wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 3, 2023 – 10:24 PM EDT

PDB ID	:	6OPE
Title	:	Crystal structure of tRNA^ Ala(GGC) U32-A38 bound to near-cognate 70S A site
Authors	:	Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on	:	2019-04-24
Resolution	:	3.10 Å(reported)

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

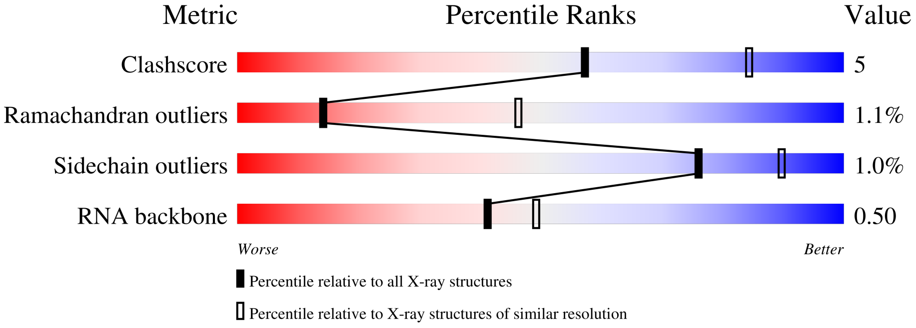
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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	1522	
1	XA	1522	
2	QB	256	
2	XB	256	
3	QC	239	
3	XC	239	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	QD	209	81% 17% •
4	XD	209	85% 14%
5	QE	162	75% 18% 7%
5	XE	162	83% 10% 7%
6	QF	101	87% 13%
6	XF	101	87% 13%
7	QG	156	88% 12% •
7	XG	156	91% 8% •
8	QH	138	88% 12%
8	XH	138	77% 23%
9	QI	128	74% 23% ••
9	XI	128	73% 27% •
10	QJ	105	70% 25% 6%
10	XJ	105	77% 17% 6%
11	QK	129	71% 21% 8%
11	XK	129	82% 9% • 8%
12	QL	131	75% 19% •• 5%
12	XL	131	76% 18% • 5%
13	QM	126	67% 28% • •
13	XM	126	78% 18% •
14	QN	61	75% 23% •
14	XN	61	85% 13% •
15	QO	89	84% 13% ••
15	XO	89	92% 7% •
16	QP	88	70% 24% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	XP	88	80% 15% • 5%
17	QQ	105	78% 17% 5%
17	XQ	105	83% 12% 5%
18	QR	88	63% 15% • 20%
18	XR	88	66% 14% 20%
19	QS	93	66% 23% • 10%
19	XS	93	69% 19% •• 10%
20	QT	106	85% 8% 7%
20	XT	106	75% 15% •• 7%
21	QU	27	70% 22% 7%
21	XU	27	78% 15% 7%
22	QV	77	70% 26% •
22	XV	77	74% 22% •
23	QX	19	26% 63% 5% 5%
23	XX	19	42% 42% 11% 5%
24	QY	76	42% 37% 17% • •
24	XY	76	54% 32% 12% ••
25	R0	85	78% 18% • •
25	Y0	85	74% 22% •
26	R1	98	81% 16% • •
26	Y1	98	80% 19% •
27	R2	72	65% 29% • •
27	Y2	72	69% 26% •
28	R3	60	83% 15% •
28	Y3	60	87% 12% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	R4	71	
29	Y4	71	
30	R5	60	
30	Y5	60	
31	R6	54	
31	Y6	54	
32	R7	49	
32	Y7	49	
33	R8	65	
33	Y8	65	
34	R9	37	
34	Y9	37	
35	RA	2915	
35	YA	2915	
36	RB	122	
36	YB	122	
37	RD	276	
37	YD	276	
38	RE	206	
38	YE	206	
39	RF	210	
39	YF	210	
40	RG	182	
40	YG	182	
41	RH	180	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	YH	180	
42	RI	148	
42	YI	148	
43	RN	140	
43	YN	140	
44	RO	122	
44	YO	122	
45	RP	150	
45	YP	150	
46	RQ	141	
46	YQ	141	
47	RR	118	
47	YR	118	
48	RS	112	
48	YS	112	
49	RT	146	
49	YT	146	
50	RU	118	
50	YU	118	
51	RV	101	
51	YV	101	
52	RW	113	
52	YW	113	
53	RX	96	
53	YX	96	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	RY	110	
54	YY	110	
55	RZ	206	
55	YZ	206	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 294981 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
1	QA	1500	Total	C	N	O	P	0	0	0
			32247	14353	5981	10414	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	XB	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	138	Total 1116	C 705	N 215	O 193	S 3	0	0	0
8	XH	138	Total 1116	C 705	N 215	O 193	S 3	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	QI	127	Total 1010	C 639	N 197	O 174	0	0	0
9	XI	127	Total 1010	C 639	N 197	O 174	0	0	0

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	QM	121	964	597	199	166	2	0	0	0
13	XM	121	964	597	199	166	2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	QO	88	734	459	147	126	2	0	0	0
15	XO	88	734	459	147	126	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	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- 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	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

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

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

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

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

- 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	0	0	0
			763	470	162	129	2			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- 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 P-site tRNAfMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total 1640	C 732	N 297	O 535	P 76	0	0	0
22	XV	77	Total 1640	C 732	N 297	O 535	P 76	0	0	0

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	18	Total 396	C 177	N 82	O 119	P 18	0	0	0
23	XX	18	Total 396	C 177	N 82	O 119	P 18	0	0	0

- Molecule 24 is a RNA chain called A-site tRNAAla(GGC) U32-A38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	75	Total 1602	C 714	N 288	O 525	P 75	0	0	0
24	XY	75	Total 1602	C 714	N 288	O 525	P 75	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	82	Total 648	C 401	N 138	O 108	S 1	0	0	0
25	Y0	82	Total 648	C 401	N 138	O 108	S 1	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R1	97	Total 763	C 481	N 150	O 131	S 1	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	Y1	97	Total C N O S 763 481 150 131 1	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L29.

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

- Molecule 28 is a protein called 50S ribosomal protein L30.

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

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	R4	71	Total C N O S 581 364 108 104 5	0	0	0
29	Y4	71	Total C N O S 581 364 108 104 5	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	R6	49	Total C N O S 424 264 87 69 4	0	0	0
31	Y6	49	Total C N O S 424 264 87 69 4	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
32	R7	49	Total C N O S 430 263 108 57 2	0	0	0
32	Y7	49	Total C N O S 430 263 108 57 2	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a RNA chain called 23S rRNA.

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

- Molecule 36 is a RNA chain called 5S rRNA.

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

- Molecule 37 is a protein called 50S ribosomal protein L2.

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

- Molecule 38 is a protein called 50S ribosomal protein L3.

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

- Molecule 39 is a protein called 50S ribosomal protein L4.

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

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

- Molecule 41 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	RH	170	1307	829	245	232	1	0	0	0
41	YH	170	1307	829	245	232	1	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L9.

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

Continued on next page...

Continued from previous page...

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

- Molecule 43 is a protein called 50S ribosomal protein L13.

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

- Molecule 44 is a protein called 50S ribosomal protein L14.

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

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RP	150	Total 1145	C 712	N 232	O 198	S 3	0	0	0
45	YP	150	Total 1145	C 712	N 232	O 198	S 3	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L16.

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

- Molecule 47 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	RR	118	Total 968	C 604	N 203	O 160	S 1	0	0	0
47	YR	118	Total 968	C 604	N 203	O 160	S 1	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L18.

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

- Molecule 49 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L21.

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

- Molecule 52 is a protein called 50S ribosomal protein L22.

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

- Molecule 53 is a protein called 50S ribosomal protein L23.

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

- Molecule 54 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	RY	102	785	505	150	125	5	0	0	0
54	YY	102	785	505	150	125	5	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L25.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
56	QA	73	73	73	0	0
56	QF	1	1	1	0	0
56	QM	1	1	1	0	0
56	QV	1	1	1	0	0
56	QX	2	2	2	0	0
56	R0	1	1	1	0	0
56	R5	1	1	1	0	0
56	R8	1	1	1	0	0
56	R9	1	1	1	0	0

Continued on next page...

Continued from previous page...

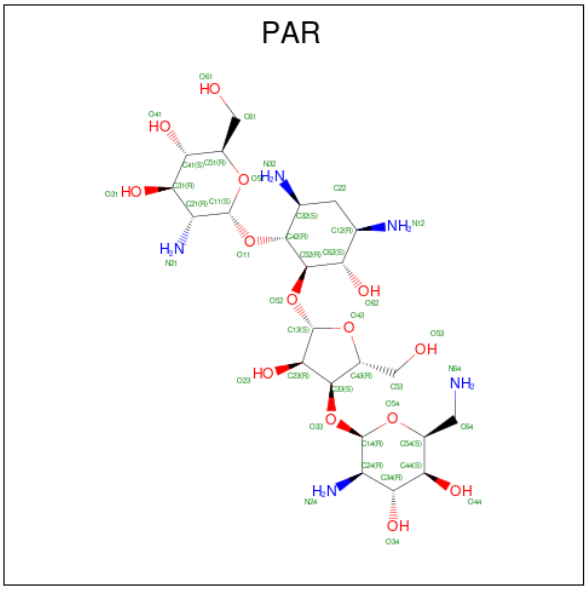
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	RA	281	Total Mg 281 281	0	0
56	RB	4	Total Mg 4 4	0	0
56	RD	1	Total Mg 1 1	0	0
56	RE	4	Total Mg 4 4	0	0
56	RF	1	Total Mg 1 1	0	0
56	RP	3	Total Mg 3 3	0	0
56	RR	1	Total Mg 1 1	0	0
56	RU	1	Total Mg 1 1	0	0
56	XA	91	Total Mg 91 91	0	0
56	XF	1	Total Mg 1 1	0	0
56	XM	1	Total Mg 1 1	0	0
56	XV	2	Total Mg 2 2	0	0
56	XX	1	Total Mg 1 1	0	0
56	Y0	1	Total Mg 1 1	0	0
56	Y1	1	Total Mg 1 1	0	0
56	Y2	1	Total Mg 1 1	0	0
56	Y5	1	Total Mg 1 1	0	0
56	Y6	2	Total Mg 2 2	0	0
56	Y8	1	Total Mg 1 1	0	0
56	Y9	1	Total Mg 1 1	0	0
56	YA	347	Total Mg 347 347	0	0

Continued on next page...

Continued from previous page...

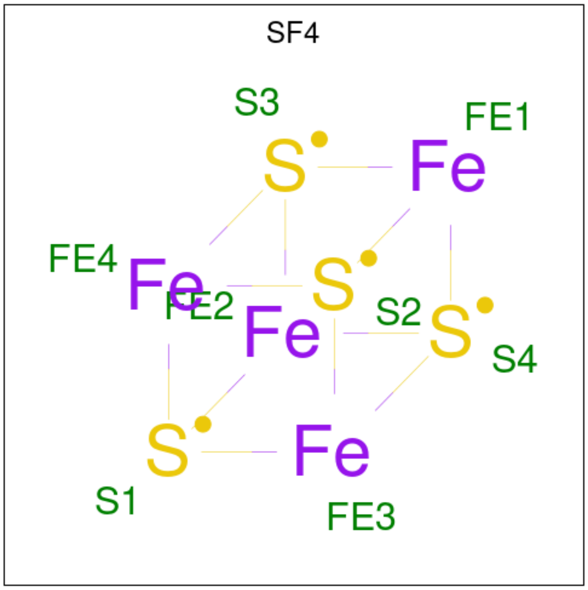
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YB	6	Total 6	Mg 6	0	0
56	YE	3	Total 3	Mg 3	0	0
56	YN	1	Total 1	Mg 1	0	0
56	YP	3	Total 3	Mg 3	0	0
56	YQ	3	Total 3	Mg 3	0	0
56	YR	1	Total 1	Mg 1	0	0
56	YX	1	Total 1	Mg 1	0	0

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	QA	1	Total 42	C 23	N 5	O 14	0	0
57	XA	1	Total 42	C 23	N 5	O 14	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	QN	1	Total Zn 1 1	0	0
59	R9	1	Total Zn 1 1	0	0
59	XN	1	Total Zn 1 1	0	0
59	Y9	1	Total Zn 1 1	0	0

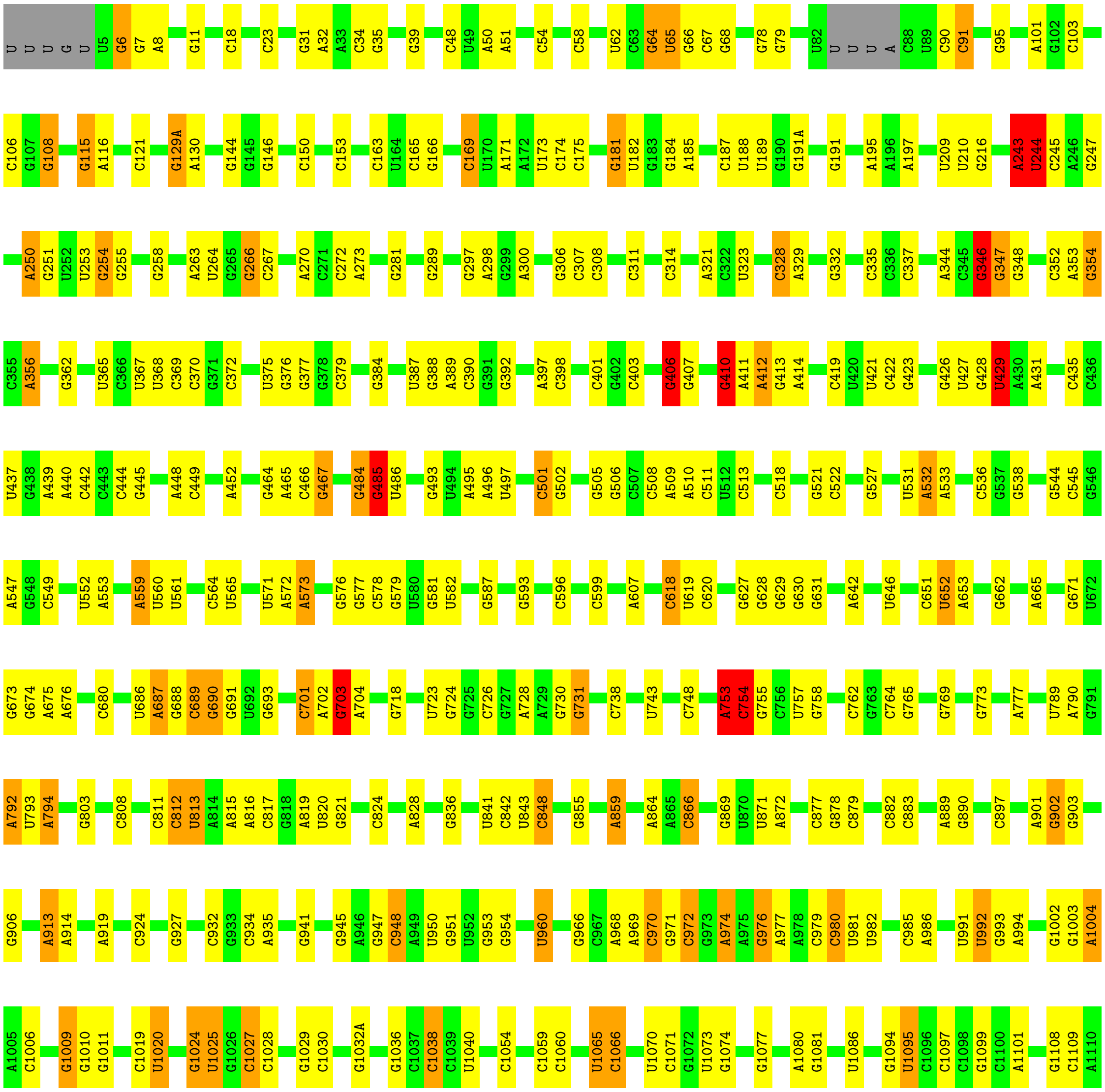
3 Residue-property plots ⓘ

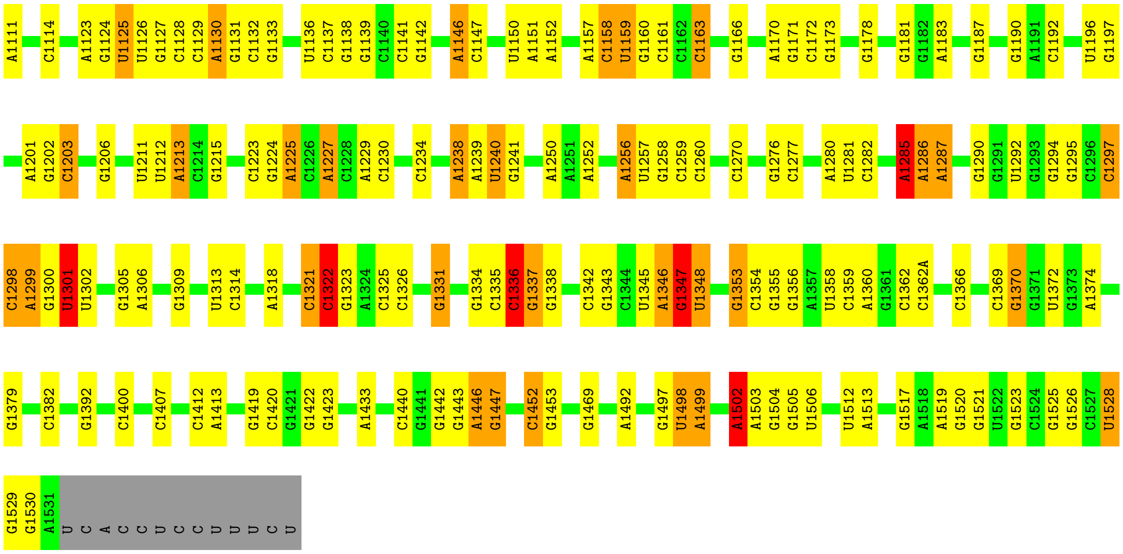
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

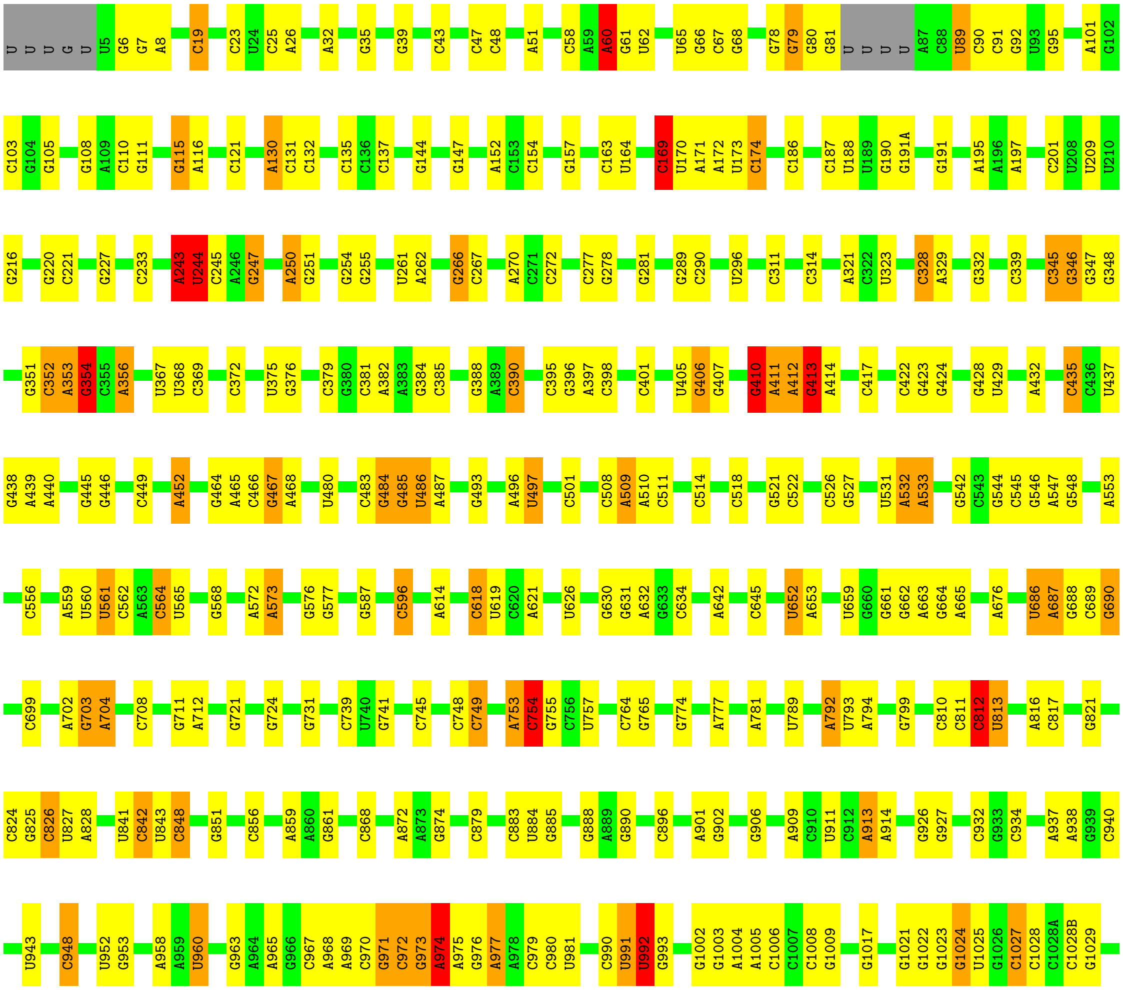
Chain QA:

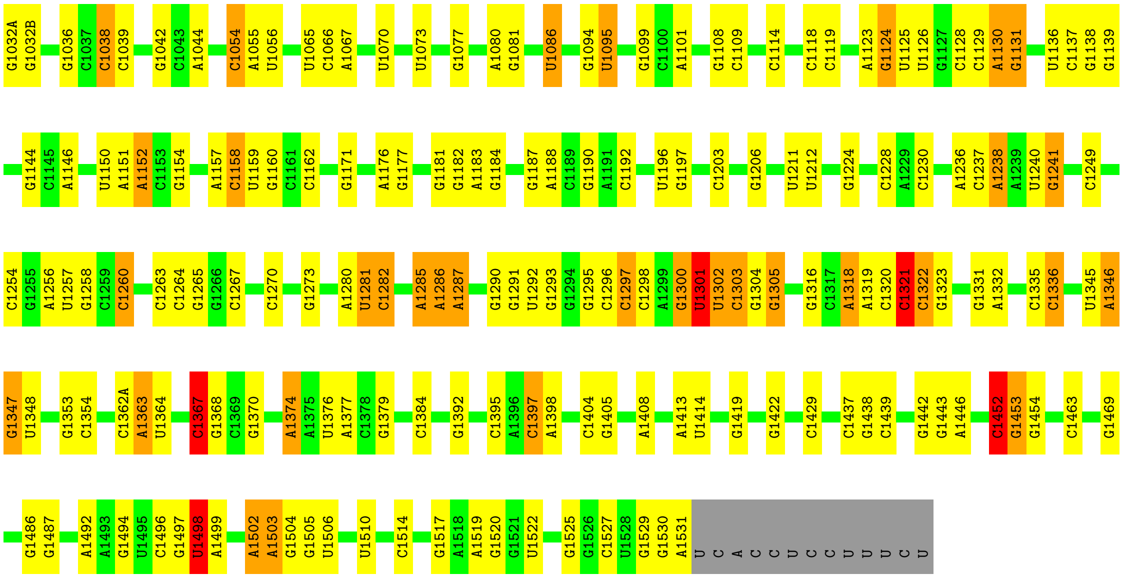




- Molecule 1: 16S rRNA

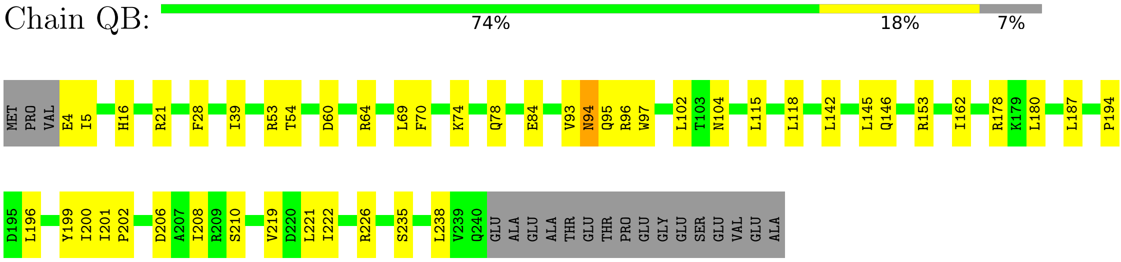
Chain XA:





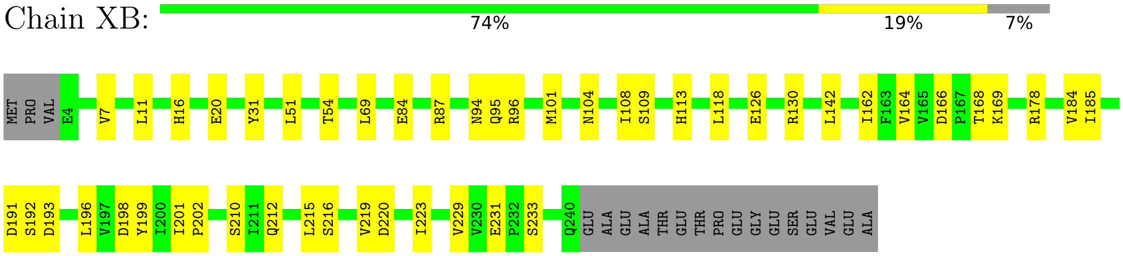
- Molecule 2: 30S ribosomal protein S2

Chain QB:



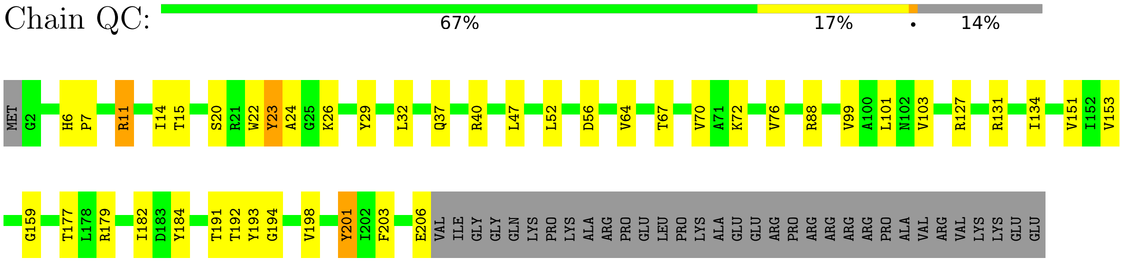
- Molecule 2: 30S ribosomal protein S2

Chain XB:

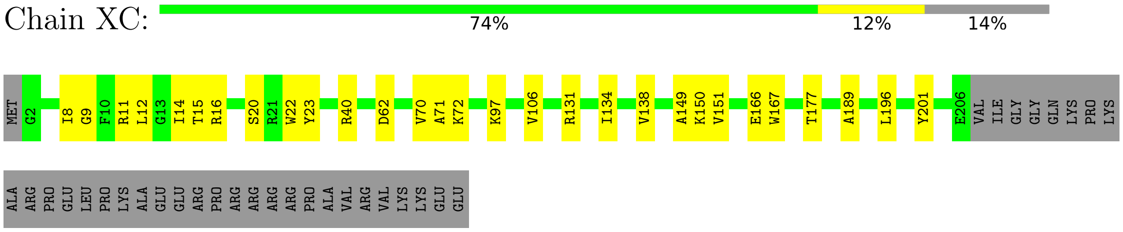


- Molecule 3: 30S ribosomal protein S3

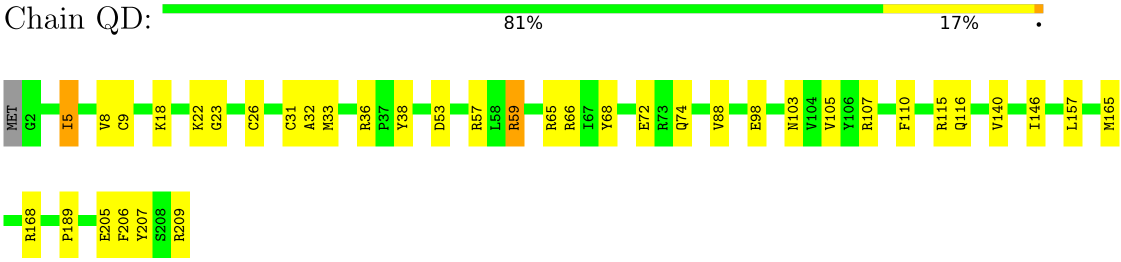
Chain QC:



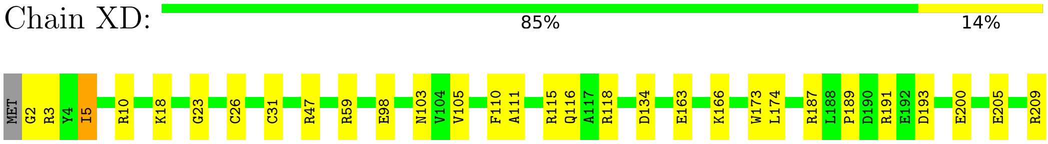
- Molecule 3: 30S ribosomal protein S3



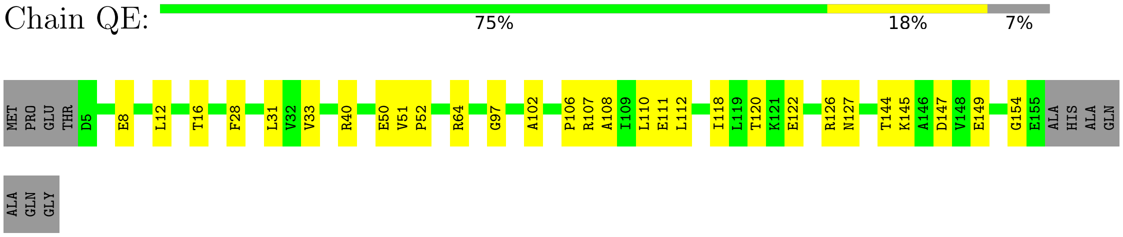
- Molecule 4: 30S ribosomal protein S4



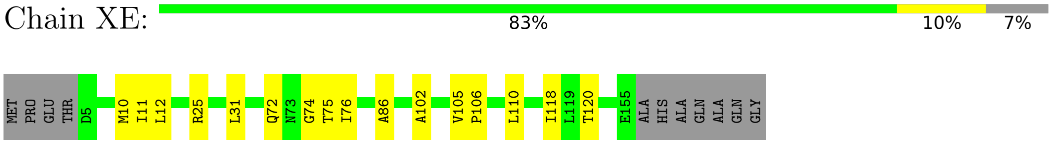
- Molecule 4: 30S ribosomal protein S4



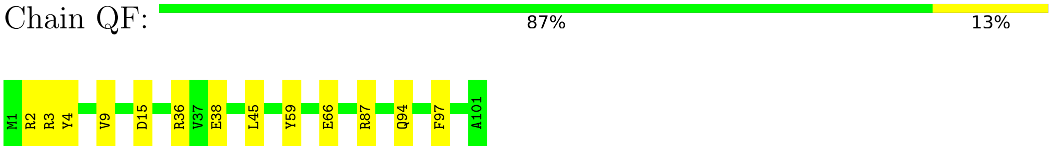
- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5

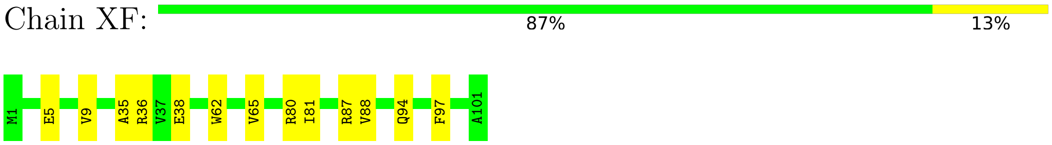


- Molecule 6: 30S ribosomal protein S6



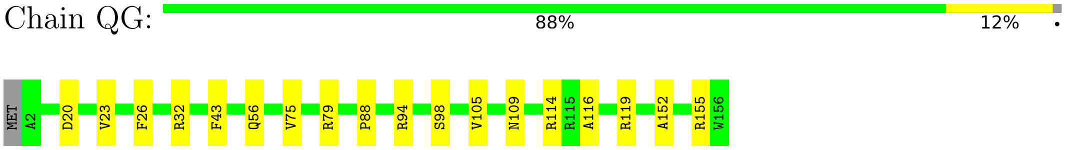
- Molecule 6: 30S ribosomal protein S6

Chain XF:



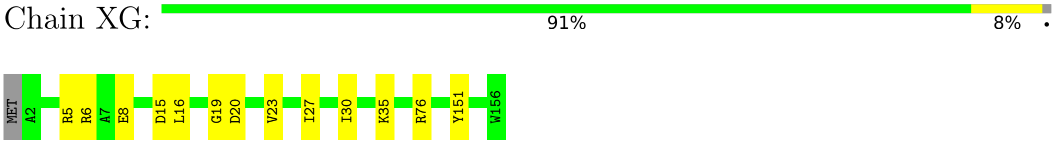
- Molecule 7: 30S ribosomal protein S7

Chain QG:



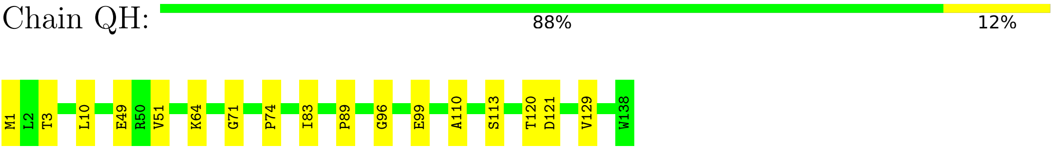
- Molecule 7: 30S ribosomal protein S7

Chain XG:



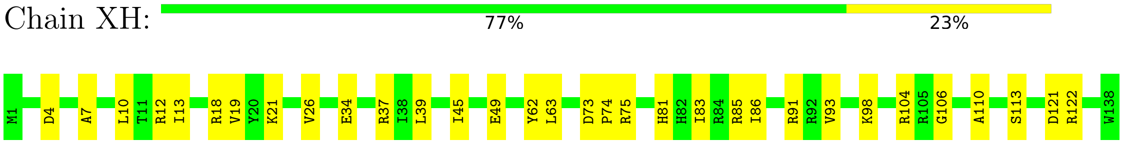
- Molecule 8: 30S ribosomal protein S8

Chain QH:



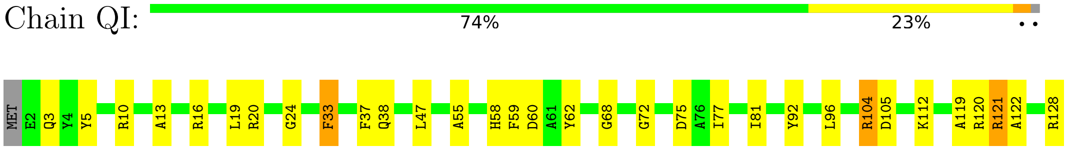
- Molecule 8: 30S ribosomal protein S8

Chain XH:



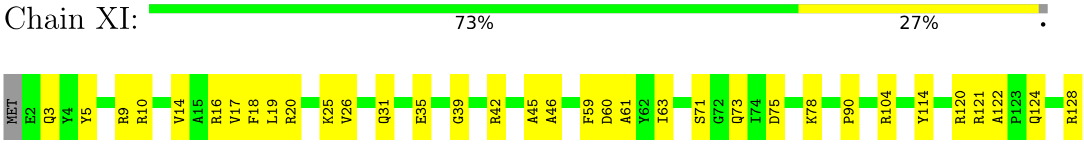
- Molecule 9: 30S ribosomal protein S9

Chain QI:



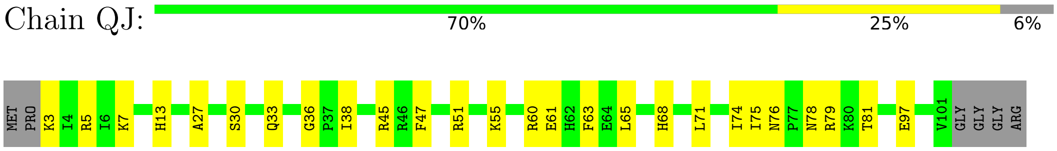
- Molecule 9: 30S ribosomal protein S9

Chain XI:



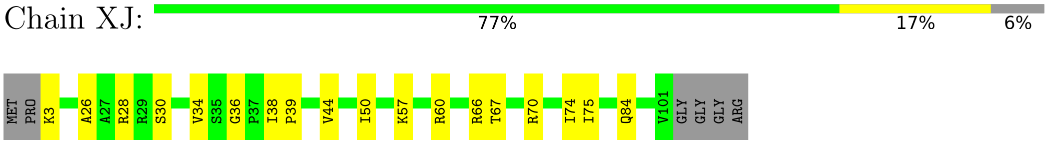
- Molecule 10: 30S ribosomal protein S10

Chain QJ:



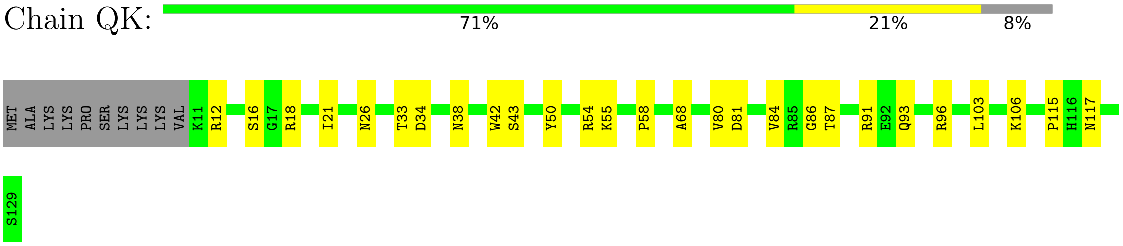
- Molecule 10: 30S ribosomal protein S10

Chain XJ:



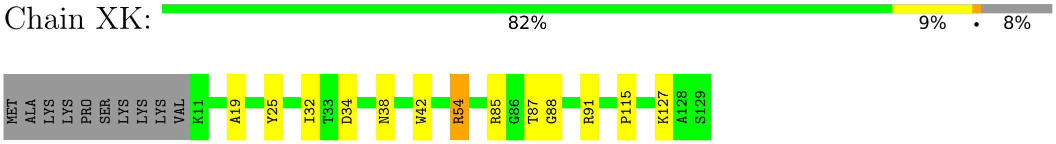
- Molecule 11: 30S ribosomal protein S11

Chain QK:



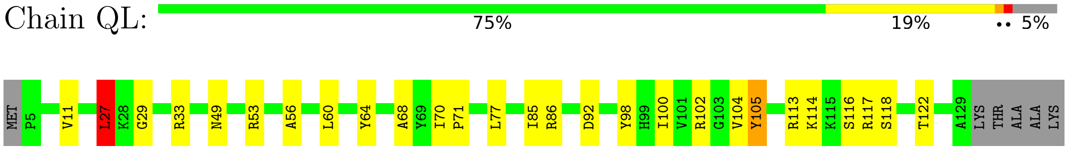
- Molecule 11: 30S ribosomal protein S11

Chain XK:



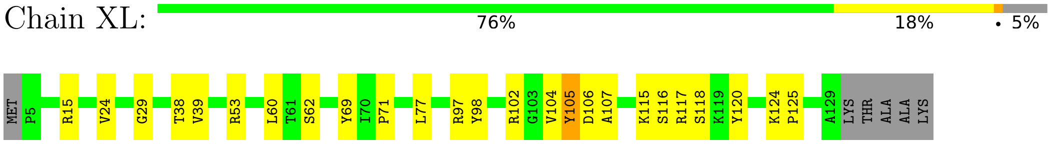
- Molecule 12: 30S ribosomal protein S12

Chain QL:



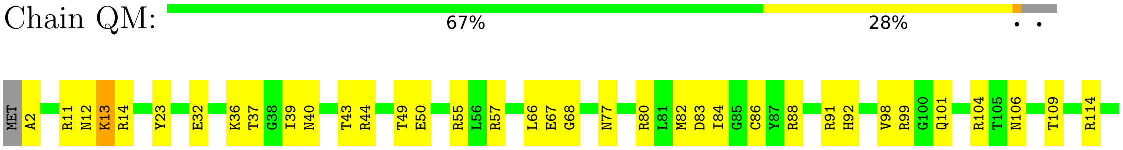
- Molecule 12: 30S ribosomal protein S12

Chain XL:



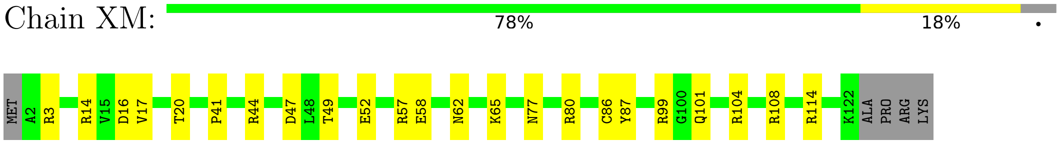
- Molecule 13: 30S ribosomal protein S13

Chain QM:



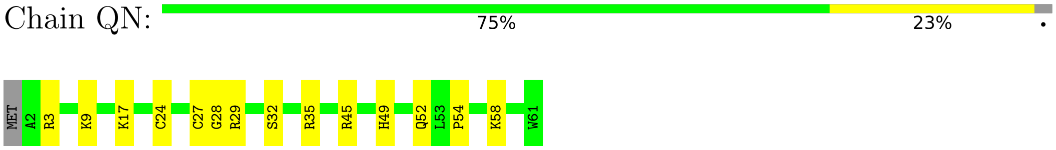
- Molecule 13: 30S ribosomal protein S13

Chain XM:



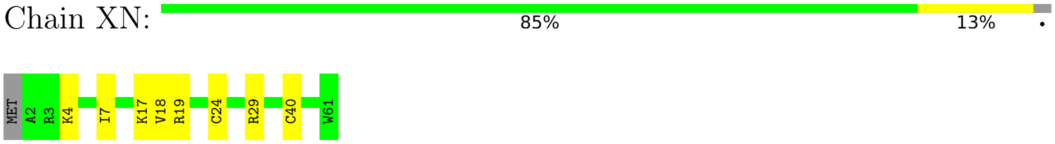
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:



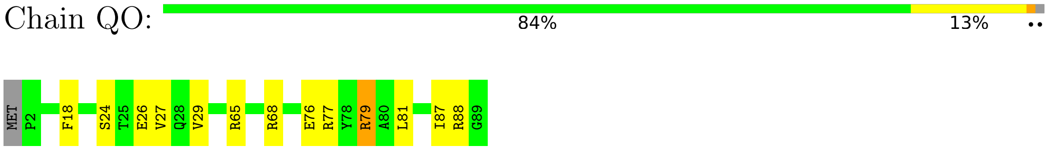
- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:



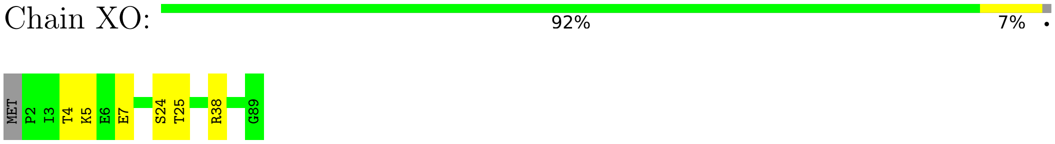
- Molecule 15: 30S ribosomal protein S15

Chain QO:



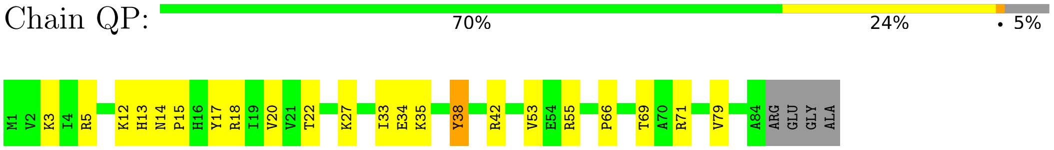
- Molecule 15: 30S ribosomal protein S15

Chain XO:



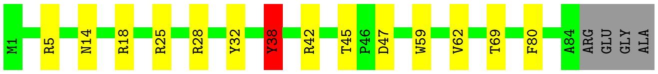
- Molecule 16: 30S ribosomal protein S16

Chain QP:



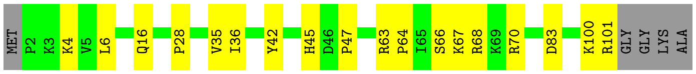
- Molecule 16: 30S ribosomal protein S16

Chain XP:



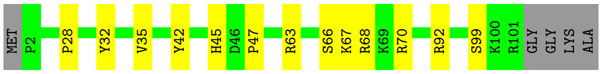
- Molecule 17: 30S ribosomal protein S17

Chain QQ:



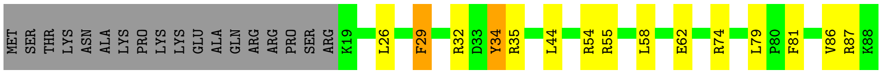
- Molecule 17: 30S ribosomal protein S17

Chain XQ:



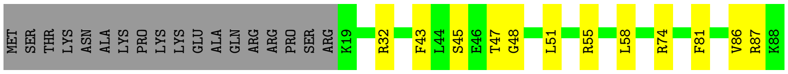
- Molecule 18: 30S ribosomal protein S18

Chain QR:



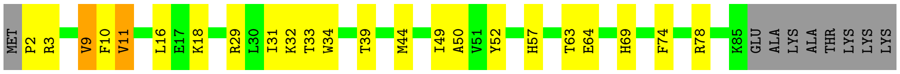
- Molecule 18: 30S ribosomal protein S18

Chain XR:



- Molecule 19: 30S ribosomal protein S19

Chain QS:

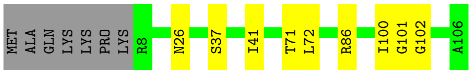


- Molecule 19: 30S ribosomal protein S19

Chain XS:

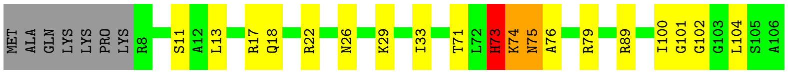
- Molecule 20: 30S ribosomal protein S20

Chain QT:



- Molecule 20: 30S ribosomal protein S20

Chain XT:

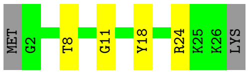


- Molecule 21: 30S ribosomal protein Thx

Chain QU:

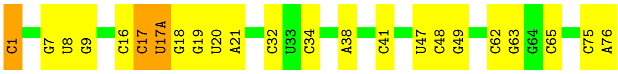
- Molecule 21: 30S ribosomal protein Thx

Chain XU:



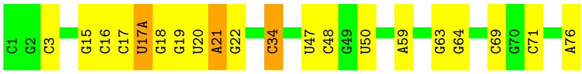
- Molecule 22: P-site tRNAfMet

Chain QV:



- Molecule 22: P-site tRNAfMet

Chain XV:



- Molecule 23: mRNA

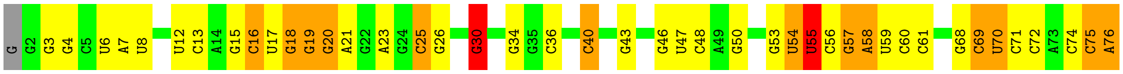
Chain QX:

- Molecule 23: mRNA

Chain XX:

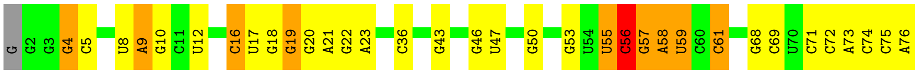
- Molecule 24: A-site tRNAAla(GGC) U32-A38

Chain QY:



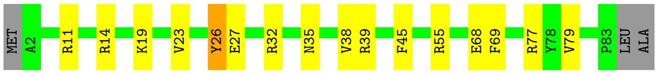
- Molecule 24: A-site tRNAAla(GGC) U32-A38

Chain XY:



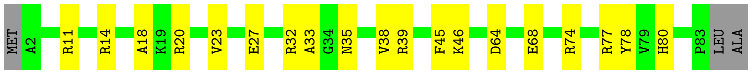
- Molecule 25: 50S ribosomal protein L27

Chain R0:



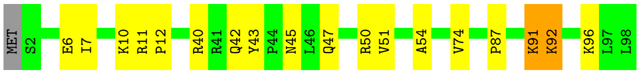
- Molecule 25: 50S ribosomal protein L27

Chain Y0:



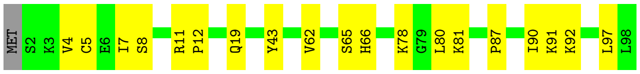
- Molecule 26: 50S ribosomal protein L28

Chain R1:



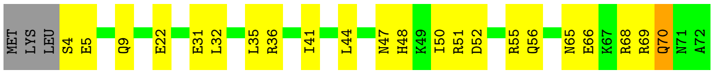
- Molecule 26: 50S ribosomal protein L28

Chain Y1:



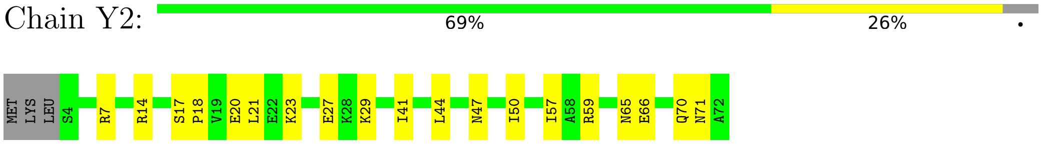
- Molecule 27: 50S ribosomal protein L29

Chain R2:



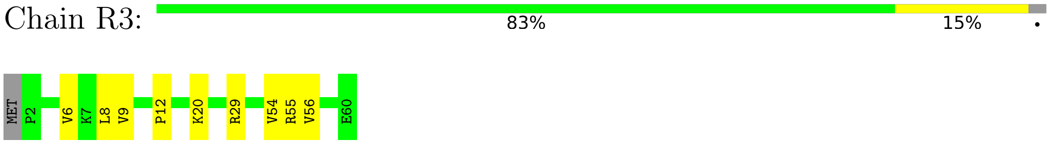
- Molecule 27: 50S ribosomal protein L29

Chain Y2:



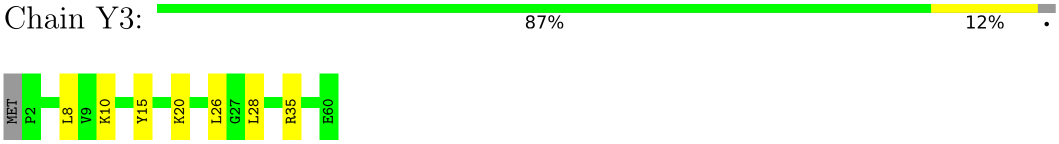
- Molecule 28: 50S ribosomal protein L30

Chain R3:



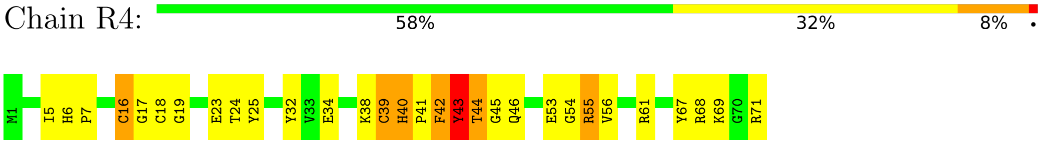
- Molecule 28: 50S ribosomal protein L30

Chain Y3:



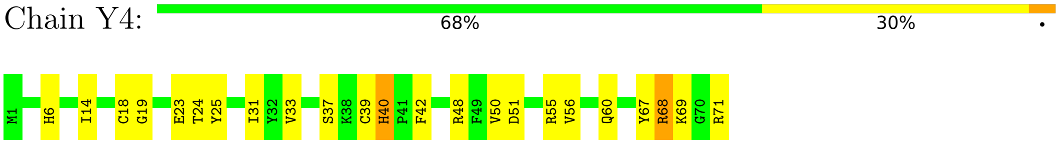
- Molecule 29: 50S ribosomal protein L31

Chain R4:



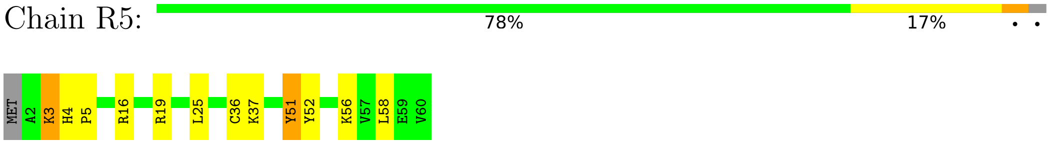
- Molecule 29: 50S ribosomal protein L31

Chain Y4:



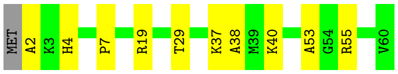
- Molecule 30: 50S ribosomal protein L32

Chain R5:



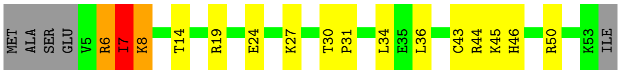
- Molecule 30: 50S ribosomal protein L32

Chain Y5:



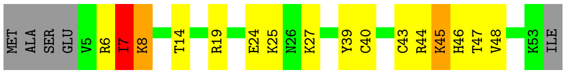
- Molecule 31: 50S ribosomal protein L33

Chain R6:



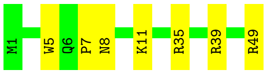
- Molecule 31: 50S ribosomal protein L33

Chain Y6:



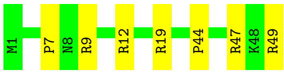
- Molecule 32: 50S ribosomal protein L34

Chain R7:



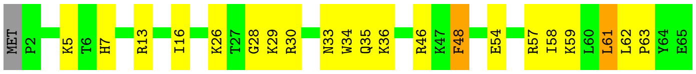
- Molecule 32: 50S ribosomal protein L34

Chain Y7:



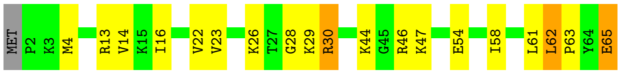
- Molecule 33: 50S ribosomal protein L35

Chain R8:



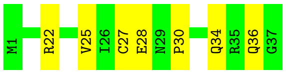
- Molecule 33: 50S ribosomal protein L35

Chain Y8:



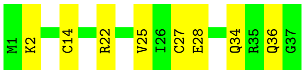
- Molecule 34: 50S ribosomal protein L36

Chain R9:



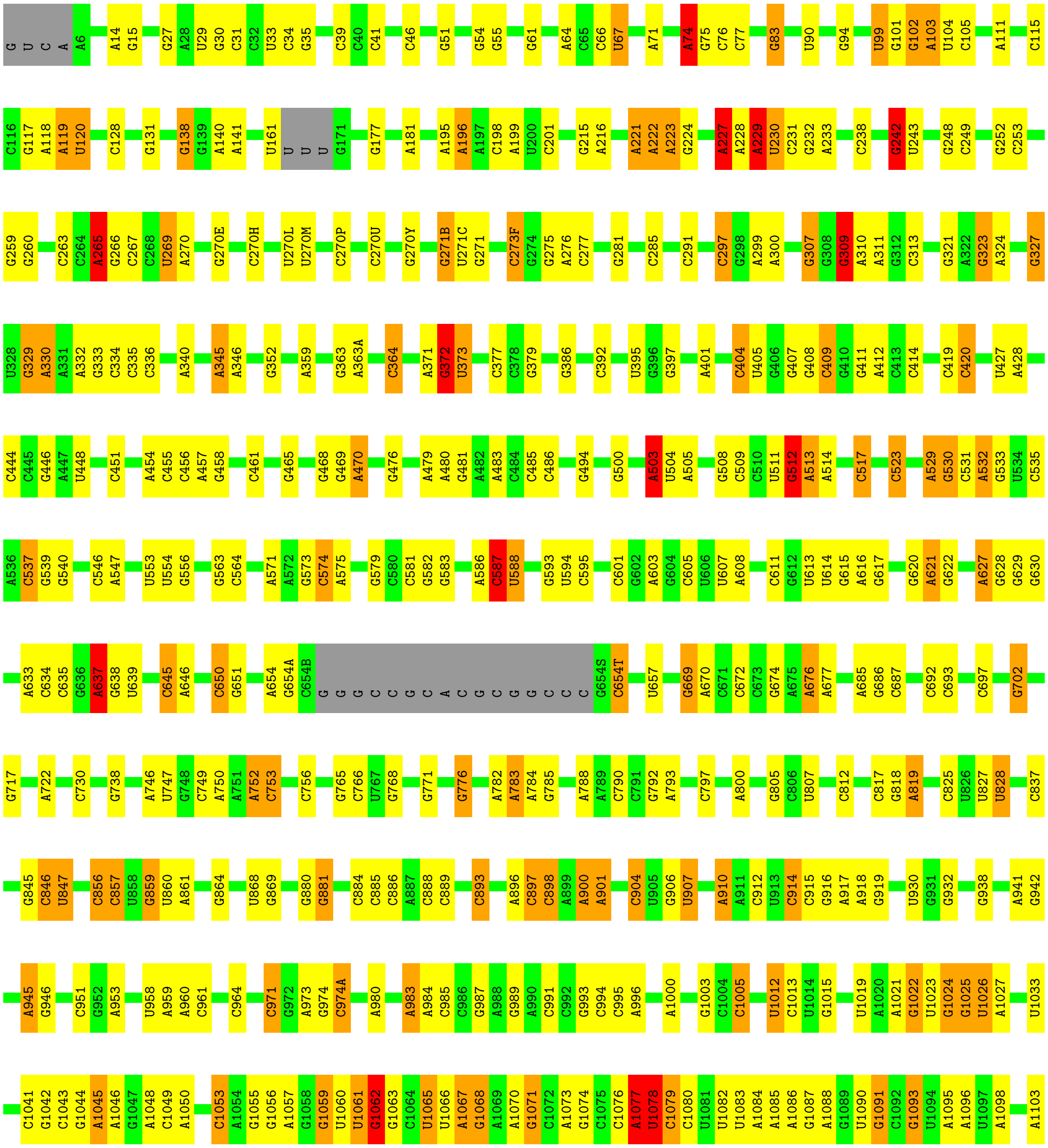
- Molecule 34: 50S ribosomal protein L36

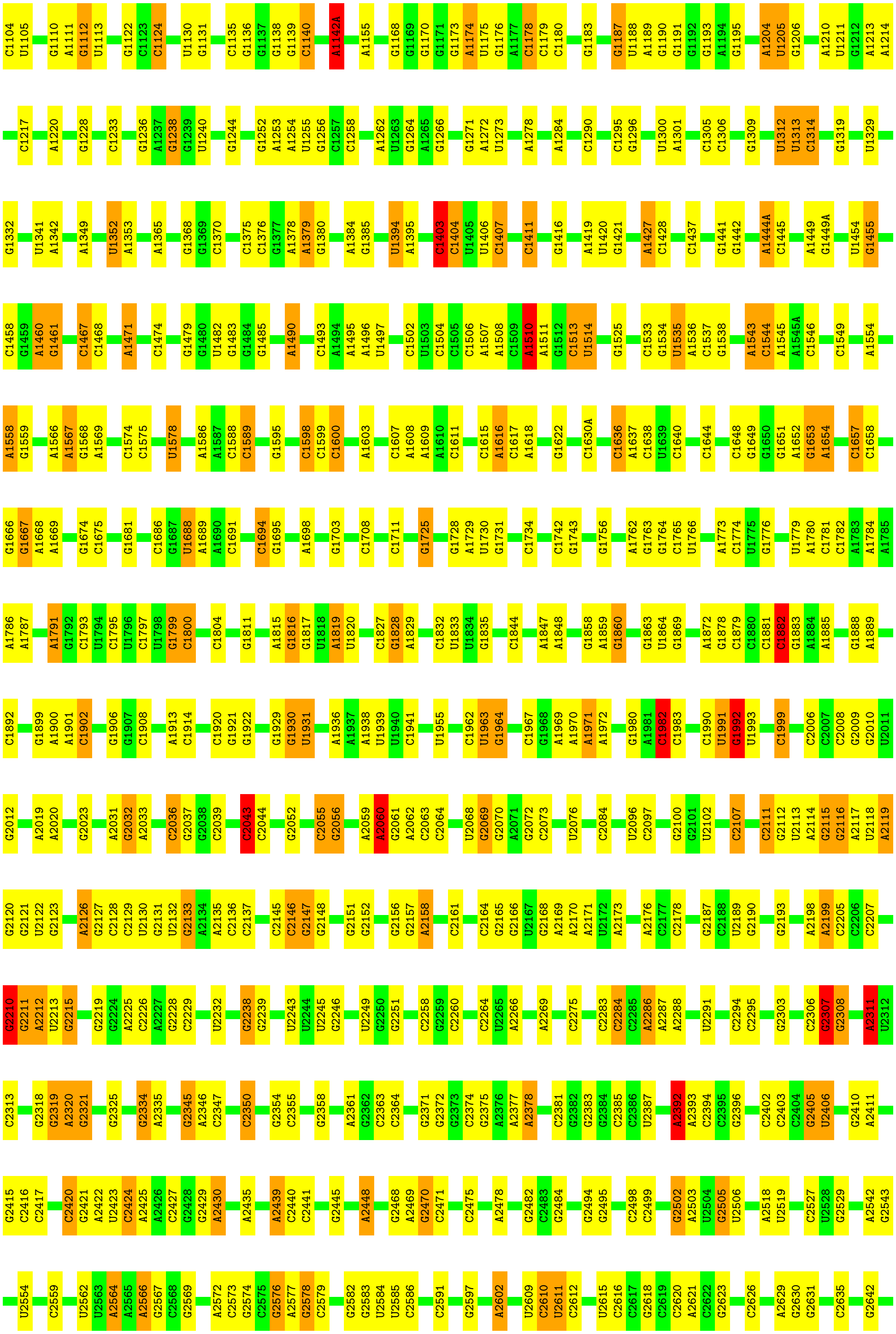
Chain Y9:

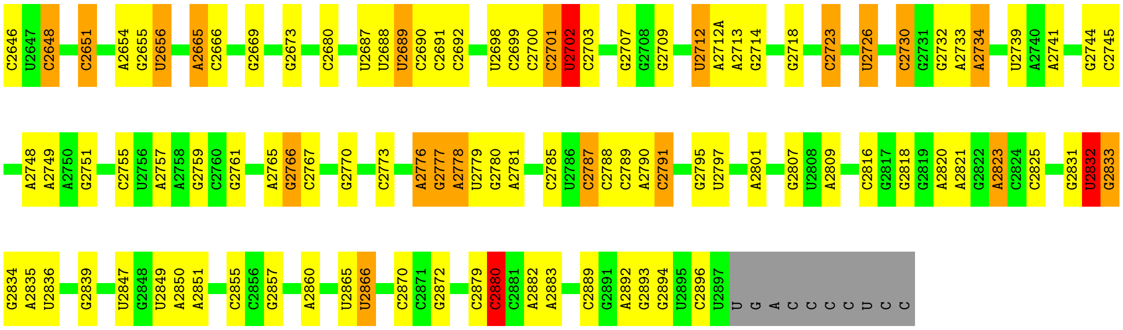


- Molecule 35: 23S rRNA

Chain RA:

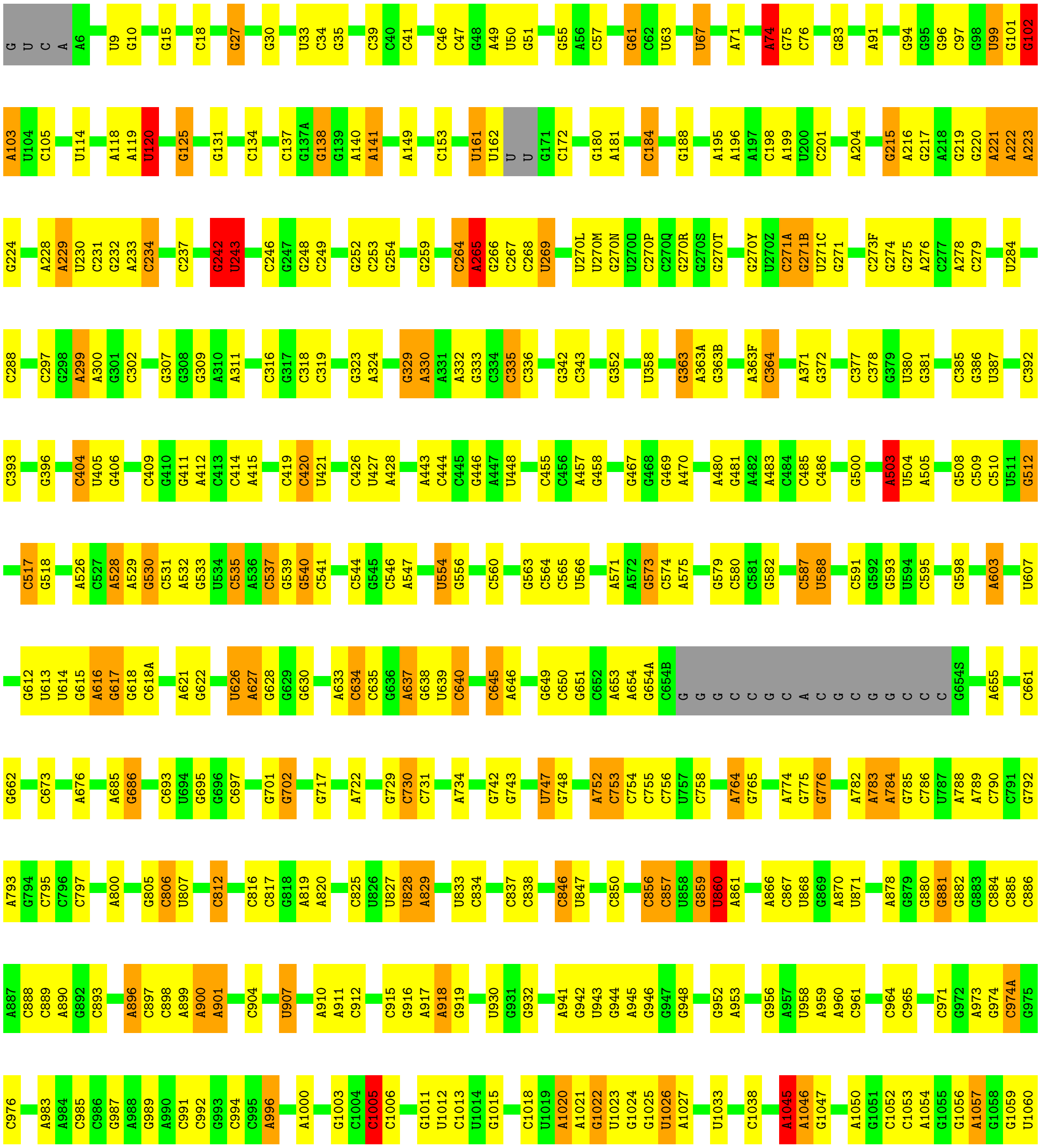


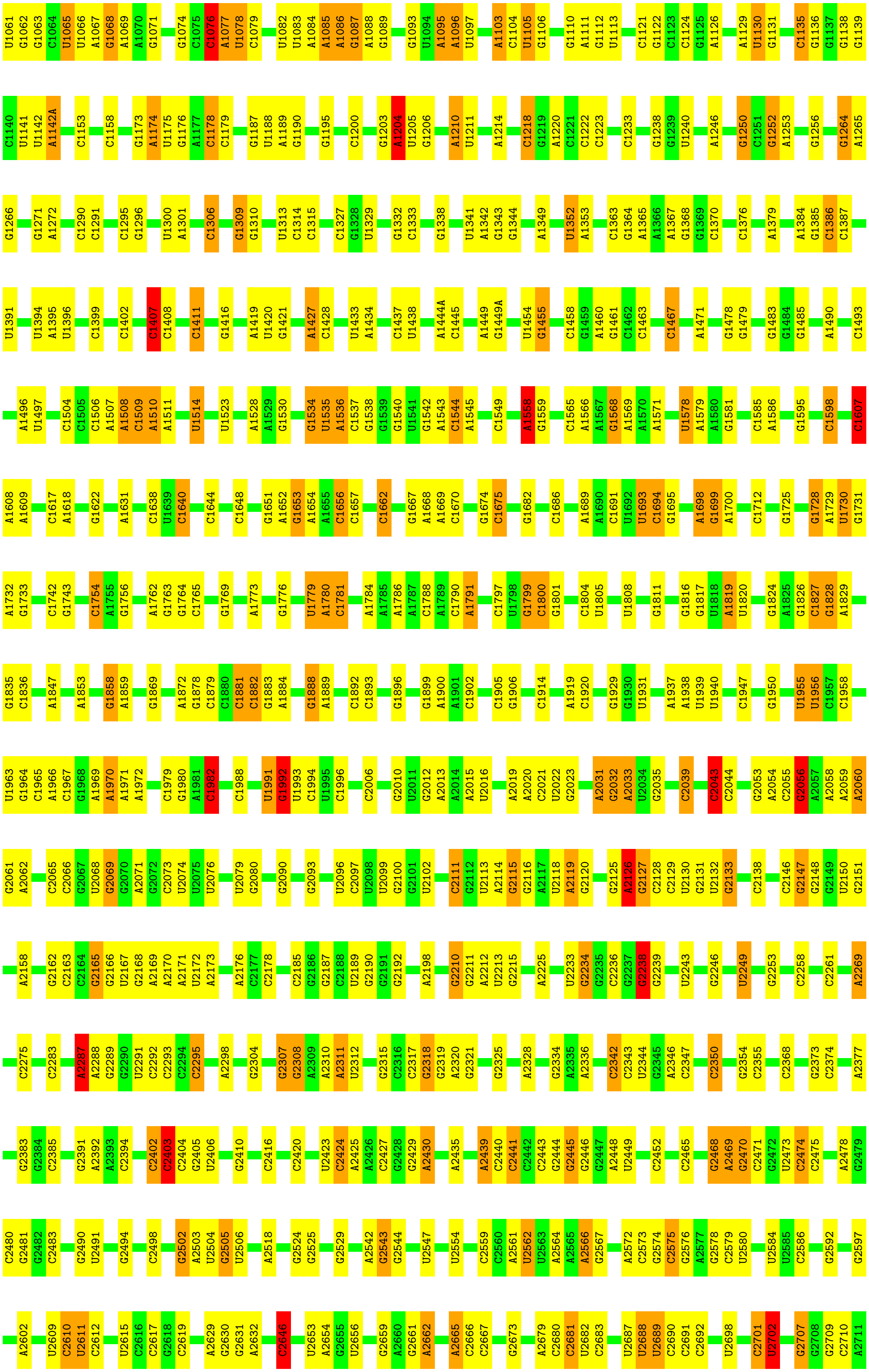

C1104 U1105 G1110 A1111 G1112 U1113 G1122 C1123 C1124 U1130 G1131 C1135 G1136 G1137 G1138 G1139 C1140 A1142A A1155 G1168 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 G1183 G1187 U1188 A1189 G1190 G1191 G1192 G1193 A1194 G1195 A1204 U1205 G1206 A1210 U1211 G1212 A1213 A1214
C1217 A1220 G1228 C1233 G1236 A1237 G1238 G1239 U1240 G1244 G1252 A1253 A1254 U1255 G1256 C1257 C1258 A1262 U1263 G1264 A1265 G1266 G1271 A1272 U1273 A1278 A1284 C1290 C1295 G1296 U1300 A1301 C1305 C1306 G1309 U1312 U1313 C1314 G1319 U1329
G1332 U1341 A1342 A1349 U1352 A1353 A1365 G1368 G1369 C1370 C1375 C1376 G1377 A1378 A1379 G1380 A1384 G1385 U1394 A1395 C1403 C1404 U1405 U1406 C1407 C1411 G1416 A1419 U1420 G1421 A1427 C1428 C1437 G1441 G1442 A1444A C1445 A1449 G1449A U1454 G1455
C1458 G1459 A1460 G1461 C1467 C1468 A1471 C1474 G1479 G1480 U1482 G1483 G1484 G1485 A1490 C1493 A1494 A1495 A1496 U1497 C1502 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1510 A1511 G1512 C1513 U1514 G1525 C1533 G1534 U1535 A1536 C1537 G1538 A1543 C1544 A1545 A1545A C1546 C1549 A1554
A1558 G1559 A1566 A1567 G1568 A1569 C1574 C1575 U1578 A1586 A1587 C1588 C1589 G1595 C1598 C1599 C1600 A1603 C1607 A1608 A1609 A1610 C1611 C1615 A1616 C1617 A1618 G1622 C1630A C1636 A1637 C1638 U1639 C1640 C1644 C1648 G1649 G1650 G1651 A1652 G1653 A1654 C1657 C1658
G1666 G1667 A1668 A1669 G1674 C1675 G1681 C1686 G1687 U1688 A1689 A1690 C1691 C1694 G1695 A1698 G1703 C1708 C1711 G1725 G1728 A1729 U1730 G1731 C1734 C1742 G1743 G1756 A1762 G1763 G1764 C1765 U1766 A1773 C1774 U1775 G1776 U1779 A1780 C1781 C1782 A1783 A1784 A1785
A1786 A1787 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 C1804 G1811 A1815 G1816 G1817 U1818 A1819 U1820 C1827 G1828 A1829 C1832 U1833 U1834 G1835 C1844 A1847 A1848 G1858 A1859 G1860 G1863 U1864 G1869 A1872 G1878 C1879 C1880 C1881 C1882 G1883 A1884 A1885 G1888 A1889
C1892 G1899 A1900 A1901 C1902 G1906 G1907 C1908 A1913 C1914 C1920 G1921 G1922 G1929 G1930 U1931 A1936 A1937 A1938 U1939 U1940 C1941 U1955 C1962 U1963 G1964 C1967 G1968 A1969 A1970 A1971 A1972 G1980 A1981 C1982 C1983 C1990 U1991 G1992 U1993 C1999 C2006 C2007 C2008 G2009 G2010 U2011
G2012 A2019 A2020 G2023 A2031 G2032 A2033 C2036 G2037 G2038 C2039 C2043 C2044 G2052 C2055 G2056 A2059 A2060 G2061 A2062 C2063 C2064 U2068 G2069 G2070 A2071 G2072 C2073 U2076 C2084 U2096 C2097 G2100 G2101 U2102 C2107 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119
G2120 G2121 U2122 G2123 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2145 C2146 G2147 G2148 G2151 G2152 G2156 G2157 A2158 C2161 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 A2176 C2177 C2178 G2187 C2188 U2189 G2190 G2193 A2198 A2199 C2205 C2206 C2207
G2210 G2211 A2212 U2213 G2215 G2219 G2224 A2225 C2226 A2227 G2228 C2229 U2232 G2238 G2239 U2243 U2244 U2245 G2246 U2249 G2250 G2251 C2258 G2259 C2260 C2264 U2265 A2266 A2269 C2275 C2283 G2284 C2285 A2286 A2287 A2288 U2291 C2294 C2295 G2303 C2306 G2307 G2308 A2311 U2312
C2313 G2318 G2319 A2320 G2321 G2325 G2334 A2335 G2345 A2346 C2347 C2350 G2354 C2355 G2358 A2361 G2362 C2363 C2364 G2371 G2372 G2373 C2374 G2375 A2376 A2377 A2378 C2381 G2382 G2383 G2384 C2385 C2386 U2387 A2392 A2393 C2394 C2395 G2396 C2402 C2403 C2404 G2405 U2406 G2410 A2411
G2415 C2416 C2417 C2420 G2421 A2422 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 A2435 A2439 C2440 C2441 G2445 A2448 G2468 A2469 G2470 C2471 C2475 A2478 G2482 C2483 G2484 G2494 G2495 C2498 C2499 G2502 A2503 U2504 G2505 U2506 A2518 U2519 C2527 U2528 G2529 A2542 G2543
U2554 C2559 U2562 U2563 A2564 A2565 A2566 G2567 C2568 G2569 A2572 C2573 G2574 C2575 G2576 A2577 G2578 C2579 G2582 G2583 U2584 U2585 C2586 C2591 G2597 A2602 U2609 C2610 U2611 C2612 U2615 C2616 C2617 G2618 C2619 C2620 A2621 C2622 G2623 C2626 A2629 G2630 G2631 C2635 G2642

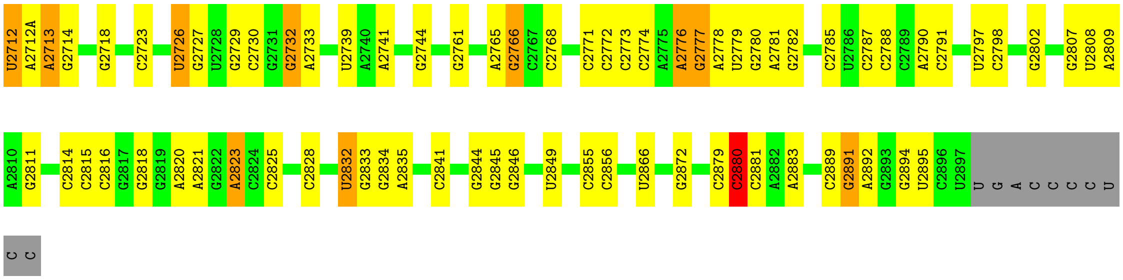


- Molecule 35: 23S rRNA

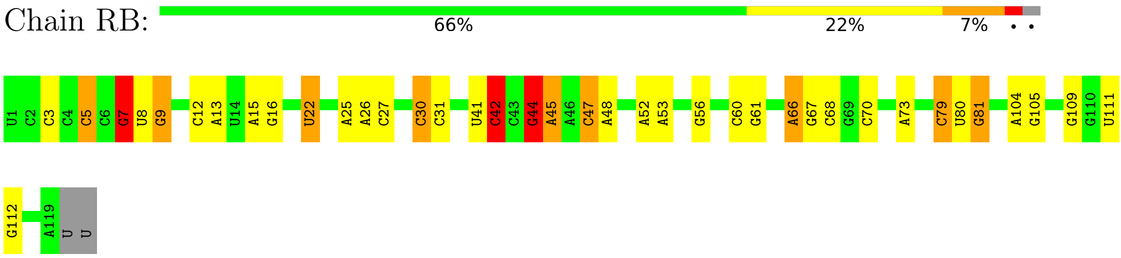
Chain YA:



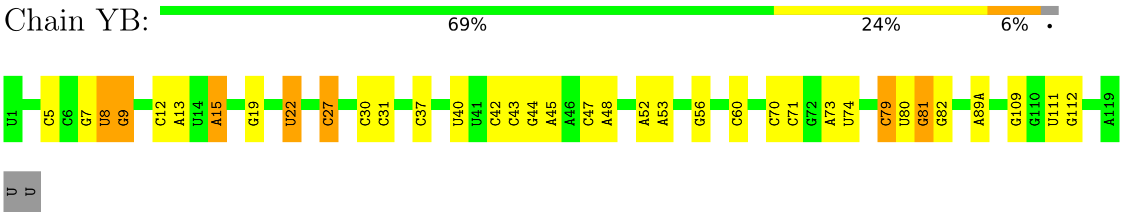

U1061
G1062
G1063
C1064
U1065
U1066
A1067
G1068
A1069
A1070
G1071
G1074
C1075
C1076
A1077
U1078
C1079
U1082
U1083
A1084
A1085
A1086
G1087
A1088
G1089
G1093
U1094
A1095
A1096
U1097
A1103
C1104
U1105
G1106
G1110
A1111
G1112
U1113
C1121
G1122
C1123
C1124
G1125
A1126
A1129
U1130
G1131
C1135
G1136
G1137
G1138
G1139
C1140
U1141
U1142
A1142A
C1153
C1158
G1173
A1174
U1175
G1176
A1177
C1178
C1179
G1187
U1188
A1189
G1190
G1195
C1200
G1203
A1204
U1205
G1206
A1210
U1211
A1214
C1218
G1219
A1220
C1221
C1222
C1223
C1233
G1238
G1239
U1240
A1246
G1250
C1251
G1252
A1253
G1256
G1264
A1265
G1266
G1271
A1272
C1290
C1291
C1295
G1296
U1300
A1301
C1306
G1309
G1310
U1313
C1314
C1315
C1327
G1328
U1329
G1332
C1333
G1338
U1341
A1342
G1343
G1344
A1349
U1352
A1353
C1363
G1364
A1365
A1366
A1367
G1368
G1369
C1370
C1376
A1379
A1384
G1385
C1386
C1387
U1391
U1394
A1395
U1396
C1399
C1402
C1407
C1408
C1411
G1416
A1419
U1420
G1421
A1427
C1428
U1433
A1434
C1437
U1438
A1444A
C1445
A1449
G1449A
U1454
G1455
C1458
G1459
A1460
G1461
C1462
C1463
C1467
A1471
G1478
G1479
G1483
G1484
G1485
A1490
C1493
A1496
U1497
C1504
C1505
C1506
A1507
A1508
C1509
A1510
A1511
U1514
U1523
A1528
A1529
G1530
G1534
U1535
A1536
C1537
G1538
G1539
G1540
U1541
G1542
A1543
C1544
A1545
C1549
A1558
G1559
C1565
A1566
A1567
G1568
A1569
A1570
A1571
U1578
A1579
A1580
G1581
C1585
A1586
G1595
C1598
C1607
A1608
A1609
C1617
A1618
G1622
A1631
C1638
U1639
C1640
C1644
C1648
G1651
A1652
G1653
A1654
A1655
C1656
C1657
C1662
G1667
A1668
A1669
C1670
G1674
C1675
G1682
C1686
A1689
A1690
C1691
U1692
U1693
C1694
G1695
A1698
G1699
A1700
C1712
G1725
G1728
A1729
U1730
G1731
A1732
G1733
C1742
G1743
C1754
A1755
G1756
A1762
G1763
G1764
C1765
G1769
A1773
G1776
U1779
A1780
C1781
A1784
A1785
A1786
A1787
C1788
A1789
C1790
A1791
C1797
U1798
G1799
C1800
G1801
C1804
U1805
U1808
G1811
G1816
G1817
U1818
A1819
U1820
G1824
A1825
G1826
C1827
G1828
A1829
G1835
C1836
A1847
A1853
G1858
A1859
G1869
A1872
G1878
C1879
C1880
C1881
C1882
G1883
A1884
G1888
A1889
C1892
C1893
G1896
G1899
A1900
A1901
C1902
C1905
G1906
C1914
A1919
C1920
G1929
G1930
U1931
A1937
A1938
U1939
U1940
C1947
G1950
U1955
U1956
C1957
C1958
U1963
G1964
C1965
A1966
C1967
G1968
A1969
A1970
A1971
A1972
C1979
G1980
A1981
C1982
C1988
U1991
G1992
U1993
C1994
U1995
C1996
C2006
G2010
U2011
G2012
A2013
A2014
A2015
U2016
A2019
A2020
C2021
U2022
G2023
A2031
G2032
A2033
U2034
G2035
C2039
C2043
C2044
G2053
A2054
C2055
G2056
A2057
A2058
A2059
A2060
G2061
A2062
C2065
C2066
G2067
U2068
G2069
G2070
A2071
G2072
C2073
U2074
U2075
U2076
U2079
G2080
G2090
G2093
U2096
C2097
U2098
U2099
G2100
G2101
U2102
C2111
G2112
U2113
A2114
G2115
G2116
A2117
U2118
A2119
G2120
G2125
A2126
G2127
C2128
C2129
U2130
G2131
U2132
G2133
C2138
C2146
G2147
G2148
G2149
U2150
G2151
A2158
G2162
C2163
C2164
G2165
G2166
U2167
G2168
A2169
A2170
A2171
U2172
A2173
A2176
C2177
C2178
C2185
G2186
G2187
C2188
U2189
G2190
G2191
G2192
A2198
G2210
G2211
A2212
U2213
G2215
A2225
U2233
G2234
G2235
C2236
G2237
U2238
G2239
U2243
G2246
U2249
G2253
C2258
C2261
A2269
C2275
C2283
A2287
A2288
G2289
G2290
U2291
C2292
C2293
C2294
C2295
A2298
G2304
G2307
G2308
A2309
A2310
A2311
U2312
G2315
C2316
C2317
G2318
G2319
A2320
G2321
G2325
A2328
G2334
A2335
A2336
C2342
C2343
U2344
G2345
A2346
C2347
C2350
G2354
C2355
C2368
G2373
C2374
A2377
G2383
G2384
C2385
G2391
A2392
A2393
C2394
C2402
C2403
C2404
G2405
U2406
G2410
C2416
C2420
U2423
C2424
A2425
A2426
C2427
G2428
G2429
A2430
A2435
A2439
C2440
C2441
C2442
C2443
G2444
G2445
G2446
G2447
A2448
U2449
C2452
C2465
G2468
A2469
G2470
C2471
G2472
U2473
C2474
C2475
A2478
G2479
C2480
G2481
G2482
C2483
G2490
U2491
G2494
C2498
G2502
A2503
U2504
G2505
U2506
A2518
G2524
G2525
G2529
A2542
G2543
G2544
U2547
U2554
C2559
C2560
A2561
U2562
U2563
A2564
A2565
A2566
G2567
A2572
G2573
G2574
C2575
G2576
A2577
G2578
C2579
U2580
U2584
U2585
C2586
G2592
G2597
A2602
U2609
C2610
U2611
C2612
U2615
C2616
C2617
G2618
C2619
A2629
G2630
G2631
A2632
C2646
U2653
A2654
G2655
U2656
G2659
A2660
G2661
A2662
A2665
C2666
C2667
G2673
A2679
C2680
C2681
U2682
C2683
U2687
U2688
U2689
C2690
C2691
C2692
U2698
C2701
U2702
G2707
G2708
G2709
C2710
A2711



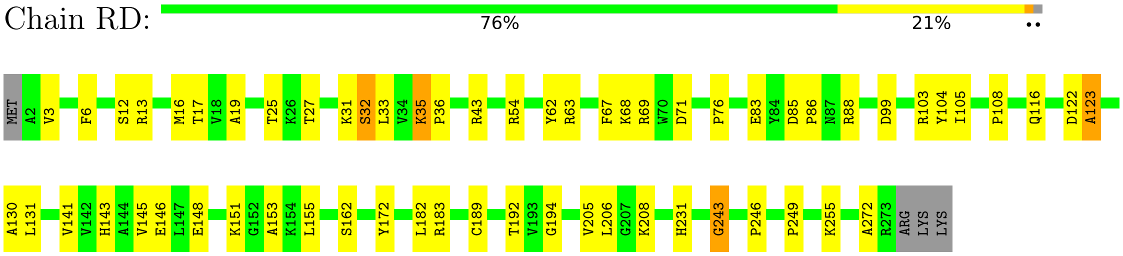
- Molecule 36: 5S rRNA



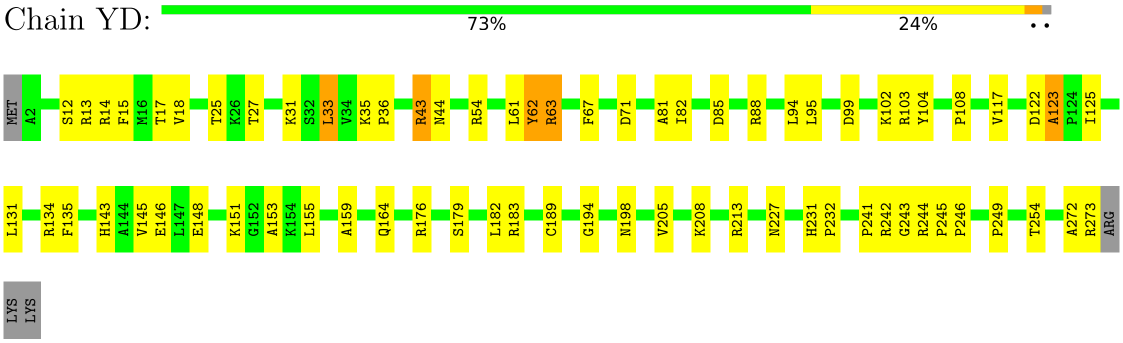
- Molecule 36: 5S rRNA



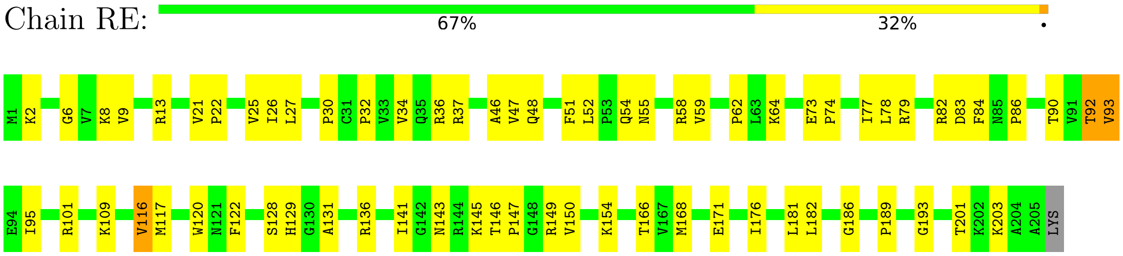
- Molecule 37: 50S ribosomal protein L2



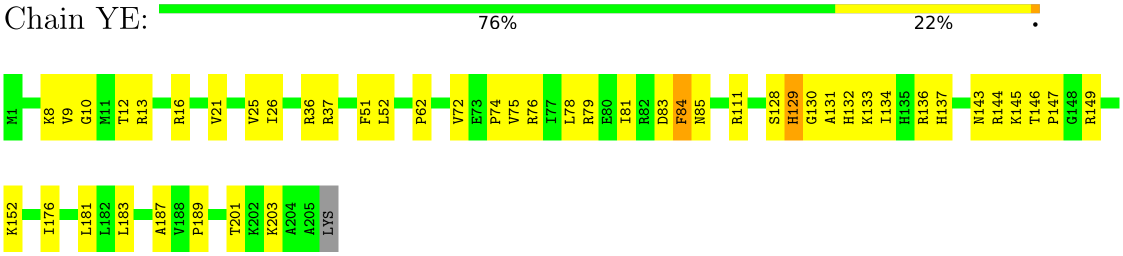
- Molecule 37: 50S ribosomal protein L2



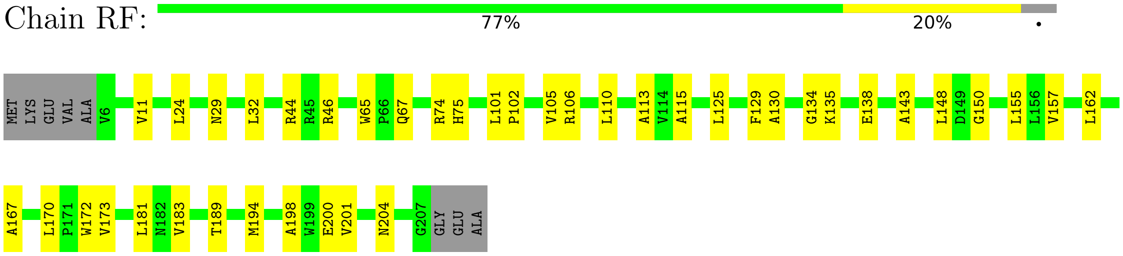
- Molecule 38: 50S ribosomal protein L3



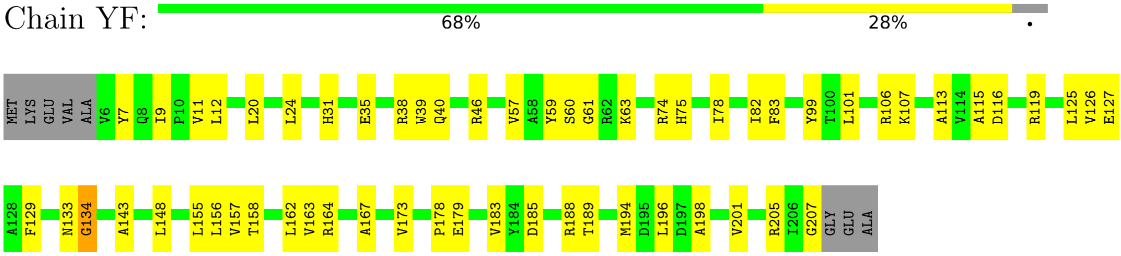
- Molecule 38: 50S ribosomal protein L3



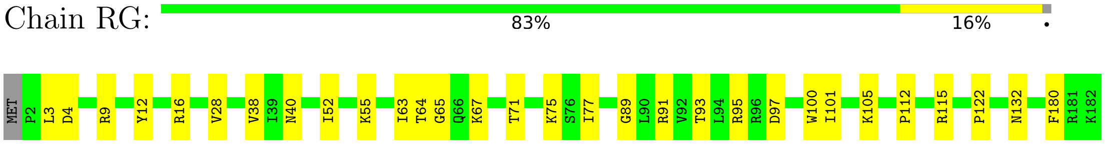
- Molecule 39: 50S ribosomal protein L4



- Molecule 39: 50S ribosomal protein L4

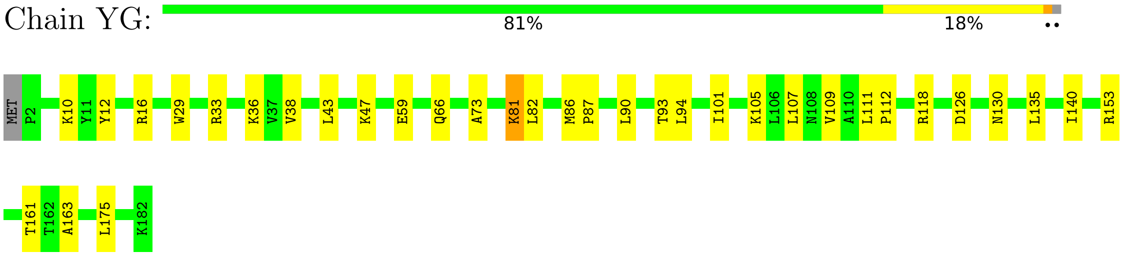


- Molecule 40: 50S ribosomal protein L5



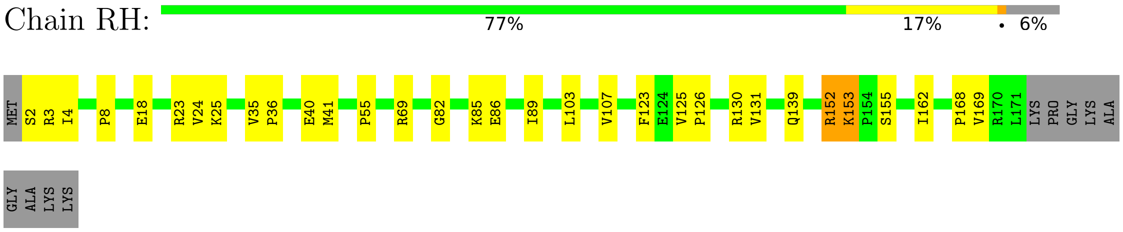
- Molecule 40: 50S ribosomal protein L5

Chain YG:



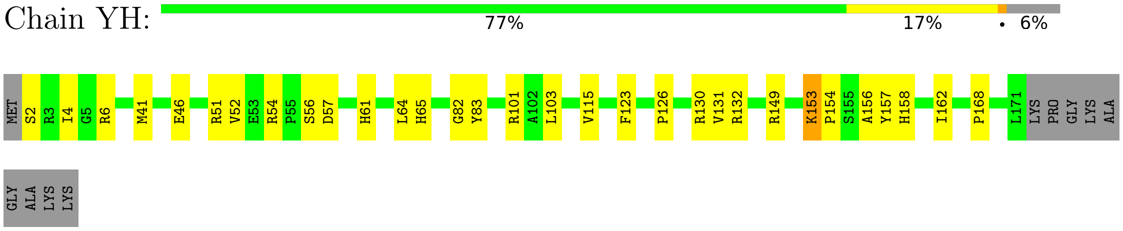
- Molecule 41: 50S ribosomal protein L6

Chain RH:



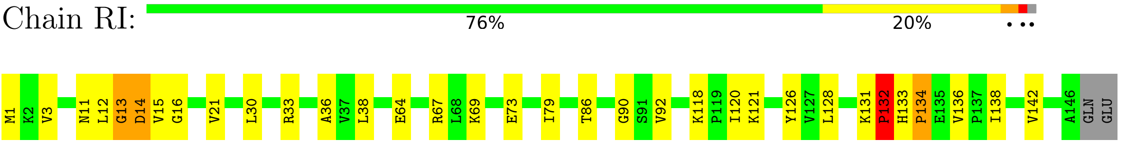
- Molecule 41: 50S ribosomal protein L6

Chain YH:



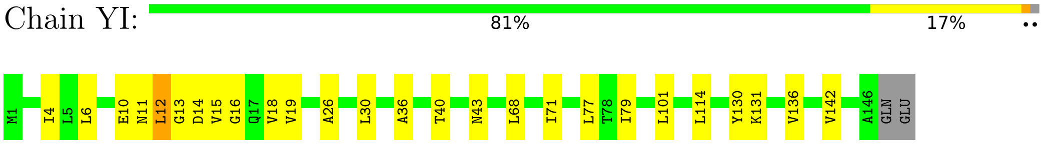
- Molecule 42: 50S ribosomal protein L9

Chain RI:



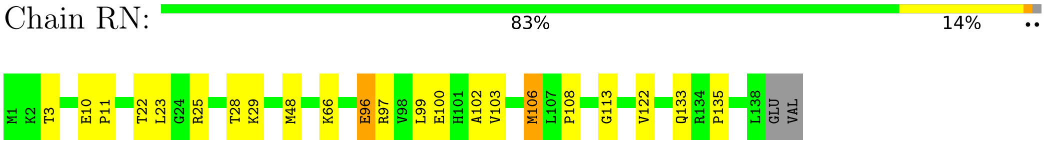
- Molecule 42: 50S ribosomal protein L9

Chain YI:



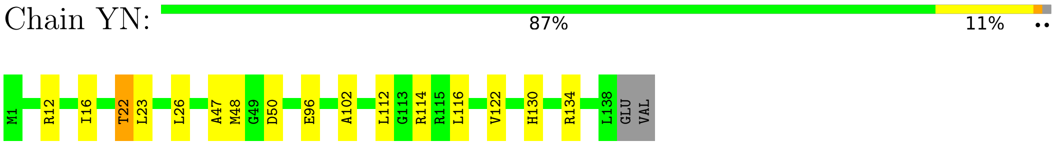
- Molecule 43: 50S ribosomal protein L13

Chain RN:



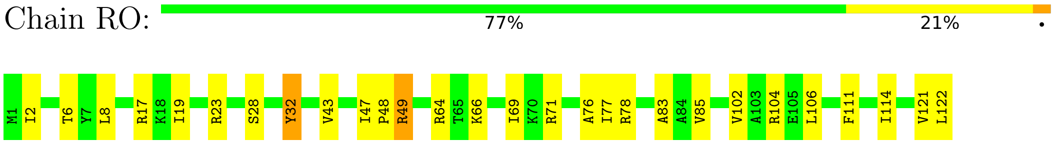
- Molecule 43: 50S ribosomal protein L13

Chain YN:



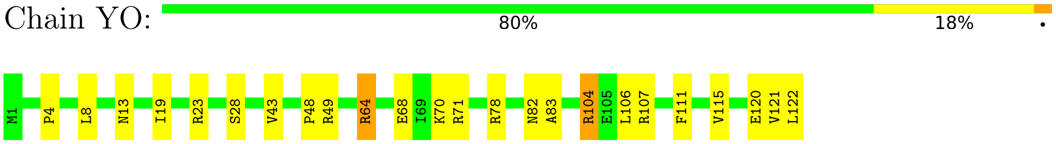
- Molecule 44: 50S ribosomal protein L14

Chain RO:



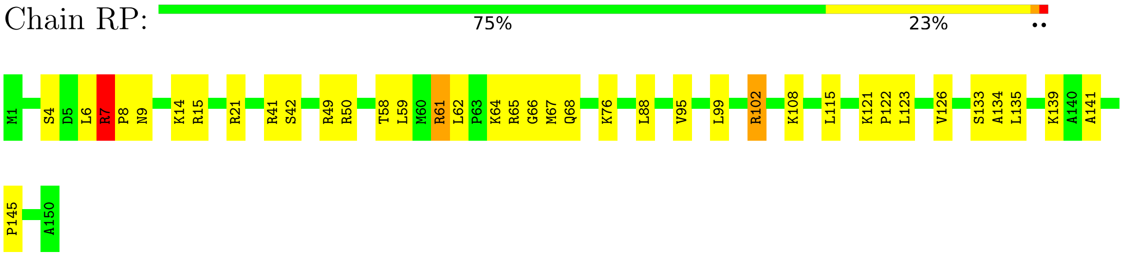
- Molecule 44: 50S ribosomal protein L14

Chain YO:



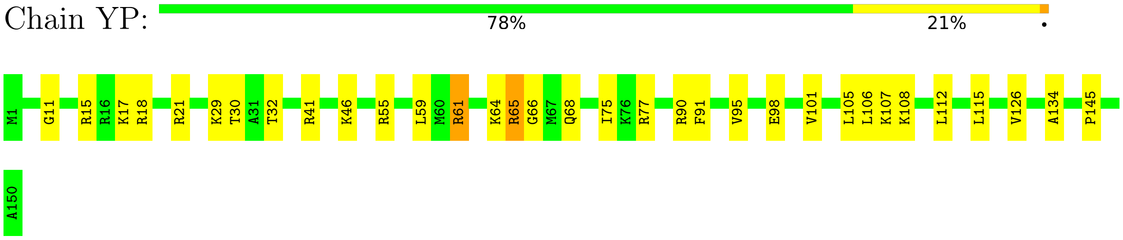
- Molecule 45: 50S ribosomal protein L15

Chain RP:



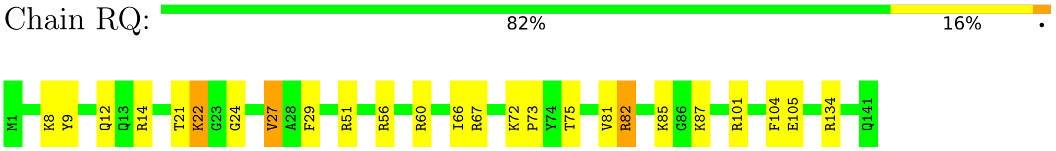
- Molecule 45: 50S ribosomal protein L15

Chain YP:



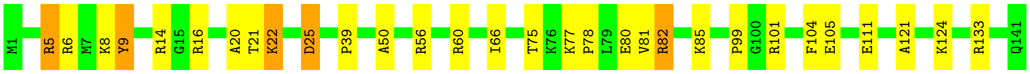
- Molecule 46: 50S ribosomal protein L16

Chain RQ:



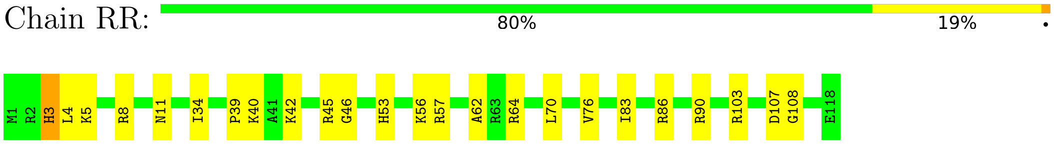
- Molecule 46: 50S ribosomal protein L16

Chain YQ:



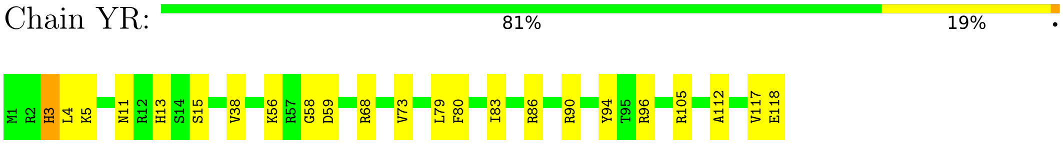
- Molecule 47: 50S ribosomal protein L17

Chain RR:



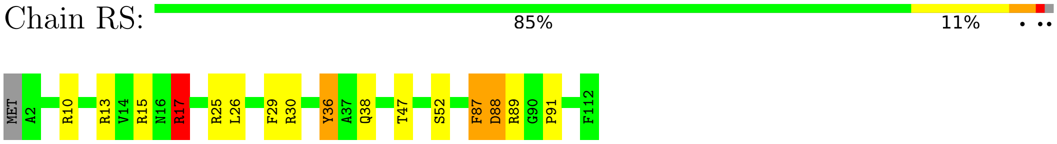
- Molecule 47: 50S ribosomal protein L17

Chain YR:



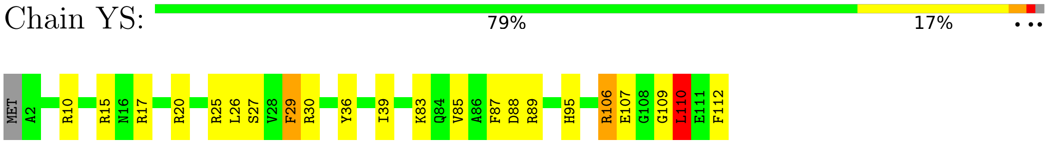
- Molecule 48: 50S ribosomal protein L18

Chain RS:



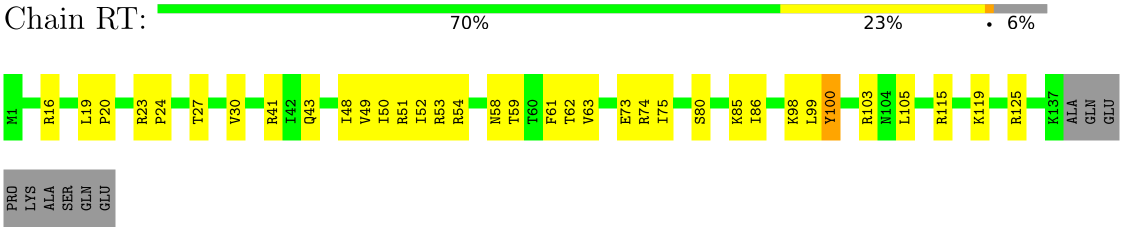
- Molecule 48: 50S ribosomal protein L18

Chain YS:



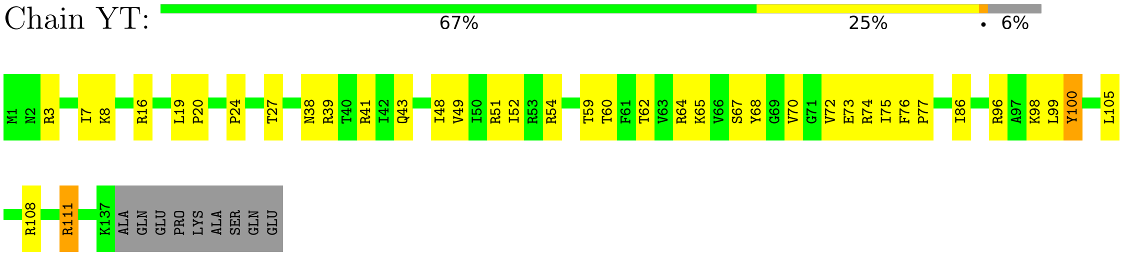
- Molecule 49: 50S ribosomal protein L19

Chain RT:



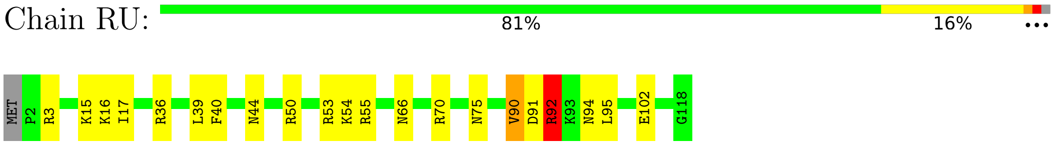
- Molecule 49: 50S ribosomal protein L19

Chain YT:



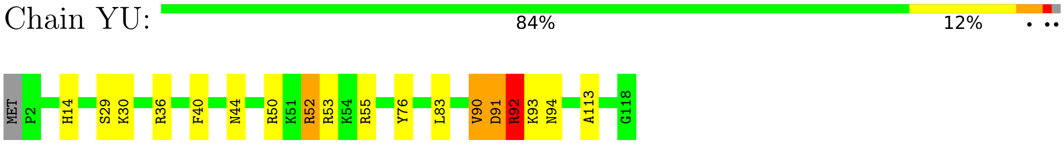
- Molecule 50: 50S ribosomal protein L20

Chain RU:



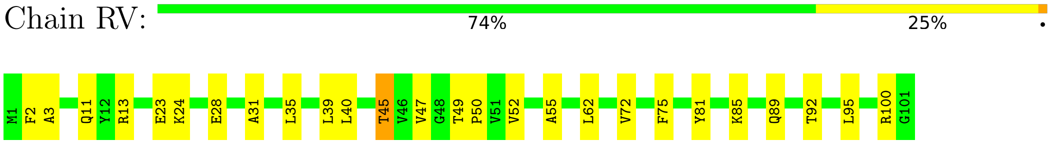
- Molecule 50: 50S ribosomal protein L20

Chain YU:



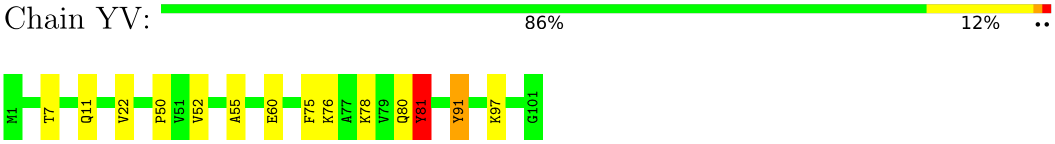
- Molecule 51: 50S ribosomal protein L21

Chain RV:



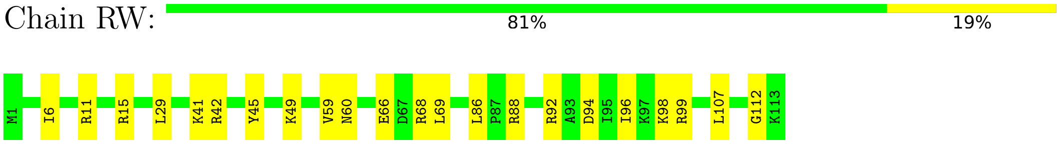
- Molecule 51: 50S ribosomal protein L21

Chain YV:



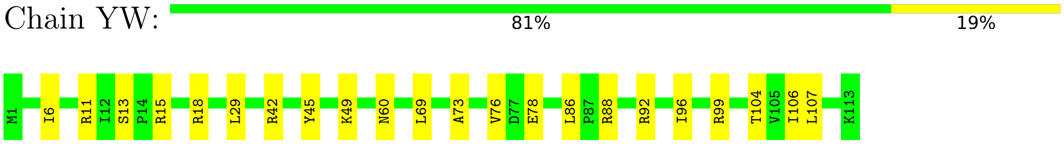
- Molecule 52: 50S ribosomal protein L22

Chain RW:



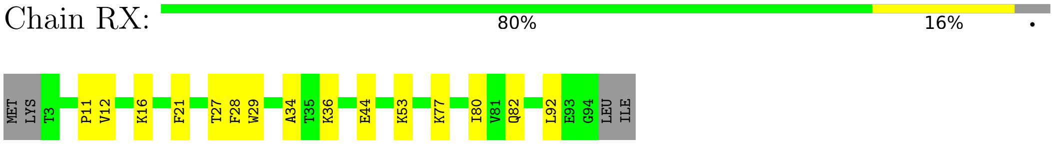
- Molecule 52: 50S ribosomal protein L22

Chain YW:



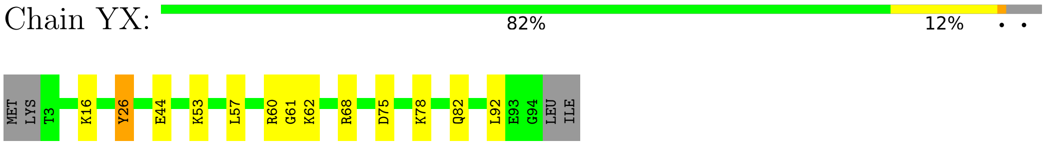
- Molecule 53: 50S ribosomal protein L23

Chain RX:



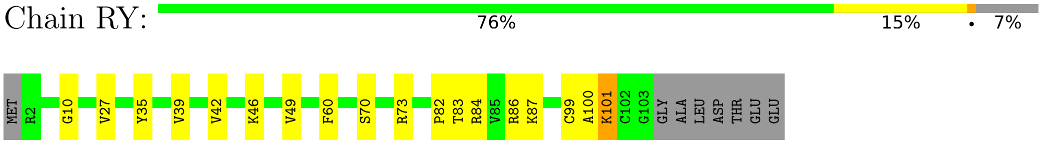
- Molecule 53: 50S ribosomal protein L23

Chain YX:



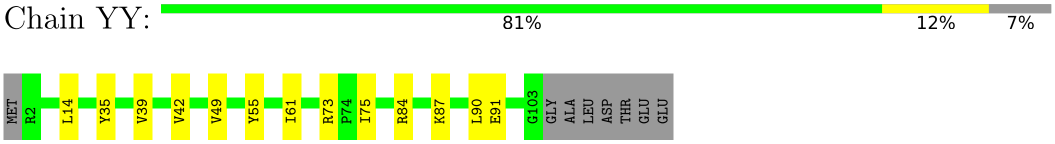
- Molecule 54: 50S ribosomal protein L24

Chain RY:



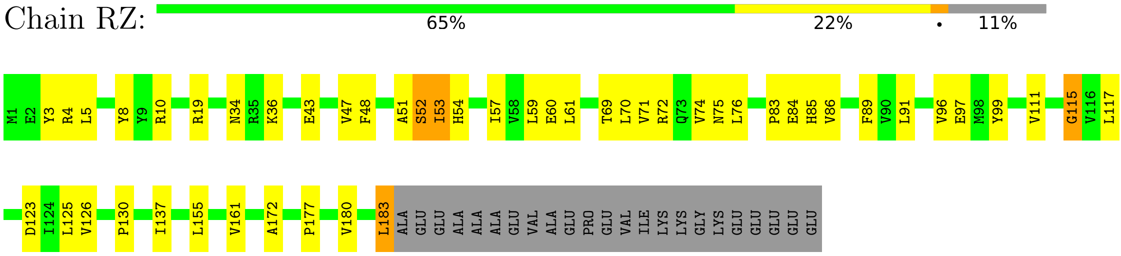
- Molecule 54: 50S ribosomal protein L24

Chain YY:



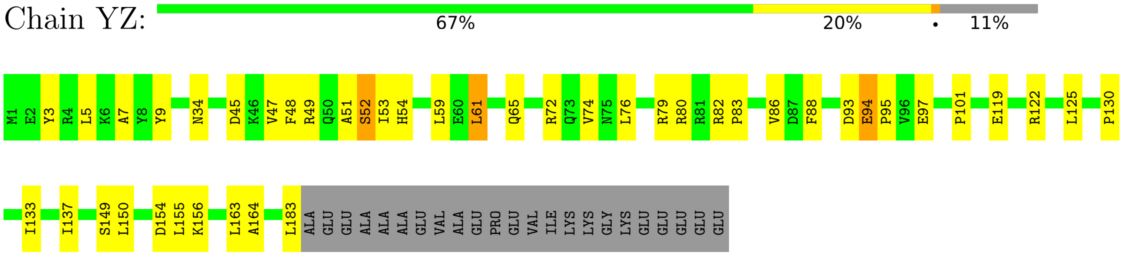
- Molecule 55: 50S ribosomal protein L25

Chain RZ:



- Molecule 55: 50S ribosomal protein L25

Chain YZ:



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	209.38Å 449.76Å 619.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 3.10	Depositor
% Data completeness (in resolution range)	97.2 (49.74-3.10)	Depositor
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.225 , 0.266	Depositor
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.328	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	294981	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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: SF4, ZN, PAR, 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	1.05	0/36098	1.14	177/56341 (0.3%)
1	XA	1.14	0/36101	1.18	234/56346 (0.4%)
2	QB	0.48	0/1959	0.68	0/2642
2	XB	0.55	0/1959	0.68	0/2642
3	QC	0.50	0/1629	0.69	2/2195 (0.1%)
3	XC	0.52	0/1629	0.66	0/2195
4	QD	0.58	0/1704	0.63	0/2284
4	XD	0.58	0/1704	0.65	0/2284
5	QE	0.55	1/1171 (0.1%)	0.67	0/1576
5	XE	0.54	0/1171	0.65	1/1576 (0.1%)
6	QF	0.60	0/856	0.62	0/1154
6	XF	0.58	0/856	0.66	0/1154
7	QG	0.51	0/1276	0.65	1/1709 (0.1%)
7	XG	0.52	0/1276	0.65	0/1709
8	QH	0.51	0/1136	0.66	0/1527
8	XH	0.59	0/1136	0.66	0/1527
9	QI	0.53	0/1029	0.77	0/1379
9	XI	0.53	0/1029	0.72	0/1379
10	QJ	0.46	0/814	0.64	0/1095
10	XJ	0.53	0/814	0.63	0/1095
11	QK	0.55	0/900	0.64	0/1213
11	XK	0.53	0/900	0.63	0/1213
12	QL	0.56	0/991	0.76	3/1327 (0.2%)
12	XL	0.63	0/991	0.75	1/1327 (0.1%)
13	QM	0.52	0/974	0.79	1/1303 (0.1%)
13	XM	0.50	0/974	0.72	0/1303
14	QN	0.55	0/501	0.67	0/664
14	XN	0.62	0/501	0.75	0/664
15	QO	0.50	0/745	0.59	0/992
15	XO	0.48	0/745	0.59	0/992
16	QP	0.58	0/721	0.75	2/970 (0.2%)
16	XP	0.55	0/721	0.76	1/970 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.60	0/847	0.65	1/1131 (0.1%)
17	XQ	0.59	0/847	0.64	1/1131 (0.1%)
18	QR	0.59	0/579	0.73	0/768
18	XR	0.57	0/579	0.65	0/768
19	QS	0.47	0/689	0.70	0/926
19	XS	0.62	0/689	0.97	2/926 (0.2%)
20	QT	0.48	0/765	0.66	0/1007
20	XT	0.44	0/765	0.71	1/1007 (0.1%)
21	QU	0.59	0/221	0.73	0/288
21	XU	0.67	0/221	0.81	1/288 (0.3%)
22	QV	0.91	0/1832	1.23	17/2855 (0.6%)
22	XV	1.07	0/1832	1.13	7/2855 (0.2%)
23	QX	0.77	0/446	1.06	2/695 (0.3%)
23	XX	0.87	0/446	1.17	1/695 (0.1%)
24	QY	0.74	0/1790	1.20	15/2789 (0.5%)
24	XY	0.78	0/1790	1.20	10/2789 (0.4%)
25	R0	0.59	0/657	0.68	1/874 (0.1%)
25	Y0	0.69	0/657	0.69	0/874
26	R1	0.63	0/770	0.79	2/1022 (0.2%)
26	Y1	0.64	0/770	0.76	1/1022 (0.1%)
27	R2	0.52	0/583	0.68	0/771
27	Y2	0.56	0/583	0.75	0/771
28	R3	0.50	0/474	0.57	0/635
28	Y3	0.57	0/474	0.58	0/635
29	R4	0.61	0/594	1.05	2/795 (0.3%)
29	Y4	0.56	0/594	1.05	3/795 (0.4%)
30	R5	0.60	0/473	0.92	2/639 (0.3%)
30	Y5	0.68	0/473	0.74	0/639
31	R6	0.70	0/431	1.14	2/575 (0.3%)
31	Y6	0.73	0/431	1.04	2/575 (0.3%)
32	R7	0.66	0/438	0.66	0/575
32	Y7	0.71	0/438	0.71	0/575
33	R8	0.64	0/525	0.86	1/691 (0.1%)
33	Y8	0.78	1/525 (0.2%)	0.84	0/691
34	R9	0.61	0/310	0.54	0/407
34	Y9	0.67	0/310	0.60	0/407
35	RA	1.23	8/69521 (0.0%)	1.22	496/108529 (0.5%)
35	YA	1.38	19/69543 (0.0%)	1.26	627/108563 (0.6%)
36	RB	0.99	0/2878	1.19	16/4490 (0.4%)
36	YB	1.23	0/2878	1.22	17/4490 (0.4%)
37	RD	0.71	0/2165	0.76	1/2919 (0.0%)
37	YD	0.75	0/2165	0.78	2/2919 (0.1%)
38	RE	0.63	0/1601	0.82	4/2160 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YE	0.71	0/1601	0.85	1/2160 (0.0%)
39	RF	0.65	0/1620	0.67	0/2194
39	YF	0.72	1/1620 (0.1%)	0.71	1/2194 (0.0%)
40	RG	0.51	0/1499	0.72	0/2016
40	YG	0.55	0/1499	0.70	1/2016 (0.0%)
41	RH	0.50	0/1332	0.81	2/1802 (0.1%)
41	YH	0.63	0/1332	0.84	3/1802 (0.2%)
42	RI	0.59	2/1151 (0.2%)	0.90	7/1558 (0.4%)
42	YI	0.52	0/1151	0.83	2/1558 (0.1%)
43	RN	0.57	0/1131	0.71	1/1525 (0.1%)
43	YN	0.63	0/1131	0.74	2/1525 (0.1%)
44	RO	0.62	0/943	0.66	1/1269 (0.1%)
44	YO	0.72	0/943	0.76	2/1269 (0.2%)
45	RP	0.59	0/1162	0.89	0/1544
45	YP	0.61	0/1162	0.85	1/1544 (0.1%)
46	RQ	0.63	0/1143	0.83	2/1527 (0.1%)
46	YQ	0.71	0/1143	0.87	3/1527 (0.2%)
47	RR	0.62	0/982	0.69	0/1312
47	YR	0.64	0/982	0.72	0/1312
48	RS	0.55	0/892	0.92	5/1187 (0.4%)
48	YS	0.59	0/892	0.78	1/1187 (0.1%)
49	RT	0.61	0/1155	0.78	3/1542 (0.2%)
49	YT	0.66	0/1155	0.82	4/1542 (0.3%)
50	RU	0.61	0/982	0.67	1/1306 (0.1%)
50	YU	0.70	0/982	0.69	1/1306 (0.1%)
51	RV	0.58	0/790	0.82	2/1057 (0.2%)
51	YV	0.76	0/790	0.88	2/1057 (0.2%)
52	RW	0.66	0/911	0.70	0/1220
52	YW	0.64	0/911	0.66	0/1220
53	RX	0.66	0/739	0.70	0/993
53	YX	0.71	0/739	0.67	0/993
54	RY	0.59	0/798	0.69	0/1064
54	YY	0.70	0/798	0.76	0/1064
55	RZ	0.52	0/1493	0.81	4/2026 (0.2%)
55	YZ	0.56	0/1493	0.78	2/2026 (0.1%)
All	All	1.08	32/319657 (0.0%)	1.11	1714/478147 (0.4%)

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
48	RS	0	1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Y8	23	VAL	CB-CG1	-8.00	1.36	1.52
35	YA	528	A	N9-C4	-7.92	1.33	1.37
35	YA	1021	A	N9-C4	-7.85	1.33	1.37
35	YA	1142(A)	A	N9-C4	-7.78	1.33	1.37
35	YA	2287	A	N9-C4	-7.34	1.33	1.37

The worst 5 of 1714 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	XS	10	PHE	CB-CG-CD1	12.46	129.52	120.80
1	QA	1301	U	N1-C2-O2	11.86	131.10	122.80
35	RA	2506	U	C2-N1-C1’	11.85	131.92	117.70
1	QA	1301	U	C2-N1-C1’	11.78	131.83	117.70
35	YA	2506	U	C2-N1-C1’	11.73	131.77	117.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	RS	17	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16277	208	0
1	XA	32249	0	16279	169	0
2	QB	1924	0	1975	27	0
2	XB	1924	0	1975	28	0
3	QC	1605	0	1668	37	0
3	XC	1605	0	1668	16	0
4	QD	1674	0	1718	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	XD	1674	0	1718	21	0
5	QE	1155	0	1213	20	0
5	XE	1155	0	1213	8	0
6	QF	843	0	857	10	0
6	XF	843	0	857	8	0
7	QG	1257	0	1296	11	0
7	XG	1257	0	1296	8	0
8	QH	1116	0	1177	13	0
8	XH	1116	0	1177	19	0
9	QI	1010	0	1037	23	0
9	XI	1010	0	1037	24	0
10	QJ	801	0	849	18	0
10	XJ	801	0	849	15	0
11	QK	885	0	904	17	0
11	XK	885	0	904	9	0
12	QL	975	0	1062	17	0
12	XL	975	0	1062	15	0
13	QM	964	0	1034	35	0
13	XM	964	0	1034	17	0
14	QN	492	0	529	14	0
14	XN	492	0	529	5	0
15	QO	734	0	771	7	0
15	XO	734	0	771	4	0
16	QP	705	0	725	14	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	11	0
17	XQ	834	0	904	9	0
18	QR	574	0	644	13	0
18	XR	574	0	644	8	0
19	QS	674	0	699	21	0
19	XS	674	0	699	13	0
20	QT	763	0	860	6	0
20	XT	763	0	861	17	0
21	QU	217	0	234	5	0
21	XU	217	0	234	1	0
22	QV	1640	0	837	4	0
22	XV	1640	0	837	3	0
23	QX	396	0	197	2	0
23	XX	396	0	197	3	0
24	QY	1602	0	811	23	0
24	XY	1602	0	811	10	0
25	R0	648	0	672	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Y0	648	0	672	10	0
26	R1	763	0	847	13	0
26	Y1	763	0	848	12	0
27	R2	581	0	629	15	0
27	Y2	581	0	629	11	0
28	R3	469	0	518	5	0
28	Y3	469	0	518	4	0
29	R4	581	0	577	17	0
29	Y4	581	0	577	16	0
30	R5	459	0	480	9	0
30	Y5	459	0	480	10	0
31	R6	424	0	450	11	0
31	Y6	424	0	450	11	0
32	R7	430	0	480	7	0
32	Y7	430	0	480	6	0
33	R8	517	0	582	17	0
33	Y8	517	0	582	30	0
34	R9	307	0	335	5	0
34	Y9	307	0	335	6	0
35	RA	62071	0	31280	341	0
35	YA	62091	0	31290	289	0
36	RB	2573	0	1306	15	0
36	YB	2573	0	1306	13	0
37	RD	2115	0	2195	43	0
37	YD	2115	0	2195	51	0
38	RE	1568	0	1633	45	0
38	YE	1568	0	1634	31	0
39	RF	1585	0	1632	22	0
39	YF	1585	0	1632	32	0
40	RG	1474	0	1535	21	0
40	YG	1474	0	1535	18	0
41	RH	1307	0	1382	20	0
41	YH	1307	0	1382	20	0
42	RI	1136	0	1223	12	0
42	YI	1136	0	1223	11	0
43	RN	1104	0	1180	23	0
43	YN	1104	0	1180	8	0
44	RO	933	0	996	23	0
44	YO	933	0	996	19	0
45	RP	1145	0	1227	30	0
45	YP	1145	0	1227	27	0
46	RQ	1122	0	1179	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	YQ	1122	0	1177	20	0
47	RR	968	0	1033	17	0
47	YR	968	0	1033	16	0
48	RS	882	0	943	9	0
48	YS	882	0	943	16	0
49	RT	1141	0	1202	29	0
49	YT	1141	0	1202	23	0
50	RU	964	0	1022	22	0
50	YU	964	0	1022	19	0
51	RV	779	0	852	17	0
51	YV	779	0	852	12	0
52	RW	900	0	964	15	0
52	YW	900	0	964	17	0
53	RX	725	0	778	9	0
53	YX	725	0	778	9	0
54	RY	785	0	878	14	0
54	YY	785	0	878	9	0
55	RZ	1461	0	1493	27	0
55	YZ	1461	0	1493	32	0
56	QA	73	0	0	0	0
56	QF	1	0	0	0	0
56	QM	1	0	0	0	0
56	QV	1	0	0	0	0
56	QX	2	0	0	0	0
56	R0	1	0	0	0	0
56	R5	1	0	0	0	0
56	R8	1	0	0	0	0
56	R9	1	0	0	0	0
56	RA	281	0	0	0	0
56	RB	4	0	0	0	0
56	RD	1	0	0	0	0
56	RE	4	0	0	0	0
56	RF	1	0	0	0	0
56	RP	3	0	0	0	0
56	RR	1	0	0	0	0
56	RU	1	0	0	0	0
56	XA	91	0	0	0	0
56	XF	1	0	0	0	0
56	XM	1	0	0	0	0
56	XV	2	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	Y1	1	0	0	0	0
56	Y2	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	2	0	0	0	0
56	Y8	1	0	0	0	0
56	Y9	1	0	0	0	0
56	YA	347	0	0	0	0
56	YB	6	0	0	0	0
56	YE	3	0	0	0	0
56	YN	1	0	0	0	0
56	YP	3	0	0	0	0
56	YQ	3	0	0	0	0
56	YR	1	0	0	0	0
56	YX	1	0	0	0	0
57	QA	42	0	45	0	0
57	XA	42	0	45	4	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	294981	0	199665	2182	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 2182 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)
55:YZ:94:GLU:CG	55:YZ:95:PRO:HD3	1.74	1.18
35:RA:1138:G:H21	43:RN:106:MET:HE1	1.13	1.11
35:RA:2055:C:H5’	35:RA:2056:G:H5”	1.35	1.07
55:YZ:94:GLU:HB3	55:YZ:95:PRO:CD	1.85	1.07
19:QS:10:PHE:HB2	19:QS:16:LEU:HD11	1.34	1.06

There are no symmetry-related clashes.

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	235/256 (92%)	206 (88%)	27 (12%)	2 (1%)	17	52
2	XB	235/256 (92%)	207 (88%)	28 (12%)	0	100	100
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
4	QD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	29	64
4	XD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	29	64
5	QE	149/162 (92%)	138 (93%)	11 (7%)	0	100	100
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	22	57
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	22	57
8	QH	136/138 (99%)	121 (89%)	15 (11%)	0	100	100
8	XH	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
9	QI	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
9	XI	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	54
10	QJ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	XJ	97/105 (92%)	84 (87%)	13 (13%)	0	100	100
11	QK	117/129 (91%)	109 (93%)	8 (7%)	0	100	100
11	XK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
12	QL	123/131 (94%)	107 (87%)	15 (12%)	1 (1%)	19	54
12	XL	123/131 (94%)	108 (88%)	10 (8%)	5 (4%)	3	16
13	QM	119/126 (94%)	99 (83%)	19 (16%)	1 (1%)	19	54
13	XM	119/126 (94%)	102 (86%)	17 (14%)	0	100	100
14	QN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	XN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	9	36
15	QO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
15	XO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	QP	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	67 (98%)	1 (2%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	82/93 (88%)	69 (84%)	13 (16%)	0	100	100
19	XS	82/93 (88%)	71 (87%)	8 (10%)	3 (4%)	3	19
20	QT	97/106 (92%)	83 (86%)	14 (14%)	0	100	100
20	XT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	4	23
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
25	R0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	Y0	80/85 (94%)	76 (95%)	4 (5%)	0	100	100
26	R1	95/98 (97%)	80 (84%)	12 (13%)	3 (3%)	4	22
26	Y1	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	7	30
27	R2	67/72 (93%)	59 (88%)	7 (10%)	1 (2%)	10	39
27	Y2	67/72 (93%)	60 (90%)	7 (10%)	0	100	100
28	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	R4	69/71 (97%)	44 (64%)	18 (26%)	7 (10%)	0	3
29	Y4	69/71 (97%)	41 (59%)	26 (38%)	2 (3%)	4	24
30	R5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
30	Y5	57/60 (95%)	48 (84%)	9 (16%)	0	100	100
31	R6	47/54 (87%)	31 (66%)	13 (28%)	3 (6%)	1	8
31	Y6	47/54 (87%)	32 (68%)	12 (26%)	3 (6%)	1	8
32	R7	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
32	Y7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	R8	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	4	22
33	Y8	62/65 (95%)	51 (82%)	10 (16%)	1 (2%)	9	37
34	R9	35/37 (95%)	35 (100%)	0	0	100	100
34	Y9	35/37 (95%)	35 (100%)	0	0	100	100
37	RD	270/276 (98%)	244 (90%)	21 (8%)	5 (2%)	8	33
37	YD	270/276 (98%)	243 (90%)	26 (10%)	1 (0%)	34	69
38	RE	203/206 (98%)	165 (81%)	35 (17%)	3 (2%)	10	39
38	YE	203/206 (98%)	168 (83%)	30 (15%)	5 (2%)	5	27
39	RF	200/210 (95%)	184 (92%)	13 (6%)	3 (2%)	10	39
39	YF	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	15	49
40	RG	179/182 (98%)	158 (88%)	21 (12%)	0	100	100
40	YG	179/182 (98%)	156 (87%)	22 (12%)	1 (1%)	25	59
41	RH	168/180 (93%)	134 (80%)	30 (18%)	4 (2%)	6	27
41	YH	168/180 (93%)	140 (83%)	26 (16%)	2 (1%)	13	44
42	RI	144/148 (97%)	115 (80%)	21 (15%)	8 (6%)	2	11
42	YI	144/148 (97%)	116 (81%)	22 (15%)	6 (4%)	3	16
43	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	22	57
43	YN	136/140 (97%)	117 (86%)	18 (13%)	1 (1%)	22	57
44	RO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
44	YO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	54
45	RP	148/150 (99%)	117 (79%)	27 (18%)	4 (3%)	5	25
45	YP	148/150 (99%)	118 (80%)	28 (19%)	2 (1%)	11	40
46	RQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	22	57
46	YQ	139/141 (99%)	116 (84%)	19 (14%)	4 (3%)	4	24
47	RR	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	9	36
47	YR	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	9	36
48	RS	109/112 (97%)	91 (84%)	15 (14%)	3 (3%)	5	25
48	YS	109/112 (97%)	92 (84%)	16 (15%)	1 (1%)	17	52
49	RT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
49	YT	135/146 (92%)	117 (87%)	17 (13%)	1 (1%)	22	57
50	RU	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	YU	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	5	26
51	RV	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	7	31
51	YV	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	15	49
52	RW	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
52	YW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
53	RX	90/96 (94%)	81 (90%)	9 (10%)	0	100	100
53	YX	90/96 (94%)	82 (91%)	7 (8%)	1 (1%)	14	46
54	RY	100/110 (91%)	91 (91%)	9 (9%)	0	100	100
54	YY	100/110 (91%)	94 (94%)	6 (6%)	0	100	100
55	RZ	181/206 (88%)	152 (84%)	24 (13%)	5 (3%)	5	25
55	YZ	181/206 (88%)	158 (87%)	19 (10%)	4 (2%)	6	29
All	All	11470/12126 (95%)	10176 (89%)	1168 (10%)	126 (1%)	14	46

5 of 126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	QD	5	ILE
26	R1	92	LYS
29	R4	24	THR
29	R4	43	TYR
31	R6	8	LYS

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	205/220 (93%)	203 (99%)	2 (1%)	76	90
2	XB	205/220 (93%)	204 (100%)	1 (0%)	88	94
3	QC	159/188 (85%)	157 (99%)	2 (1%)	69	87
3	XC	159/188 (85%)	159 (100%)	0	100	100
4	QD	173/181 (96%)	171 (99%)	2 (1%)	71	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	XD	173/181 (96%)	172 (99%)	1 (1%)	86	94
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	91
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	91
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%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	119/119 (100%)	119 (100%)	0	100	100
8	XH	119/119 (100%)	118 (99%)	1 (1%)	81	92
9	QI	98/99 (99%)	95 (97%)	3 (3%)	40	70
9	XI	98/99 (99%)	97 (99%)	1 (1%)	76	90
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	89/92 (97%)	88 (99%)	1 (1%)	73	89
11	QK	90/99 (91%)	89 (99%)	1 (1%)	73	89
11	XK	90/99 (91%)	89 (99%)	1 (1%)	73	89
12	QL	104/108 (96%)	103 (99%)	1 (1%)	76	90
12	XL	104/108 (96%)	104 (100%)	0	100	100
13	QM	97/101 (96%)	96 (99%)	1 (1%)	76	90
13	XM	97/101 (96%)	97 (100%)	0	100	100
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	77 (98%)	2 (2%)	47	75
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%)	71 (99%)	1 (1%)	67	86
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	73	89
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	59 (97%)	2 (3%)	38	69
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	73/80 (91%)	70 (96%)	3 (4%)	30	64
19	XS	73/80 (91%)	71 (97%)	2 (3%)	44	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	57
25	R0	65/67 (97%)	64 (98%)	1 (2%)	65	85
25	Y0	65/67 (97%)	62 (95%)	3 (5%)	27	59
26	R1	82/83 (99%)	82 (100%)	0	100	100
26	Y1	82/83 (99%)	82 (100%)	0	100	100
27	R2	64/67 (96%)	64 (100%)	0	100	100
27	Y2	64/67 (96%)	62 (97%)	2 (3%)	40	70
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	51/52 (98%)	51 (100%)	0	100	100
29	R4	63/63 (100%)	59 (94%)	4 (6%)	18	48
29	Y4	63/63 (100%)	62 (98%)	1 (2%)	62	84
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	51/52 (98%)	50 (98%)	1 (2%)	55	80
31	R6	48/52 (92%)	47 (98%)	1 (2%)	53	79
31	Y6	48/52 (92%)	48 (100%)	0	100	100
32	R7	42/42 (100%)	42 (100%)	0	100	100
32	Y7	42/42 (100%)	41 (98%)	1 (2%)	49	76
33	R8	54/55 (98%)	53 (98%)	1 (2%)	57	81
33	Y8	54/55 (98%)	52 (96%)	2 (4%)	34	66
34	R9	34/34 (100%)	34 (100%)	0	100	100
34	Y9	34/34 (100%)	34 (100%)	0	100	100
37	RD	214/218 (98%)	212 (99%)	2 (1%)	78	91
37	YD	214/218 (98%)	211 (99%)	3 (1%)	67	86
38	RE	165/166 (99%)	163 (99%)	2 (1%)	71	88
38	YE	165/166 (99%)	163 (99%)	2 (1%)	71	88
39	RF	161/166 (97%)	160 (99%)	1 (1%)	86	94
39	YF	161/166 (97%)	160 (99%)	1 (1%)	86	94
40	RG	155/156 (99%)	154 (99%)	1 (1%)	86	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	YG	155/156 (99%)	154 (99%)	1 (1%)	86	94
41	RH	142/148 (96%)	141 (99%)	1 (1%)	84	93
41	YH	142/148 (96%)	141 (99%)	1 (1%)	84	93
42	RI	122/124 (98%)	121 (99%)	1 (1%)	81	92
42	YI	122/124 (98%)	122 (100%)	0	100	100
43	RN	117/119 (98%)	116 (99%)	1 (1%)	78	91
43	YN	117/119 (98%)	117 (100%)	0	100	100
44	RO	100/100 (100%)	98 (98%)	2 (2%)	55	80
44	YO	100/100 (100%)	98 (98%)	2 (2%)	55	80
45	RP	116/116 (100%)	113 (97%)	3 (3%)	46	74
45	YP	116/116 (100%)	115 (99%)	1 (1%)	78	91
46	RQ	111/111 (100%)	109 (98%)	2 (2%)	59	82
46	YQ	111/111 (100%)	108 (97%)	3 (3%)	44	74
47	RR	101/101 (100%)	101 (100%)	0	100	100
47	YR	101/101 (100%)	100 (99%)	1 (1%)	76	90
48	RS	87/88 (99%)	85 (98%)	2 (2%)	50	77
48	YS	87/88 (99%)	84 (97%)	3 (3%)	37	69
49	RT	120/127 (94%)	118 (98%)	2 (2%)	60	83
49	YT	120/127 (94%)	117 (98%)	3 (2%)	47	75
50	RU	93/94 (99%)	92 (99%)	1 (1%)	73	89
50	YU	93/94 (99%)	92 (99%)	1 (1%)	73	89
51	RV	82/82 (100%)	81 (99%)	1 (1%)	71	88
51	YV	82/82 (100%)	80 (98%)	2 (2%)	49	76
52	RW	92/92 (100%)	91 (99%)	1 (1%)	73	89
52	YW	92/92 (100%)	92 (100%)	0	100	100
53	RX	74/78 (95%)	74 (100%)	0	100	100
53	YX	74/78 (95%)	73 (99%)	1 (1%)	67	86
54	RY	85/91 (93%)	84 (99%)	1 (1%)	71	88
54	YY	85/91 (93%)	85 (100%)	0	100	100
55	RZ	162/179 (90%)	161 (99%)	1 (1%)	86	94
55	YZ	162/179 (90%)	160 (99%)	2 (1%)	71	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9688/10064 (96%)	9587 (99%)	101 (1%)	76 90

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	XI	18	PHE
32	Y7	49	ARG
55	YZ	93	ASP
11	XK	54	ARG
25	Y0	45	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
8	XH	78	GLN
19	XS	23	ASN
9	XI	31	GLN
10	XJ	84	GLN
39	YF	40	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	270 (18%)	29 (1%)
1	XA	1498/1522 (98%)	279 (18%)	27 (1%)
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	14 (18%)	0
23	QX	17/19 (89%)	8 (47%)	1 (5%)
23	XX	17/19 (89%)	7 (41%)	1 (5%)
24	QY	74/76 (97%)	28 (37%)	0
24	XY	74/76 (97%)	25 (33%)	0
35	RA	2879/2915 (98%)	587 (20%)	47 (1%)
35	YA	2880/2915 (98%)	587 (20%)	44 (1%)
36	RB	119/122 (97%)	21 (17%)	1 (0%)
36	YB	119/122 (97%)	18 (15%)	0
All	All	9327/9462 (98%)	1859 (19%)	150 (1%)

5 of 1859 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	31	G
1	QA	32	A
1	QA	39	G
1	QA	48	C

5 of 150 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	YA	503	A
35	YA	2566	A
35	YA	752	A
35	YA	1210	A
35	RA	752	A

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 855 ligands modelled in this entry, 851 are monoatomic - leaving 4 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 $\vert Z\vert > 2$ 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	$\#\vert Z\vert > 2$	Counts	RMSZ	$\#\vert Z\vert > 2$
57	PAR	XA	1670	-	45,45,45	0.86	1 (2%)	64,67,67	1.28	7 (10%)
57	PAR	QA	1663	-	45,45,45	0.80	0	64,67,67	1.30	8 (12%)
58	SF4	QD	501	-	0,12,12	-	-	-		
58	SF4	XD	501	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	PAR	XA	1670	-	-	3/18/94/94	0/4/4/4
57	PAR	QA	1663	-	-	3/18/94/94	0/4/4/4
58	SF4	QD	501	-	-	-	0/6/5/5
58	SF4	XD	501	4	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	XA	1670	PAR	C24-N24	-2.01	1.44	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	QA	1663	PAR	C13-O52-C52	-3.20	110.03	117.96
57	XA	1670	PAR	O11-C42-C32	-2.97	102.08	109.18
57	XA	1670	PAR	C13-O52-C52	-2.87	110.85	117.96
57	QA	1663	PAR	C64-C54-C44	-2.68	107.82	113.10
57	QA	1663	PAR	O62-C62-C12	-2.58	105.08	109.81

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	QA	1663	PAR	O54-C54-C64-N64
57	XA	1670	PAR	O54-C14-O33-C33
57	QA	1663	PAR	O51-C51-C61-O61
57	QA	1663	PAR	C23-C33-O33-C14
57	XA	1670	PAR	C43-C33-O33-C14

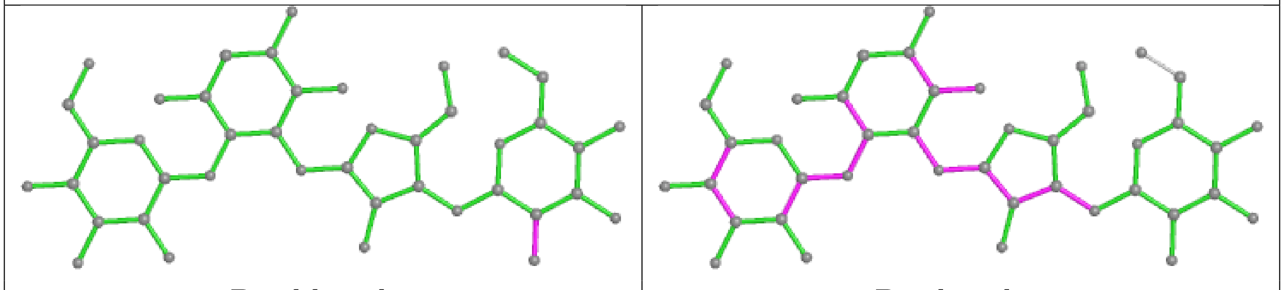
There are no ring outliers.

1 monomer is involved in 4 short contacts:

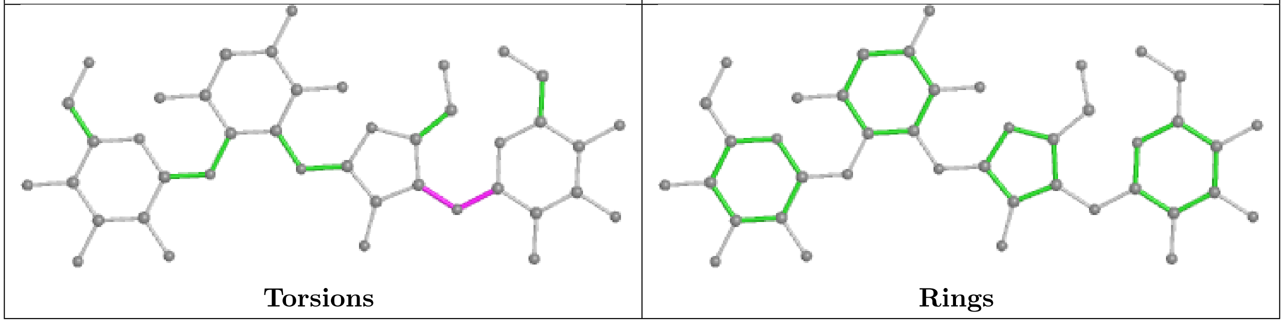
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	XA	1670	PAR	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PAR XA 1670

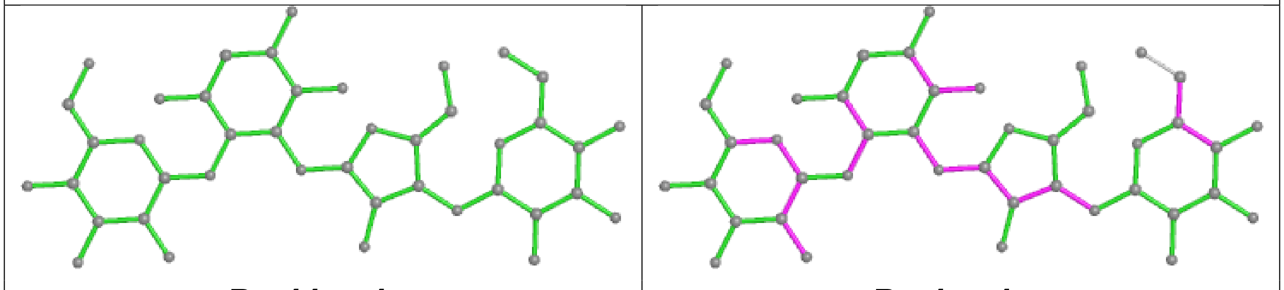


Bond lengths **Bond angles**

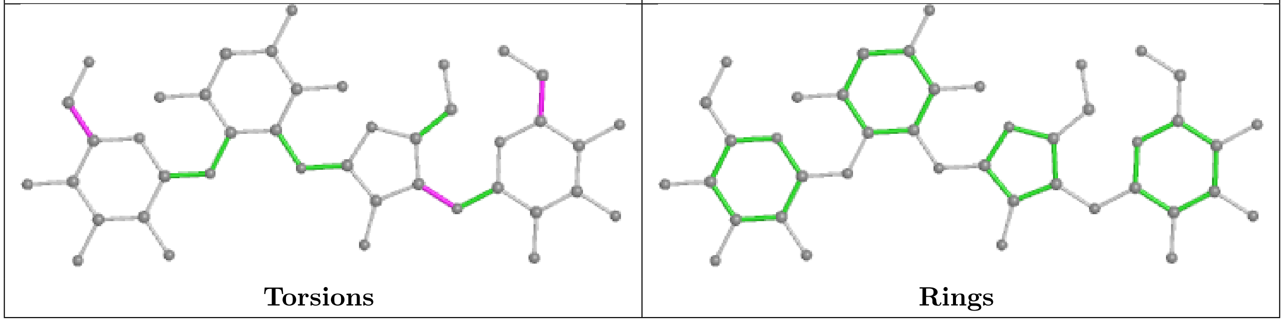


Torsions **Rings**

Ligand PAR QA 1663



Bond lengths **Bond angles**



Torsions **Rings**

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.