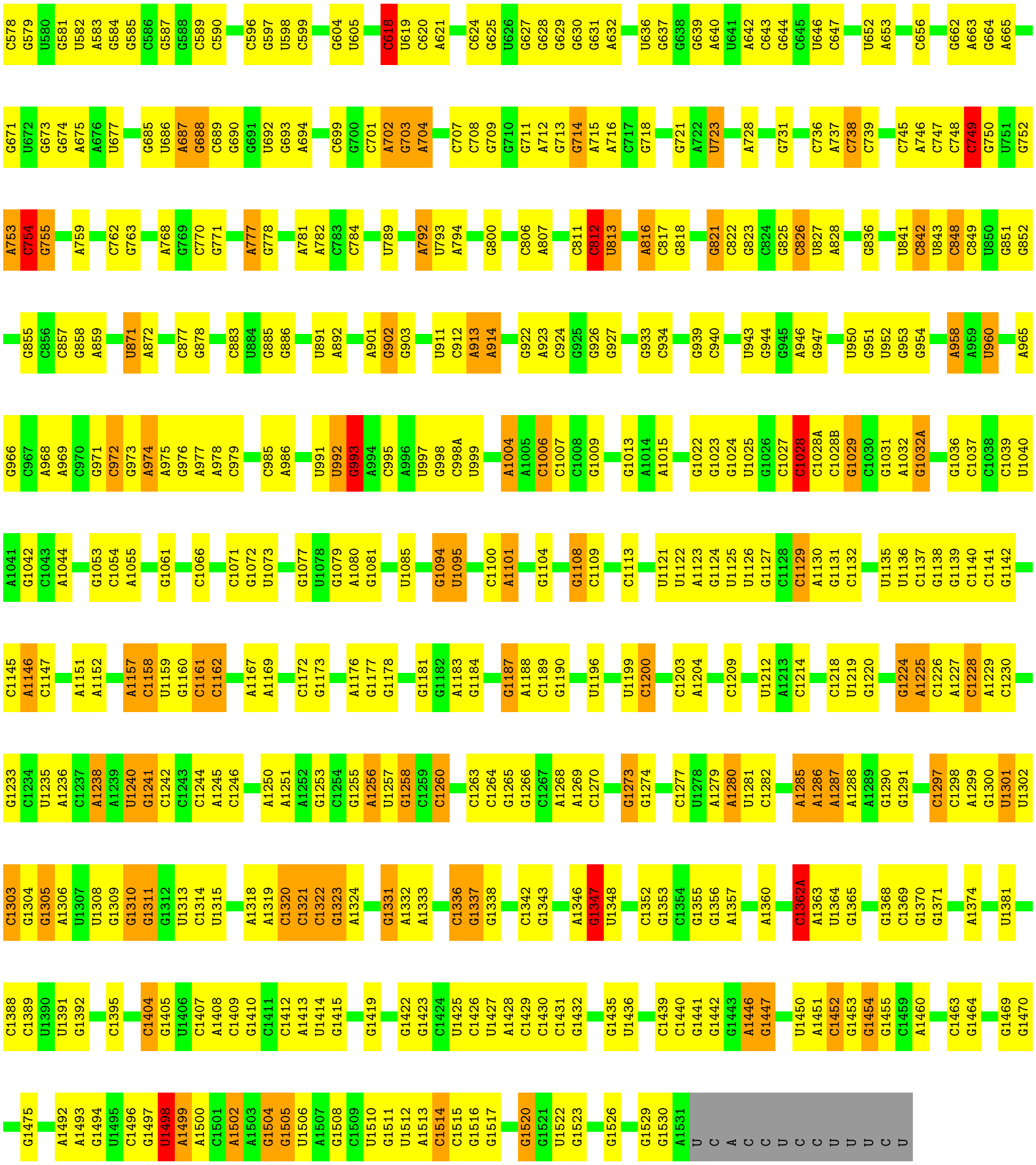




- Molecule 1: 16S rRNA

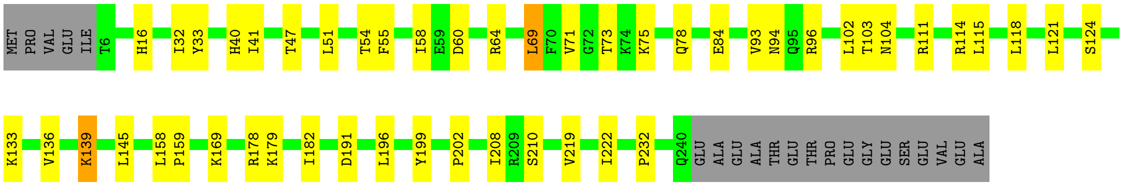
Chain XA:





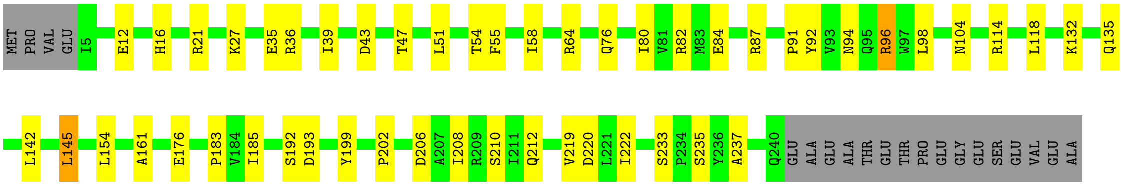
- Molecule 2: 30S ribosomal protein S2

Chain QB:



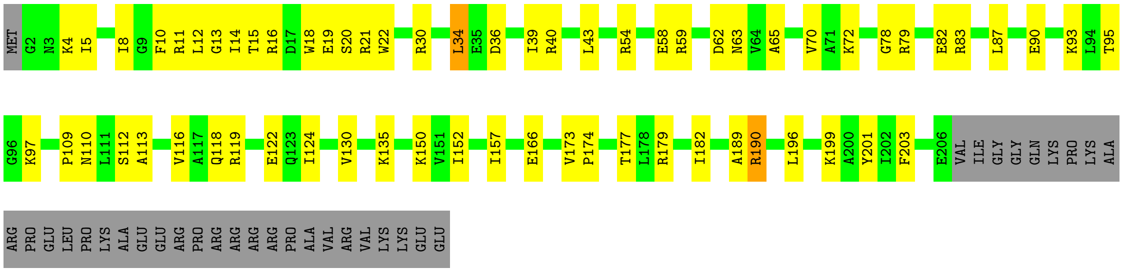
- Molecule 2: 30S ribosomal protein S2

Chain XB:



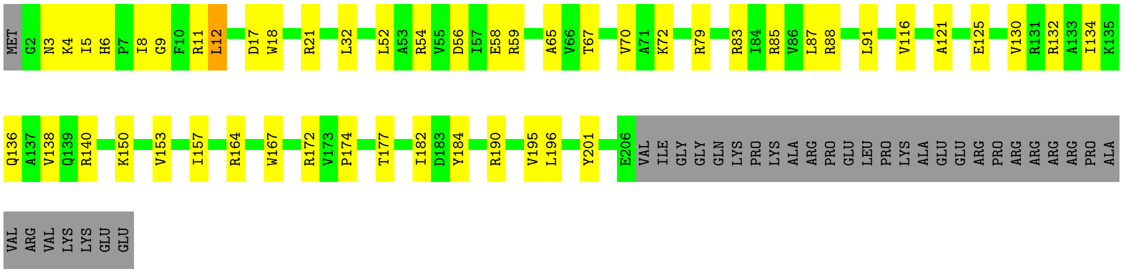
- Molecule 3: 30S ribosomal protein S3

Chain QC:



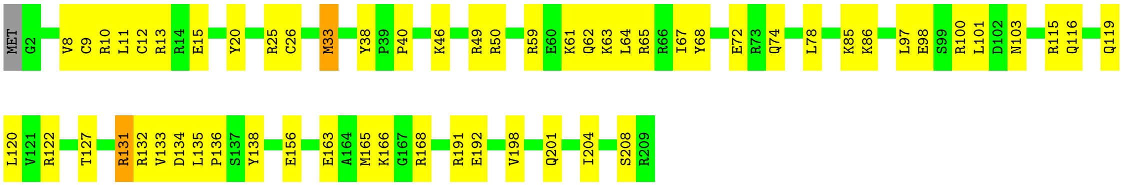
- Molecule 3: 30S ribosomal protein S3

Chain XC:



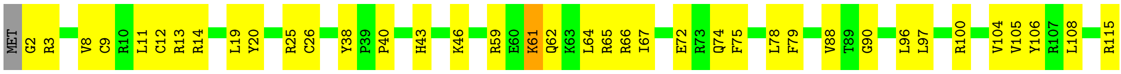
- Molecule 4: 30S ribosomal protein S4

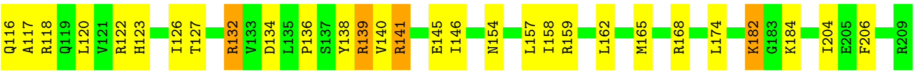
Chain QD:



- Molecule 4: 30S ribosomal protein S4

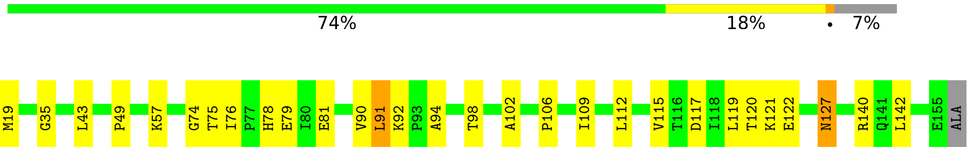
Chain XD:





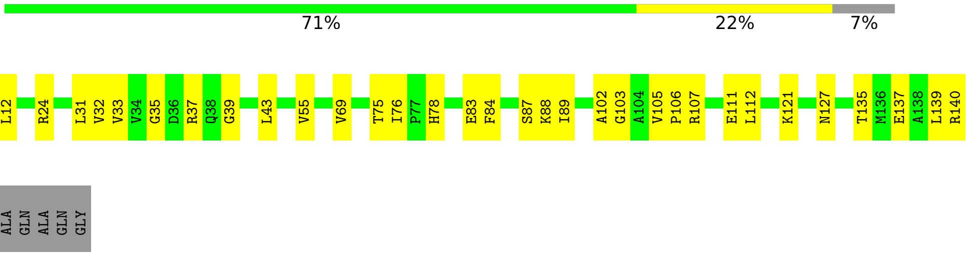
- Molecule 5: 30S ribosomal protein S5

Chain QE:



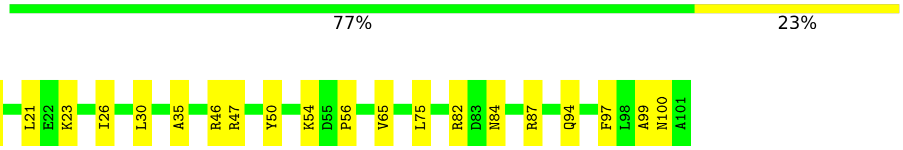
- Molecule 5: 30S ribosomal protein S5

Chain XE:



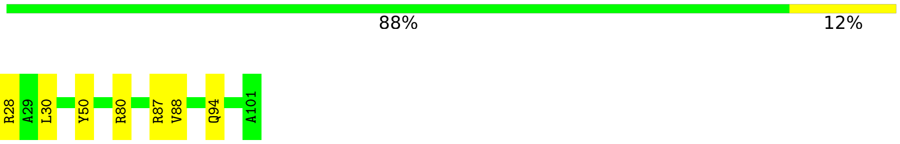
- Molecule 6: 30S ribosomal protein S6

Chain QF:



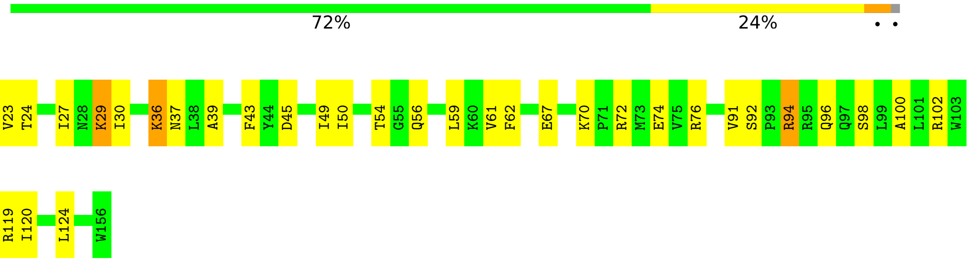
- Molecule 6: 30S ribosomal protein S6

Chain XF:



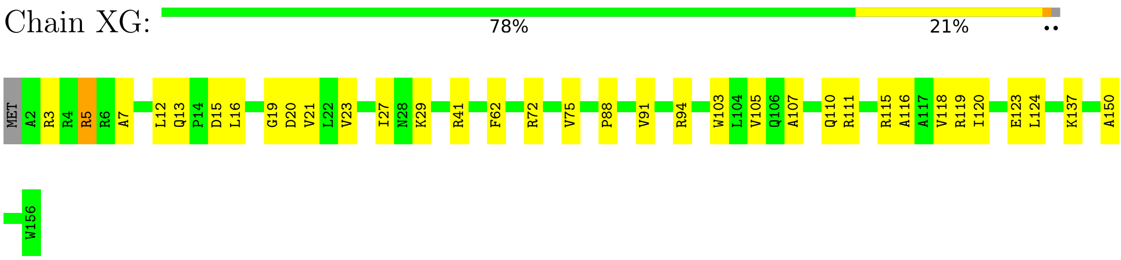
- Molecule 7: 30S ribosomal protein S7

Chain QG:



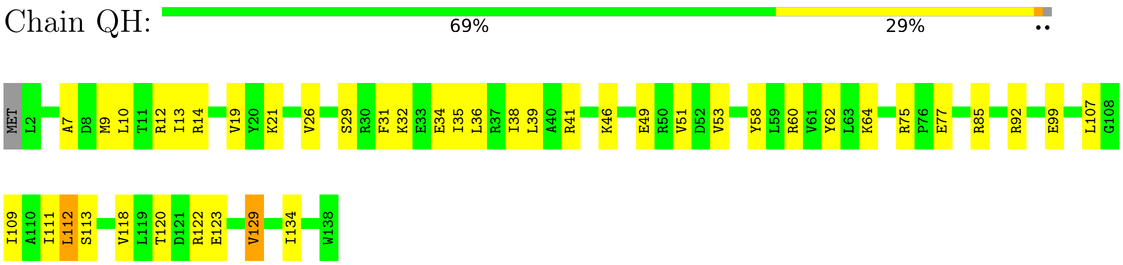
- Molecule 7: 30S ribosomal protein S7

Chain XG:



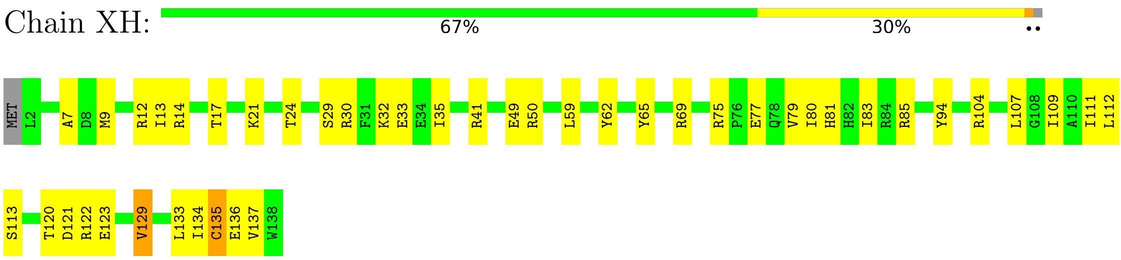
- Molecule 8: 30S ribosomal protein S8

Chain QH:



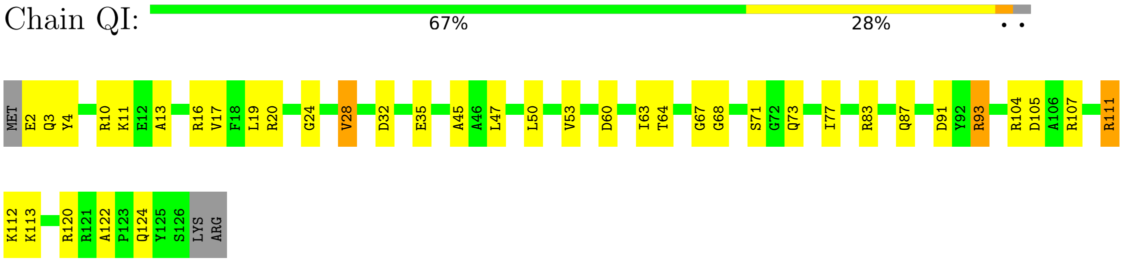
- Molecule 8: 30S ribosomal protein S8

Chain XH:



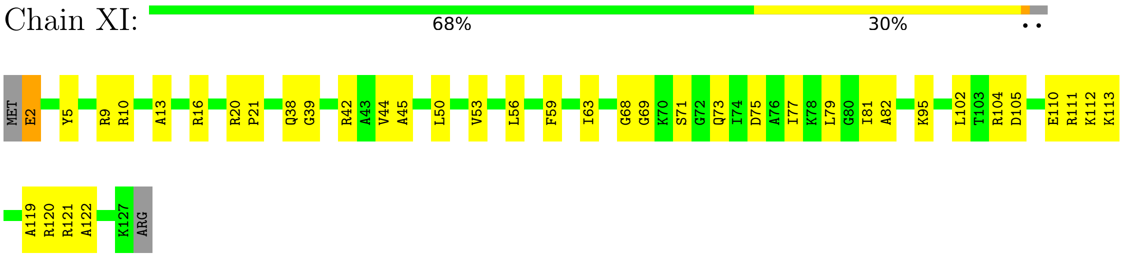
- Molecule 9: 30S ribosomal protein S9

Chain QI:

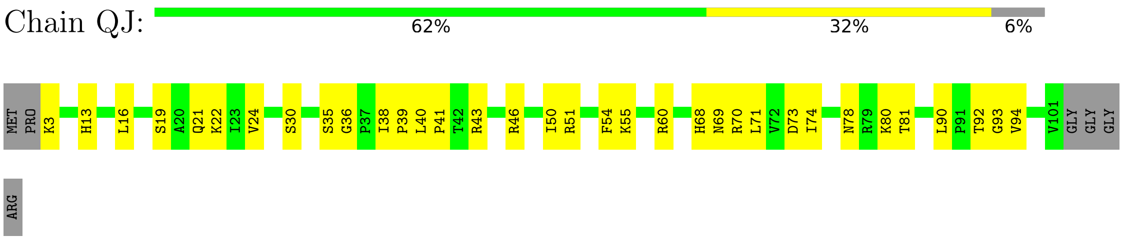


- Molecule 9: 30S ribosomal protein S9

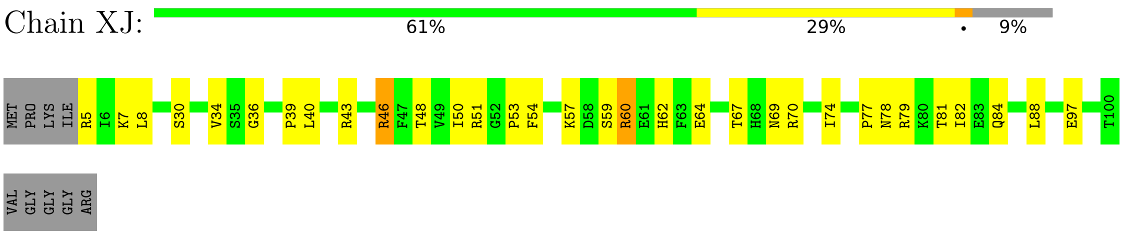
Chain XI:



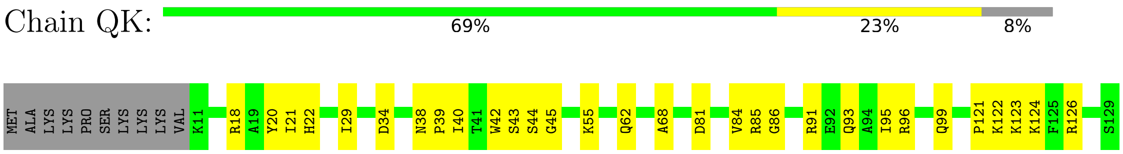
- Molecule 10: 30S ribosomal protein S10



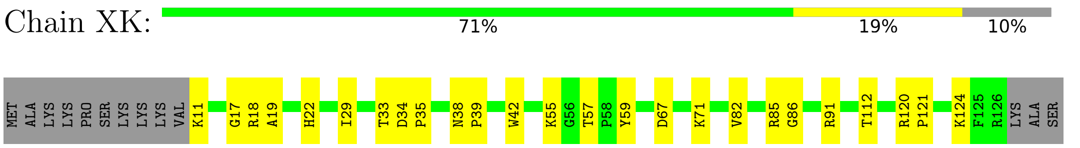
- Molecule 10: 30S ribosomal protein S10



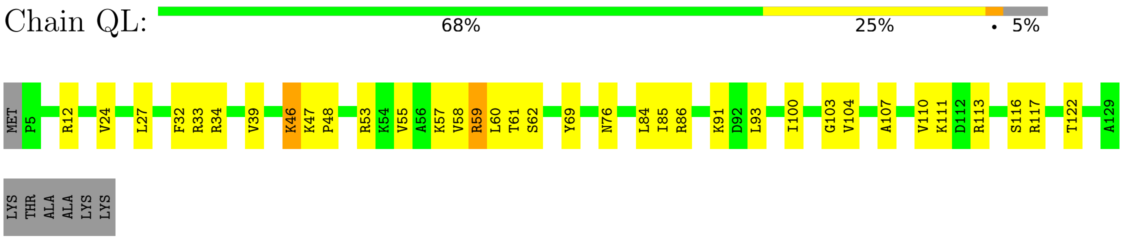
- Molecule 11: 30S ribosomal protein S11



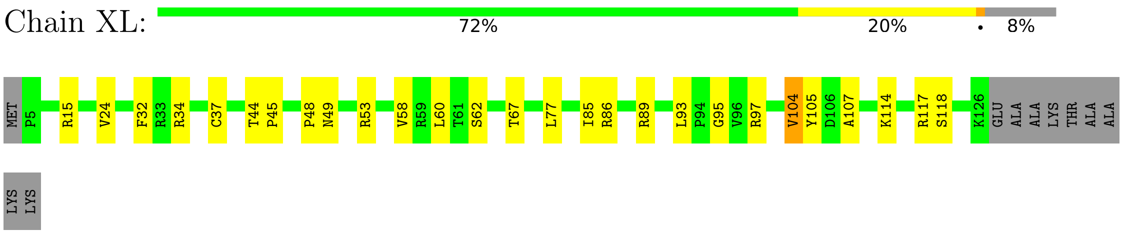
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

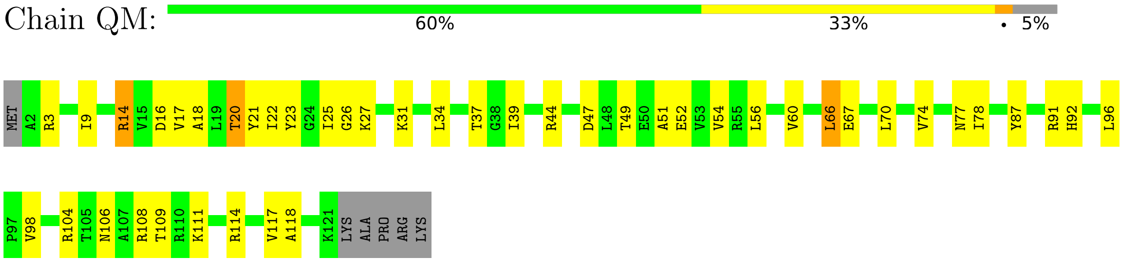


- Molecule 12: 30S ribosomal protein S12



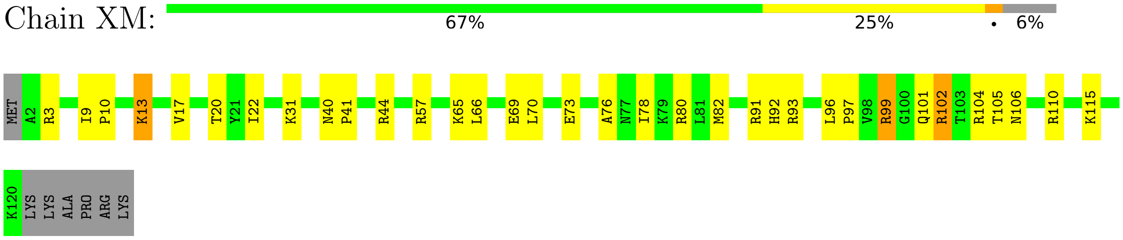
- Molecule 13: 30S ribosomal protein S13

Chain QM:



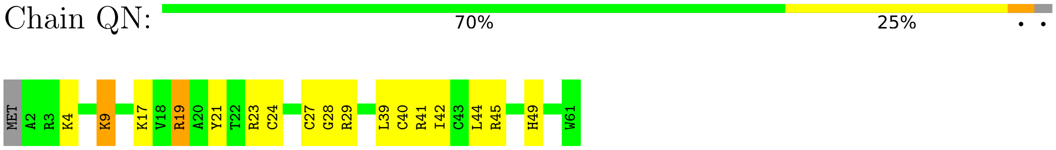
- Molecule 13: 30S ribosomal protein S13

Chain XM:



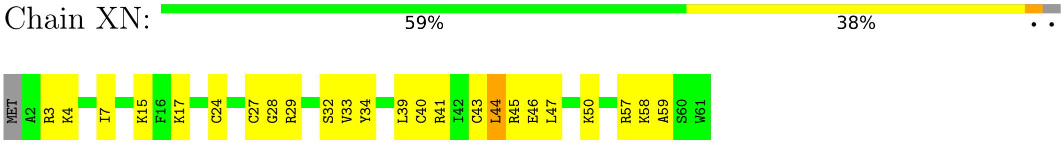
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:



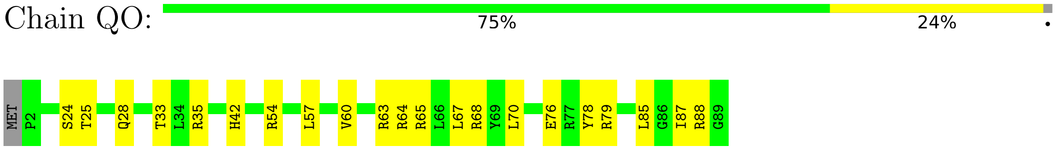
- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:



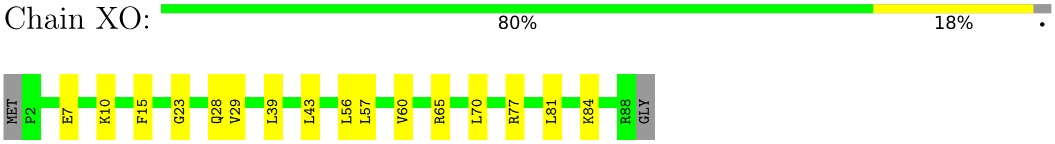
- Molecule 15: 30S ribosomal protein S15

Chain QO:

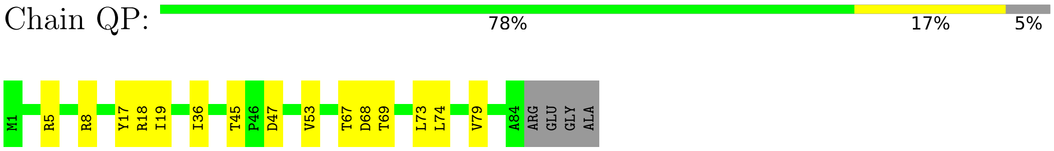


- Molecule 15: 30S ribosomal protein S15

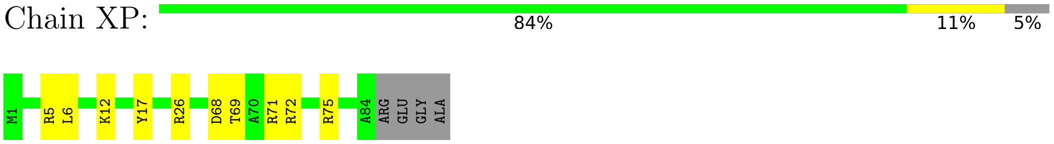
Chain XO:



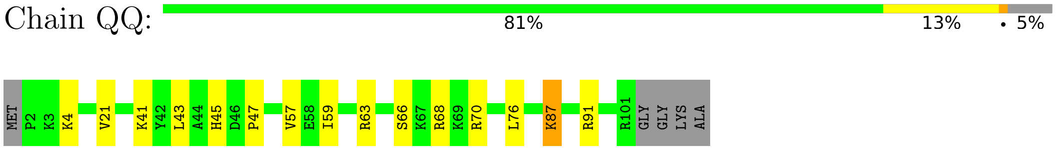
- Molecule 16: 30S ribosomal protein S16



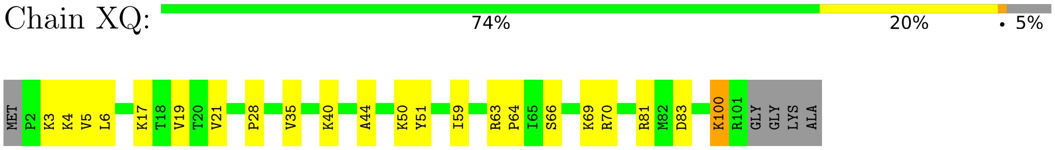
- Molecule 16: 30S ribosomal protein S16



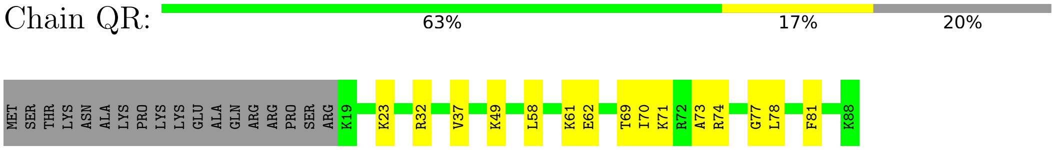
- Molecule 17: 30S ribosomal protein S17



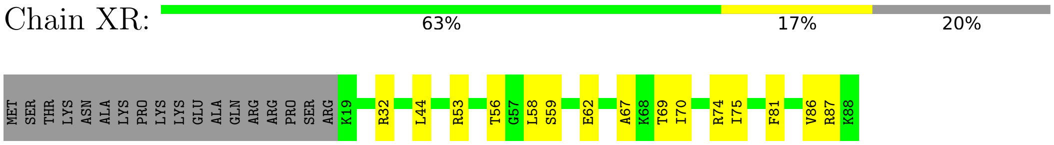
- Molecule 17: 30S ribosomal protein S17



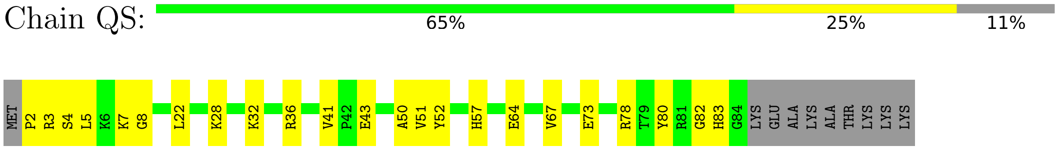
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

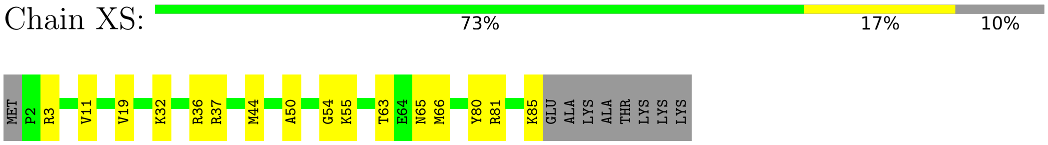


- Molecule 19: 30S ribosomal protein S19



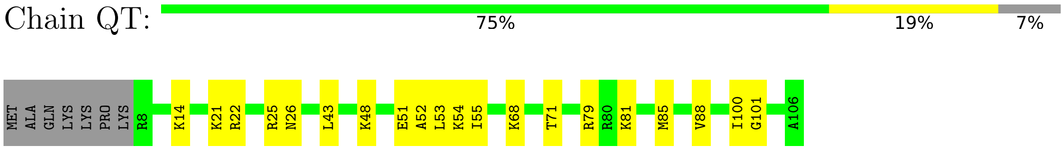
- Molecule 19: 30S ribosomal protein S19

Chain XS:



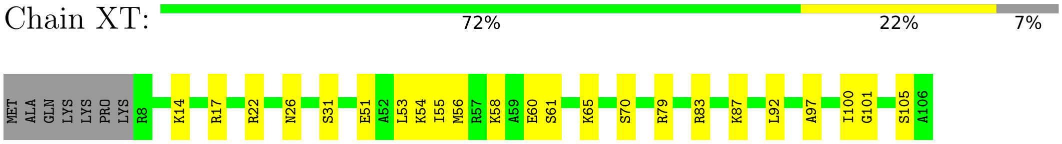
- Molecule 20: 30S ribosomal protein S20

Chain QT:



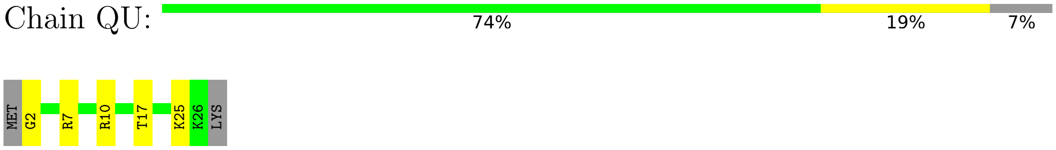
- Molecule 20: 30S ribosomal protein S20

Chain XT:



- Molecule 21: 30S ribosomal protein Thx

Chain QU:

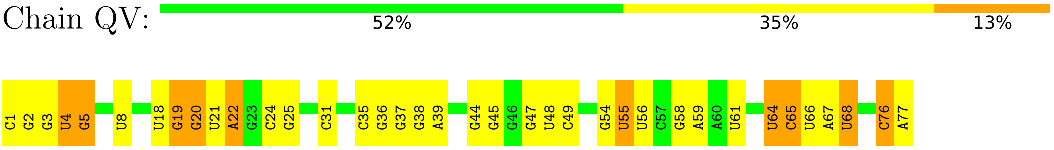


- Molecule 21: 30S ribosomal protein Thx

Chain XU:

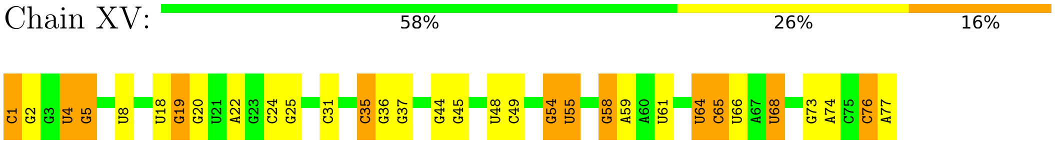
- Molecule 22: P-site ASLPro

Chain QV:



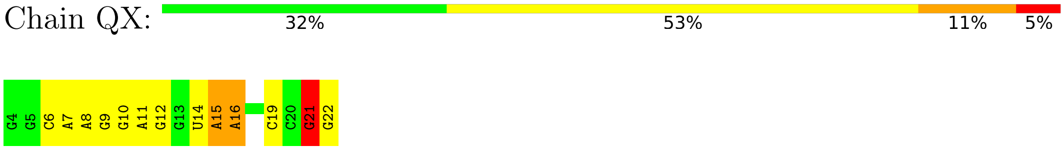
- Molecule 22: P-site ASLPro

Chain XV:



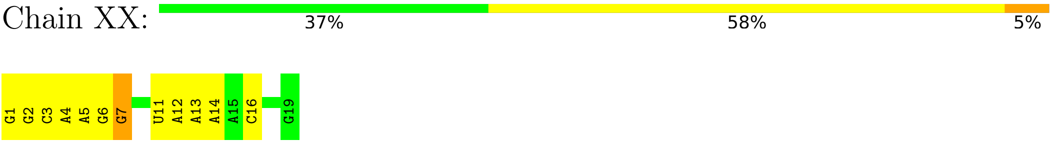
- Molecule 23: mRNA

Chain QX:



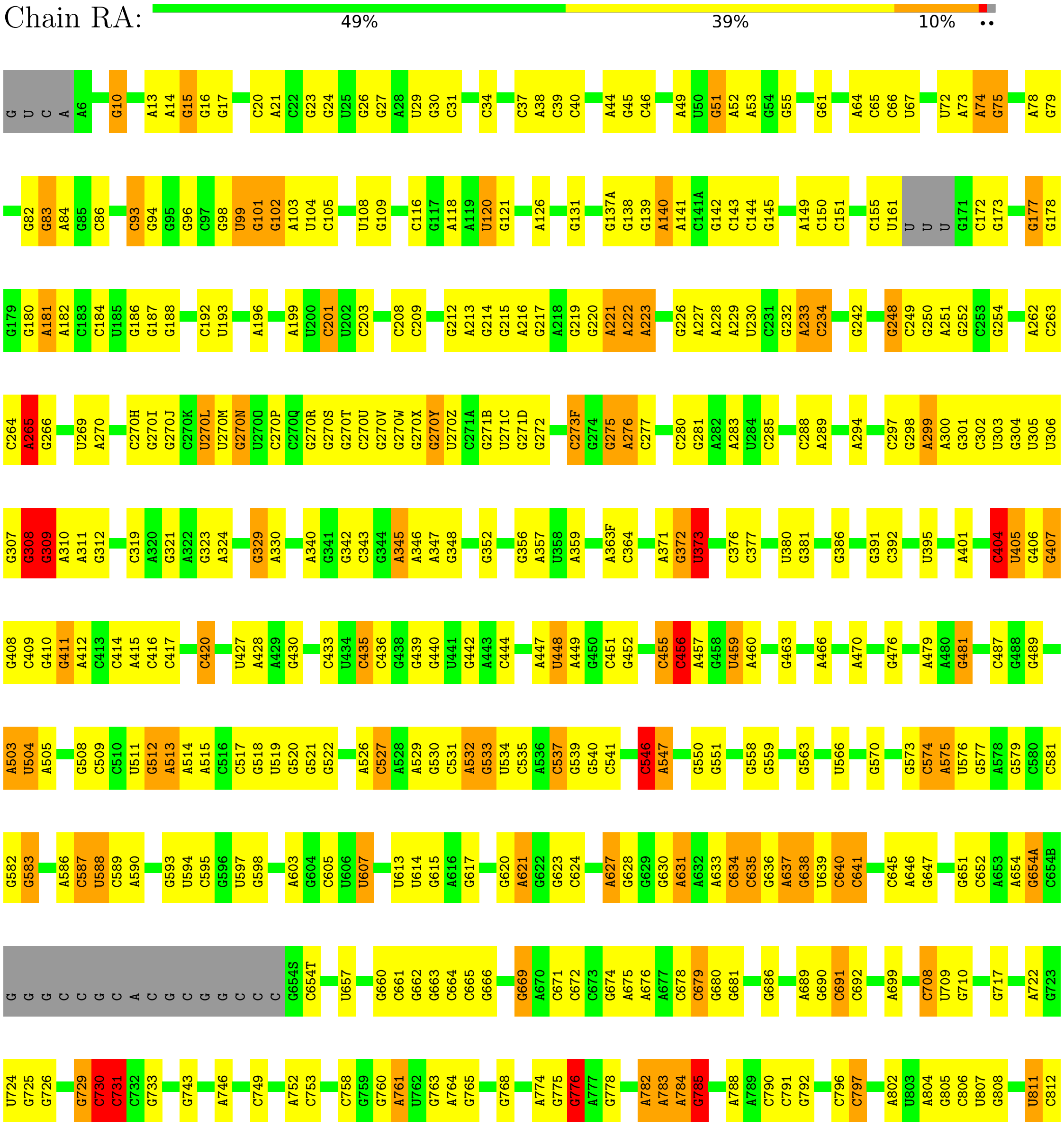
- Molecule 23: mRNA

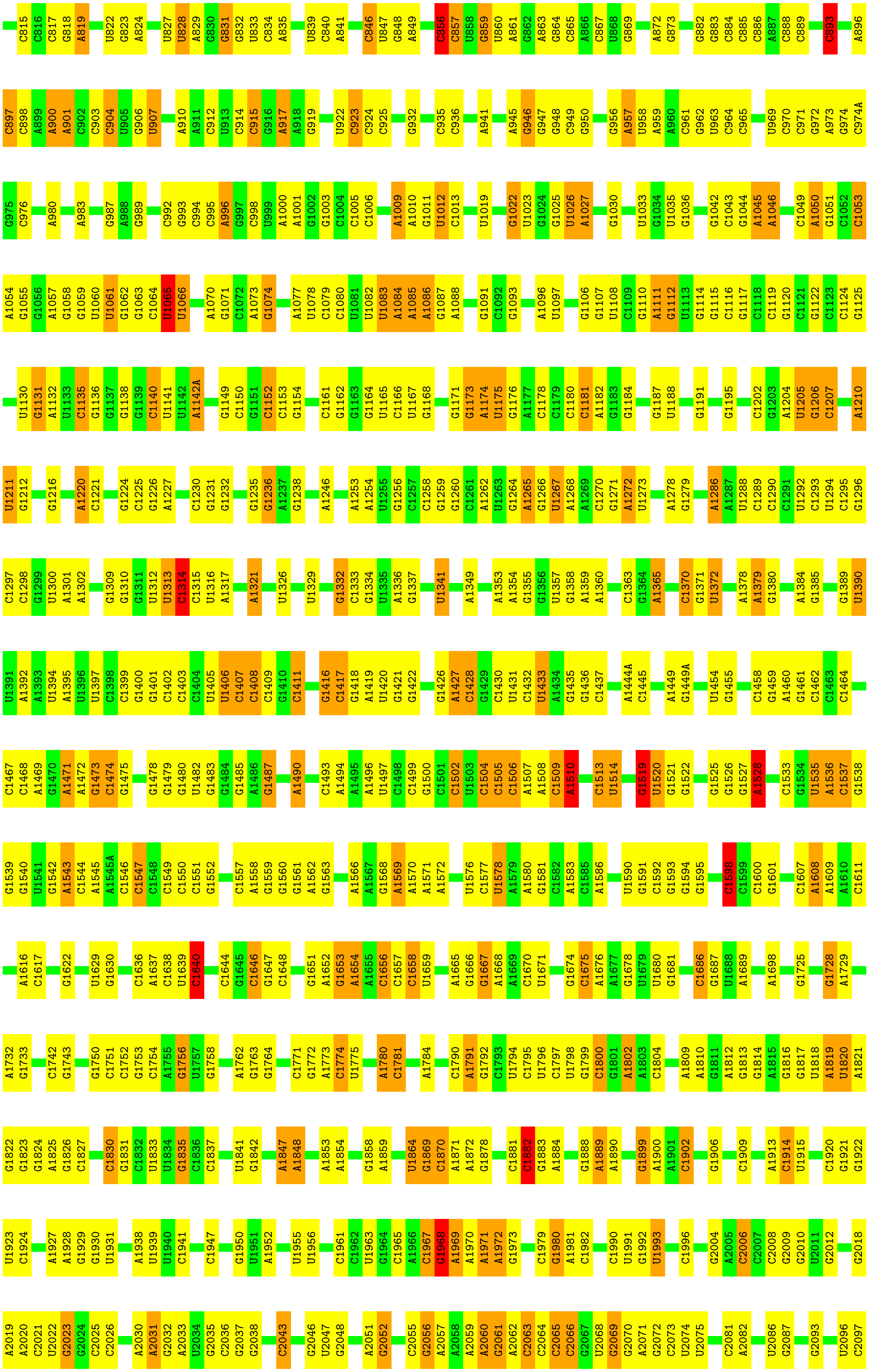
Chain XX:



- Molecule 24: 23S rRNA

Chain RA:




C815 C816 C817 G818 A819 U822 G823 A824 U827 U828 A829 G830 G831 G832 U833 C834 A835 U839 C840 A841 C846 U847 G848 A849 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865 A866 C867 U868 G869 A872 G873 G882 G883 C884 C885 C886 A887 C888 C889 C893 A896
C897 C898 A899 A900 A901 C902 C903 C904 U905 G906 U907 A910 A911 C912 U913 C914 C915 G916 A917 A918 G919 U922 C923 C924 C925 G932 C935 C936 A941 A945 G946 G947 G948 C949 G950 G956 A957 U958 A959 A960 C961 G962 U963 C964 C965 U969 C970 C971 G972 A973 G974 C974A
G975 C976 A980 A983 G987 A988 G989 C992 G993 C994 C995 A996 G997 C998 U999 A1000 A1001 G1002 C1003 C1004 C1005 C1006 A1009 A1010 G1011 U1012 C1013 U1019 G1022 U1023 G1024 C1025 U1026 A1027 G1030 U1033 G1034 U1035 G1036 G1042 C1043 G1044 A1045 A1046 C1049 A1050 G1051 C1052 C1053
A1054 G1055 G1056 A1057 G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1070 G1071 C1072 A1073 G1074 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1091 C1092 G1093 A1096 U1097 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1117 C1118 C1119 G1120 C1121 G1122 C1123 C1124 G1125
U1130 G1131 A1132 U1133 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A G1149 C1150 G1151 C1152 C1153 G1154 C1161 G1162 G1163 G1164 U1165 C1166 U1167 G1168 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1184 G1187 U1188 G1191 G1195 C1202 G1203 A1204 U1205 G1206 C1207 A1210
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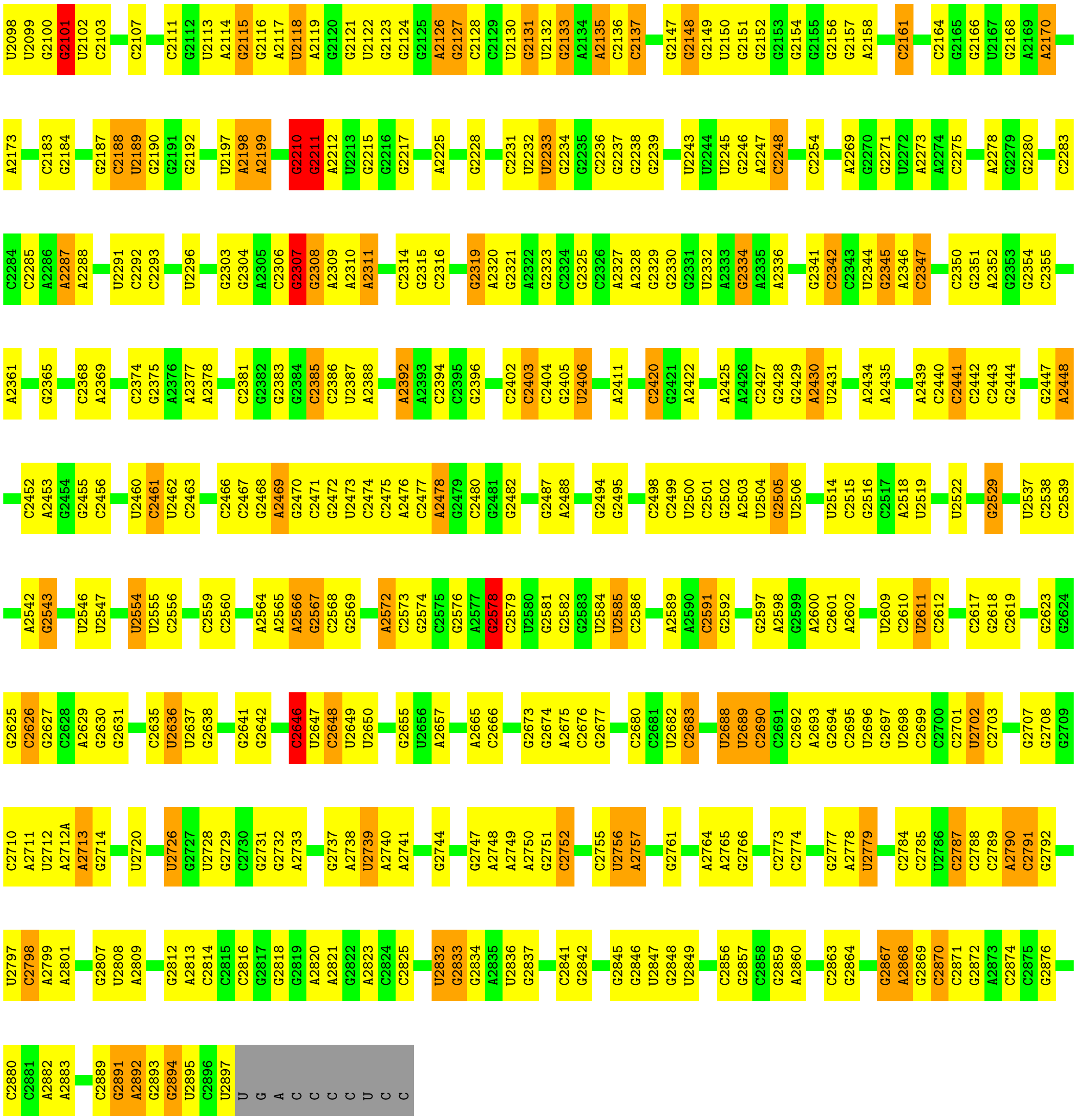

- Molecule 24: 23S rRNA

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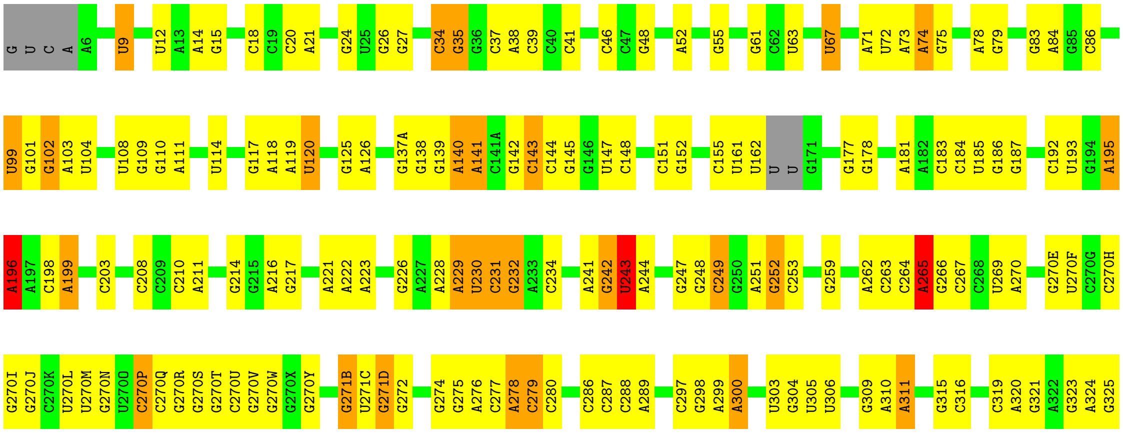

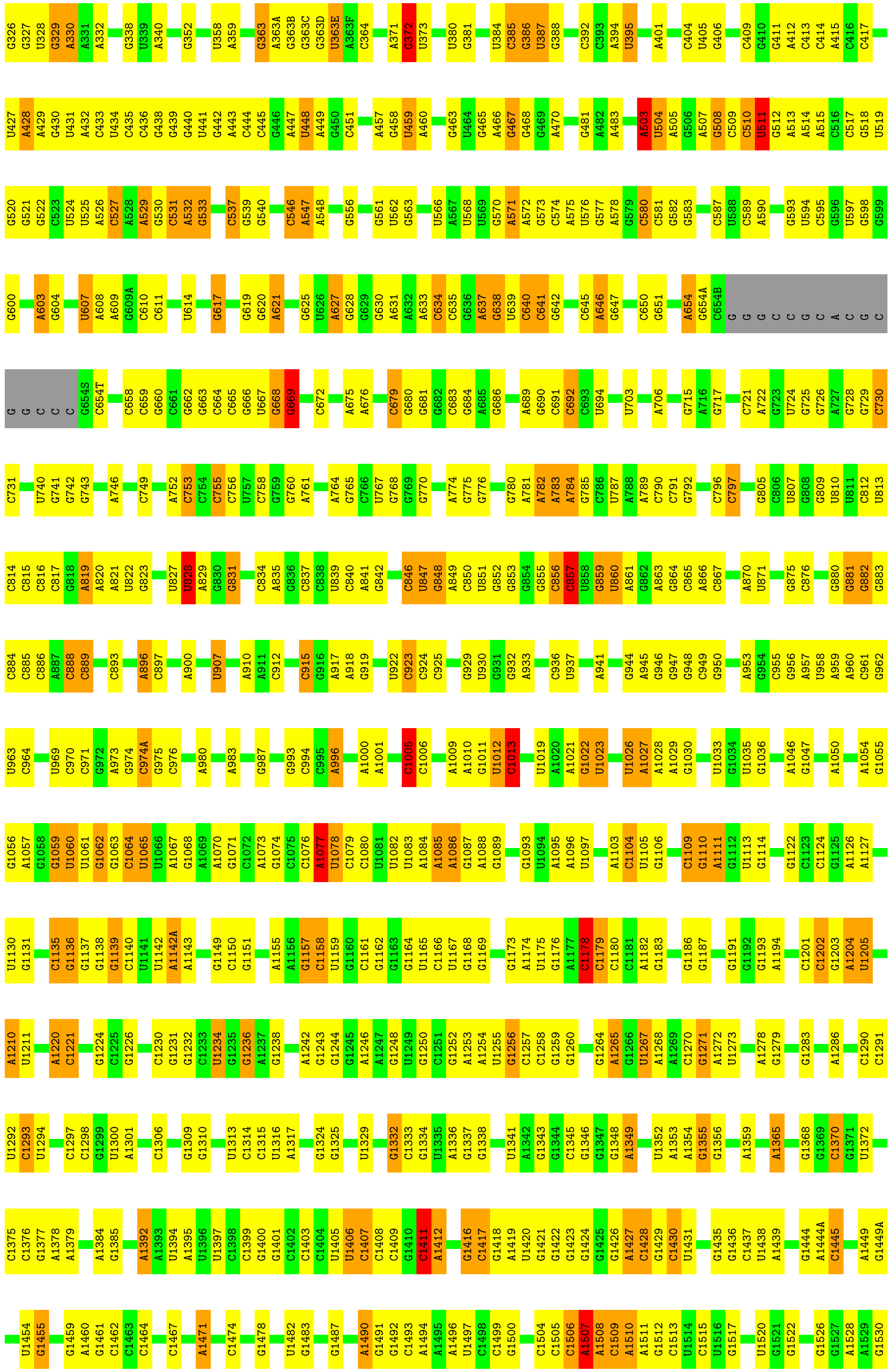
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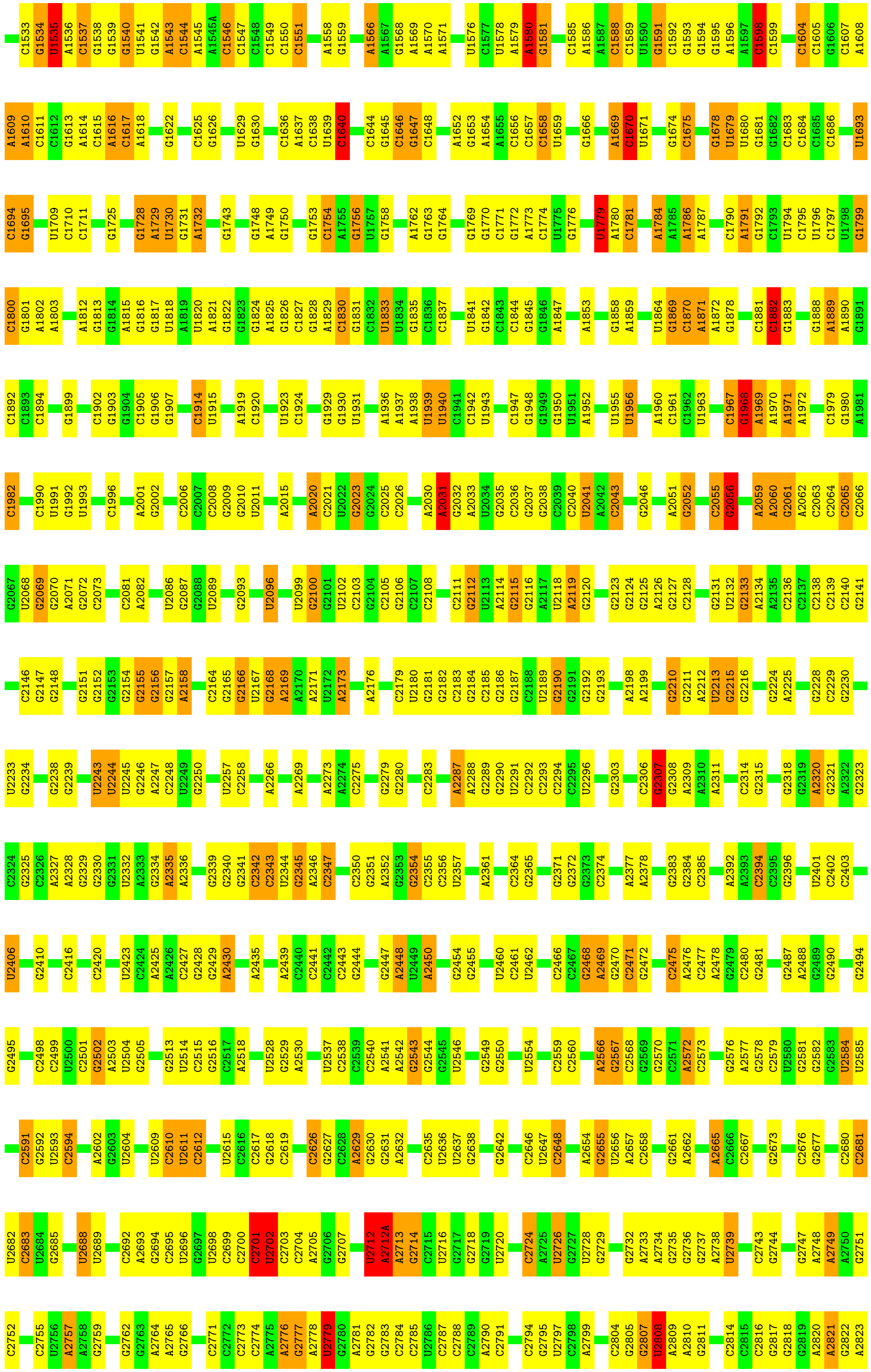
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- Molecule 25: 5S rRNA

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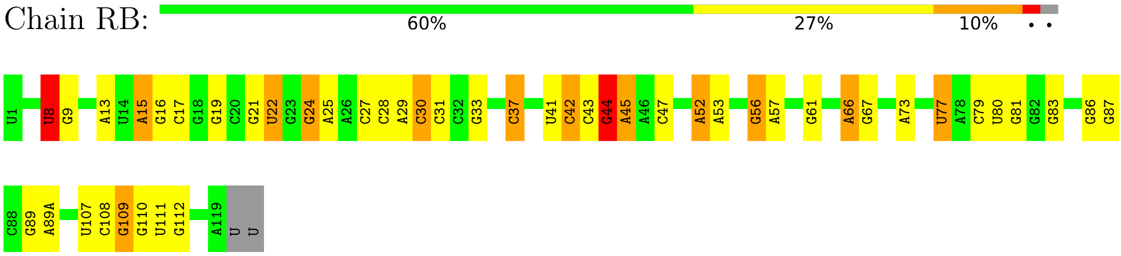

- Molecule 25: 5S rRNA

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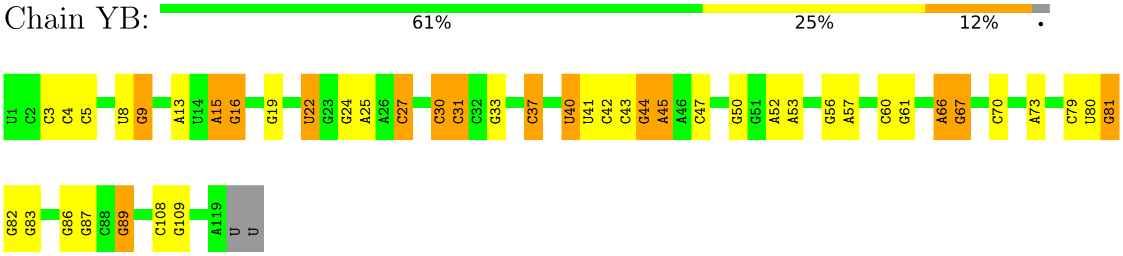

- Molecule 26: 50S ribosomal protein L2

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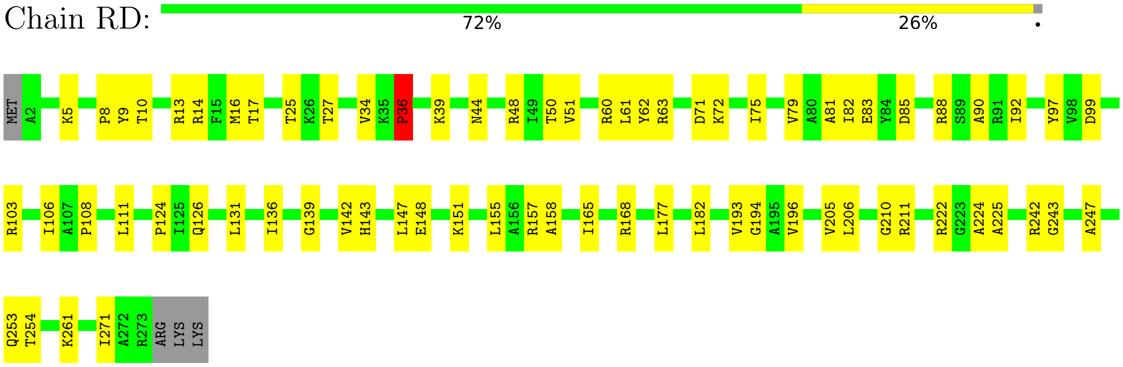

- Molecule 26: 50S ribosomal protein L2

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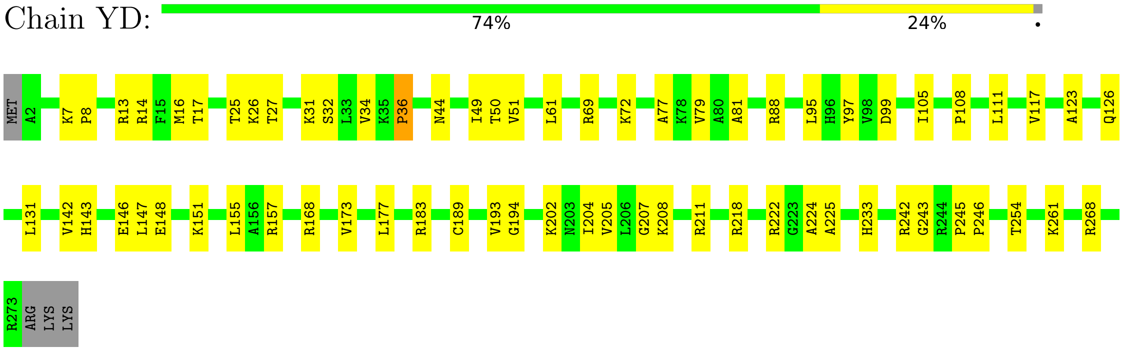

- Molecule 27: 50S ribosomal protein L3

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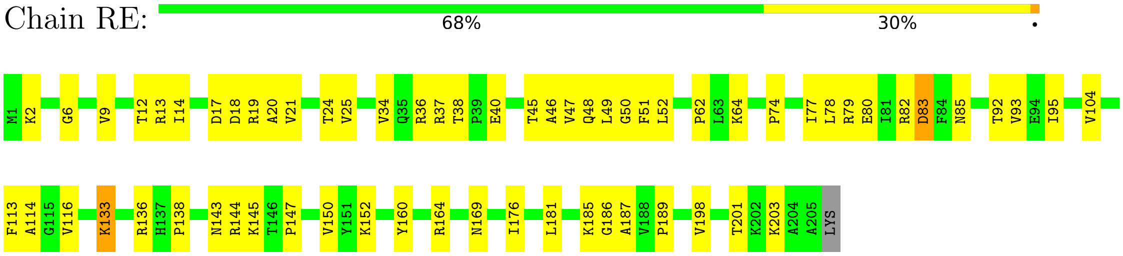

- Molecule 27: 50S ribosomal protein L3

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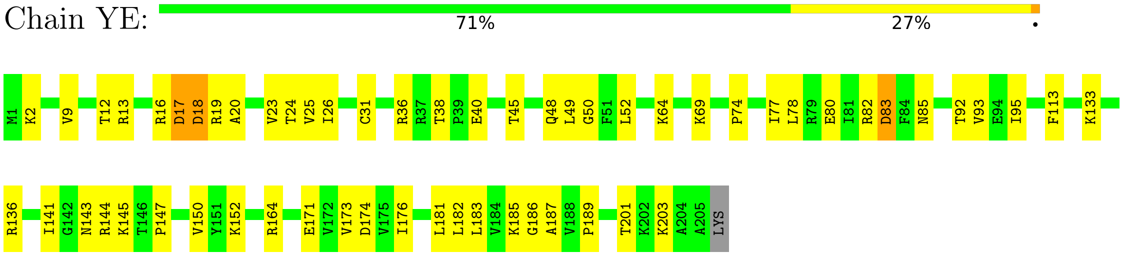

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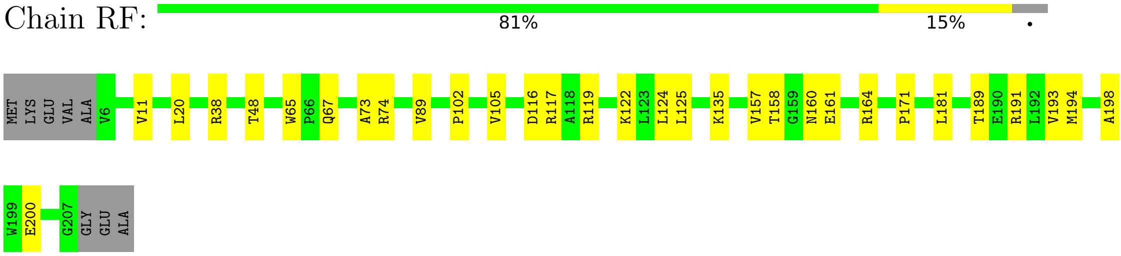

- Molecule 28: 50S ribosomal protein L4

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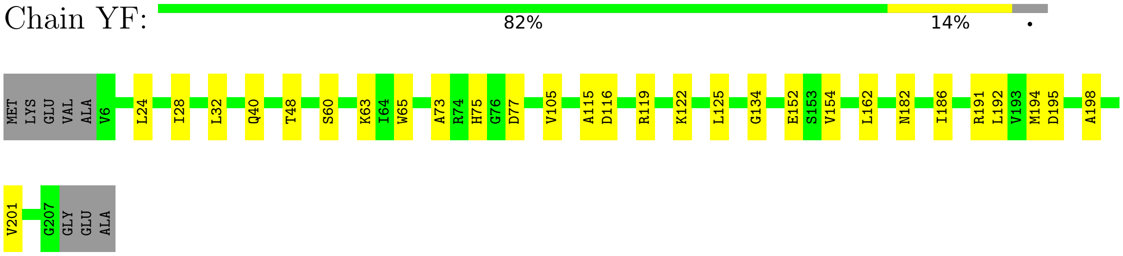

- Molecule 29: 50S ribosomal protein L5

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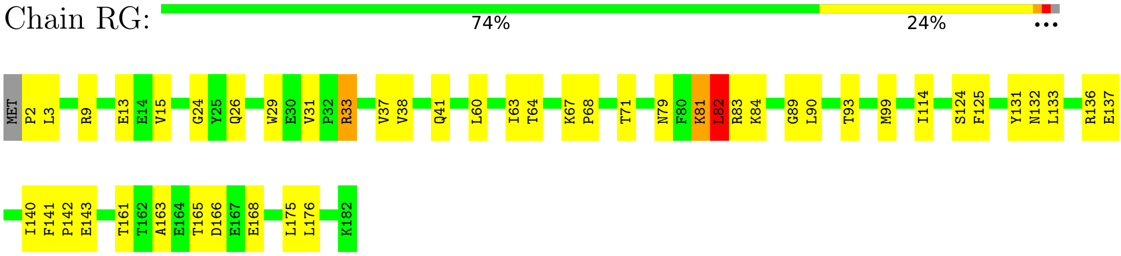

- Molecule 29: 50S ribosomal protein L5

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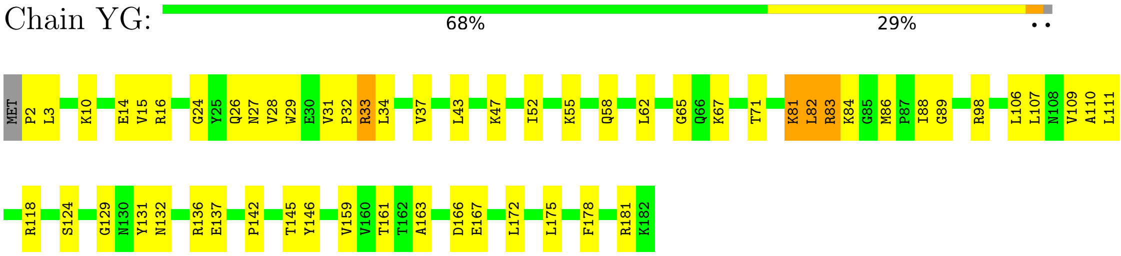

- Molecule 30: 50S ribosomal protein L6

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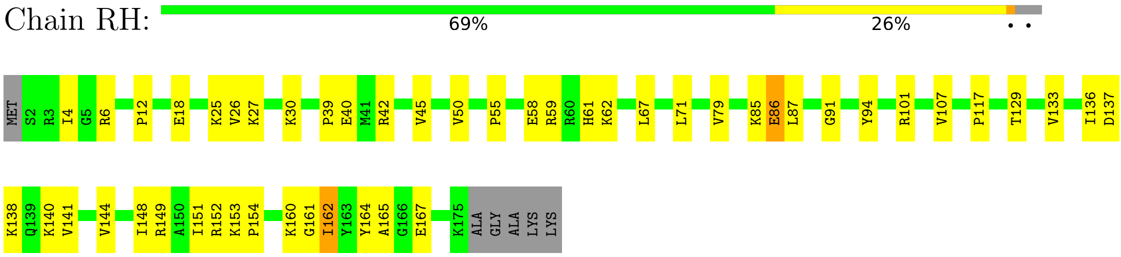

- Molecule 30: 50S ribosomal protein L6

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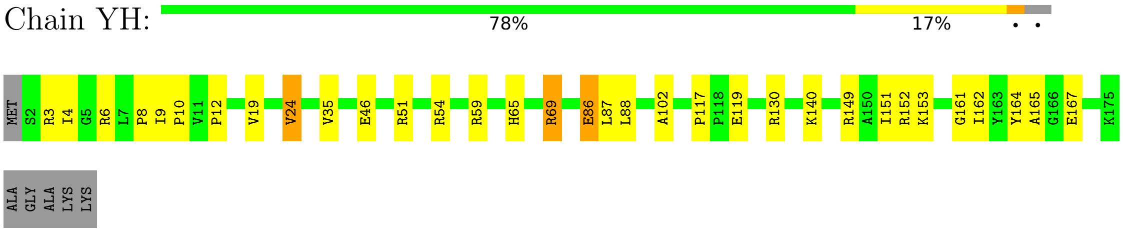

- Molecule 31: 50S ribosomal protein L9

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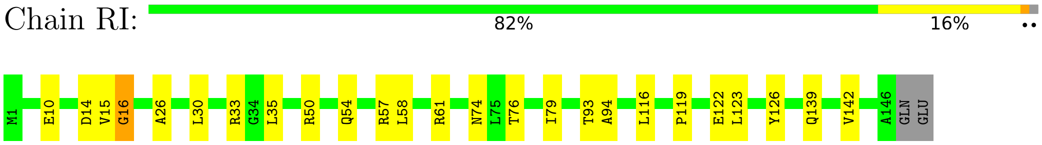

- Molecule 31: 50S ribosomal protein L9

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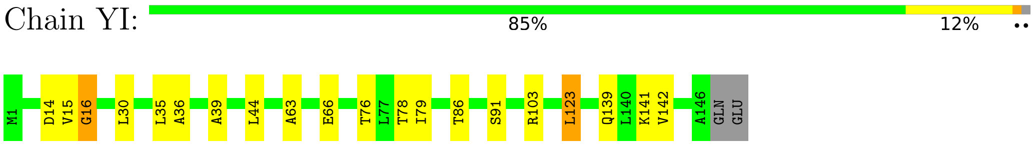

- Molecule 32: 50S ribosomal protein L13

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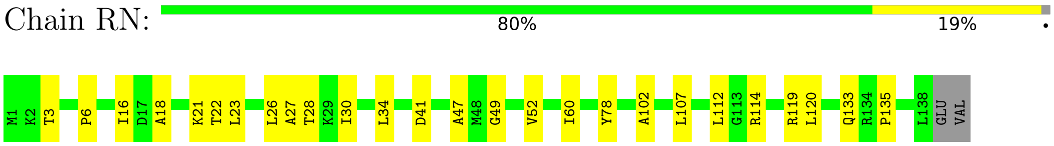

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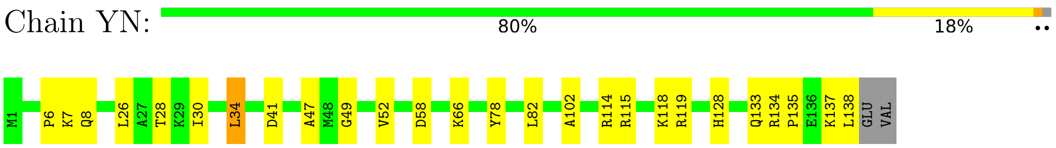
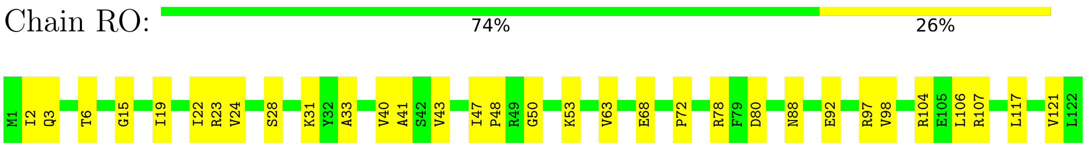
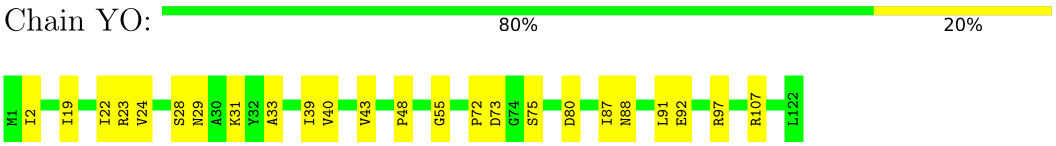


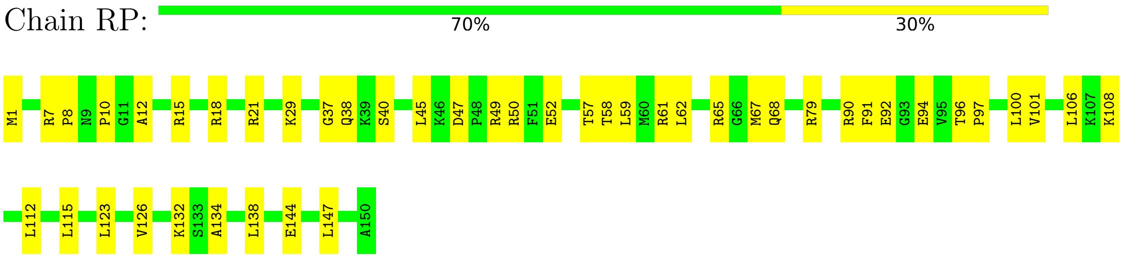
- Molecule 33: 50S ribosomal protein L14



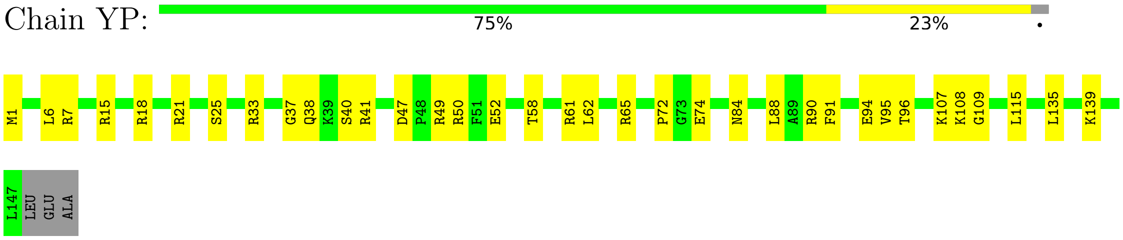
- Molecule 33: 50S ribosomal protein L14



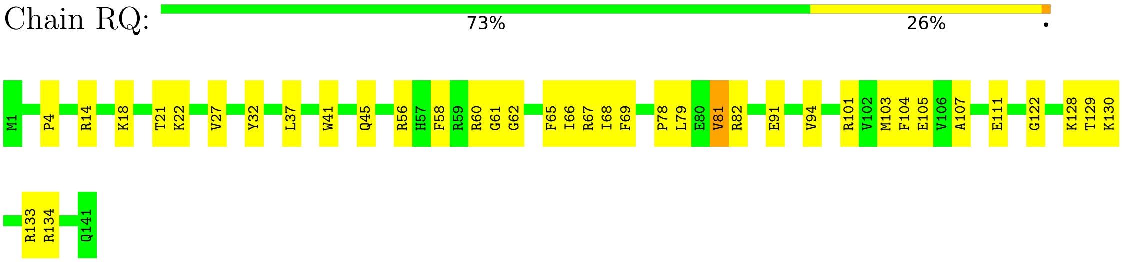
- Molecule 34: 50S ribosomal protein L15



- Molecule 34: 50S ribosomal protein L15

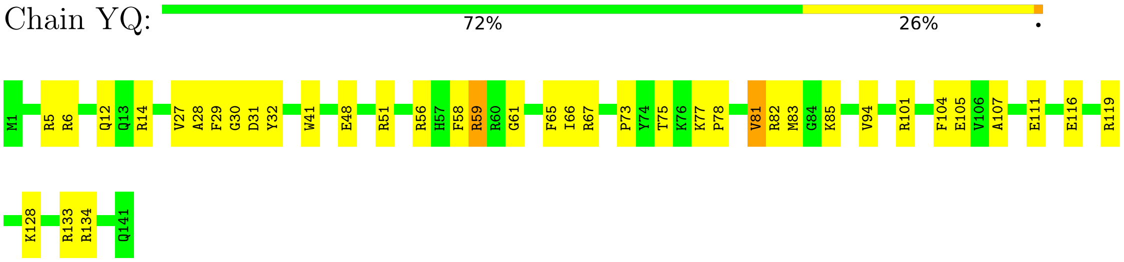


- Molecule 35: 50S ribosomal protein L16



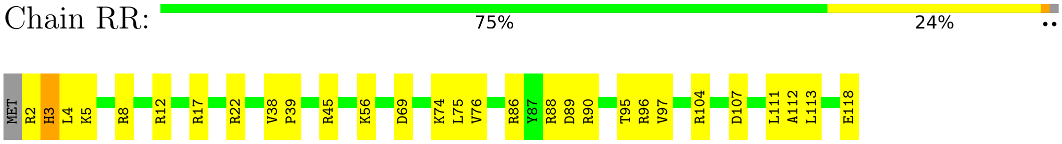
- Molecule 35: 50S ribosomal protein L16

Chain YQ:



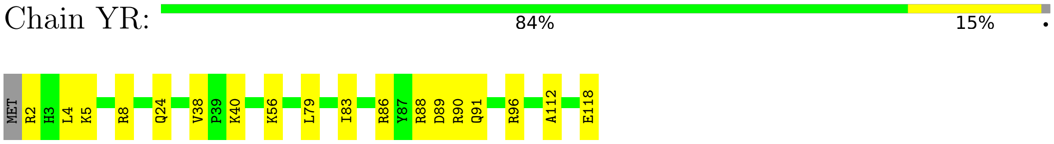
- Molecule 36: 50S ribosomal protein L17

Chain RR:



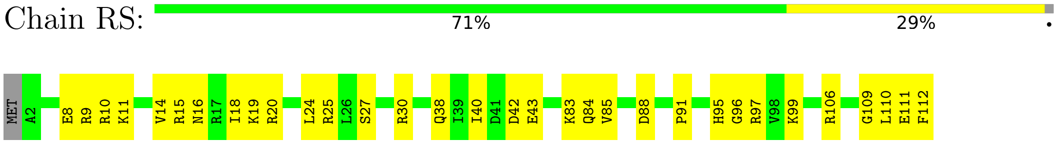
- Molecule 36: 50S ribosomal protein L17

Chain YR:



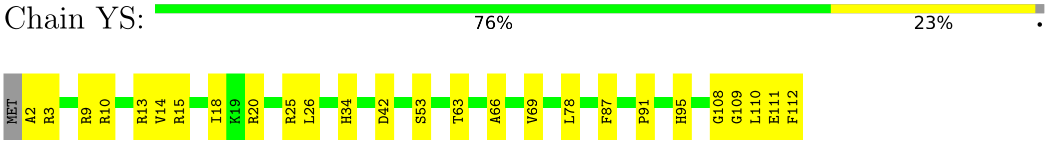
- Molecule 37: 50S ribosomal protein L18

Chain RS:



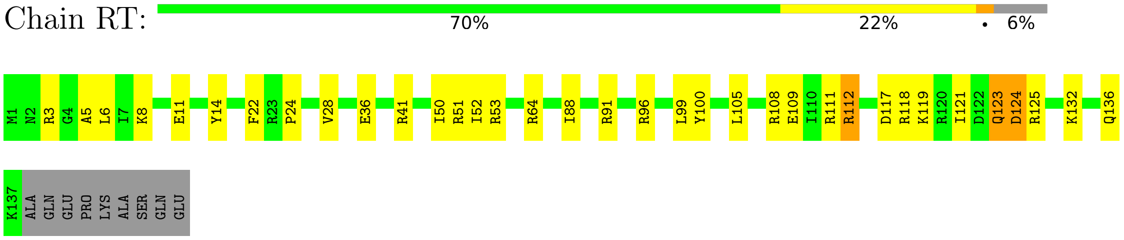
- Molecule 37: 50S ribosomal protein L18

Chain YS:



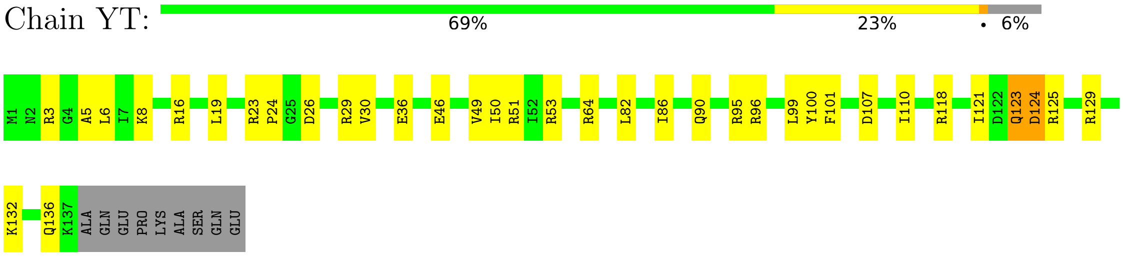
- Molecule 38: 50S ribosomal protein L19

Chain RT:



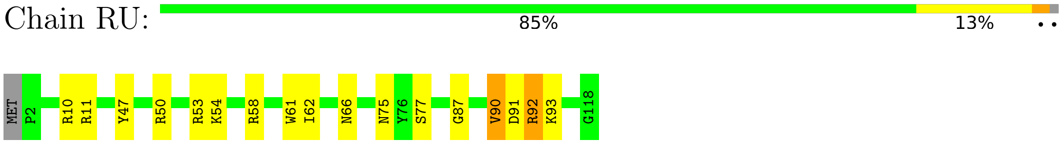
- Molecule 38: 50S ribosomal protein L19

Chain YT:



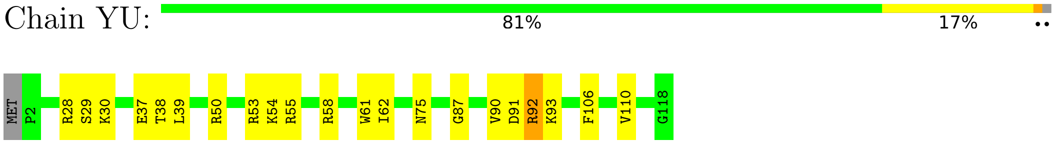
• Molecule 39: 50S ribosomal protein L20

Chain RU:



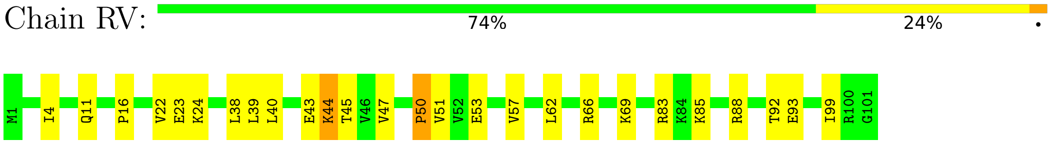
• Molecule 39: 50S ribosomal protein L20

Chain YU:



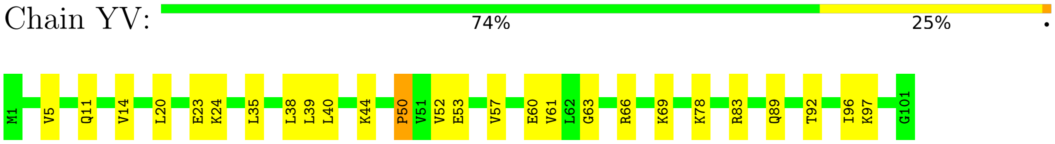
• Molecule 40: 50S ribosomal protein L21

Chain RV:



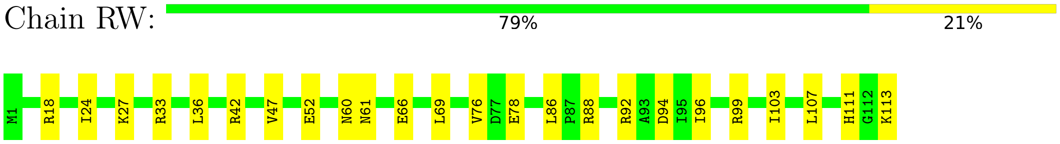
• Molecule 40: 50S ribosomal protein L21

Chain YV:



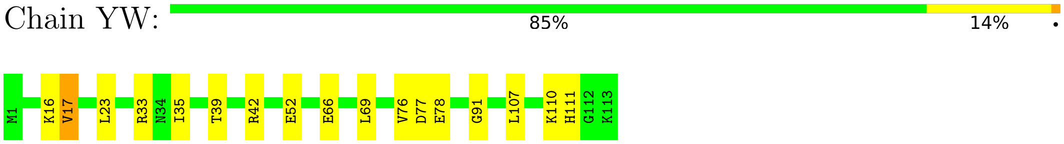
• Molecule 41: 50S ribosomal protein L22

Chain RW:



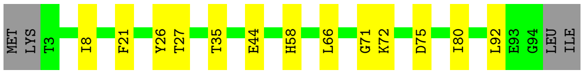
• Molecule 41: 50S ribosomal protein L22

Chain YW:



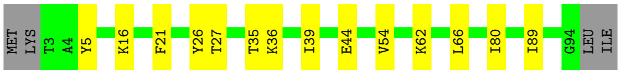
- Molecule 42: 50S ribosomal protein L23

Chain RX:



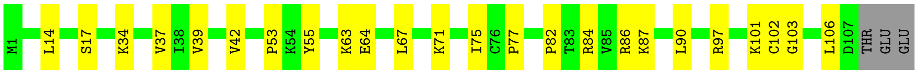
- Molecule 42: 50S ribosomal protein L23

Chain YX:



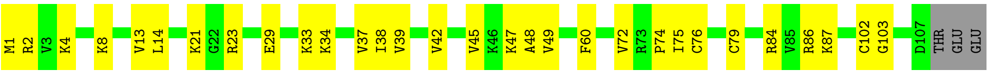
- Molecule 43: 50S ribosomal protein L24

Chain RY:



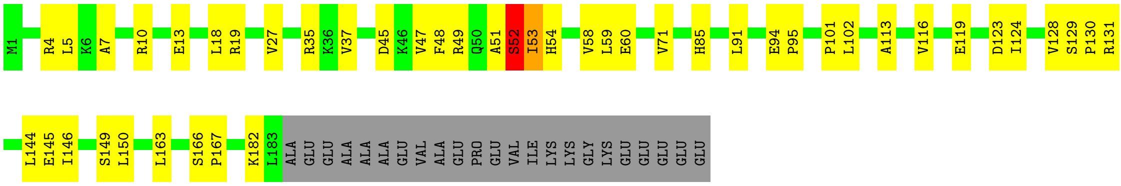
- Molecule 43: 50S ribosomal protein L24

Chain YY:



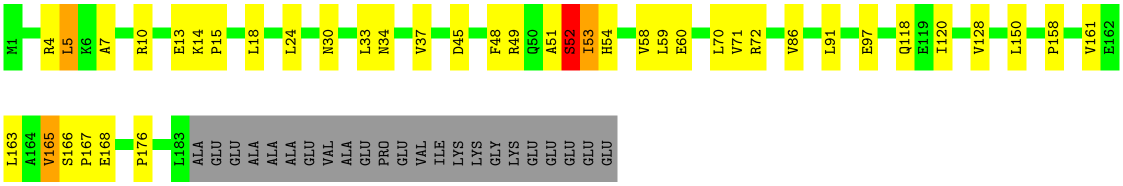
- Molecule 44: 50S ribosomal protein L25

Chain RZ:

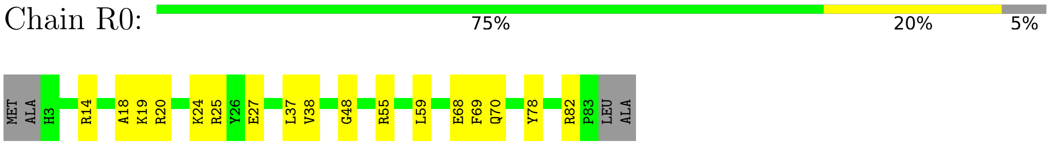


- Molecule 44: 50S ribosomal protein L25

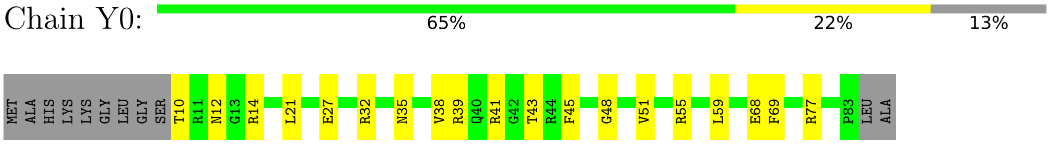
Chain YZ:



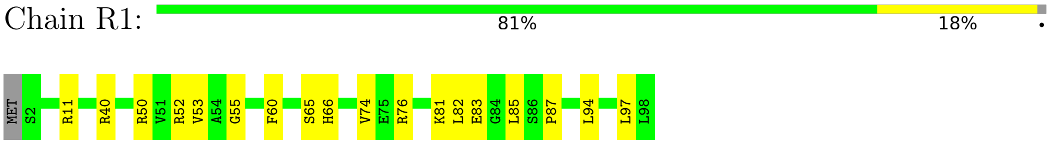
- Molecule 45: 50S ribosomal protein L27



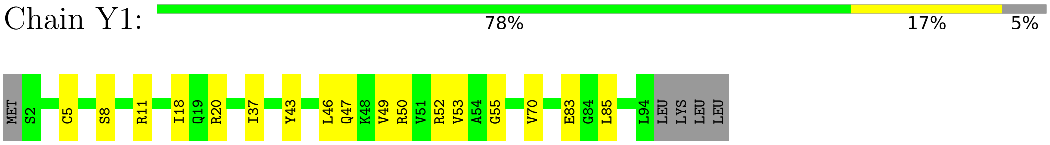
- Molecule 45: 50S ribosomal protein L27



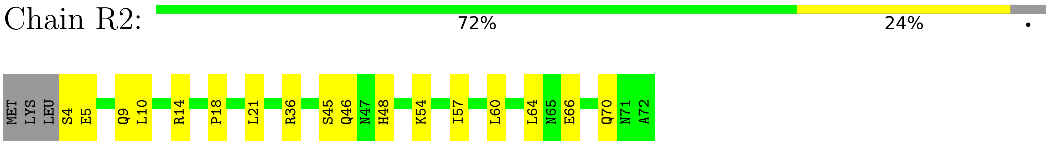
- Molecule 46: 50S ribosomal protein L28



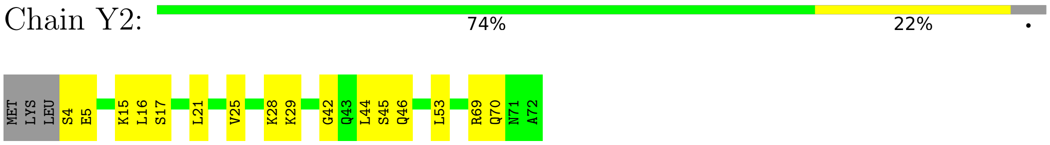
- Molecule 46: 50S ribosomal protein L28



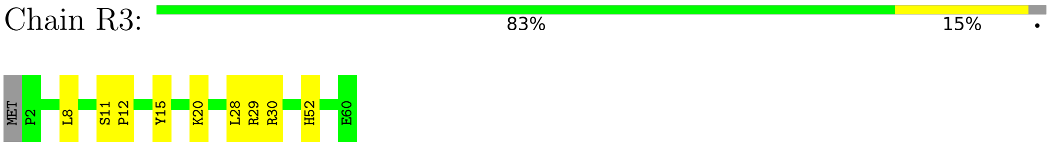
- Molecule 47: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L29

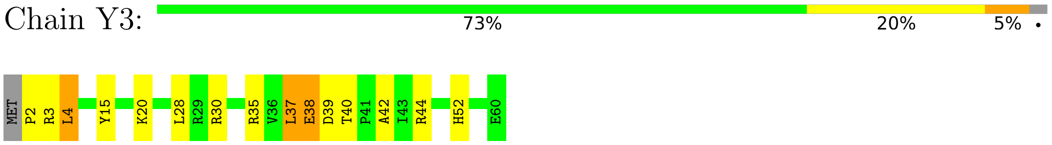


- Molecule 48: 50S ribosomal protein L30



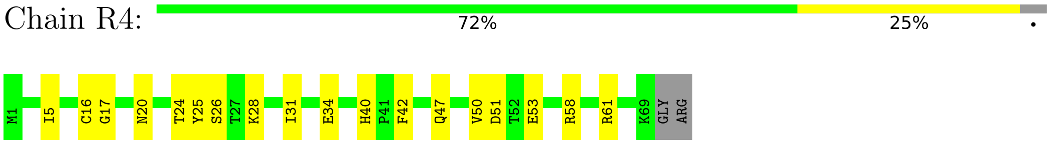
- Molecule 48: 50S ribosomal protein L30

Chain Y3:



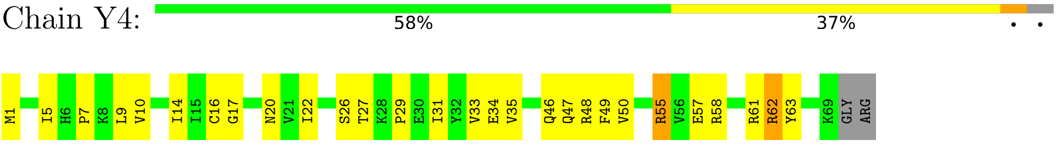
- Molecule 49: 50S ribosomal protein L31

Chain R4:



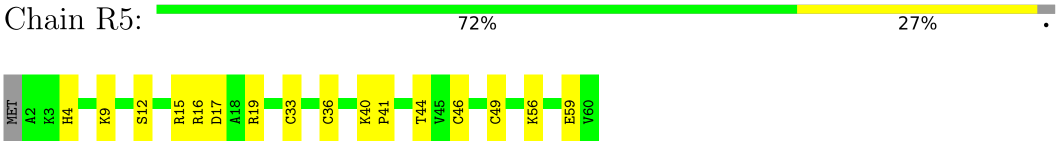
- Molecule 49: 50S ribosomal protein L31

Chain Y4:



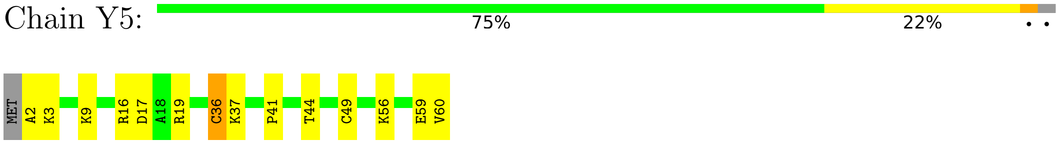
- Molecule 50: 50S ribosomal protein L32

Chain R5:



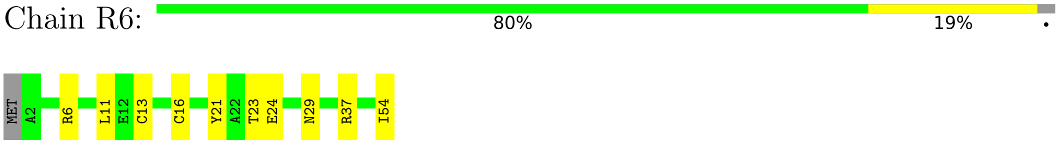
- Molecule 50: 50S ribosomal protein L32

Chain Y5:



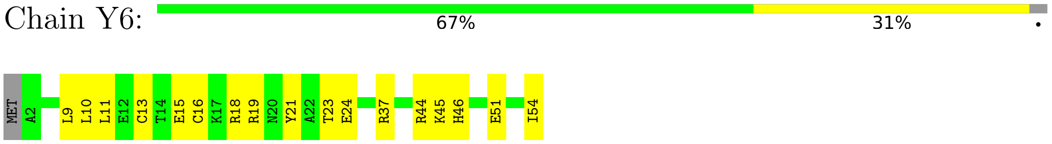
- Molecule 51: 50S ribosomal protein L33

Chain R6:



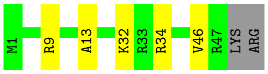
- Molecule 51: 50S ribosomal protein L33

Chain Y6:



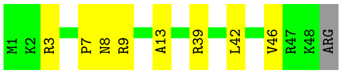
- Molecule 52: 50S ribosomal protein L34

Chain R7:



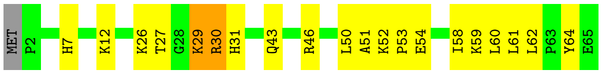
- Molecule 52: 50S ribosomal protein L34

Chain Y7:



- Molecule 53: 50S ribosomal protein L35

Chain R8:

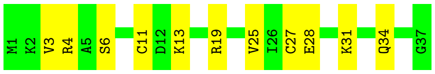


- Molecule 53: 50S ribosomal protein L35

Chain Y8:

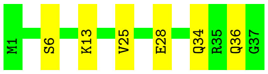
- Molecule 54: 50S ribosomal protein L36

Chain R9:



- Molecule 54: 50S ribosomal protein L36

Chain Y9:



4 Data and refinement statistics ⓘ

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.97Å 450.71Å 619.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.82 – 3.97	Depositor
% Data completeness (in resolution range)	98.7 (49.82-3.97)	Depositor
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.228 , 0.255	Depositor
Wilson B-factor (Å^2)	146.0	Xtriage
Anisotropy	0.246	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	291782	wwPDB-VP
Average B, all atoms (Å^2)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	QA	0.59	0/36098	1.09	116/56341 (0.2%)
1	XA	0.59	0/36101	1.09	126/56346 (0.2%)
2	QB	0.44	0/1942	0.69	1/2619 (0.0%)
2	XB	0.46	0/1950	0.68	0/2630
3	QC	0.46	0/1629	0.72	0/2195
3	XC	0.44	0/1629	0.72	0/2195
4	QD	0.47	1/1733 (0.1%)	0.67	0/2318
4	XD	0.53	1/1733 (0.1%)	0.65	0/2318
5	QE	0.46	1/1171 (0.1%)	0.68	1/1576 (0.1%)
5	XE	0.45	0/1171	0.69	0/1576
6	QF	0.46	0/856	0.69	0/1154
6	XF	0.41	0/856	0.66	0/1154
7	QG	0.46	0/1276	0.67	0/1709
7	XG	0.45	0/1276	0.70	0/1709
8	QH	0.45	0/1128	0.64	1/1517 (0.1%)
8	XH	0.41	0/1128	0.63	0/1517
9	QI	0.46	0/1008	0.77	3/1354 (0.2%)
9	XI	0.45	0/1017	0.79	2/1365 (0.1%)
10	QJ	0.45	0/814	0.69	1/1095 (0.1%)
10	XJ	0.46	0/790	0.71	0/1063
11	QK	0.42	0/900	0.59	0/1213
11	XK	0.42	0/879	0.66	0/1187
12	QL	0.44	0/991	0.69	0/1327
12	XL	0.43	0/972	0.70	0/1301
13	QM	0.46	0/965	0.74	0/1292
13	XM	0.49	0/956	0.83	1/1281 (0.1%)
14	QN	0.42	0/501	0.70	1/664 (0.2%)
14	XN	0.51	0/501	0.76	1/664 (0.2%)
15	QO	0.40	0/745	0.56	0/992
15	XO	0.41	0/740	0.62	0/987
16	QP	0.46	0/721	0.63	0/970
16	XP	0.43	0/721	0.70	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.38	0/847	0.61	0/1131
17	XQ	0.39	0/847	0.63	0/1131
18	QR	0.40	0/579	0.61	0/768
18	XR	0.44	0/579	0.65	0/768
19	QS	0.39	0/680	0.74	1/915 (0.1%)
19	XS	0.46	0/689	0.75	0/926
20	QT	0.37	0/765	0.61	0/1007
20	XT	0.49	0/765	0.75	0/1007
21	QU	0.41	0/221	0.68	0/288
21	XU	0.40	0/221	0.71	0/288
22	QV	0.47	1/1840 (0.1%)	1.02	6/2866 (0.2%)
22	XV	0.42	1/1840 (0.1%)	1.02	9/2866 (0.3%)
23	QX	0.28	0/470	0.86	1/733 (0.1%)
23	XX	0.33	0/470	0.90	0/733
24	RA	0.76	1/69521 (0.0%)	1.14	353/108529 (0.3%)
24	YA	0.89	3/69543 (0.0%)	1.17	381/108563 (0.4%)
25	RB	0.56	0/2878	1.14	22/4490 (0.5%)
25	YB	0.78	0/2878	1.19	15/4490 (0.3%)
26	RD	0.51	0/2165	0.71	2/2919 (0.1%)
26	YD	0.53	0/2165	0.68	2/2919 (0.1%)
27	RE	0.45	0/1601	0.72	0/2160
27	YE	0.47	0/1601	0.68	0/2160
28	RF	0.49	0/1620	0.64	0/2194
28	YF	0.55	0/1620	0.66	0/2194
29	RG	0.44	0/1499	0.73	0/2016
29	YG	0.46	0/1499	0.73	0/2016
30	RH	0.48	0/1362	0.75	0/1841
30	YH	0.49	0/1362	0.74	0/1841
31	RI	0.43	0/1151	0.76	0/1558
31	YI	0.46	0/1151	0.76	1/1558 (0.1%)
32	RN	0.42	0/1131	0.67	0/1525
32	YN	0.50	0/1131	0.69	0/1525
33	RO	0.52	0/943	0.67	0/1269
33	YO	0.51	0/943	0.67	0/1269
34	RP	0.47	0/1162	0.78	0/1544
34	YP	0.47	0/1139	0.73	0/1514
35	RQ	0.45	0/1143	0.70	0/1527
35	YQ	0.51	0/1143	0.71	0/1527
36	RR	0.45	0/974	0.67	0/1302
36	YR	0.46	0/974	0.67	0/1302
37	RS	0.43	0/892	0.76	0/1187
37	YS	0.44	0/892	0.72	0/1187
38	RT	0.46	0/1155	0.75	2/1542 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YT	0.48	0/1155	0.74	2/1542 (0.1%)
39	RU	0.46	0/982	0.65	0/1306
39	YU	0.55	0/982	0.64	0/1306
40	RV	0.48	0/790	0.72	0/1057
40	YV	0.49	0/790	0.70	0/1057
41	RW	0.50	0/911	0.67	0/1220
41	YW	0.50	0/911	0.64	0/1220
42	RX	0.43	0/739	0.64	1/993 (0.1%)
42	YX	0.50	0/739	0.67	1/993 (0.1%)
43	RY	0.44	0/831	0.60	0/1108
43	YY	0.46	0/831	0.58	0/1108
44	RZ	0.49	0/1493	0.79	0/2026
44	YZ	0.44	0/1493	0.74	2/2026 (0.1%)
45	R0	0.41	0/652	0.61	0/867
45	Y0	0.44	0/601	0.60	0/801
46	R1	0.46	0/770	0.66	0/1022
46	Y1	0.50	0/736	0.69	0/978
47	R2	0.49	0/583	0.68	0/771
47	Y2	0.46	0/583	0.68	0/771
48	R3	0.43	0/474	0.65	0/635
48	Y3	0.49	0/474	0.66	0/635
49	R4	0.44	0/578	0.73	0/776
49	Y4	0.48	0/578	0.76	0/776
50	R5	0.46	0/473	0.62	0/639
50	Y5	0.50	0/473	0.78	1/639 (0.2%)
51	R6	0.40	0/460	0.60	0/613
51	Y6	0.45	0/460	0.62	0/613
52	R7	0.44	0/417	0.65	0/550
52	Y7	0.49	0/426	0.64	0/561
53	R8	0.52	0/525	0.75	0/691
53	Y8	0.59	0/525	0.76	0/691
54	R9	0.37	0/310	0.62	0/407
54	Y9	0.42	0/310	0.59	0/407
All	All	0.68	9/316004 (0.0%)	1.03	1056/472499 (0.2%)

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
4	QD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	XL	0	1
27	YE	0	1
29	RG	0	1
29	YG	0	1
44	RZ	0	1
44	YZ	0	1
All	All	0	7

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	XD	61	LYS	CE-NZ	11.17	1.76	1.49
22	QV	1	C	OP3-P	-10.43	1.48	1.61
22	XV	1	C	OP3-P	-10.41	1.48	1.61
4	QD	13	ARG	CZ-NH1	7.36	1.42	1.33
5	QE	57	LYS	CD-CE	5.31	1.64	1.51

The worst 5 of 1056 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	RA	1774	C	C2-N1-C1'	19.55	140.31	118.80
24	RA	1774	C	C6-N1-C1'	-15.44	102.27	120.80
1	XA	359	U	C2-N1-C1'	13.62	134.05	117.70
24	YA	1158	C	C2-N1-C1'	13.17	133.29	118.80
1	QA	1301	U	N1-C2-O2	12.01	131.21	122.80

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	QD	33	MET	Peptide
29	RG	82	LEU	Peptide
44	RZ	52	SER	Peptide
12	XL	104	VAL	Peptide
27	YE	17	ASP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16276	508	0
1	XA	32249	0	16279	516	1
2	QB	1907	0	1958	28	0
2	XB	1915	0	1969	33	0
3	QC	1605	0	1668	40	0
3	XC	1605	0	1668	27	1
4	QD	1703	0	1763	39	0
4	XD	1703	0	1763	53	1
5	QE	1155	0	1213	21	0
5	XE	1155	0	1213	24	0
6	QF	843	0	857	17	0
6	XF	843	0	857	9	0
7	QG	1257	0	1296	27	0
7	XG	1257	0	1296	22	0
8	QH	1108	0	1165	29	0
8	XH	1108	0	1165	30	0
9	QI	989	0	1011	29	0
9	XI	998	0	1024	26	0
10	QJ	801	0	849	26	0
10	XJ	777	0	816	27	0
11	QK	885	0	904	24	1
11	XK	864	0	881	17	0
12	QL	975	0	1062	29	0
12	XL	956	0	1046	18	0
13	QM	955	0	1021	38	0
13	XM	946	0	1008	20	0
14	QN	492	0	528	16	0
14	XN	492	0	531	36	0
15	QO	734	0	771	14	0
15	XO	729	0	768	11	0
16	QP	705	0	725	10	0
16	XP	705	0	725	9	0
17	QQ	834	0	904	11	0
17	XQ	834	0	904	18	0
18	QR	574	0	644	14	0
18	XR	574	0	644	12	0
19	QS	665	0	686	18	0
19	XS	674	0	699	14	0
20	QT	763	0	861	15	0
20	XT	763	0	861	21	0
21	QU	217	0	234	5	0
21	XU	217	0	234	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	QV	1647	0	832	20	0
22	XV	1647	0	832	18	0
23	QX	418	0	209	10	0
23	XX	418	0	209	9	0
24	RA	62071	0	31291	830	4
24	YA	62091	0	31297	821	0
25	RB	2573	0	1306	27	0
25	YB	2573	0	1306	26	0
26	RD	2115	0	2195	50	0
26	YD	2115	0	2195	52	0
27	RE	1568	0	1634	53	0
27	YE	1568	0	1634	41	0
28	RF	1585	0	1632	25	0
28	YF	1585	0	1632	21	0
29	RG	1474	0	1535	33	0
29	YG	1474	0	1535	42	0
30	RH	1336	0	1418	33	0
30	YH	1336	0	1418	20	1
31	RI	1136	0	1223	15	0
31	YI	1136	0	1223	10	0
32	RN	1104	0	1180	23	0
32	YN	1104	0	1180	21	0
33	RO	933	0	996	23	0
33	YO	933	0	996	17	0
34	RP	1145	0	1228	35	0
34	YP	1122	0	1206	29	0
35	RQ	1122	0	1179	27	0
35	YQ	1122	0	1179	29	0
36	RR	960	0	1021	20	0
36	YR	960	0	1021	11	0
37	RS	882	0	942	19	0
37	YS	882	0	943	19	0
38	RT	1141	0	1202	26	0
38	YT	1141	0	1202	24	0
39	RU	964	0	1022	19	0
39	YU	964	0	1022	22	0
40	RV	779	0	852	18	0
40	YV	779	0	852	16	1
41	RW	900	0	964	16	0
41	YW	900	0	964	10	0
42	RX	725	0	778	9	0
42	YX	725	0	778	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	RY	818	0	909	16	0
43	YY	818	0	909	18	1
44	RZ	1461	0	1493	32	0
44	YZ	1461	0	1493	24	0
45	R0	643	0	667	12	0
45	Y0	593	0	612	15	0
46	R1	763	0	848	11	0
46	Y1	729	0	802	11	0
47	R2	581	0	629	11	0
47	Y2	581	0	629	9	2
48	R3	469	0	518	6	0
48	Y3	469	0	518	9	0
49	R4	565	0	557	12	0
49	Y4	565	0	557	21	0
50	R5	459	0	476	16	0
50	Y5	459	0	477	13	1
51	R6	453	0	473	9	0
51	Y6	453	0	473	11	0
52	R7	409	0	454	4	0
52	Y7	418	0	467	7	0
53	R8	517	0	582	17	0
53	Y8	517	0	582	19	0
54	R9	307	0	335	9	0
54	Y9	307	0	335	5	0
55	QA	69	0	0	0	0
55	QE	1	0	0	0	0
55	QH	1	0	0	0	0
55	QV	1	0	0	0	0
55	R1	1	0	0	0	0
55	RA	381	0	0	0	0
55	RB	9	0	0	0	0
55	RD	1	0	0	0	0
55	RE	1	0	0	0	0
55	RQ	1	0	0	0	0
55	XA	67	0	0	0	0
55	XE	1	0	0	0	0
55	Y0	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	2	0	0	0	0
55	YA	454	0	0	0	0
55	YB	8	0	0	0	0
55	YD	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	YE	1	0	0	0	0
55	YP	1	0	0	0	0
55	YQ	2	0	0	0	0
55	YR	2	0	0	0	0
56	QD	8	0	0	1	0
56	XD	8	0	0	3	0
57	QN	1	0	0	0	0
57	R4	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y4	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	0	0
All	All	291782	0	197805	4186	7

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 9.

The worst 5 of 4186 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:XN:24:CYS:SG	14:XN:40:CYS:HB2	1.54	1.47
4:XD:61:LYS:NZ	4:XD:61:LYS:CE	1.77	1.47
14:XN:29:ARG:HD2	14:XN:40:CYS:SG	1.67	1.33
14:XN:24:CYS:SG	14:XN:40:CYS:CB	2.36	1.14
14:XN:29:ARG:CD	14:XN:40:CYS:SG	2.36	1.13

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:YV:53:GLU:CB	50:Y5:59:GLU:OE1[4_445]	1.95	0.25
11:QK:99:GLN:OE1	3:XC:79:ARG:CD[4_555]	2.01	0.19
24:RA:2137:C:OP1	1:XA:999:U:O2'[4_555]	2.05	0.15
30:YH:46:GLU:OE2	43:YY:23:ARG:NH1[4_445]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:RA:306:U:O3'	47:Y2:17:SER:OG[3_555]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
2	QB	233/256 (91%)	204 (88%)	27 (12%)	2 (1%)	17	54
2	XB	234/256 (91%)	207 (88%)	27 (12%)	0	100	100
3	QC	203/239 (85%)	189 (93%)	13 (6%)	1 (0%)	29	66
3	XC	203/239 (85%)	184 (91%)	18 (9%)	1 (0%)	29	66
4	QD	206/209 (99%)	188 (91%)	18 (9%)	0	100	100
4	XD	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
5	QE	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	22	60
5	XE	149/162 (92%)	138 (93%)	11 (7%)	0	100	100
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
8	XH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
9	QI	123/128 (96%)	113 (92%)	9 (7%)	1 (1%)	19	57
9	XI	124/128 (97%)	116 (94%)	8 (6%)	0	100	100
10	QJ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
10	XJ	94/105 (90%)	83 (88%)	11 (12%)	0	100	100
11	QK	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
11	XK	114/129 (88%)	110 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	QL	123/132 (93%)	111 (90%)	11 (9%)	1 (1%)	19	57
12	XL	120/132 (91%)	104 (87%)	15 (12%)	1 (1%)	19	57
13	QM	118/126 (94%)	102 (86%)	15 (13%)	1 (1%)	19	57
13	XM	117/126 (93%)	99 (85%)	17 (14%)	1 (1%)	17	54
14	QN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9	42
14	XN	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9	42
15	QO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	QP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
16	XP	82/88 (93%)	81 (99%)	1 (1%)	0	100	100
17	QQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	62 (91%)	6 (9%)	0	100	100
19	QS	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
19	XS	82/93 (88%)	68 (83%)	14 (17%)	0	100	100
20	QT	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
20	XT	97/106 (92%)	90 (93%)	6 (6%)	1 (1%)	15	52
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
26	RD	270/276 (98%)	245 (91%)	23 (8%)	2 (1%)	22	60
26	YD	270/276 (98%)	248 (92%)	20 (7%)	2 (1%)	22	60
27	RE	203/206 (98%)	170 (84%)	31 (15%)	2 (1%)	15	52
27	YE	203/206 (98%)	166 (82%)	35 (17%)	2 (1%)	15	52
28	RF	200/210 (95%)	189 (94%)	11 (6%)	0	100	100
28	YF	200/210 (95%)	189 (94%)	11 (6%)	0	100	100
29	RG	179/182 (98%)	148 (83%)	29 (16%)	2 (1%)	14	50
29	YG	179/182 (98%)	150 (84%)	27 (15%)	2 (1%)	14	50
30	RH	172/180 (96%)	147 (86%)	20 (12%)	5 (3%)	4	32
30	YH	172/180 (96%)	150 (87%)	18 (10%)	4 (2%)	6	37
31	RI	144/148 (97%)	121 (84%)	20 (14%)	3 (2%)	7	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	YI	144/148 (97%)	120 (83%)	21 (15%)	3 (2%)	7	38
32	RN	136/140 (97%)	120 (88%)	15 (11%)	1 (1%)	22	60
32	YN	136/140 (97%)	119 (88%)	17 (12%)	0	100	100
33	RO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
33	YO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
34	RP	148/150 (99%)	120 (81%)	26 (18%)	2 (1%)	11	45
34	YP	145/150 (97%)	119 (82%)	25 (17%)	1 (1%)	22	60
35	RQ	139/141 (99%)	119 (86%)	19 (14%)	1 (1%)	22	60
35	YQ	139/141 (99%)	117 (84%)	21 (15%)	1 (1%)	22	60
36	RR	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	9	42
36	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	54
37	RS	109/112 (97%)	93 (85%)	15 (14%)	1 (1%)	17	54
37	YS	109/112 (97%)	92 (84%)	17 (16%)	0	100	100
38	RT	135/146 (92%)	118 (87%)	15 (11%)	2 (2%)	10	45
38	YT	135/146 (92%)	114 (84%)	19 (14%)	2 (2%)	10	45
39	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	54
39	YU	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	17	54
40	RV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15	52
40	YV	99/101 (98%)	86 (87%)	12 (12%)	1 (1%)	15	52
41	RW	111/113 (98%)	105 (95%)	5 (4%)	1 (1%)	17	54
41	YW	111/113 (98%)	101 (91%)	9 (8%)	1 (1%)	17	54
42	RX	90/96 (94%)	89 (99%)	1 (1%)	0	100	100
42	YX	90/96 (94%)	88 (98%)	2 (2%)	0	100	100
43	RY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
43	YY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
44	RZ	181/206 (88%)	146 (81%)	32 (18%)	3 (2%)	9	42
44	YZ	181/206 (88%)	149 (82%)	29 (16%)	3 (2%)	9	42
45	R0	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
45	Y0	72/85 (85%)	69 (96%)	3 (4%)	0	100	100
46	R1	95/98 (97%)	86 (90%)	9 (10%)	0	100	100
46	Y1	91/98 (93%)	83 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	R2	67/72 (93%)	63 (94%)	3 (4%)	1 (2%)	10	45
47	Y2	67/72 (93%)	63 (94%)	3 (4%)	1 (2%)	10	45
48	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
48	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	R4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	45
49	Y4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	45
50	R5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	Y5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
51	R6	51/54 (94%)	51 (100%)	0	0	100	100
51	Y6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
52	R7	45/49 (92%)	45 (100%)	0	0	100	100
52	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	R8	62/65 (95%)	48 (77%)	11 (18%)	3 (5%)	2	23
53	Y8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	4	31
54	R9	35/37 (95%)	35 (100%)	0	0	100	100
54	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
All	All	11449/12128 (94%)	10319 (90%)	1055 (9%)	75 (1%)	22	60

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	RE	18	ASP
31	RI	15	VAL
38	RT	124	ASP
44	RZ	53	ILE
53	R8	30	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
2	QB	203/220 (92%)	200 (98%)	3 (2%)	65	79
2	XB	204/220 (93%)	201 (98%)	3 (2%)	65	79
3	QC	159/188 (85%)	154 (97%)	5 (3%)	40	63
3	XC	159/188 (85%)	157 (99%)	2 (1%)	69	81
4	QD	180/181 (99%)	176 (98%)	4 (2%)	52	71
4	XD	180/181 (99%)	175 (97%)	5 (3%)	43	65
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	87
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	87
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	122 (97%)	4 (3%)	39	62
7	XG	126/127 (99%)	124 (98%)	2 (2%)	62	79
8	QH	118/119 (99%)	116 (98%)	2 (2%)	60	78
8	XH	118/119 (99%)	116 (98%)	2 (2%)	60	78
9	QI	96/99 (97%)	94 (98%)	2 (2%)	53	72
9	XI	97/99 (98%)	95 (98%)	2 (2%)	53	72
10	QJ	89/92 (97%)	88 (99%)	1 (1%)	73	84
10	XJ	86/92 (94%)	83 (96%)	3 (4%)	36	61
11	QK	90/99 (91%)	89 (99%)	1 (1%)	73	84
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	103 (99%)	1 (1%)	76	85
12	XL	103/109 (94%)	102 (99%)	1 (1%)	76	85
13	QM	96/101 (95%)	93 (97%)	3 (3%)	40	63
13	XM	95/101 (94%)	92 (97%)	3 (3%)	39	62
14	QN	49/50 (98%)	47 (96%)	2 (4%)	30	57
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	73	84
17	XQ	95/97 (98%)	94 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	71 (99%)	1 (1%)	67	80
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	75 (99%)	1 (1%)	69	81
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	19 (95%)	1 (5%)	24	52
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	52
26	RD	214/218 (98%)	212 (99%)	2 (1%)	78	87
26	YD	214/218 (98%)	212 (99%)	2 (1%)	78	87
27	RE	165/166 (99%)	164 (99%)	1 (1%)	86	91
27	YE	165/166 (99%)	165 (100%)	0	100	100
28	RF	161/166 (97%)	161 (100%)	0	100	100
28	YF	161/166 (97%)	161 (100%)	0	100	100
29	RG	155/156 (99%)	154 (99%)	1 (1%)	86	91
29	YG	155/156 (99%)	154 (99%)	1 (1%)	86	91
30	RH	145/148 (98%)	144 (99%)	1 (1%)	84	90
30	YH	145/148 (98%)	143 (99%)	2 (1%)	67	80
31	RI	122/124 (98%)	122 (100%)	0	100	100
31	YI	122/124 (98%)	121 (99%)	1 (1%)	81	88
32	RN	117/119 (98%)	117 (100%)	0	100	100
32	YN	117/119 (98%)	116 (99%)	1 (1%)	78	87
33	RO	100/100 (100%)	100 (100%)	0	100	100
33	YO	100/100 (100%)	100 (100%)	0	100	100
34	RP	116/116 (100%)	114 (98%)	2 (2%)	60	78
34	YP	114/116 (98%)	114 (100%)	0	100	100
35	RQ	111/111 (100%)	109 (98%)	2 (2%)	59	77
35	YQ	111/111 (100%)	109 (98%)	2 (2%)	59	77
36	RR	100/101 (99%)	100 (100%)	0	100	100
36	YR	100/101 (99%)	100 (100%)	0	100	100
37	RS	87/88 (99%)	86 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	YS	87/88 (99%)	87 (100%)	0	100	100
38	RT	120/127 (94%)	119 (99%)	1 (1%)	81	88
38	YT	120/127 (94%)	120 (100%)	0	100	100
39	RU	93/94 (99%)	92 (99%)	1 (1%)	73	84
39	YU	93/94 (99%)	93 (100%)	0	100	100
40	RV	82/82 (100%)	81 (99%)	1 (1%)	71	83
40	YV	82/82 (100%)	80 (98%)	2 (2%)	49	69
41	RW	92/92 (100%)	92 (100%)	0	100	100
41	YW	92/92 (100%)	90 (98%)	2 (2%)	52	71
42	RX	74/78 (95%)	74 (100%)	0	100	100
42	YX	74/78 (95%)	74 (100%)	0	100	100
43	RY	88/91 (97%)	87 (99%)	1 (1%)	73	84
43	YY	88/91 (97%)	86 (98%)	2 (2%)	50	70
44	RZ	162/179 (90%)	162 (100%)	0	100	100
44	YZ	162/179 (90%)	160 (99%)	2 (1%)	71	83
45	R0	65/67 (97%)	64 (98%)	1 (2%)	65	79
45	Y0	60/67 (90%)	59 (98%)	1 (2%)	60	78
46	R1	82/83 (99%)	81 (99%)	1 (1%)	71	83
46	Y1	78/83 (94%)	78 (100%)	0	100	100
47	R2	64/67 (96%)	64 (100%)	0	100	100
47	Y2	64/67 (96%)	64 (100%)	0	100	100
48	R3	51/52 (98%)	50 (98%)	1 (2%)	55	73
48	Y3	51/52 (98%)	45 (88%)	6 (12%)	5	24
49	R4	62/63 (98%)	61 (98%)	1 (2%)	62	79
49	Y4	62/63 (98%)	60 (97%)	2 (3%)	39	62
50	R5	51/52 (98%)	51 (100%)	0	100	100
50	Y5	51/52 (98%)	50 (98%)	1 (2%)	55	73
51	R6	51/52 (98%)	51 (100%)	0	100	100
51	Y6	51/52 (98%)	50 (98%)	1 (2%)	55	73
52	R7	40/42 (95%)	40 (100%)	0	100	100
52	Y7	41/42 (98%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	R8	54/55 (98%)	53 (98%)	1 (2%)	57	75
53	Y8	54/55 (98%)	54 (100%)	0	100	100
54	R9	34/34 (100%)	34 (100%)	0	100	100
54	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9684/10066 (96%)	9578 (99%)	106 (1%)	73	84

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

Mol	Chain	Res	Type
4	XD	19	LEU
10	XJ	60	ARG
48	Y3	37	LEU
4	XD	139	ARG
8	XH	129	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
27	YE	66	HIS
39	YU	94	ASN
29	YG	40	ASN
2	XB	95	GLN
26	YD	126	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1521 (98%)	271 (18%)	37 (2%)
1	XA	1498/1521 (98%)	254 (16%)	30 (2%)
22	QV	76/77 (98%)	15 (19%)	1 (1%)
22	XV	76/77 (98%)	17 (22%)	1 (1%)
23	QX	18/19 (94%)	5 (27%)	2 (11%)
23	XX	18/19 (94%)	5 (27%)	1 (5%)
24	RA	2879/2915 (98%)	571 (19%)	41 (1%)
24	YA	2880/2915 (98%)	576 (20%)	42 (1%)
25	RB	119/122 (97%)	18 (15%)	1 (0%)
25	YB	119/122 (97%)	21 (17%)	1 (0%)
All	All	9182/9308 (98%)	1753 (19%)	157 (1%)

5 of 1753 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

5 of 157 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	YA	221	A
24	YA	1786	A
24	YA	278	A
24	YA	1022	G
24	YA	2681	C

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1022 ligands modelled in this entry, 1020 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
56	SF4	QD	301	4	0,12,12	-	-	-		
56	SF4	XD	301	4	0,12,12	-	-	-		

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
56	SF4	QD	301	4	-	-	0/6/5/5
56	SF4	XD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	QD	301	SF4	1	0
56	XD	301	SF4	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.