wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 12:21 AM EDT

PDB ID	:	6BZ7
Title	:	Thermus thermophilus 70S containing 16S G299A point mutation and near-cognate ASL Leucine in A site.
Authors	:	Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on	:	2017-12-22
Resolution	:	3.68 Å(reported)

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

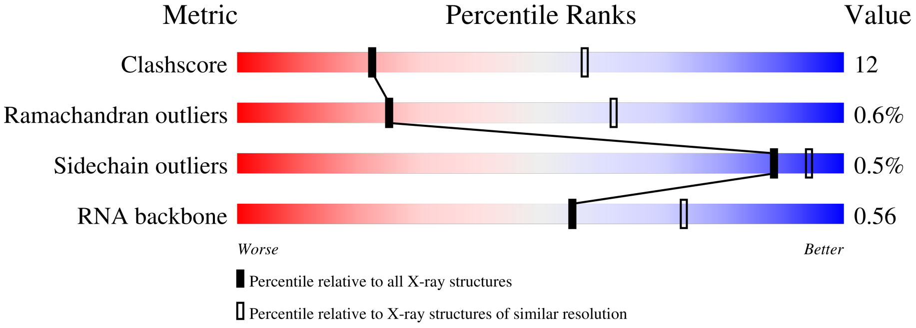
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.68 Å.

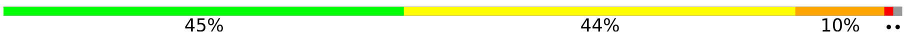
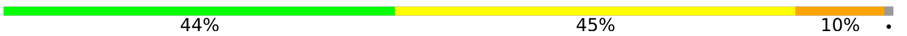
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1070 (3.84-3.52)
Ramachandran outliers	138981	1036 (3.84-3.52)
Sidechain outliers	138945	1033 (3.84-3.52)
RNA backbone	3102	1024 (4.30-3.00)

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	1508	
1	XA	1508	
2	QB	256	
2	XB	256	
3	QC	239	
3	XC	239	

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Mol	Chain	Length	Quality of chain
4	QD	209	68% 31%
4	XD	209	70% 29% •
5	QE	162	71% 22% 7%
5	XE	162	77% 17% 7%
6	QF	101	74% 24% •
6	XF	101	68% 32%
7	QG	156	81% 18% •
7	XG	156	83% 16% •
8	QH	138	74% 25% •
8	XH	138	80% 20% •
9	QI	128	65% 33% • •
9	XI	128	62% 36% •
10	QJ	105	60% 33% • 6%
10	XJ	105	69% 23% 9%
11	QK	129	65% 27% 8%
11	XK	129	66% 24% 10%
12	QL	132	72% 23% 5%
12	XL	132	70% 20% • 8%
13	QM	126	59% 36% • 5%
13	XM	126	61% 33% • 6%
14	QN	61	72% 25% • •
14	XN	61	72% 25% • •
15	QO	89	80% 19% •
15	XO	89	72% 26% •
16	QP	88	66% 30% 5%

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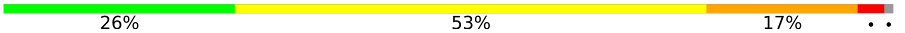
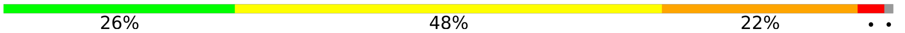
Mol	Chain	Length	Quality of chain
16	XP	88	 66% 30% 5%
17	QQ	105	 74% 21% 5%
17	XQ	105	 69% 27% 5%
18	QR	88	 58% 22% 20%
18	XR	88	 53% 26% 20%
19	QS	93	 58% 30% • 11%
19	XS	93	 65% 25% • 10%
20	QT	106	 69% 25% 7%
20	XT	106	 72% 22% 7%
21	QU	27	 67% 26% 7%
21	XU	27	 52% 41% 7%
22	QV	77	 56% 34% 10%
22	QW	77	 26% 53% 17% • •
22	XV	77	 58% 30% 12%
22	XW	77	 26% 48% 22% • •
23	QX	25	 32% 68%
23	XX	25	 28% 8% • 60%
24	QY	17	 59% 35% 6%
24	XY	17	 41% 53% 6%
25	RA	2915	 48% 40% 10% •
25	YA	2915	 46% 43% 9% ••
26	RB	122	 64% 28% 7% •
26	YB	122	 54% 38% 7% •
27	RD	276	 58% 40% ••
27	YD	276	 59% 39% •

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Mol	Chain	Length	Quality of chain
28	RE	206	61% 37% •
28	YE	206	59% 40% •
29	RF	210	66% 30% •
29	YF	210	63% 32% •
30	RG	182	59% 40% ••
30	YG	182	54% 44% • •
31	RH	180	68% 26% • •
31	YH	180	64% 29% • •
32	RI	148	68% 30% ••
32	YI	148	70% 27% ••
33	RN	140	65% 33% ••
33	YN	140	71% 26% ••
34	RO	122	71% 28% •
34	YO	122	78% 21% •
35	RP	150	69% 31% •
35	YP	150	61% 37% • •
36	RQ	141	62% 38%
36	YQ	141	60% 40%
37	RR	118	66% 33% •
37	YR	118	65% 34% •
38	RS	112	72% 26% ••
38	YS	112	71% 28% ••
39	RT	146	56% 37% • 6%
39	YT	146	55% 38% • 6%
40	RU	118	70% 27% • •

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Mol	Chain	Length	Quality of chain
40	YU	118	70% 27% • •
41	RV	101	64% 35% •
41	YV	101	71% 29%
42	RW	113	74% 24% •
42	YW	113	75% 23% •
43	RX	96	71% 25% •
43	YX	96	63% 33% •
44	RY	110	78% 19% •
44	YY	110	76% 21% •
45	RZ	206	56% 32% • 11%
45	YZ	206	59% 29% • 11%
46	R0	85	66% 29% 5%
46	Y0	85	59% 28% • 12%
47	R1	98	73% 26% •
47	Y1	98	61% 34% 5%
48	R2	72	71% 25% •
48	Y2	72	67% 29% •
49	R3	60	67% 32% •
49	Y3	60	63% 35% •
50	R4	71	69% 25% • •
50	Y4	71	66% 27% • •
51	R5	60	90% 8% •
51	Y5	60	85% 13% •
52	R6	54	81% 17% •
52	Y6	54	89% 9% •

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Mol	Chain	Length	Quality of chain
53	R7	49	
53	Y7	49	
54	R8	65	
54	Y8	65	
55	R9	37	
55	Y9	37	

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 295575 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	32246	14353	5981	10413	1499	0	0	0
1	XA	1500	32248	14354	5984	10411	1499	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	299	A	G	engineered mutation	GB 55771382
XA	299	A	G	engineered mutation	GB 55771382

- 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

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

- 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	127	Total	C	N	O	0	0	0
			1010	639	197	174			
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			
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 734 459 147 126 2	0	0	0
15	XO	87	Total C N O S 729 457 146 124 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	QP	84	Total C N O S 705 446 140 118 1	0	0	0
16	XP	84	Total C N O S 705 446 140 118 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 C N O S 834 534 155 143 2	0	0	0
17	XQ	100	Total C N O S 834 534 155 143 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 C N O 574 367 112 95	0	0	0
18	XR	70	Total C N O 574 367 112 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 C N O S 665 424 124 115 2	0	0	0
19	XS	84	Total C N O S 674 430 126 116 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 C N O S 763 470 162 129 2	0	0	0

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

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

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

- Molecule 22 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total 1644	C 732	N 297	O 538	P 77	0	0	0
22	QW	76	Total 1618	C 722	N 292	O 529	P 75	0	0	0
22	XV	77	Total 1644	C 732	N 297	O 538	P 77	0	0	0
22	XW	76	Total 1618	C 722	N 292	O 529	P 75	0	0	0

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total 169	C 76	N 29	O 56	P 8	0	0	0
23	XX	10	Total 210	C 96	N 39	O 66	P 9	0	0	0

- Molecule 24 is a RNA chain called ASL Leu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	17	Total 358	C 162	N 64	O 116	P 16	0	0	0
24	XY	17	Total 358	C 162	N 64	O 116	P 16	0	0	0

- Molecule 25 is a RNA chain called 23S rRNA.

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

- Molecule 26 is a RNA chain called 5S rRNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	Y0	75	Total 599	C 370	N 127	O 101	S 1	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L36.

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	QA	68	Total Mg 68 68	0	0
56	QC	1	Total Mg 1 1	0	0
56	QE	1	Total Mg 1 1	0	0
56	QF	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	QH	1	Total Mg 1 1	0	0
56	QQ	1	Total Mg 1 1	0	0
56	QV	6	Total Mg 6 6	0	0
56	QY	1	Total Mg 1 1	0	0
56	RA	508	Total Mg 508 508	0	0
56	RB	7	Total Mg 7 7	0	0
56	RE	2	Total Mg 2 2	0	0
56	RF	1	Total Mg 1 1	0	0
56	RN	1	Total Mg 1 1	0	0
56	RO	2	Total Mg 2 2	0	0
56	RP	2	Total Mg 2 2	0	0
56	RQ	2	Total Mg 2 2	0	0
56	RR	1	Total Mg 1 1	0	0
56	RT	1	Total Mg 1 1	0	0
56	RU	1	Total Mg 1 1	0	0
56	RY	1	Total Mg 1 1	0	0
56	R0	4	Total Mg 4 4	0	0
56	R1	2	Total Mg 2 2	0	0
56	R4	1	Total Mg 1 1	0	0
56	R8	1	Total Mg 1 1	0	0
56	R9	1	Total Mg 1 1	0	0

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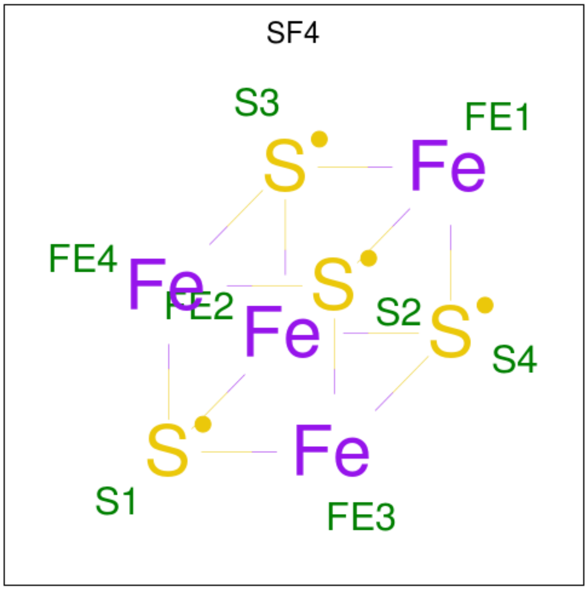
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	XA	82	Total Mg 82 82	0	0
56	XE	1	Total Mg 1 1	0	0
56	XL	1	Total Mg 1 1	0	0
56	XM	1	Total Mg 1 1	0	0
56	XQ	1	Total Mg 1 1	0	0
56	XS	1	Total Mg 1 1	0	0
56	XV	6	Total Mg 6 6	0	0
56	YA	546	Total Mg 546 546	0	0
56	YB	12	Total Mg 12 12	0	0
56	YD	2	Total Mg 2 2	0	0
56	YE	2	Total Mg 2 2	0	0
56	YO	1	Total Mg 1 1	0	0
56	YP	3	Total Mg 3 3	0	0
56	YQ	3	Total Mg 3 3	0	0
56	YX	2	Total Mg 2 2	0	0
56	YY	1	Total Mg 1 1	0	0
56	Y0	1	Total Mg 1 1	0	0
56	Y7	1	Total Mg 1 1	0	0
56	Y8	1	Total Mg 1 1	0	0
56	Y9	1	Total Mg 1 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	Y6	1	Total Zn 1 1	0	0
58	Y9	1	Total Zn 1 1	0	0

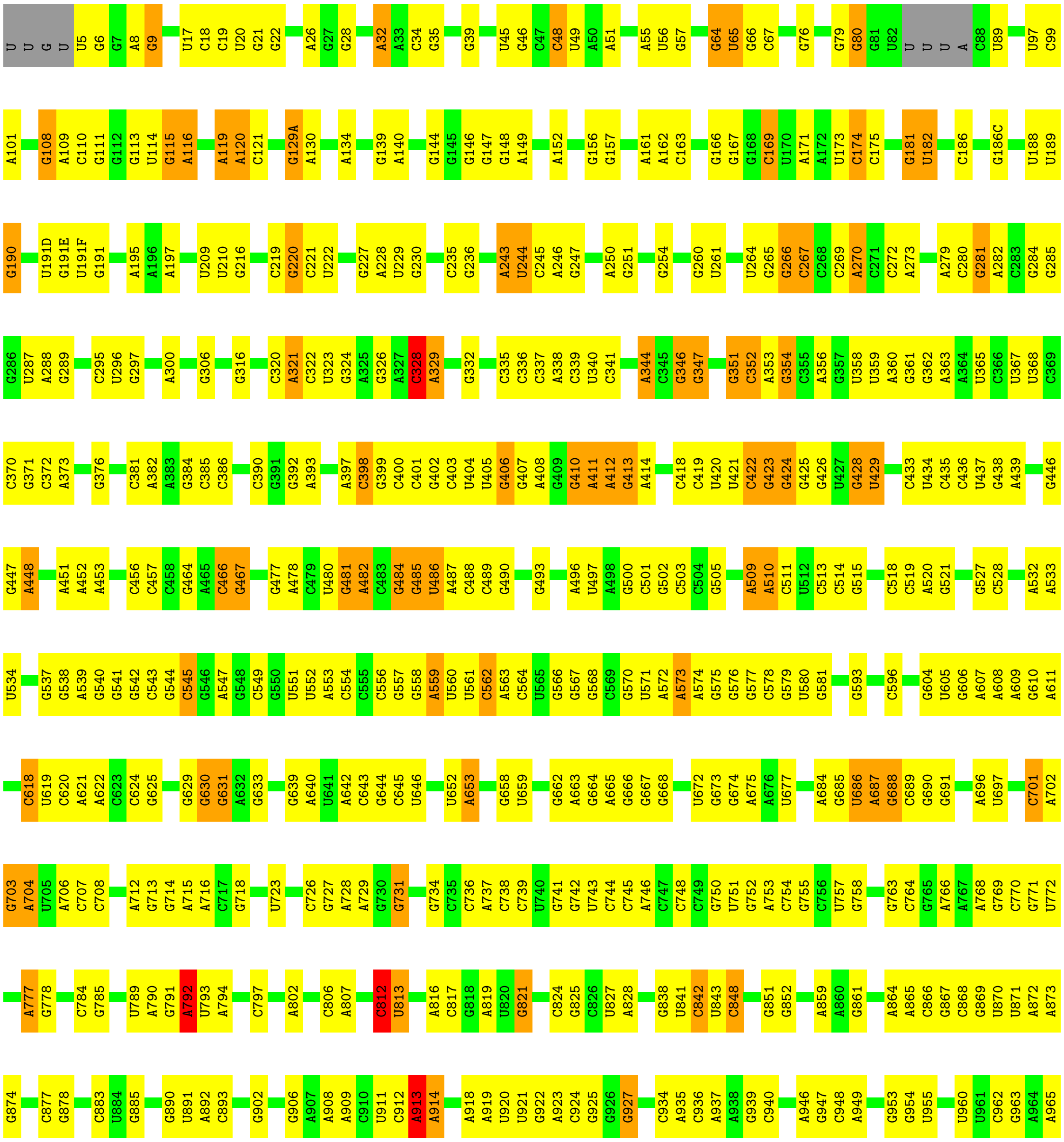
3 Residue-property plots (i)

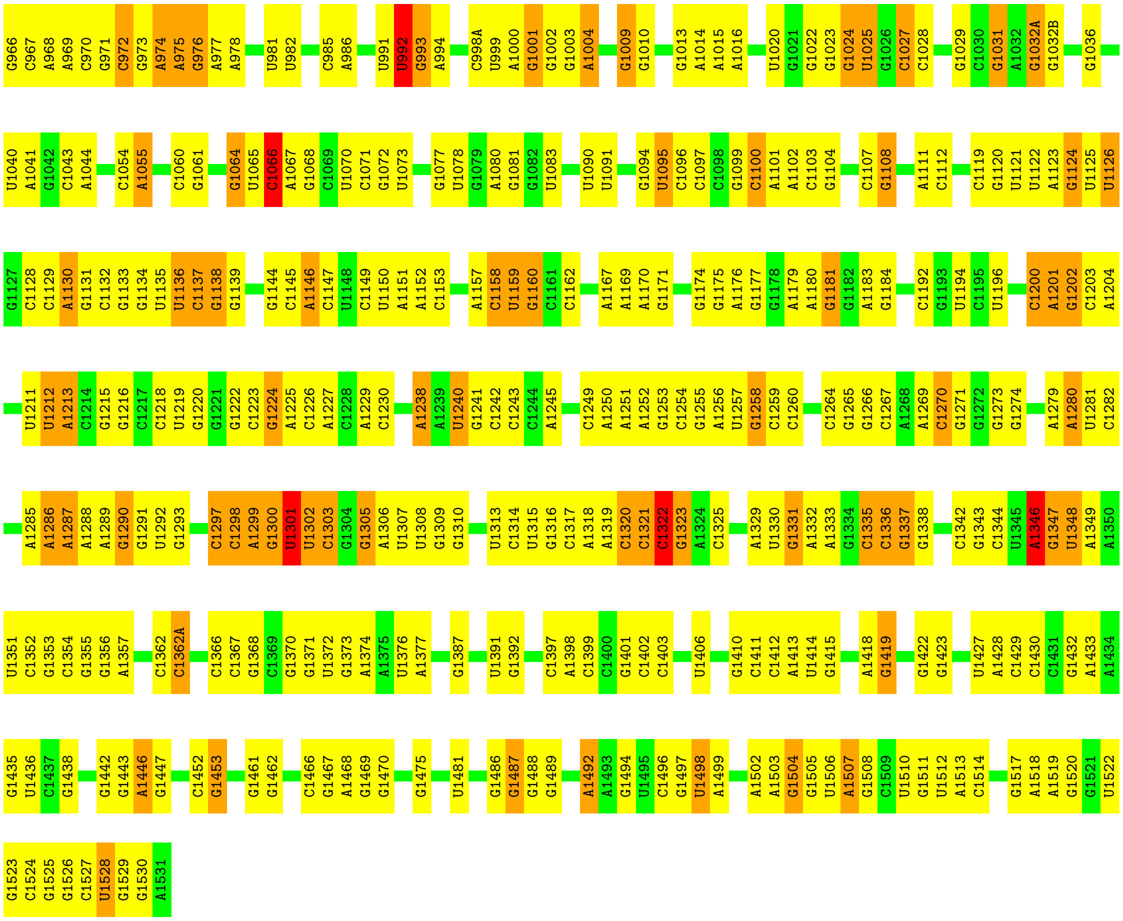
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

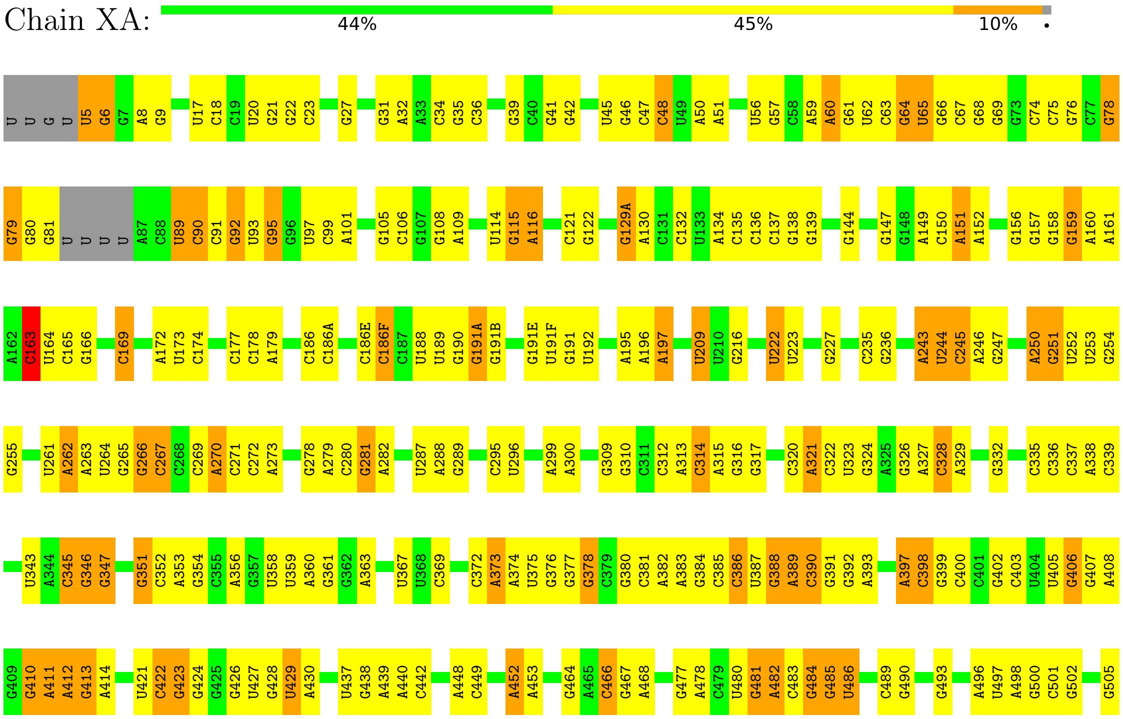
Chain QA:

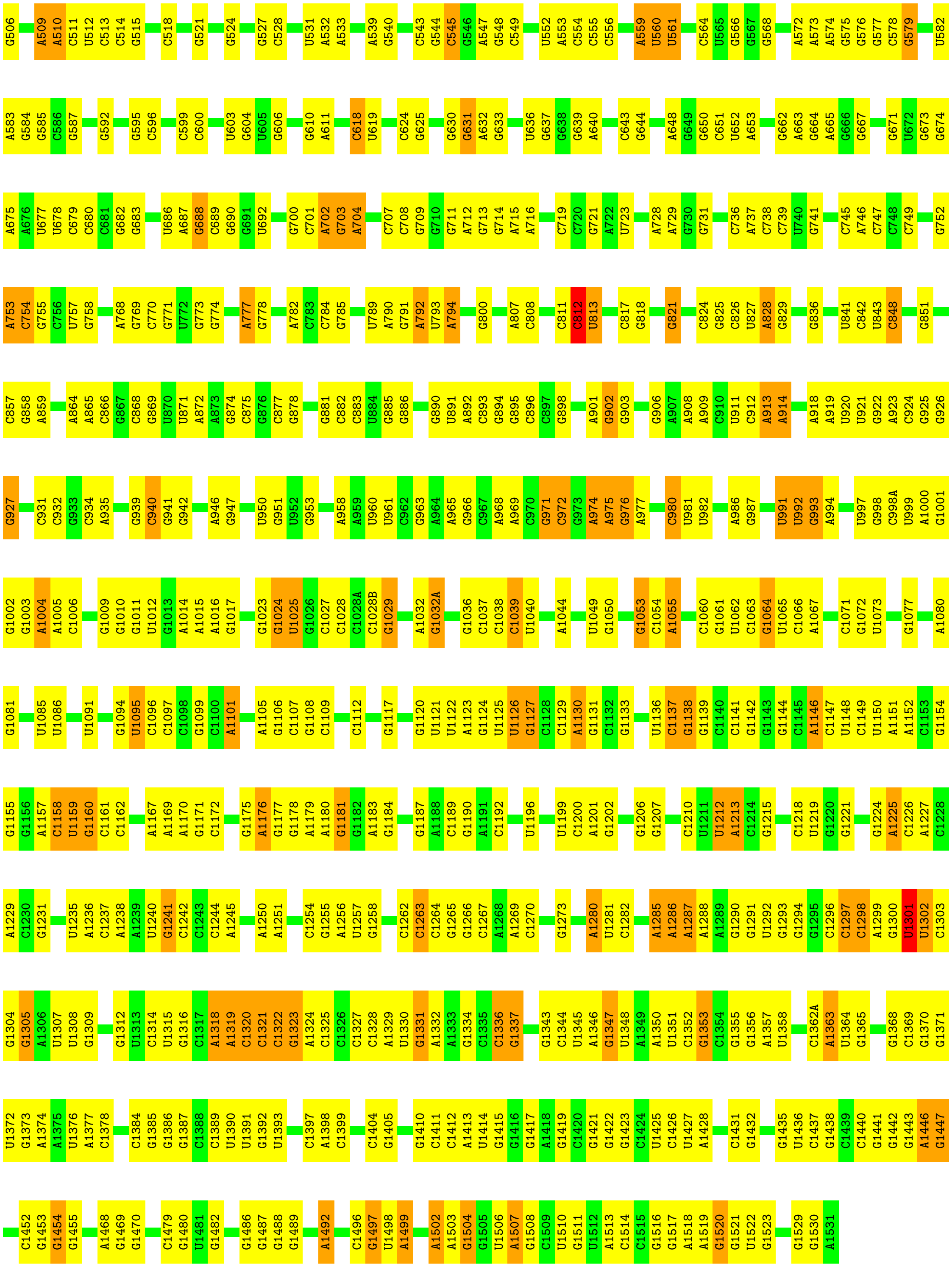




- Molecule 1: 16S rRNA

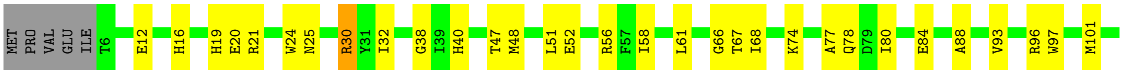
Chain XA:

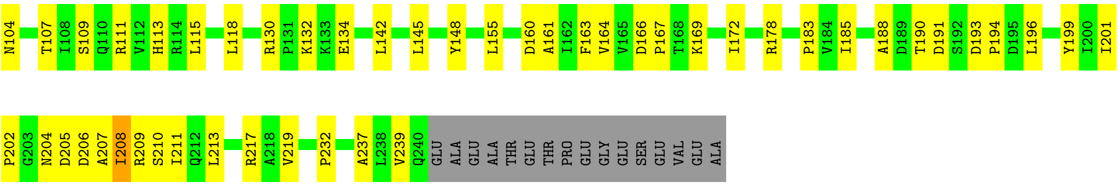




- Molecule 2: 30S ribosomal protein S2

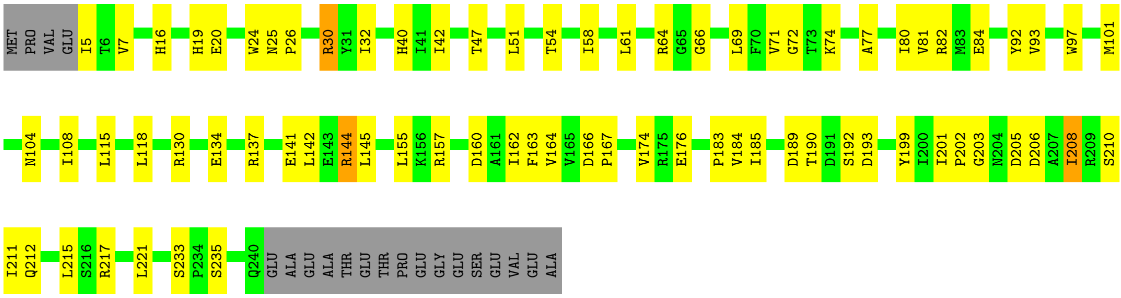
Chain QB:





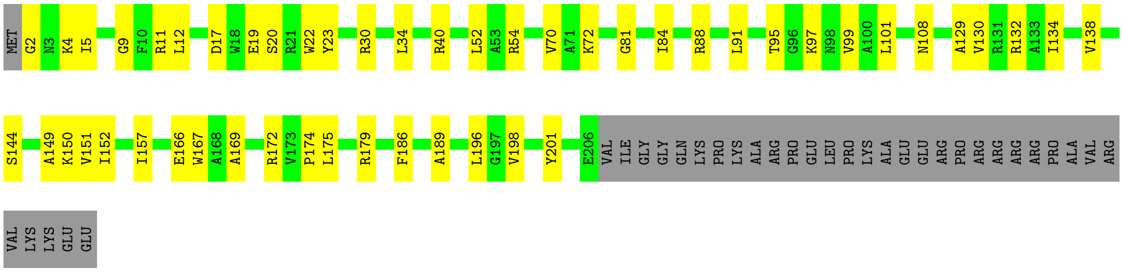
- Molecule 2: 30S ribosomal protein S2

Chain XB:



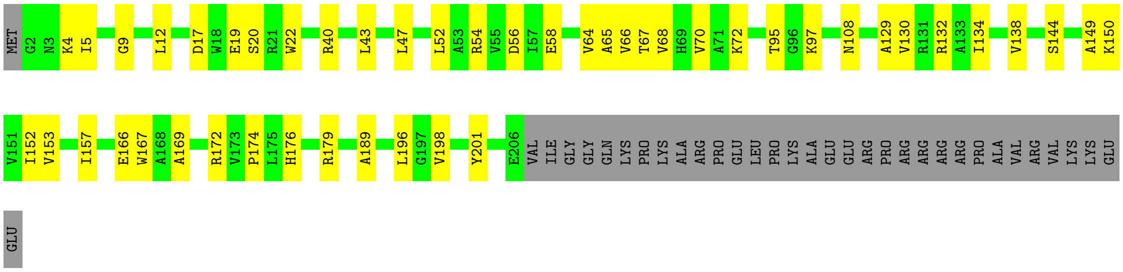
- Molecule 3: 30S ribosomal protein S3

Chain QC:



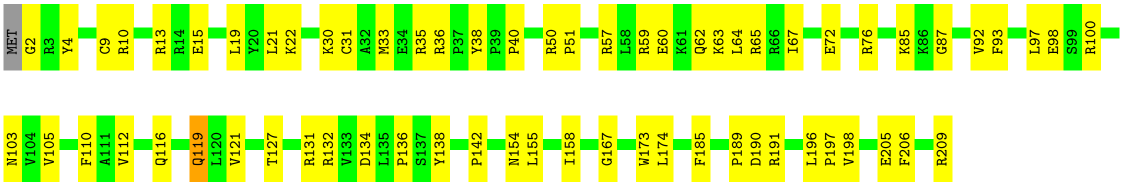
- Molecule 3: 30S ribosomal protein S3

Chain XC:



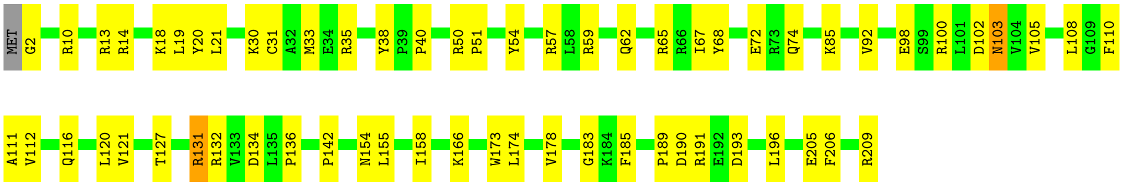
- Molecule 4: 30S ribosomal protein S4

Chain QD:



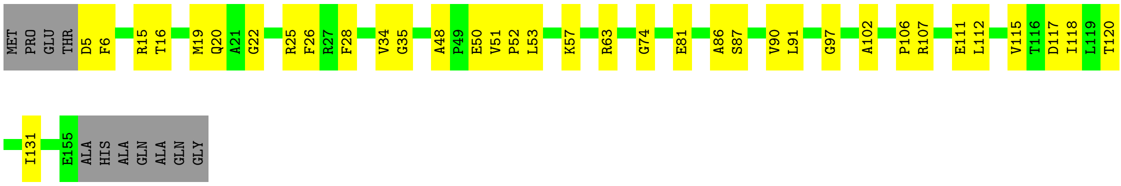
- Molecule 4: 30S ribosomal protein S4

Chain XD:



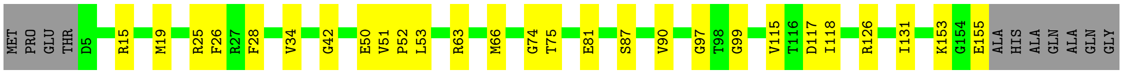
- Molecule 5: 30S ribosomal protein S5

Chain QE:



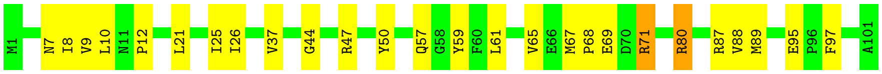
- Molecule 5: 30S ribosomal protein S5

Chain XE:



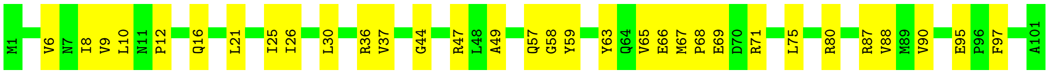
- Molecule 6: 30S ribosomal protein S6

Chain QF:

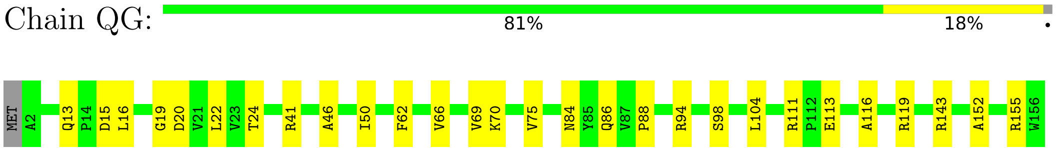


- Molecule 6: 30S ribosomal protein S6

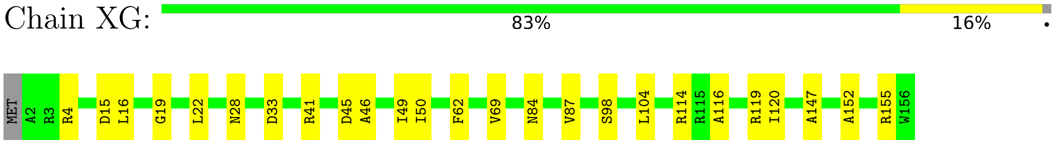
Chain XF:



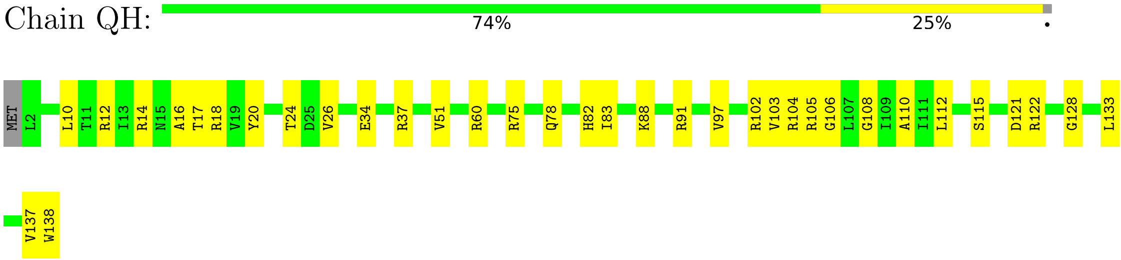
- Molecule 7: 30S ribosomal protein S7



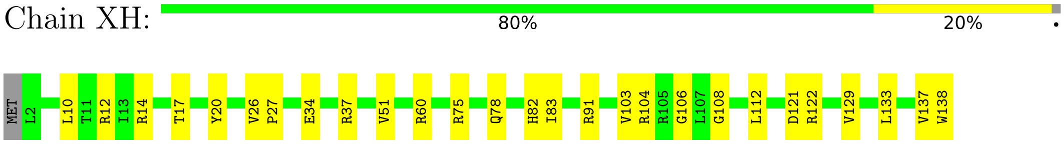
- Molecule 7: 30S ribosomal protein S7



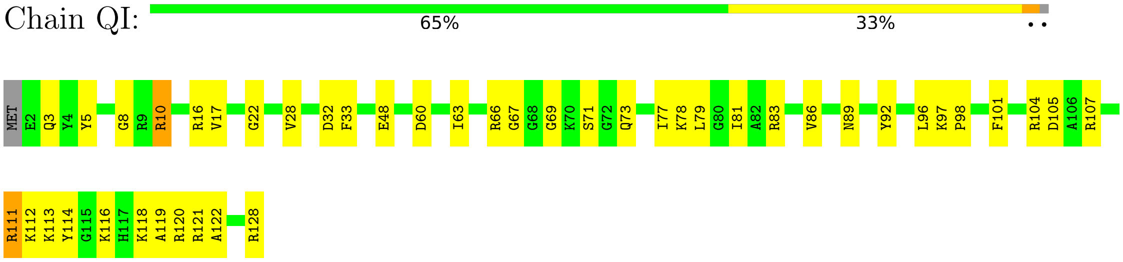
- Molecule 8: 30S ribosomal protein S8



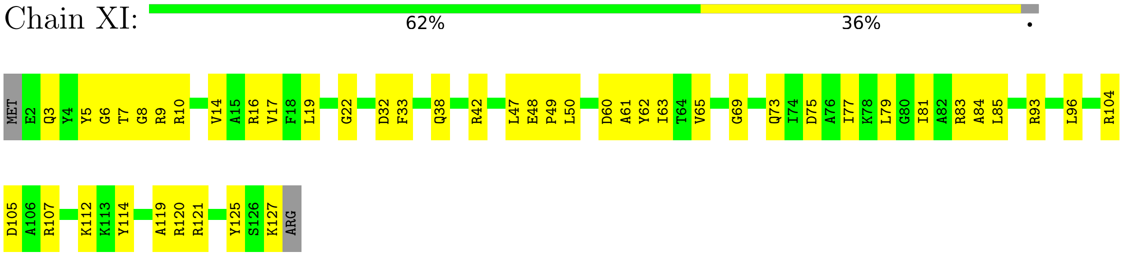
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9

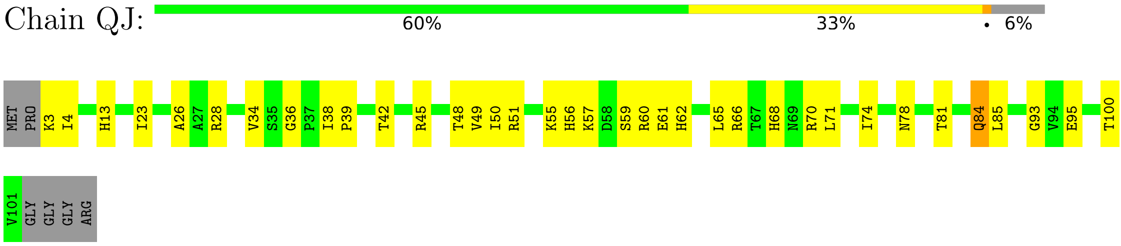


- Molecule 9: 30S ribosomal protein S9



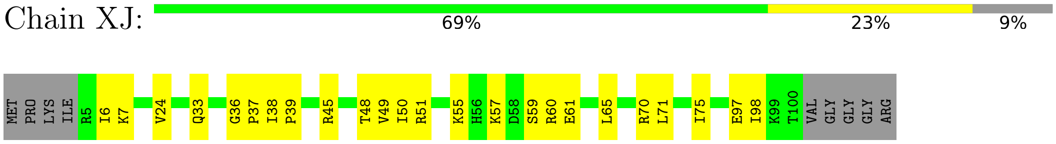
- Molecule 10: 30S ribosomal protein S10

Chain QJ:



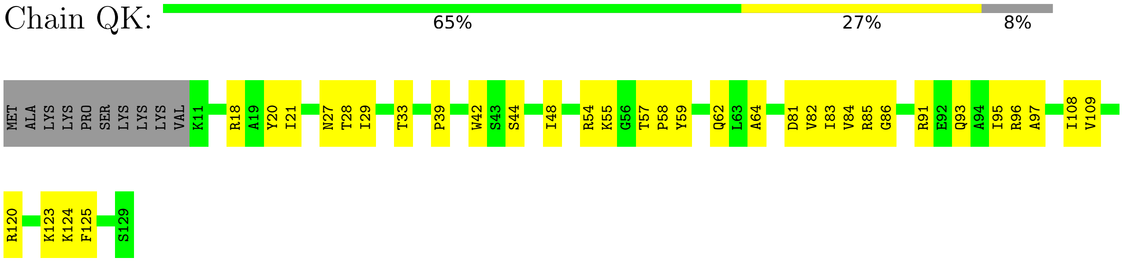
- Molecule 10: 30S ribosomal protein S10

Chain XJ:



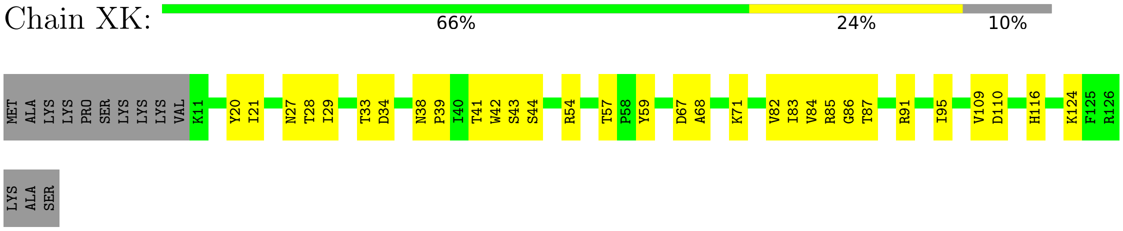
- Molecule 11: 30S ribosomal protein S11

Chain QK:



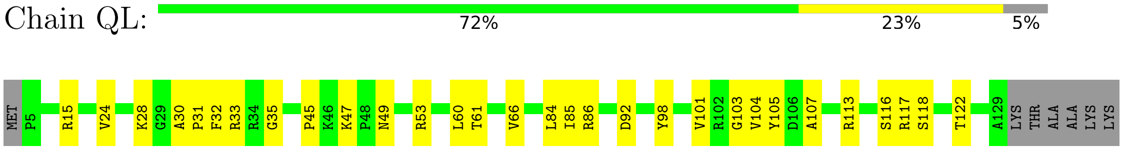
- Molecule 11: 30S ribosomal protein S11

Chain XK:



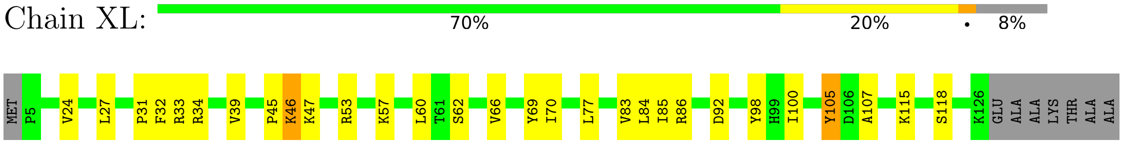
- Molecule 12: 30S ribosomal protein S12

Chain QL:



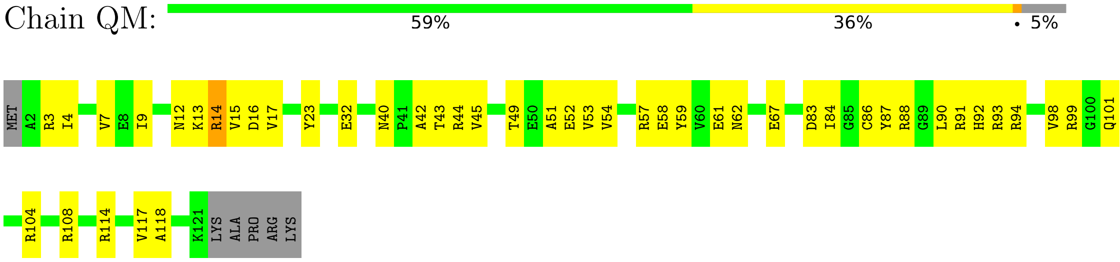
- Molecule 12: 30S ribosomal protein S12

Chain XL:



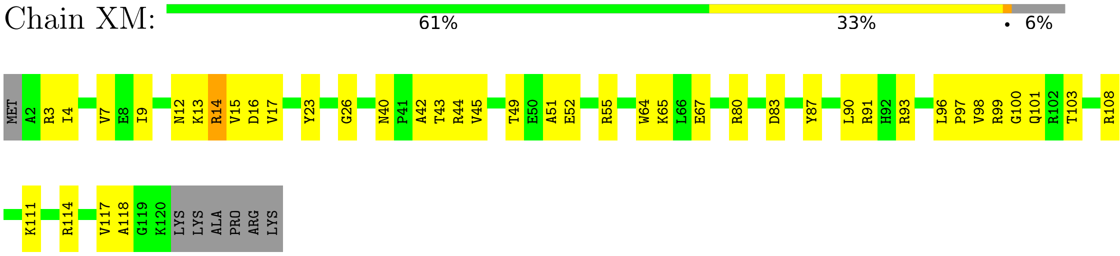
- Molecule 13: 30S ribosomal protein S13

Chain QM:



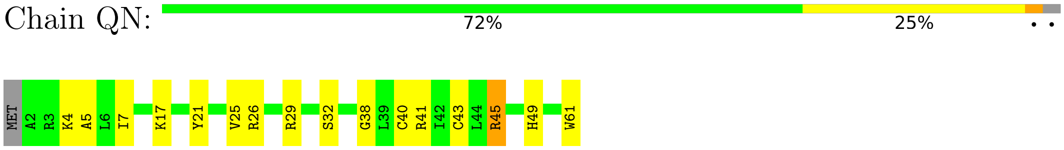
- Molecule 13: 30S ribosomal protein S13

Chain XM:



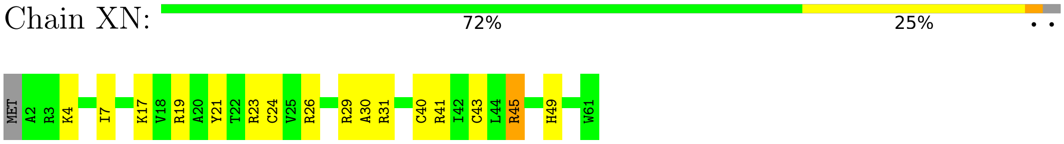
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:



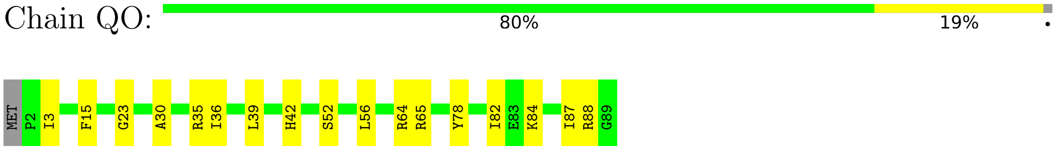
- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:



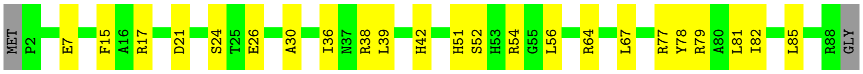
- Molecule 15: 30S ribosomal protein S15

Chain QO:



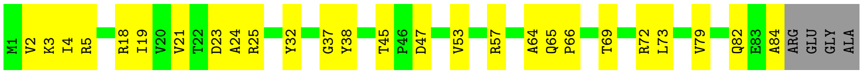
- Molecule 15: 30S ribosomal protein S15

Chain XO:



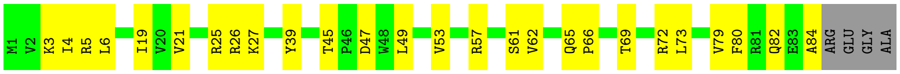
- Molecule 16: 30S ribosomal protein S16

Chain QP:



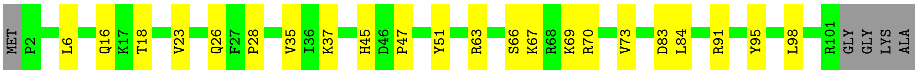
- Molecule 16: 30S ribosomal protein S16

Chain XP:



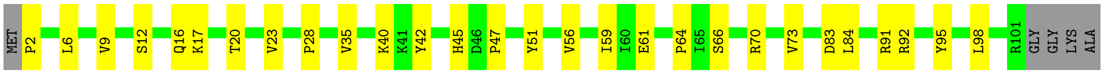
- Molecule 17: 30S ribosomal protein S17

Chain QQ:



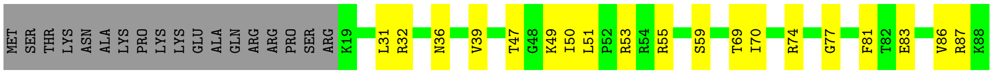
- Molecule 17: 30S ribosomal protein S17

Chain XQ:



- Molecule 18: 30S ribosomal protein S18

Chain QR:

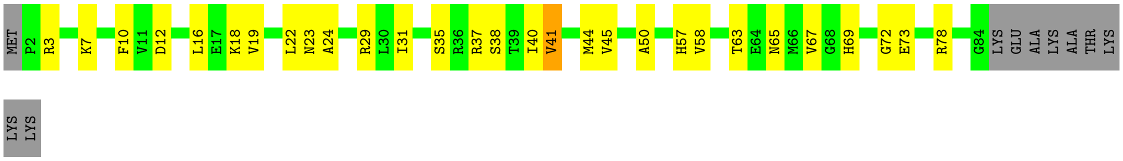


- Molecule 18: 30S ribosomal protein S18

Chain XR:

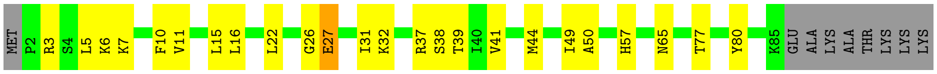
- Molecule 19: 30S ribosomal protein S19

Chain QS:



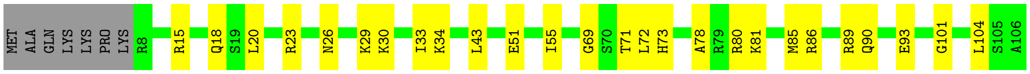
- Molecule 19: 30S ribosomal protein S19

Chain XS:



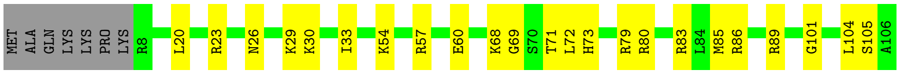
- Molecule 20: 30S ribosomal protein S20

Chain QT:



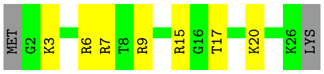
- Molecule 20: 30S ribosomal protein S20

Chain XT:



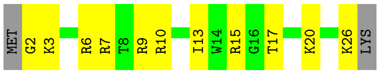
- Molecule 21: 30S ribosomal protein Thx

Chain QU:



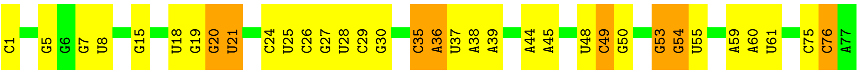
- Molecule 21: 30S ribosomal protein Thx

Chain XU:



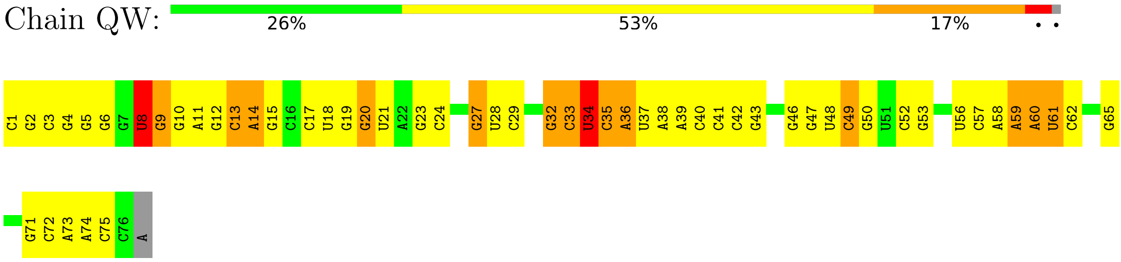
- Molecule 22: tRNA fMet

Chain QV:



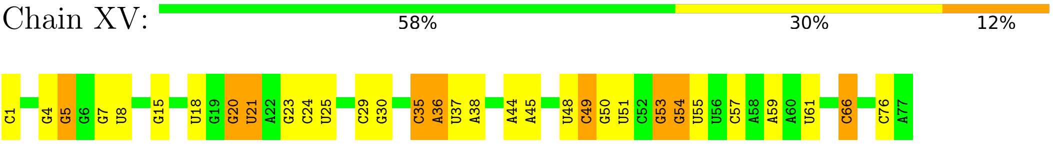
- Molecule 22: tRNA fMet

Chain QW:



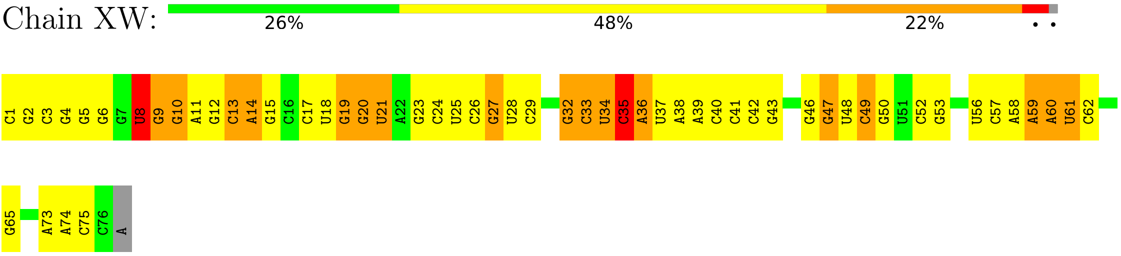
- Molecule 22: tRNA fMet

Chain XV:



- Molecule 22: tRNA fMet

Chain XW:

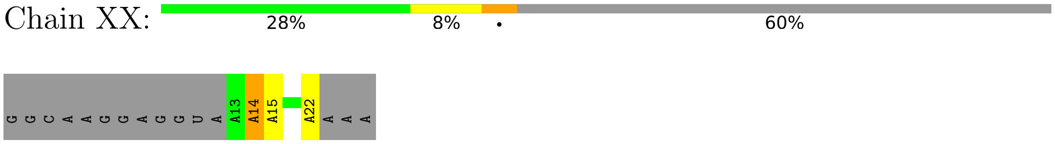


- Molecule 23: messenger RNA

Chain QX:

- Molecule 23: messenger RNA

Chain XX:

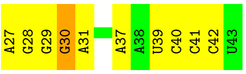


- Molecule 24: ASL Leu

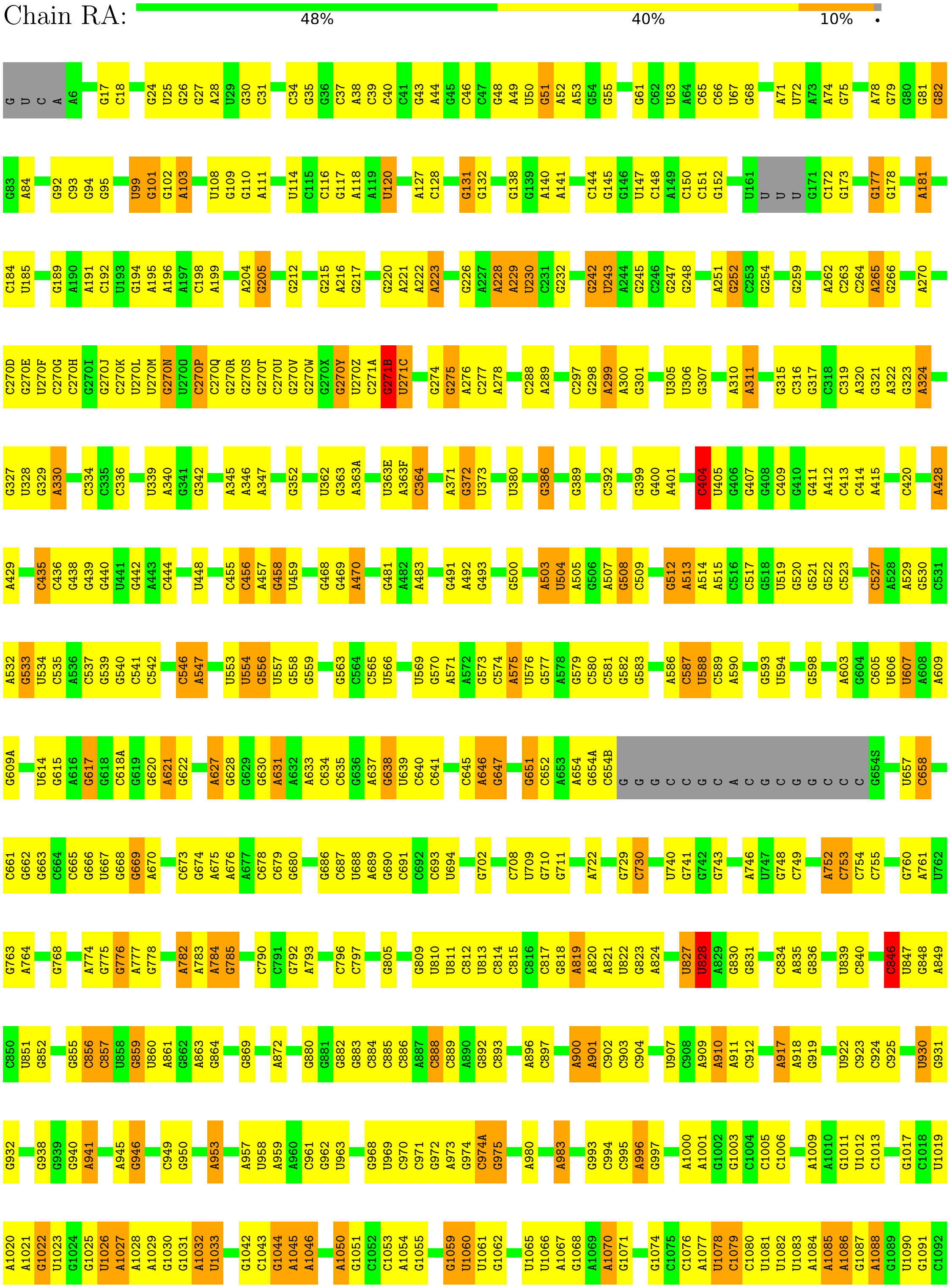
Chain QY:

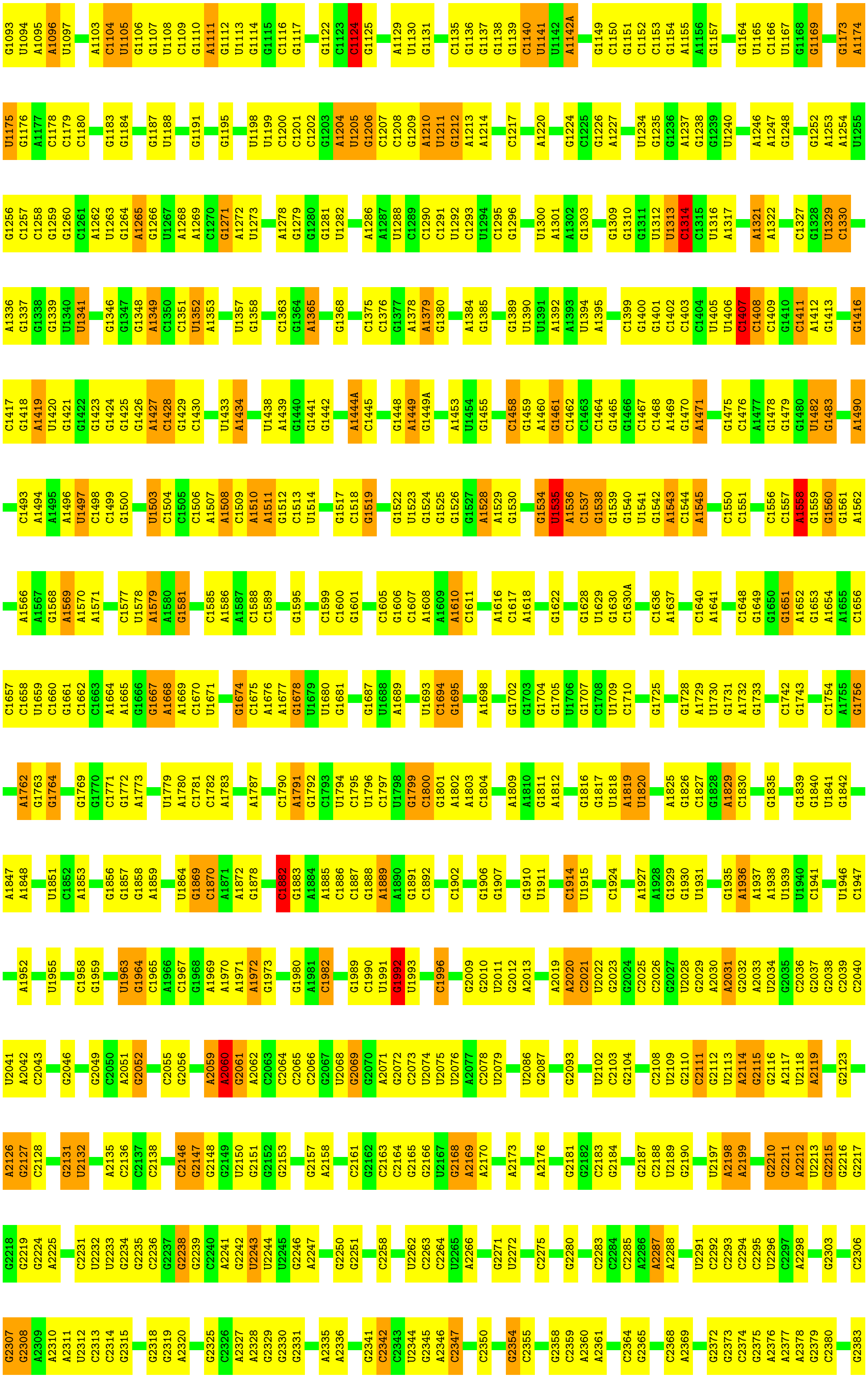
- Molecule 24: ASL Leu

Chain XY:



- Molecule 25: 23S rRNA

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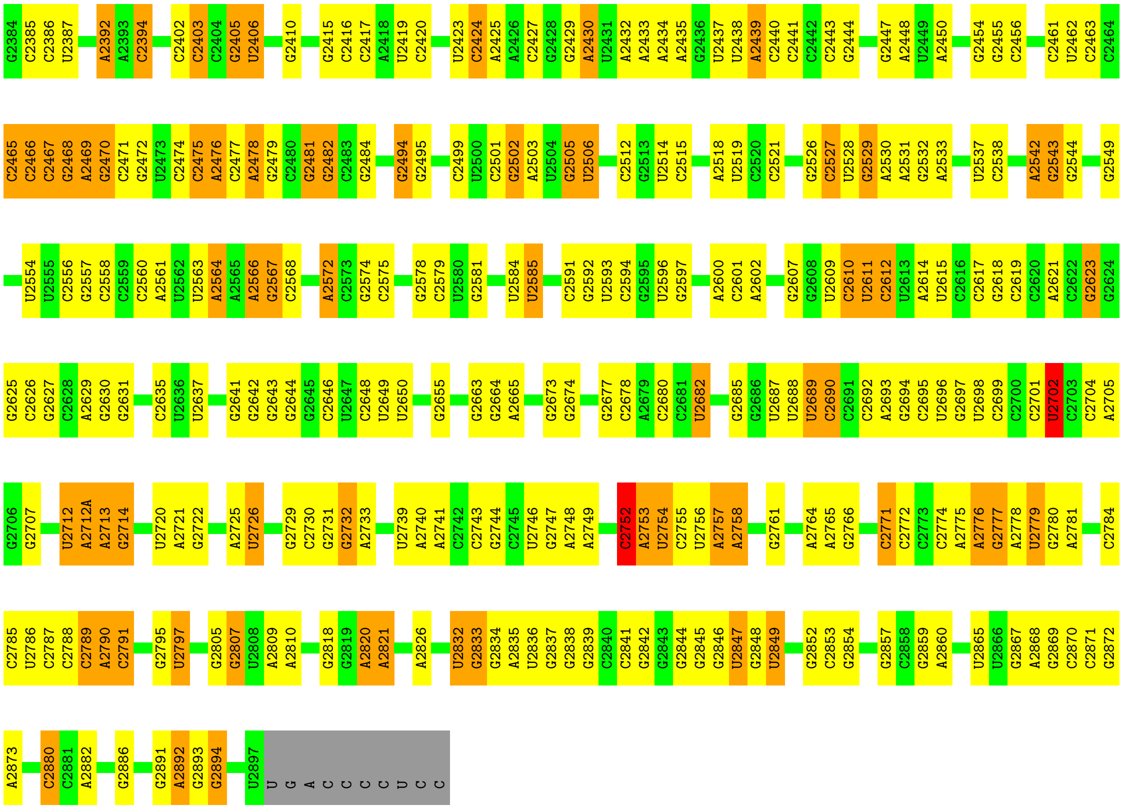
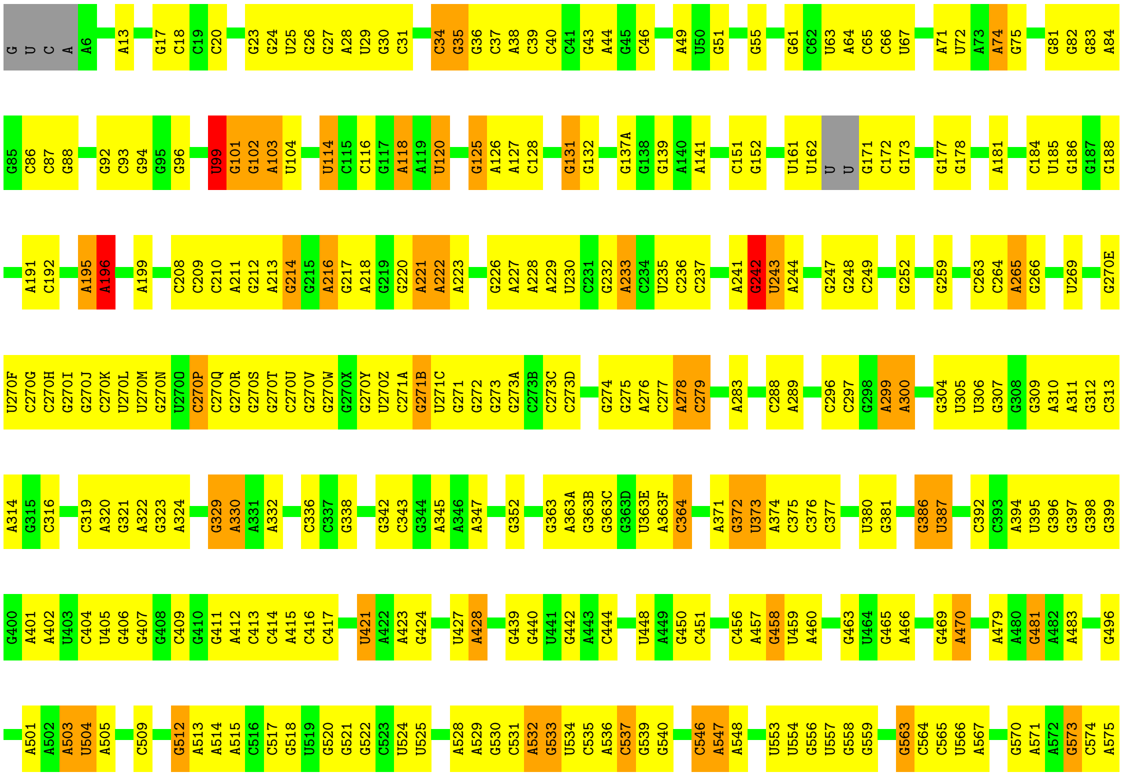
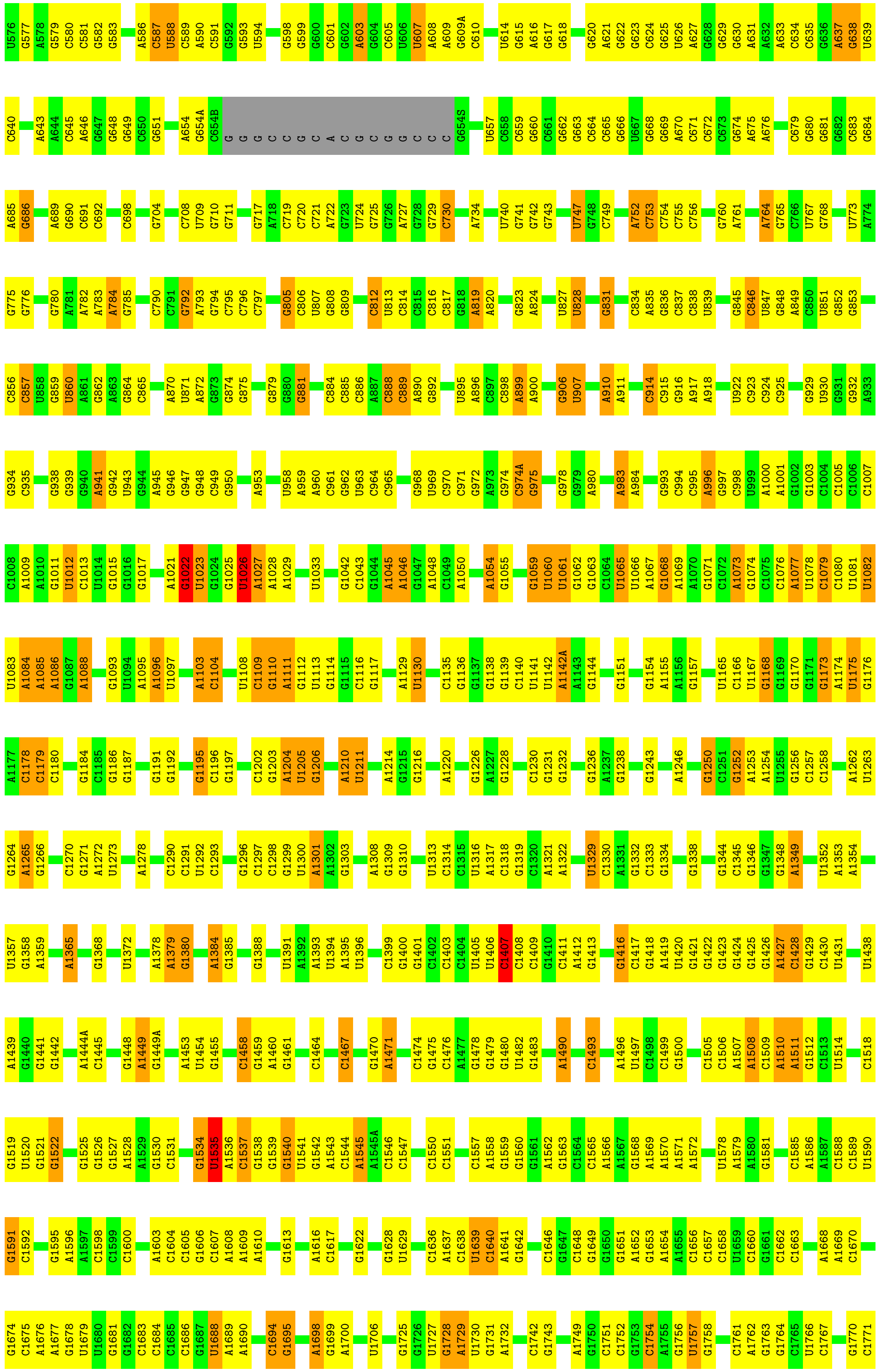


- Molecule 25: 23S rRNA

Chain YA:

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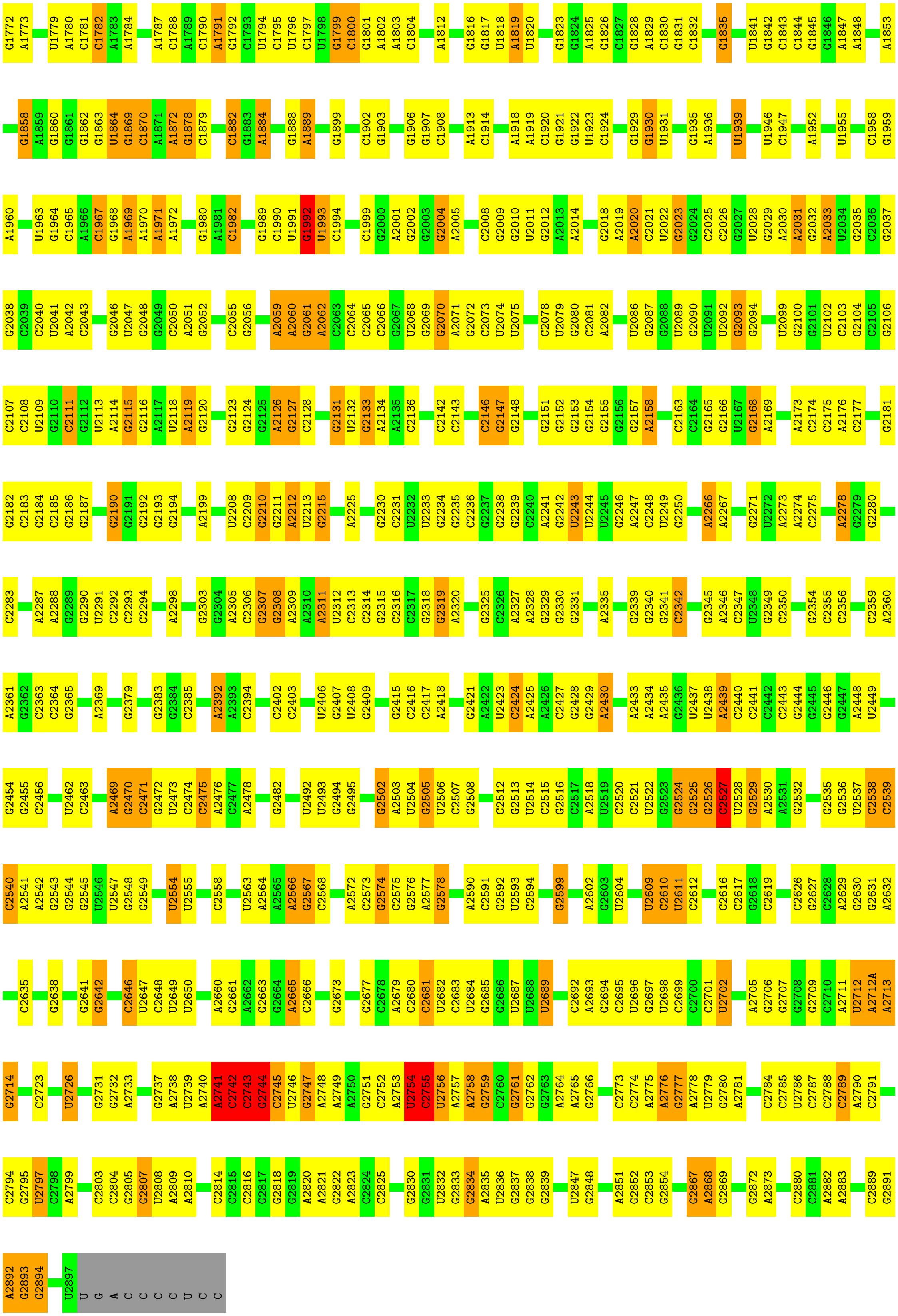
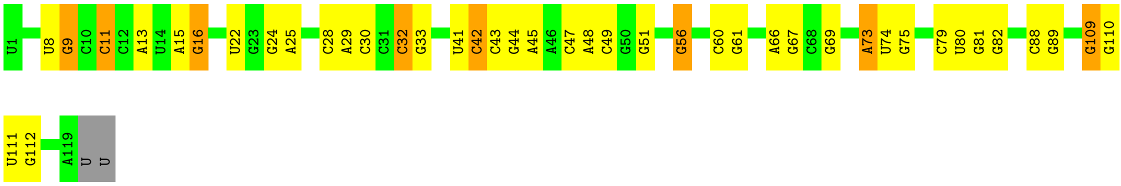


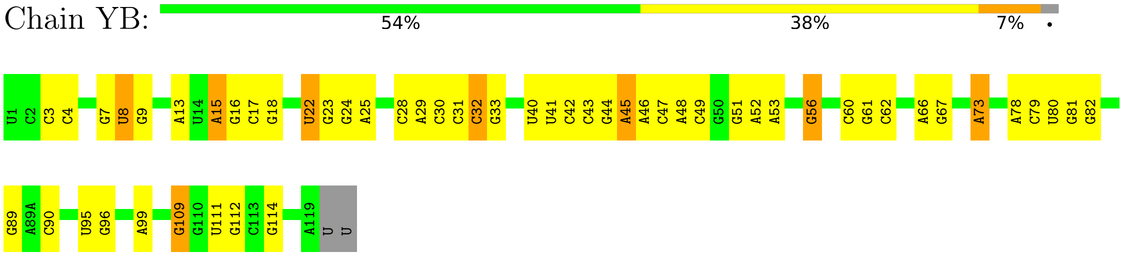
- Molecule 26: 5S rRNA

Chain RB:



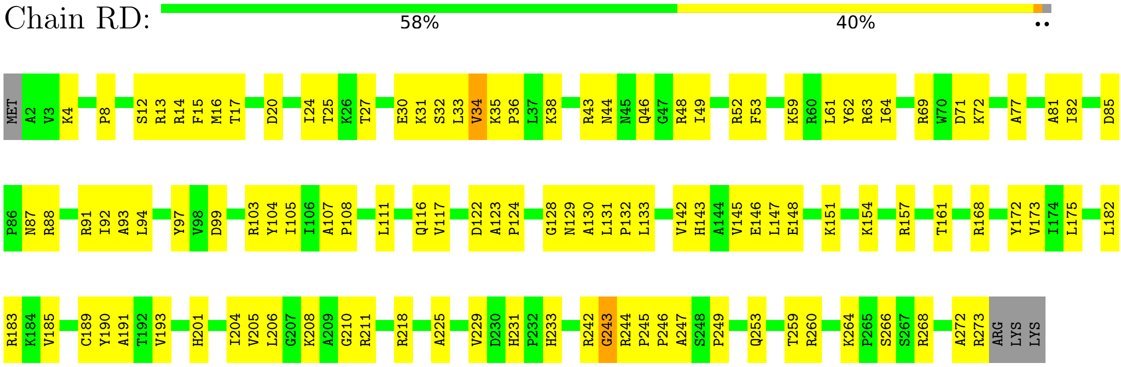
- Molecule 26: 5S rRNA

Chain YB:



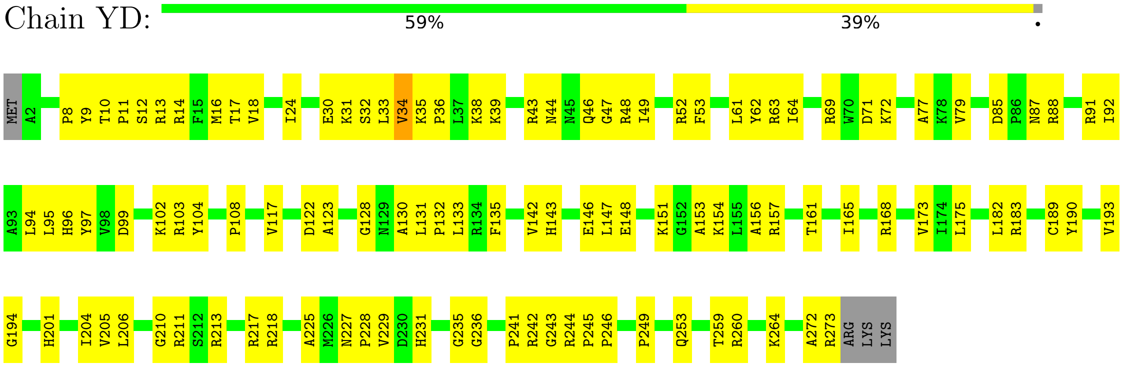
- Molecule 27: 50S ribosomal protein L2

Chain RD:



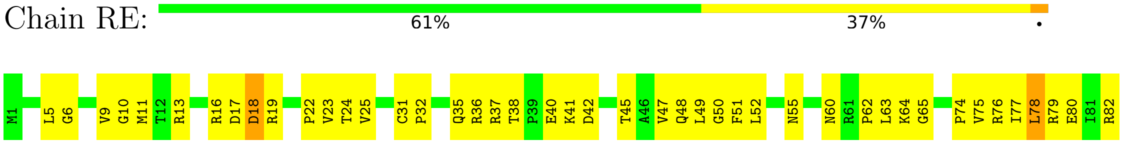
- Molecule 27: 50S ribosomal protein L2

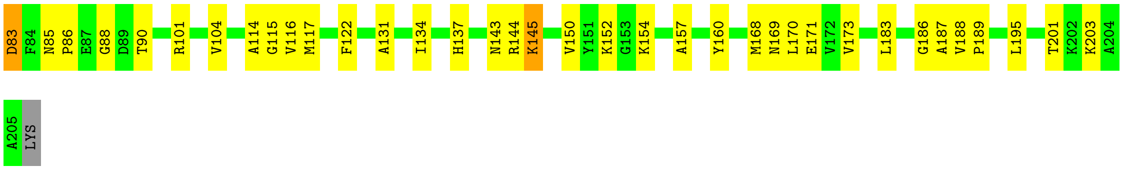
Chain YD:



- Molecule 28: 50S ribosomal protein L3

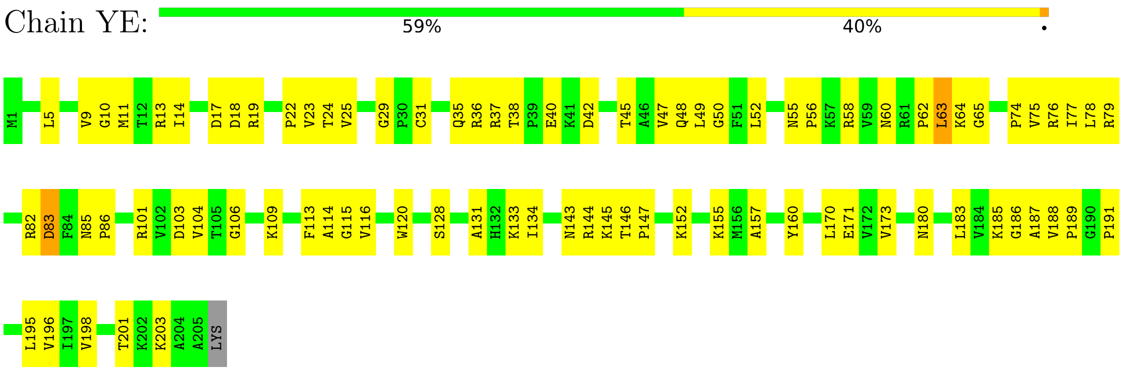
Chain RE:





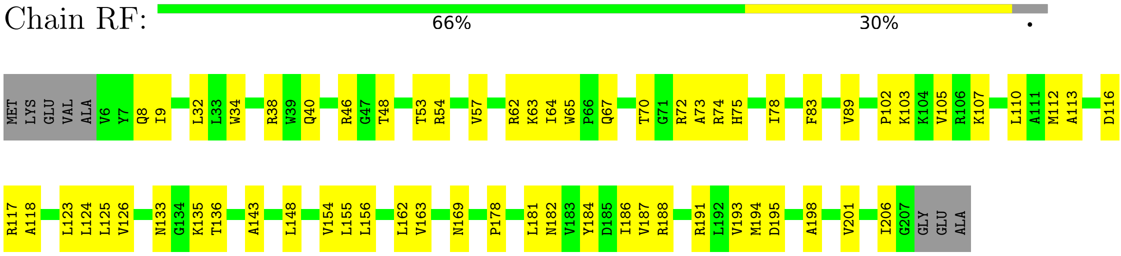
- Molecule 28: 50S ribosomal protein L3

Chain YE:



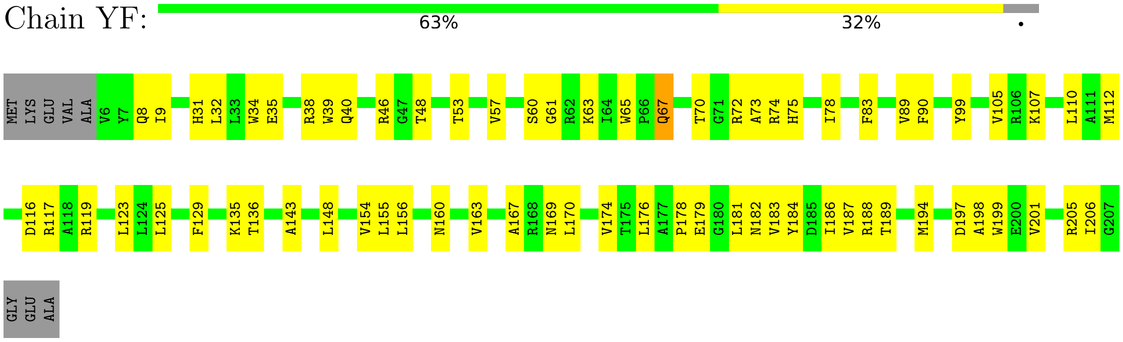
- Molecule 29: 50S ribosomal protein L4

Chain RF:



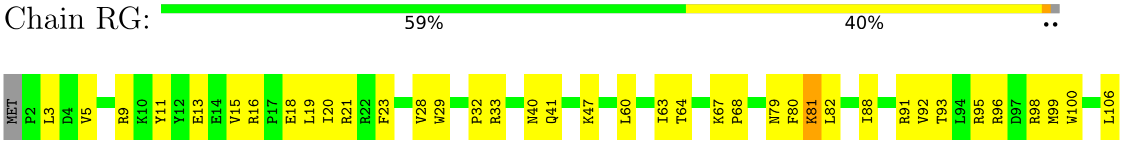
- Molecule 29: 50S ribosomal protein L4

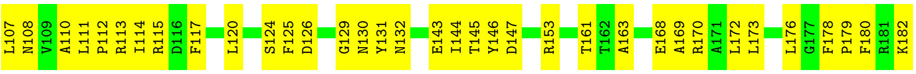
Chain YF:



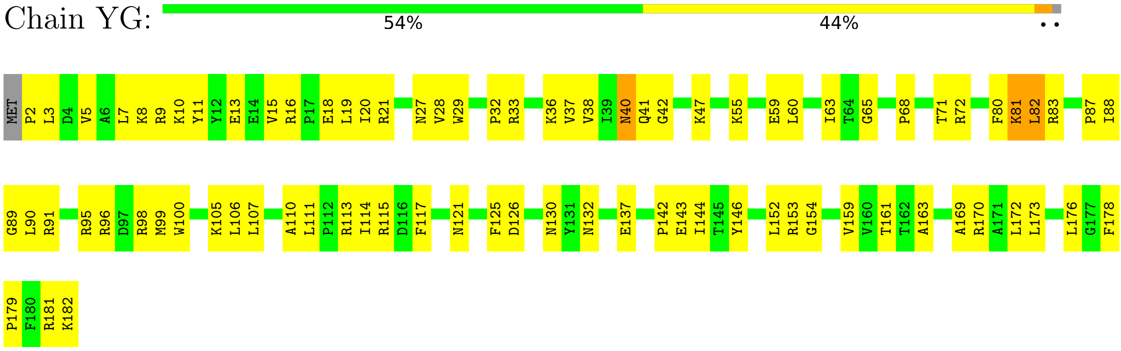
- Molecule 30: 50S ribosomal protein L5

Chain RG:

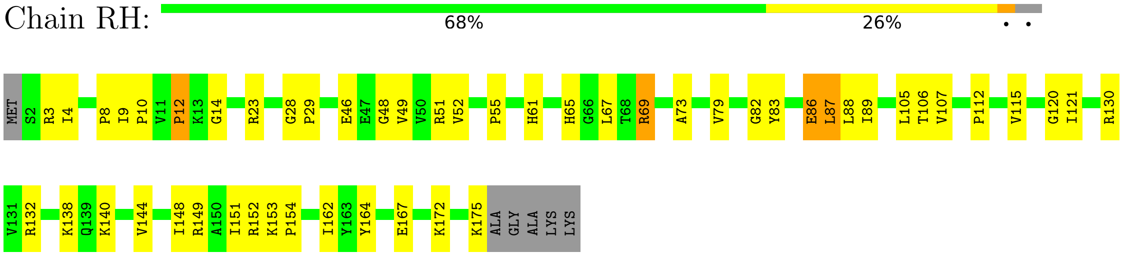




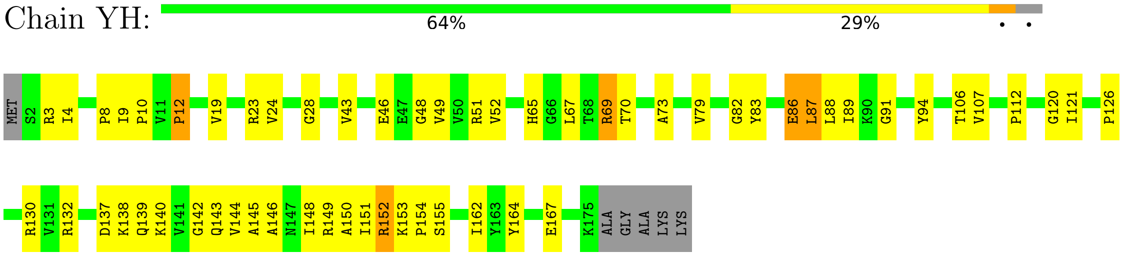
- Molecule 30: 50S ribosomal protein L5



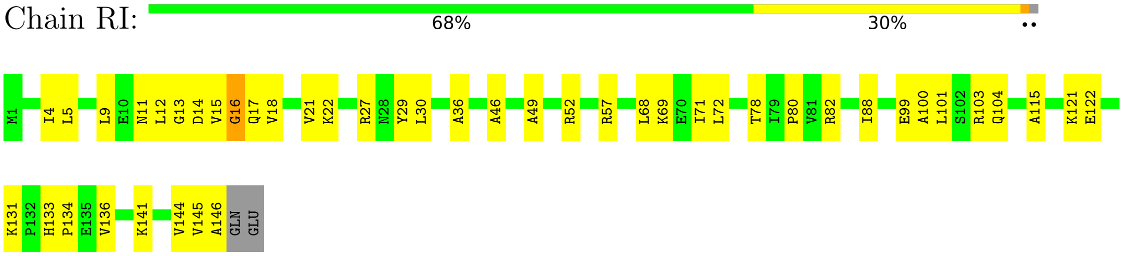
- Molecule 31: 50S ribosomal protein L6



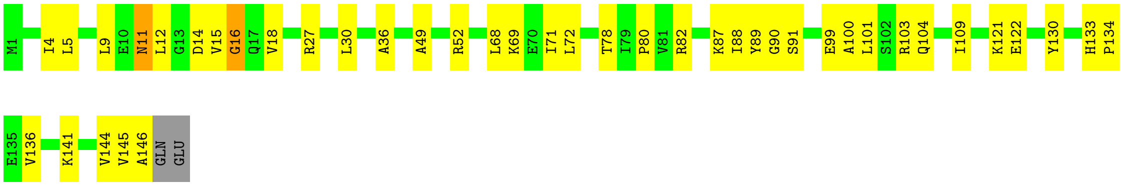
- Molecule 31: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L9

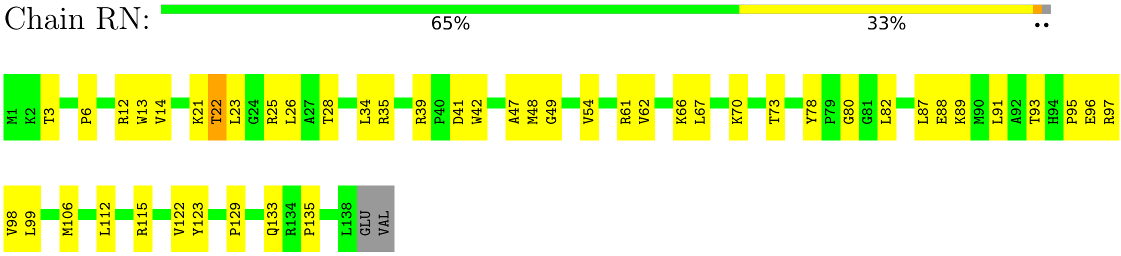


- Molecule 32: 50S ribosomal protein L9



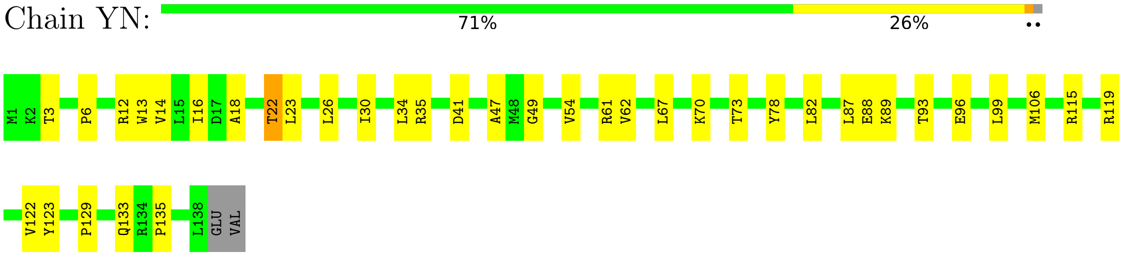
- Molecule 33: 50S ribosomal protein L13

Chain RN:



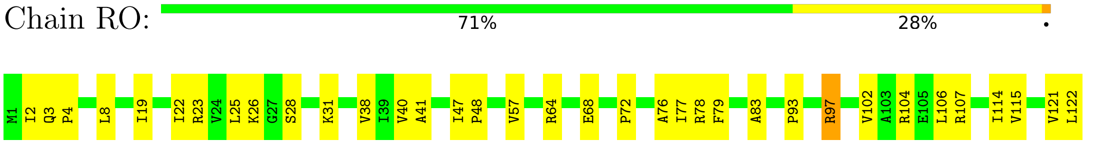
- Molecule 33: 50S ribosomal protein L13

Chain YN:



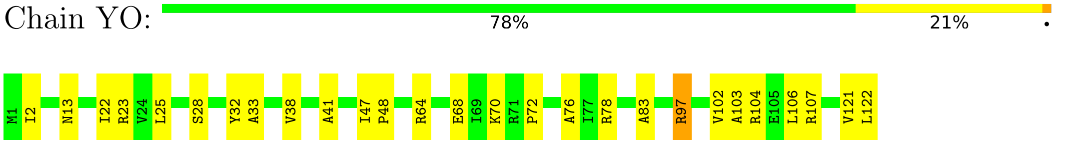
- Molecule 34: 50S ribosomal protein L14

Chain RO:



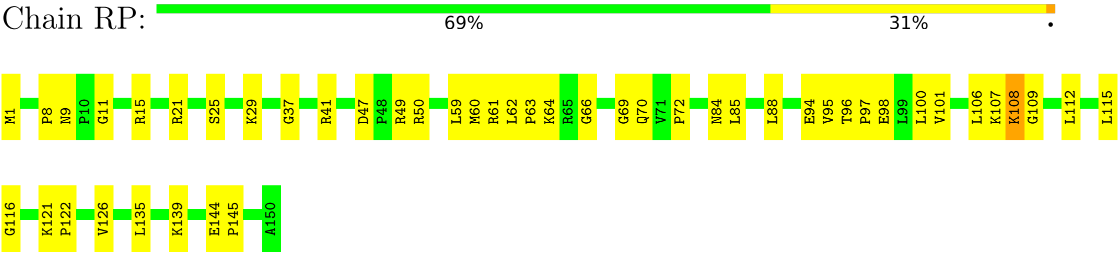
- Molecule 34: 50S ribosomal protein L14

Chain YO:

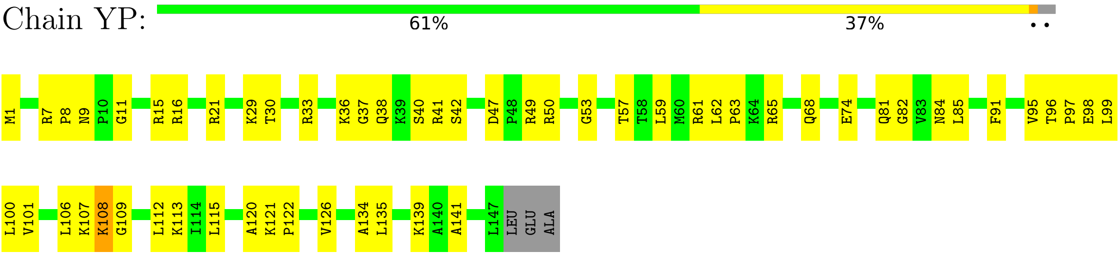


- Molecule 35: 50S ribosomal protein L15

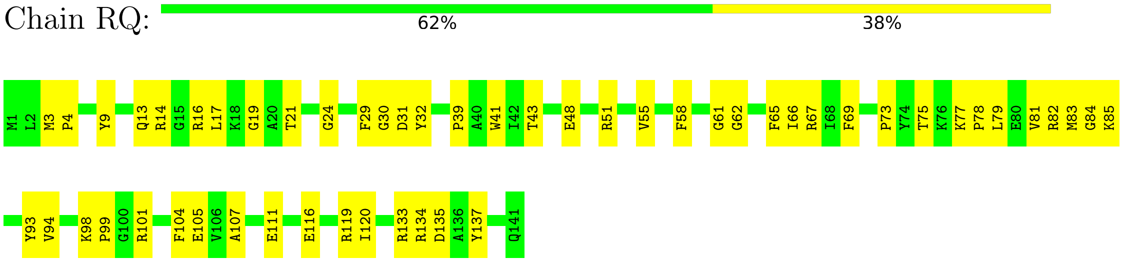
Chain RP:



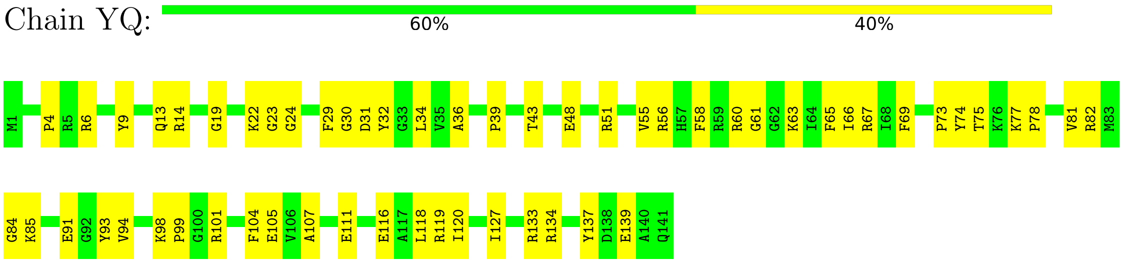
- Molecule 35: 50S ribosomal protein L15



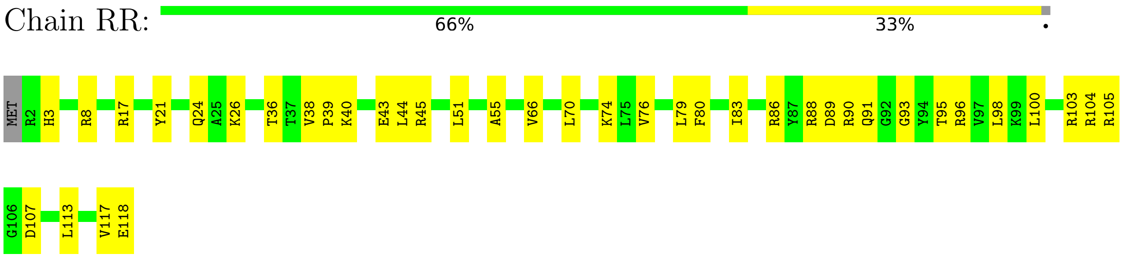
- Molecule 36: 50S ribosomal protein L16



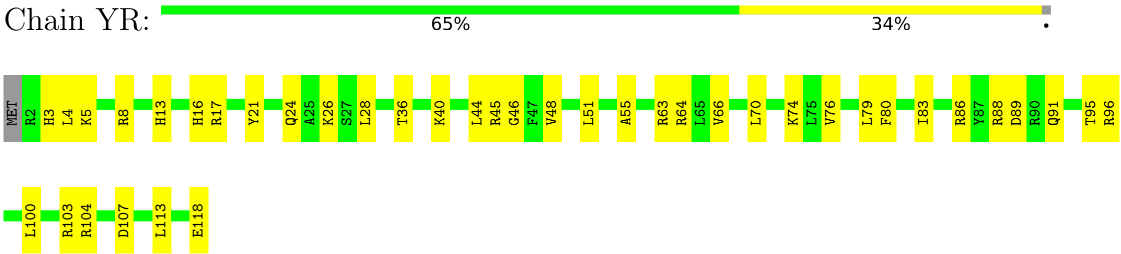
- Molecule 36: 50S ribosomal protein L16



- Molecule 37: 50S ribosomal protein L17

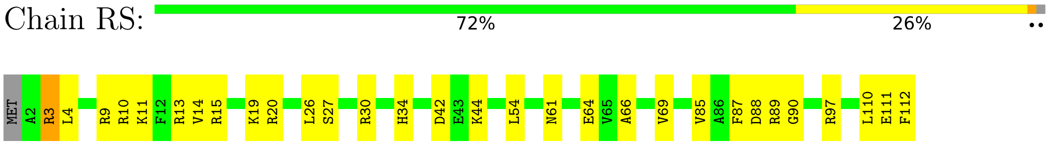


- Molecule 37: 50S ribosomal protein L17



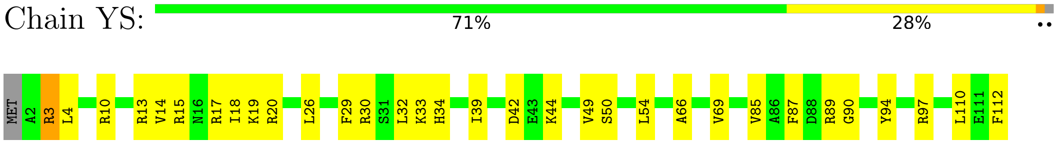
- Molecule 38: 50S ribosomal protein L18

Chain RS:



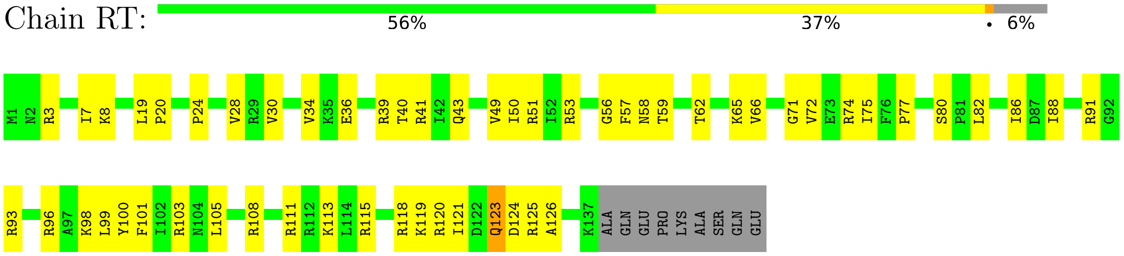
- Molecule 38: 50S ribosomal protein L18

Chain YS:



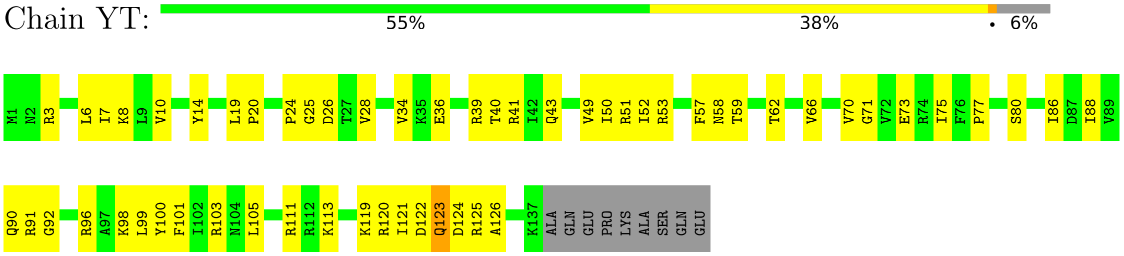
- Molecule 39: 50S ribosomal protein L19

Chain RT:



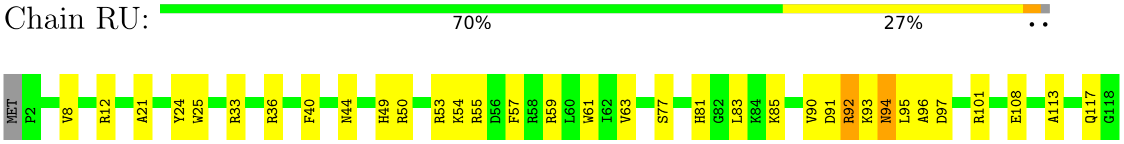
- Molecule 39: 50S ribosomal protein L19

Chain YT:



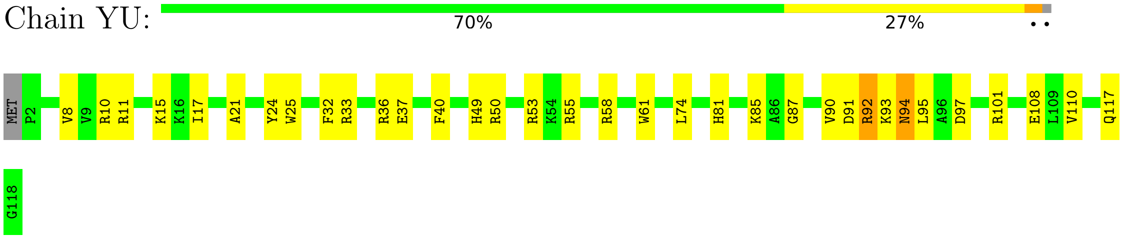
- Molecule 40: 50S ribosomal protein L20

Chain RU:



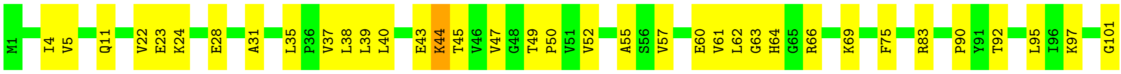
- Molecule 40: 50S ribosomal protein L20

Chain YU:



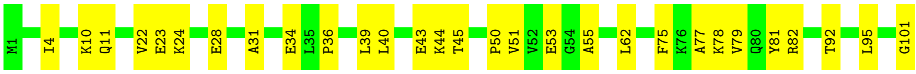
- Molecule 41: 50S ribosomal protein L21

Chain RV:



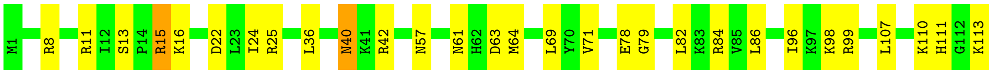
- Molecule 41: 50S ribosomal protein L21

Chain YV:



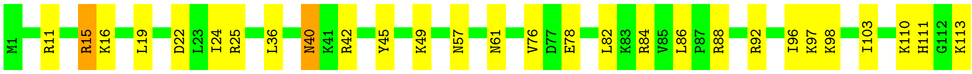
- Molecule 42: 50S ribosomal protein L22

Chain RW:



- Molecule 42: 50S ribosomal protein L22

Chain YW:

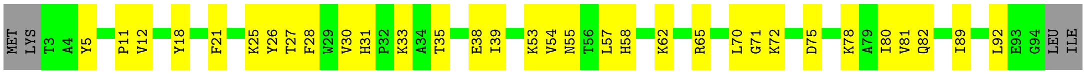


- Molecule 43: 50S ribosomal protein L23

Chain RX:

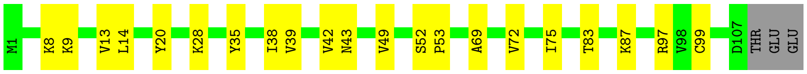
- Molecule 43: 50S ribosomal protein L23

Chain YX:



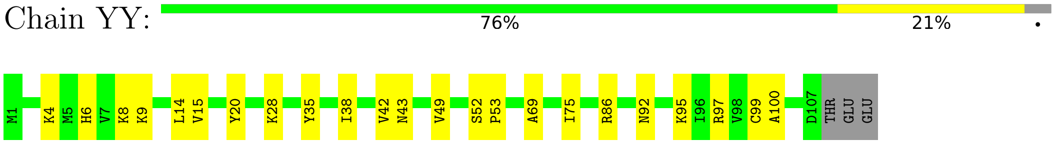
- Molecule 44: 50S ribosomal protein L24

Chain RY:



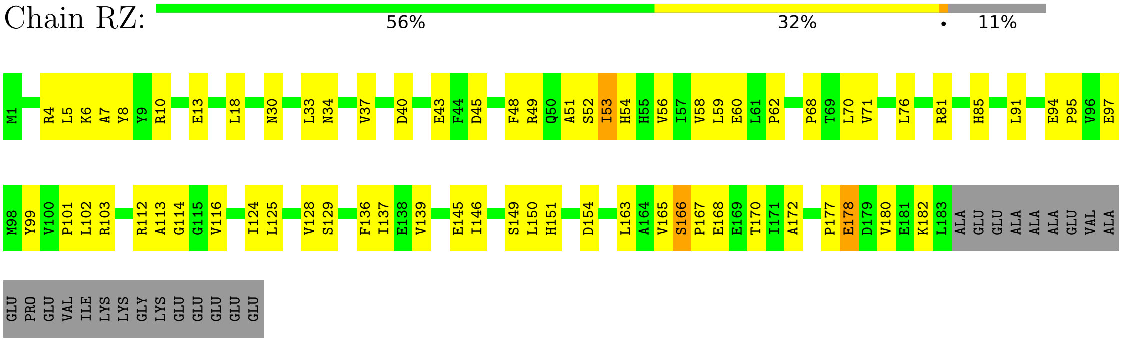
- Molecule 44: 50S ribosomal protein L24

Chain YY:



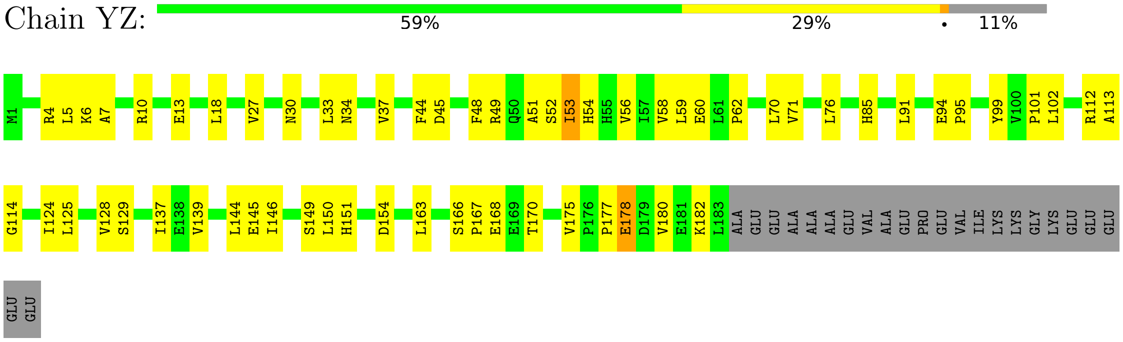
- Molecule 45: 50S ribosomal protein L25

Chain RZ:



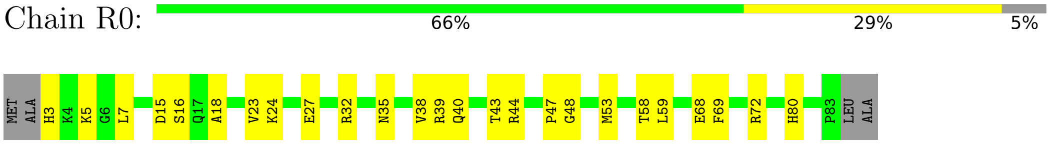
- Molecule 45: 50S ribosomal protein L25

Chain YZ:



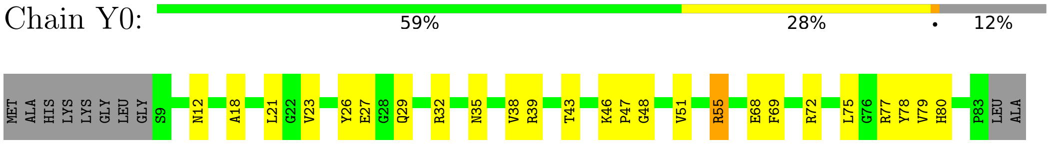
- Molecule 46: 50S ribosomal protein L27

Chain R0:



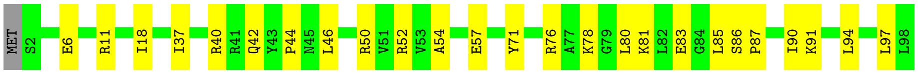
- Molecule 46: 50S ribosomal protein L27

Chain Y0:



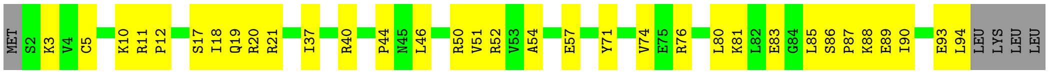
- Molecule 47: 50S ribosomal protein L28

Chain R1:



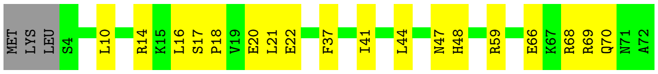
- Molecule 47: 50S ribosomal protein L28

Chain Y1:



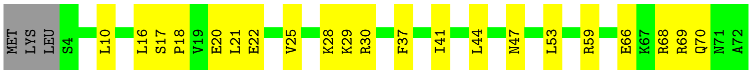
- Molecule 48: 50S ribosomal protein L29

Chain R2:



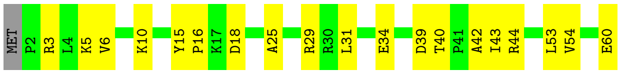
- Molecule 48: 50S ribosomal protein L29

Chain Y2:



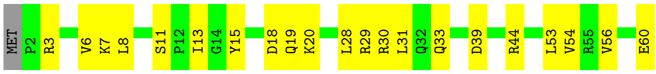
- Molecule 49: 50S ribosomal protein L30

Chain R3:



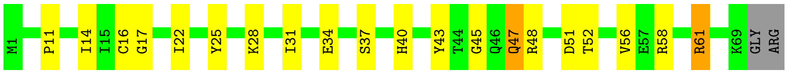
- Molecule 49: 50S ribosomal protein L30

Chain Y3:



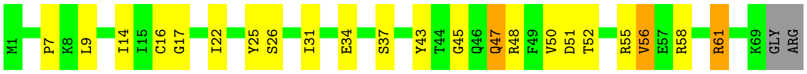
- Molecule 50: 50S ribosomal protein L31

Chain R4:



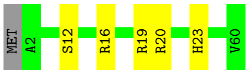
- Molecule 50: 50S ribosomal protein L31

Chain Y4:



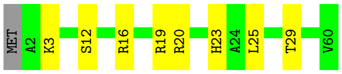
- Molecule 51: 50S ribosomal protein L32

Chain R5:



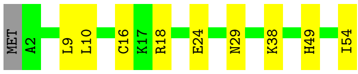
- Molecule 51: 50S ribosomal protein L32

Chain Y5:



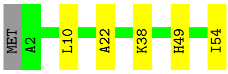
- Molecule 52: 50S ribosomal protein L33

Chain R6:



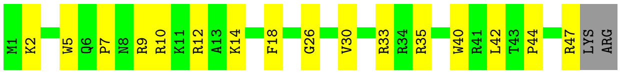
- Molecule 52: 50S ribosomal protein L33

Chain Y6:



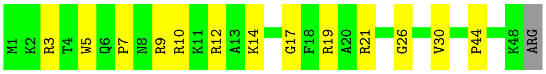
- Molecule 53: 50S ribosomal protein L34

Chain R7:



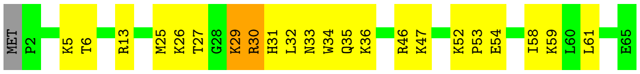
- Molecule 53: 50S ribosomal protein L34

Chain Y7:



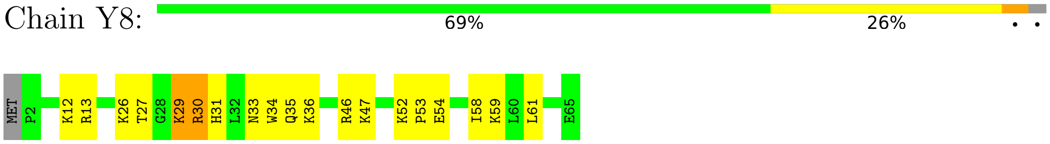
- Molecule 54: 50S ribosomal protein L35

Chain R8:



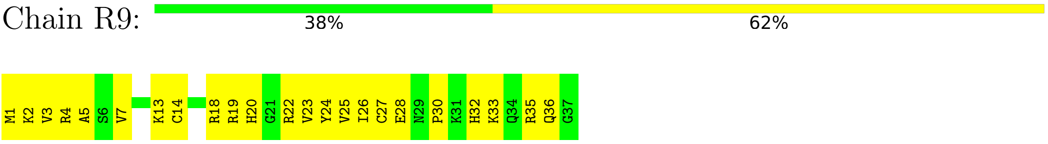
- Molecule 54: 50S ribosomal protein L35

Chain Y8:



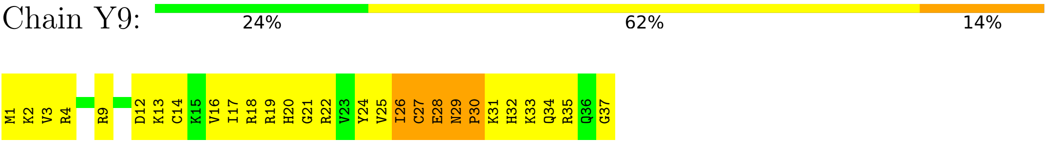
- Molecule 55: 50S ribosomal protein L36

Chain R9:



- Molecule 55: 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	210.70Å 446.14Å 616.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.57 – 3.68	Depositor
% Data completeness (in resolution range)	99.3 (145.57-3.68)	Depositor
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.228 , 0.274	Depositor
Wilson B-factor (Å^2)	89.7	Xtriage
Anisotropy	0.196	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	295575	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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	0.22	0/36097	0.80	21/56339 (0.0%)
1	XA	0.22	0/36100	0.82	27/56344 (0.0%)
2	QB	0.26	0/1942	0.50	0/2619
2	XB	0.25	0/1950	0.49	0/2630
3	QC	0.25	0/1629	0.47	0/2195
3	XC	0.24	0/1629	0.46	0/2195
4	QD	0.35	1/1733 (0.1%)	0.49	1/2318 (0.0%)
4	XD	0.26	0/1733	0.47	0/2318
5	QE	0.24	0/1171	0.48	0/1576
5	XE	0.25	0/1171	0.49	0/1576
6	QF	0.24	0/856	0.49	0/1154
6	XF	0.24	0/856	0.48	0/1154
7	QG	0.24	0/1276	0.43	0/1709
7	XG	0.24	0/1276	0.42	0/1709
8	QH	0.24	0/1128	0.45	0/1517
8	XH	0.24	0/1128	0.46	0/1517
9	QI	0.26	0/1029	0.50	0/1379
9	XI	0.27	0/1017	0.52	0/1365
10	QJ	0.45	1/814 (0.1%)	0.63	3/1095 (0.3%)
10	XJ	0.24	0/790	0.49	0/1063
11	QK	0.25	0/900	0.46	0/1213
11	XK	0.24	0/879	0.47	0/1187
12	QL	0.26	0/991	0.59	0/1327
12	XL	0.26	0/972	0.63	1/1301 (0.1%)
13	QM	0.25	0/965	0.53	0/1292
13	XM	0.24	0/956	0.53	0/1281
14	QN	0.26	0/501	0.46	0/664
14	XN	0.25	0/501	0.46	0/664
15	QO	0.24	0/745	0.43	0/992
15	XO	0.23	0/740	0.40	0/987
16	QP	0.24	0/721	0.49	0/970
16	XP	0.24	0/721	0.49	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.24	0/847	0.46	0/1131
17	XQ	0.24	0/847	0.45	0/1131
18	QR	0.24	0/579	0.48	0/768
18	XR	0.24	0/579	0.49	0/768
19	QS	0.25	0/680	0.57	0/915
19	XS	0.26	0/689	0.57	0/926
20	QT	0.25	0/765	0.52	0/1007
20	XT	0.25	0/765	0.50	0/1007
21	QU	0.22	0/221	0.45	0/288
21	XU	0.23	0/221	0.46	0/288
22	QV	0.33	1/1836 (0.1%)	0.83	0/2859
22	QW	0.26	0/1807	0.92	2/2816 (0.1%)
22	XV	0.33	1/1836 (0.1%)	0.84	1/2859 (0.0%)
22	XW	0.26	0/1807	0.91	2/2816 (0.1%)
23	QX	0.19	0/188	0.73	0/290
23	XX	0.19	0/235	0.73	0/364
24	QY	0.19	0/400	0.80	0/621
24	XY	0.20	0/400	0.79	0/621
25	RA	0.24	0/69521	0.83	34/108529 (0.0%)
25	YA	0.27	6/69543 (0.0%)	0.85	91/108563 (0.1%)
26	RB	0.22	0/2878	0.81	1/4490 (0.0%)
26	YB	0.23	0/2878	0.82	0/4490
27	RD	0.28	0/2165	0.56	0/2919
27	YD	0.28	0/2165	0.56	0/2919
28	RE	0.26	0/1601	0.60	1/2160 (0.0%)
28	YE	0.26	0/1601	0.60	0/2160
29	RF	0.26	0/1620	0.50	0/2194
29	YF	0.27	0/1620	0.51	0/2194
30	RG	0.26	0/1499	0.55	0/2016
30	YG	0.26	0/1499	0.54	0/2016
31	RH	0.26	0/1362	0.57	1/1841 (0.1%)
31	YH	0.29	0/1362	0.62	1/1841 (0.1%)
32	RI	0.25	0/1151	0.56	0/1558
32	YI	0.25	0/1151	0.56	0/1558
33	RN	0.26	0/1131	0.58	0/1525
33	YN	0.26	0/1131	0.56	0/1525
34	RO	0.26	0/943	0.48	0/1269
34	YO	0.26	0/943	0.50	0/1269
35	RP	0.27	0/1162	0.61	0/1544
35	YP	0.27	0/1139	0.62	0/1514
36	RQ	0.26	0/1143	0.55	0/1527
36	YQ	0.26	0/1143	0.57	0/1527
37	RR	0.26	0/974	0.52	0/1302

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\lvert Z\rvert$ >5	RMSZ	#$\lvert Z\rvert$ >5
37	YR	0.25	0/974	0.49	0/1302
38	RS	0.25	0/892	0.54	0/1187
38	YS	0.25	0/892	0.54	0/1187
39	RT	0.25	0/1155	0.53	0/1542
39	YT	0.25	0/1155	0.54	0/1542
40	RU	0.26	0/982	0.51	0/1306
40	YU	0.26	0/982	0.51	0/1306
41	RV	0.26	0/790	0.58	0/1057
41	YV	0.26	0/790	0.58	0/1057
42	RW	0.25	0/911	0.50	0/1220
42	YW	0.25	0/911	0.50	0/1220
43	RX	0.26	0/739	0.48	0/993
43	YX	0.26	0/739	0.48	0/993
44	RY	0.26	0/831	0.48	0/1108
44	YY	0.26	0/831	0.51	0/1108
45	RZ	0.25	0/1493	0.63	0/2026
45	YZ	0.26	0/1493	0.64	0/2026
46	R0	0.24	0/652	0.47	0/867
46	Y0	0.25	0/607	0.48	0/809
47	R1	0.27	0/770	0.55	0/1022
47	Y1	0.29	0/736	0.53	0/978
48	R2	0.24	0/583	0.49	0/771
48	Y2	0.24	0/583	0.51	0/771
49	R3	0.24	0/474	0.48	0/635
49	Y3	0.25	0/474	0.48	0/635
50	R4	0.25	0/578	0.53	0/776
50	Y4	0.27	0/578	0.54	0/776
51	R5	0.26	0/473	0.48	0/639
51	Y5	0.25	0/473	0.46	0/639
52	R6	0.22	0/460	0.47	0/613
52	Y6	0.22	0/460	0.47	0/613
53	R7	0.24	0/417	0.48	0/550
53	Y7	0.24	0/426	0.49	0/561
54	R8	0.33	0/525	0.67	0/691
54	Y8	0.33	0/525	0.67	0/691
55	R9	0.27	0/310	0.64	0/407
55	Y9	0.63	0/310	1.20	2/407 (0.5%)
All	All	0.25	10/319918 (0.0%)	0.76	189/478576 (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
28	YE	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	XV	1	C	OP3-P	-10.62	1.48	1.61
22	QV	1	C	OP3-P	-10.59	1.48	1.61
10	QJ	84	GLN	CD-NE2	9.70	1.57	1.32
4	QD	119	GLN	CB-CG	9.68	1.78	1.52
25	YA	2743	C	P-O5'	7.27	1.67	1.59

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	YA	2743	C	O4'-C1'-N1	17.82	122.46	108.20
25	YA	2755	C	OP1-P-OP2	12.48	138.32	119.60
25	YA	2754	U	OP1-P-O3'	-11.78	79.29	105.20
25	YA	2525	G	O4'-C1'-N9	11.27	117.22	108.20
25	YA	2754	U	OP2-P-O3'	-11.23	80.50	105.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	YE	146	THR	Peptide,Mainchain

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	QA	32246	0	16278	644	0
1	XA	32248	0	16279	617	0
2	QB	1907	0	1958	51	0
2	XB	1915	0	1969	47	0
3	QC	1605	0	1668	37	0
3	XC	1605	0	1668	33	0
4	QD	1703	0	1766	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	XD	1703	0	1767	46	0
5	QE	1155	0	1213	23	0
5	XE	1155	0	1213	18	0
6	QF	843	0	857	18	0
6	XF	843	0	857	22	0
7	QG	1257	0	1296	20	0
7	XG	1257	0	1296	18	0
8	QH	1108	0	1165	23	0
8	XH	1108	0	1165	20	0
9	QI	1010	0	1037	35	0
9	XI	998	0	1024	39	0
10	QJ	801	0	849	39	0
10	XJ	777	0	816	24	0
11	QK	885	0	904	33	0
11	XK	864	0	881	25	0
12	QL	975	0	1062	26	0
12	XL	956	0	1046	28	0
13	QM	955	0	1021	46	0
13	XM	946	0	1007	36	0
14	QN	492	0	529	15	0
14	XN	492	0	529	12	0
15	QO	734	0	771	13	0
15	XO	729	0	768	17	0
16	QP	705	0	725	19	0
16	XP	705	0	725	22	0
17	QQ	834	0	904	14	0
17	XQ	834	0	904	21	0
18	QR	574	0	644	19	0
18	XR	574	0	644	22	0
19	QS	665	0	686	26	0
19	XS	674	0	699	21	0
20	QT	763	0	861	17	0
20	XT	763	0	861	19	0
21	QU	217	0	234	6	0
21	XU	217	0	234	10	0
22	QV	1644	0	836	21	0
22	QW	1618	0	826	45	0
22	XV	1644	0	836	19	0
22	XW	1618	0	826	44	0
23	QX	169	0	86	0	0
23	XX	210	0	109	3	0
24	QY	358	0	183	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	XY	358	0	184	5	0
25	RA	62071	0	31291	1006	0
25	YA	62091	0	31297	1166	0
26	RB	2573	0	1306	29	0
26	YB	2573	0	1306	42	0
27	RD	2115	0	2195	101	0
27	YD	2115	0	2195	102	0
28	RE	1568	0	1634	67	0
28	YE	1568	0	1634	64	0
29	RF	1585	0	1632	53	0
29	YF	1585	0	1632	55	0
30	RG	1474	0	1535	58	0
30	YG	1474	0	1535	69	0
31	RH	1336	0	1418	37	0
31	YH	1336	0	1418	72	0
32	RI	1136	0	1223	28	0
32	YI	1136	0	1223	27	0
33	RN	1104	0	1180	30	0
33	YN	1104	0	1180	25	0
34	RO	933	0	996	32	0
34	YO	933	0	996	26	0
35	RP	1145	0	1228	48	0
35	YP	1122	0	1206	50	0
36	RQ	1122	0	1179	49	0
36	YQ	1122	0	1179	47	0
37	RR	960	0	1021	30	0
37	YR	960	0	1021	27	0
38	RS	882	0	943	23	0
38	YS	882	0	943	27	0
39	RT	1141	0	1202	46	0
39	YT	1141	0	1202	49	0
40	RU	964	0	1022	47	0
40	YU	964	0	1022	45	0
41	RV	779	0	852	31	0
41	YV	779	0	852	24	0
42	RW	900	0	964	21	1
42	YW	900	0	964	21	0
43	RX	725	0	778	17	0
43	YX	725	0	778	25	0
44	RY	818	0	910	13	0
44	YY	818	0	912	14	1
45	RZ	1461	0	1493	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	YZ	1461	0	1493	46	0
46	R0	643	0	667	20	0
46	Y0	599	0	617	23	0
47	R1	763	0	848	18	0
47	Y1	729	0	802	22	0
48	R2	581	0	629	12	0
48	Y2	581	0	629	14	0
49	R3	469	0	518	14	0
49	Y3	469	0	518	16	0
50	R4	565	0	557	18	0
50	Y4	565	0	558	25	0
51	R5	459	0	477	5	0
51	Y5	459	0	480	10	0
52	R6	453	0	474	7	0
52	Y6	453	0	473	3	0
53	R7	409	0	454	12	0
53	Y7	418	0	467	9	0
54	R8	517	0	582	22	0
54	Y8	517	0	582	21	0
55	R9	307	0	338	22	0
55	Y9	307	0	338	141	0
56	QA	68	0	0	0	0
56	QC	1	0	0	0	0
56	QE	1	0	0	0	0
56	QF	1	0	0	0	0
56	QH	1	0	0	0	0
56	QQ	1	0	0	0	0
56	QV	6	0	0	0	0
56	QY	1	0	0	0	0
56	R0	4	0	0	0	0
56	R1	2	0	0	0	0
56	R4	1	0	0	0	0
56	R8	1	0	0	0	0
56	R9	1	0	0	0	0
56	RA	508	0	0	0	0
56	RB	7	0	0	0	0
56	RE	2	0	0	0	0
56	RF	1	0	0	0	0
56	RN	1	0	0	0	0
56	RO	2	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	RR	1	0	0	0	0
56	RT	1	0	0	0	0
56	RU	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	82	0	0	0	0
56	XE	1	0	0	0	0
56	XL	1	0	0	0	0
56	XM	1	0	0	0	0
56	XQ	1	0	0	0	0
56	XS	1	0	0	0	0
56	XV	6	0	0	0	0
56	Y0	1	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YA	546	0	0	0	0
56	YB	12	0	0	0	0
56	YD	2	0	0	0	0
56	YE	2	0	0	0	0
56	YO	1	0	0	0	0
56	YP	3	0	0	0	0
56	YQ	3	0	0	0	0
56	YX	2	0	0	0	0
56	YY	1	0	0	0	0
57	QD	8	0	0	1	0
57	XD	8	0	0	0	0
58	QN	1	0	0	0	0
58	R4	1	0	0	0	0
58	R5	1	0	0	0	0
58	R6	1	0	0	0	0
58	R9	1	0	0	0	0
58	RY	1	0	0	0	0
58	XN	1	0	0	0	0
58	Y4	1	0	0	0	0
58	Y5	1	0	0	0	0
58	Y6	1	0	0	0	0
58	Y9	1	0	0	0	0
58	YY	1	0	0	0	0
All	All	295575	0	199664	5705	1

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 12.

The worst 5 of 5705 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)
4:QD:119:GLN:CG	4:QD:119:GLN:CB	1.78	1.55
25:YA:2755:C:H42	55:Y9:1:MET:HG2	1.08	1.16
25:RA:2747:G:N2	25:RA:2757:A:H62	1.43	1.15
25:YA:2742:C:H1'	55:Y9:26:ILE:HA	1.33	1.10
25:RA:2747:G:H21	25:RA:2757:A:N6	1.52	1.05

All (1) 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)
42:RW:63:ASP:OD1	44:YY:92:ASN:ND2[3_555]	2.18	0.02

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%)	202 (87%)	29 (12%)	2 (1%)	17	54
2	XB	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	34	69
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	190 (94%)	13 (6%)	0	100	100
4	QD	206/209 (99%)	189 (92%)	17 (8%)	0	100	100
4	XD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	QE	149/162 (92%)	141 (95%)	7 (5%)	1 (1%)	22	59
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	22	59
6	QF	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	XH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
9	QI	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
9	XI	124/128 (97%)	112 (90%)	12 (10%)	0	100	100
10	QJ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
10	XJ	94/105 (90%)	84 (89%)	10 (11%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	114/129 (88%)	108 (95%)	6 (5%)	0	100	100
12	QL	123/132 (93%)	105 (85%)	18 (15%)	0	100	100
12	XL	120/132 (91%)	97 (81%)	22 (18%)	1 (1%)	19	56
13	QM	118/126 (94%)	96 (81%)	21 (18%)	1 (1%)	19	56
13	XM	117/126 (93%)	94 (80%)	22 (19%)	1 (1%)	17	54
14	QN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	42
14	XN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	42
15	QO	86/89 (97%)	81 (94%)	5 (6%)	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%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
17	XQ	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
18	QR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
19	XS	82/93 (88%)	70 (85%)	11 (13%)	1 (1%)	13	49
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
21	QU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	XU	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
27	RD	270/276 (98%)	235 (87%)	33 (12%)	2 (1%)	22	59
27	YD	270/276 (98%)	239 (88%)	29 (11%)	2 (1%)	22	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	RE	203/206 (98%)	163 (80%)	37 (18%)	3 (2%)	10	44
28	YE	203/206 (98%)	158 (78%)	42 (21%)	3 (2%)	10	44
29	RF	200/210 (95%)	183 (92%)	17 (8%)	0	100	100
29	YF	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	15	51
30	RG	179/182 (98%)	149 (83%)	29 (16%)	1 (1%)	25	62
30	YG	179/182 (98%)	148 (83%)	29 (16%)	2 (1%)	14	50
31	RH	172/180 (96%)	141 (82%)	28 (16%)	3 (2%)	9	42
31	YH	172/180 (96%)	137 (80%)	32 (19%)	3 (2%)	9	42
32	RI	144/148 (97%)	119 (83%)	22 (15%)	3 (2%)	7	38
32	YI	144/148 (97%)	117 (81%)	24 (17%)	3 (2%)	7	38
33	RN	136/140 (97%)	117 (86%)	17 (12%)	2 (2%)	10	44
33	YN	136/140 (97%)	117 (86%)	18 (13%)	1 (1%)	22	59
34	RO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
34	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	RP	148/150 (99%)	114 (77%)	33 (22%)	1 (1%)	22	59
35	YP	145/150 (97%)	112 (77%)	32 (22%)	1 (1%)	22	59
36	RQ	139/141 (99%)	114 (82%)	24 (17%)	1 (1%)	22	59
36	YQ	139/141 (99%)	116 (84%)	21 (15%)	2 (1%)	11	45
37	RR	115/118 (98%)	102 (89%)	13 (11%)	0	100	100
37	YR	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	17	54
38	RS	109/112 (97%)	86 (79%)	23 (21%)	0	100	100
38	YS	109/112 (97%)	87 (80%)	22 (20%)	0	100	100
39	RT	135/146 (92%)	115 (85%)	18 (13%)	2 (2%)	10	44
39	YT	135/146 (92%)	115 (85%)	18 (13%)	2 (2%)	10	44
40	RU	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	17	54
40	YU	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	17	54
41	RV	99/101 (98%)	86 (87%)	12 (12%)	1 (1%)	15	51
41	YV	99/101 (98%)	86 (87%)	13 (13%)	0	100	100
42	RW	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
42	YW	111/113 (98%)	98 (88%)	13 (12%)	0	100	100
43	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	YX	90/96 (94%)	88 (98%)	2 (2%)	0	100	100
44	RY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
44	YY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	RZ	181/206 (88%)	144 (80%)	33 (18%)	4 (2%)	6	37
45	YZ	181/206 (88%)	142 (78%)	36 (20%)	3 (2%)	9	42
46	R0	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
46	Y0	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
47	R1	95/98 (97%)	85 (90%)	9 (10%)	1 (1%)	14	50
47	Y1	91/98 (93%)	77 (85%)	13 (14%)	1 (1%)	14	50
48	R2	67/72 (93%)	62 (92%)	4 (6%)	1 (2%)	10	44
48	Y2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	10	44
49	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
49	Y3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	R4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	44
50	Y4	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	10	44
51	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
51	Y5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
52	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	Y6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
53	R7	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
53	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
54	R8	62/65 (95%)	46 (74%)	14 (23%)	2 (3%)	4	31
54	Y8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	4	31
55	R9	35/37 (95%)	25 (71%)	10 (29%)	0	100	100
55	Y9	35/37 (95%)	18 (51%)	15 (43%)	2 (6%)	1	19
All	All	11452/12128 (94%)	10130 (88%)	1249 (11%)	73 (1%)	25	62

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	RE	18	ASP
31	RH	87	LEU
32	RI	15	VAL

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Mol	Chain	Res	Type
35	RP	108	LYS
39	RT	124	ASP

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%)	202 (100%)	1 (0%)	88	94
2	XB	204/220 (93%)	201 (98%)	3 (2%)	65	81
3	QC	159/188 (85%)	159 (100%)	0	100	100
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	180/181 (99%)	178 (99%)	2 (1%)	73	85
4	XD	180/181 (99%)	178 (99%)	2 (1%)	73	85
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	116 (100%)	0	100	100
6	QF	90/90 (100%)	88 (98%)	2 (2%)	52	72
6	XF	90/90 (100%)	90 (100%)	0	100	100
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	117 (99%)	1 (1%)	81	89
8	XH	118/119 (99%)	117 (99%)	1 (1%)	81	89
9	QI	98/99 (99%)	96 (98%)	2 (2%)	55	74
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55	74
14	XN	49/50 (98%)	48 (98%)	1 (2%)	55	74
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	85
17	XQ	95/97 (98%)	94 (99%)	1 (1%)	73	85
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	82
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	75 (99%)	1 (1%)	69	83
20	XT	76/82 (93%)	75 (99%)	1 (1%)	69	83
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
27	RD	214/218 (98%)	213 (100%)	1 (0%)	88	94
27	YD	214/218 (98%)	213 (100%)	1 (0%)	88	94
28	RE	165/166 (99%)	165 (100%)	0	100	100
28	YE	165/166 (99%)	165 (100%)	0	100	100
29	RF	161/166 (97%)	160 (99%)	1 (1%)	86	93
29	YF	161/166 (97%)	160 (99%)	1 (1%)	86	93
30	RG	155/156 (99%)	154 (99%)	1 (1%)	86	93
30	YG	155/156 (99%)	154 (99%)	1 (1%)	86	93
31	RH	145/148 (98%)	142 (98%)	3 (2%)	53	73
31	YH	145/148 (98%)	142 (98%)	3 (2%)	53	73
32	RI	122/124 (98%)	122 (100%)	0	100	100
32	YI	122/124 (98%)	122 (100%)	0	100	100
33	RN	117/119 (98%)	116 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	YN	117/119 (98%)	116 (99%)	1 (1%)	78	88
34	RO	100/100 (100%)	99 (99%)	1 (1%)	76	86
34	YO	100/100 (100%)	99 (99%)	1 (1%)	76	86
35	RP	116/116 (100%)	116 (100%)	0	100	100
35	YP	114/116 (98%)	114 (100%)	0	100	100
36	RQ	111/111 (100%)	111 (100%)	0	100	100
36	YQ	111/111 (100%)	111 (100%)	0	100	100
37	RR	100/101 (99%)	100 (100%)	0	100	100
37	YR	100/101 (99%)	100 (100%)	0	100	100
38	RS	87/88 (99%)	86 (99%)	1 (1%)	73	85
38	YS	87/88 (99%)	86 (99%)	1 (1%)	73	85
39	RT	120/127 (94%)	120 (100%)	0	100	100
39	YT	120/127 (94%)	120 (100%)	0	100	100
40	RU	93/94 (99%)	92 (99%)	1 (1%)	73	85
40	YU	93/94 (99%)	92 (99%)	1 (1%)	73	85
41	RV	82/82 (100%)	82 (100%)	0	100	100
41	YV	82/82 (100%)	82 (100%)	0	100	100
42	RW	92/92 (100%)	90 (98%)	2 (2%)	52	72
42	YW	92/92 (100%)	90 (98%)	2 (2%)	52	72
43	RX	74/78 (95%)	74 (100%)	0	100	100
43	YX	74/78 (95%)	74 (100%)	0	100	100
44	RY	88/91 (97%)	88 (100%)	0	100	100
44	YY	88/91 (97%)	88 (100%)	0	100	100
45	RZ	162/179 (90%)	161 (99%)	1 (1%)	86	93
45	YZ	162/179 (90%)	161 (99%)	1 (1%)	86	93
46	R0	65/67 (97%)	65 (100%)	0	100	100
46	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	79
47	R1	82/83 (99%)	82 (100%)	0	100	100
47	Y1	78/83 (94%)	78 (100%)	0	100	100
48	R2	64/67 (96%)	64 (100%)	0	100	100
48	Y2	64/67 (96%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	R3	51/52 (98%)	51 (100%)	0	100	100
49	Y3	51/52 (98%)	51 (100%)	0	100	100
50	R4	62/63 (98%)	61 (98%)	1 (2%)	62	79
50	Y4	62/63 (98%)	60 (97%)	2 (3%)	39	64
51	R5	51/52 (98%)	51 (100%)	0	100	100
51	Y5	51/52 (98%)	51 (100%)	0	100	100
52	R6	51/52 (98%)	51 (100%)	0	100	100
52	Y6	51/52 (98%)	51 (100%)	0	100	100
53	R7	40/42 (95%)	40 (100%)	0	100	100
53	Y7	41/42 (98%)	41 (100%)	0	100	100
54	R8	54/55 (98%)	54 (100%)	0	100	100
54	Y8	54/55 (98%)	54 (100%)	0	100	100
55	R9	34/34 (100%)	34 (100%)	0	100	100
55	Y9	34/34 (100%)	33 (97%)	1 (3%)	42	66
All	All	9687/10066 (96%)	9635 (100%)	52 (0%)	88	94

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	XB	144	ARG
27	YD	273	ARG
50	Y4	56	VAL
4	XD	103	ASN
14	XN	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
31	YH	74	ASN
44	YY	6	HIS
37	RR	71	GLN
39	RT	58	ASN
42	RW	111	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1508 (99%)	252 (16%)	34 (2%)
1	XA	1499/1508 (99%)	272 (18%)	37 (2%)
22	QV	76/77 (98%)	17 (22%)	3 (3%)
22	QW	75/77 (97%)	31 (41%)	2 (2%)
22	XV	76/77 (98%)	18 (23%)	3 (3%)
22	XW	75/77 (97%)	32 (42%)	2 (2%)
23	QX	7/25 (28%)	0	0
23	XX	9/25 (36%)	3 (33%)	0
24	QY	16/17 (94%)	2 (12%)	0
24	XY	16/17 (94%)	2 (12%)	0
25	RA	2879/2915 (98%)	599 (20%)	47 (1%)
25	YA	2880/2915 (98%)	570 (19%)	48 (1%)
26	RB	119/122 (97%)	17 (14%)	1 (0%)
26	YB	119/122 (97%)	19 (15%)	1 (0%)
All	All	9344/9482 (98%)	1834 (19%)	178 (1%)

5 of 1834 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	48	C

5 of 178 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	1027	C
25	YA	752	A
1	XA	1297	C
25	YA	195	A
25	YA	1026	U

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 1301 ligands modelled in this entry, 1299 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	$\#\|Z\| > 2$
57	SF4	XD	301	4	0,12,12	-	-	-		
57	SF4	QD	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**
57	SF4	XD	301	4	-	-	0/6/5/5
57	SF4	QD	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.

1 monomer is involved in 1 short contact:

Mol	**Chain**	**Res**	**Type**	**Clashes**	**Symm-Clashes**
57	QD	301	SF4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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.