wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2023 – 06:36 PM EST

PDB ID	:	4P70
Title	:	Crystal Structure of Unmodified tRNA Proline (CGG) Bound to Codon CCG on the Ribosome
Authors	:	Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on	:	2014-03-25
Resolution	:	3.68 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

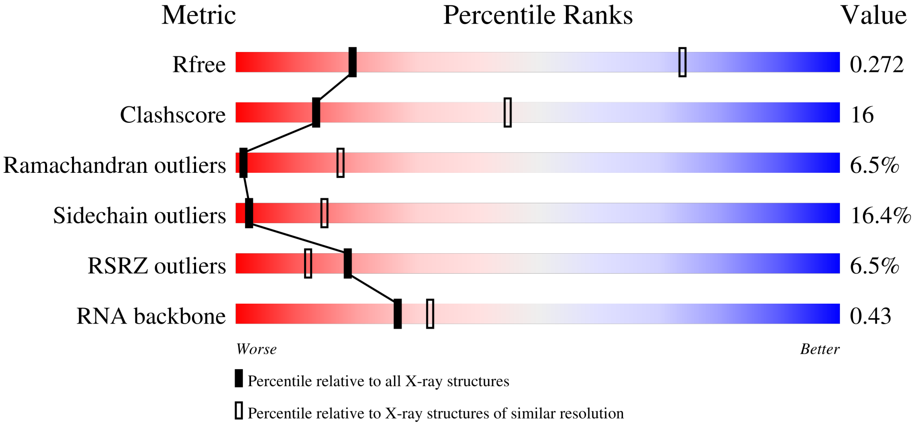
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

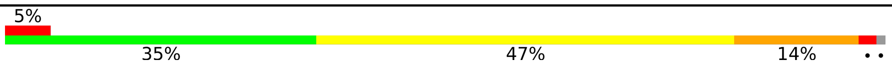
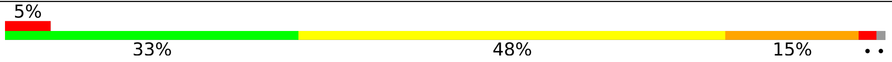
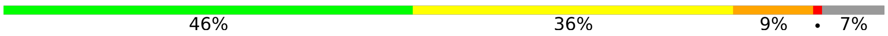
The reported resolution of this entry is 3.68 Å.

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.



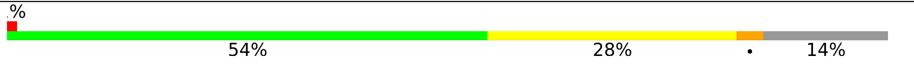
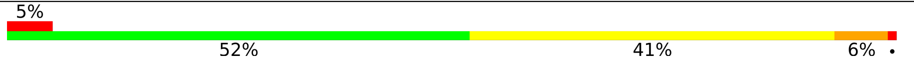
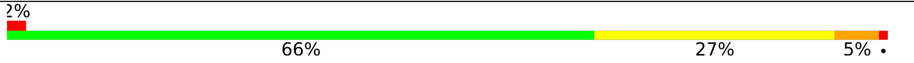
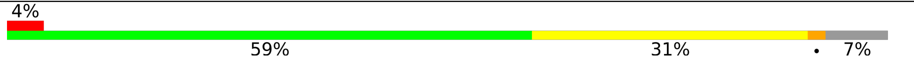
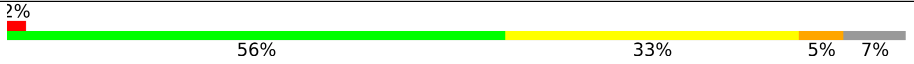
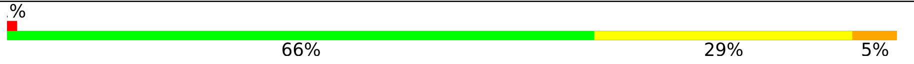
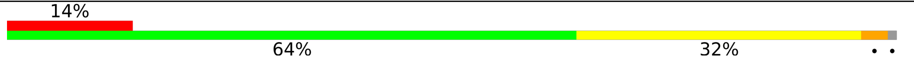
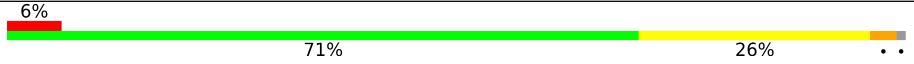
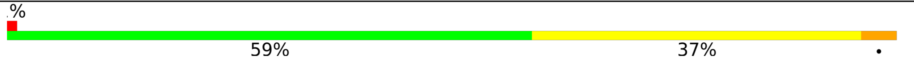
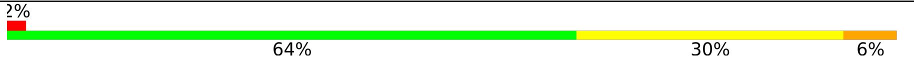
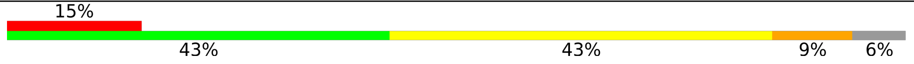
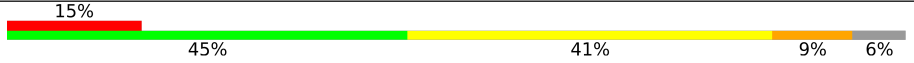
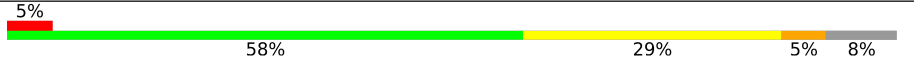
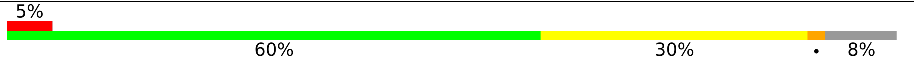
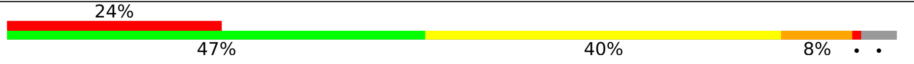
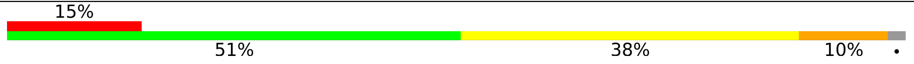
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1013 (3.84-3.52)
Clashscore	141614	1070 (3.84-3.52)
Ramachandran outliers	138981	1036 (3.84-3.52)
Sidechain outliers	138945	1033 (3.84-3.52)
RSRZ outliers	127900	1471 (3.86-3.50)
RNA backbone	3102	1024 (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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	QA	1522	 5% 35% 47% 14% • •
1	XA	1522	 5% 33% 48% 15% • •
2	QB	256	 4% 49% 36% 7% • 7%
2	XB	256	 46% 36% 9% • 7%

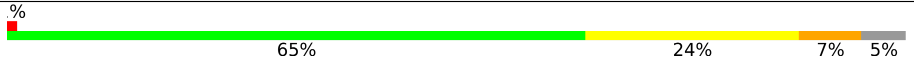
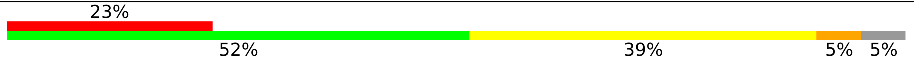
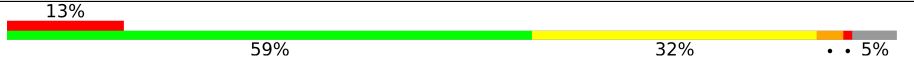
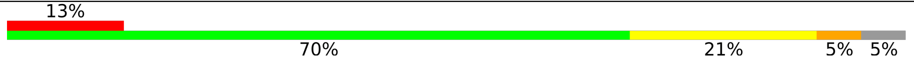
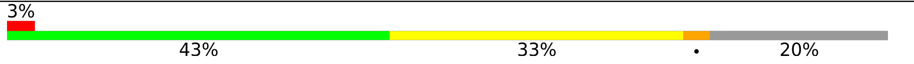
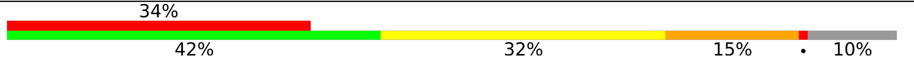
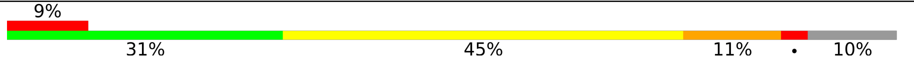
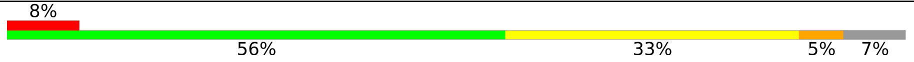
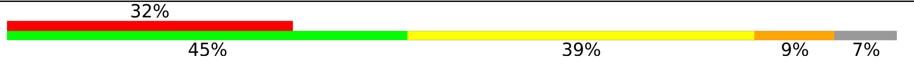
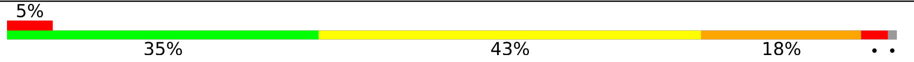
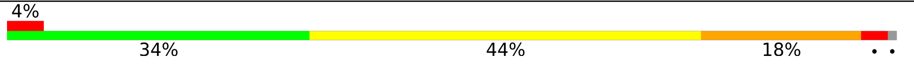
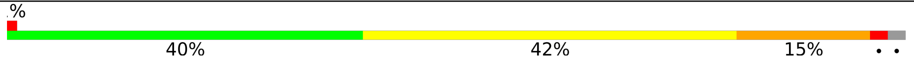
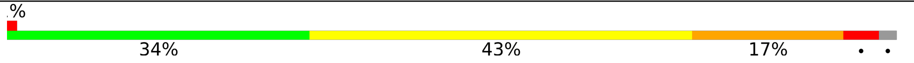
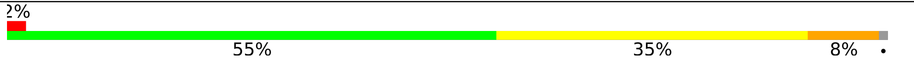
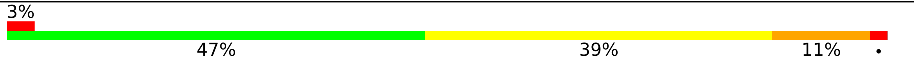
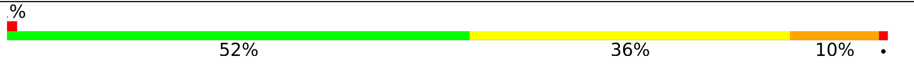
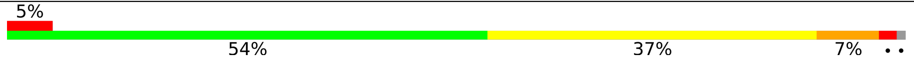
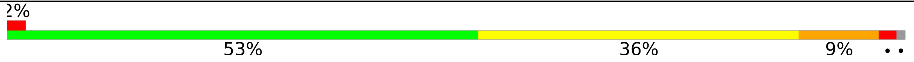
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	

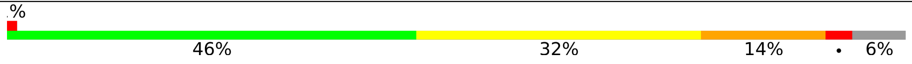
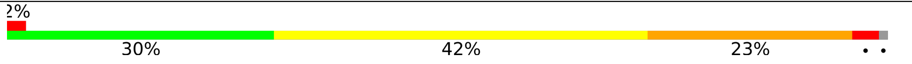
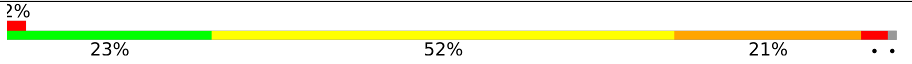
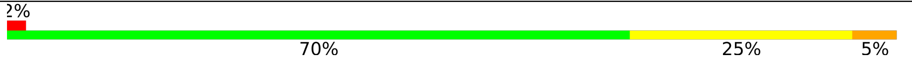
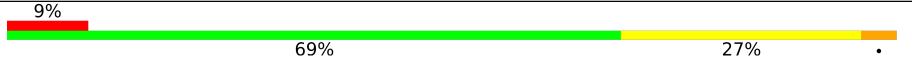
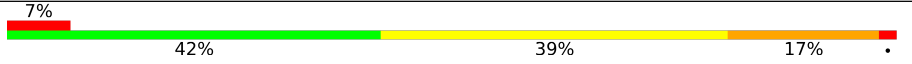
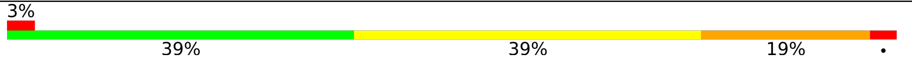
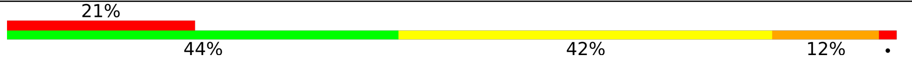
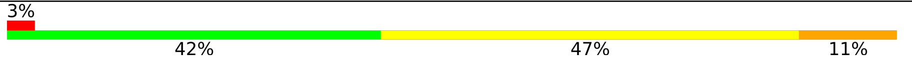
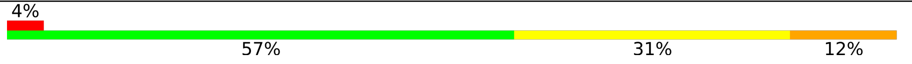
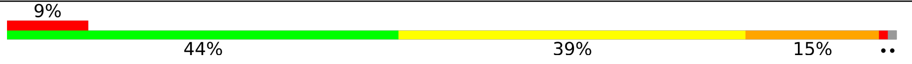
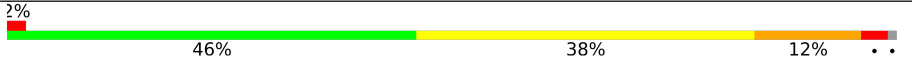
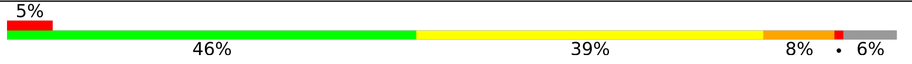
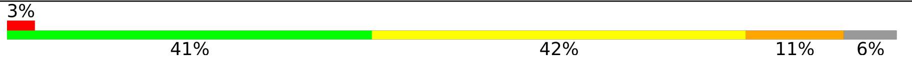
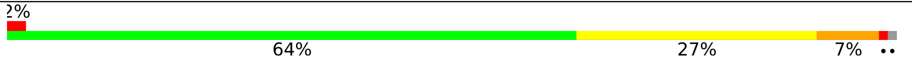
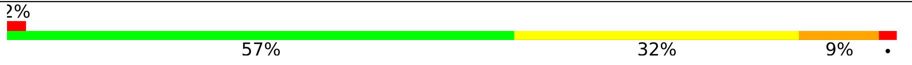
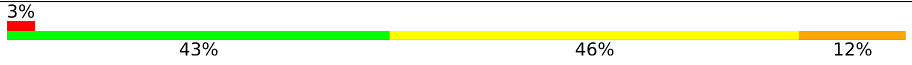
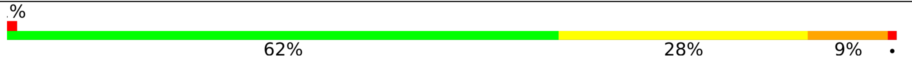
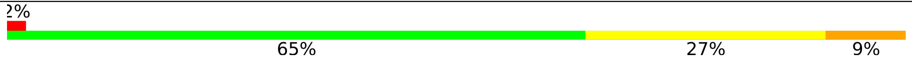
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	RA	2916	
22	YA	2916	
23	RB	122	
23	YB	122	
24	RD	276	
24	YD	276	
25	RE	206	
25	YE	206	
26	RF	210	
26	YF	210	
27	RG	182	
27	YG	182	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	RH	180	
28	YH	180	
29	RI	148	
29	YI	148	
30	RN	140	
30	YN	140	
31	RO	122	
31	YO	122	
32	RP	150	
32	YP	150	
33	RQ	141	
33	YQ	141	
34	RR	118	
34	YR	118	
35	RS	112	
35	YS	112	
36	RT	146	
36	YT	146	
37	RU	118	
37	YU	118	
38	RV	101	
38	YV	101	
39	RW	113	
39	YW	113	
40	RX	96	

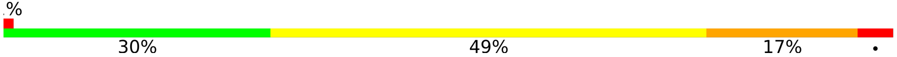
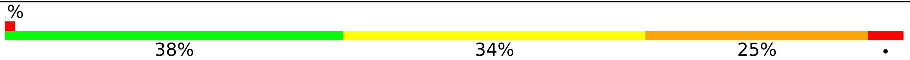
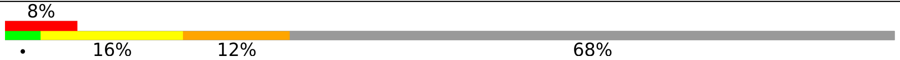
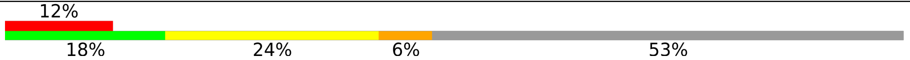
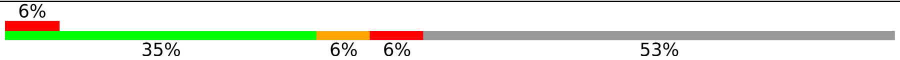
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	YX	96	52% 39% 5% •
41	RY	110	% 28% 49% 15% 7%
41	YY	110	% 45% 32% 15% • 7%
42	RZ	206	6% 31% 39% 16% • 11%
42	YZ	206	30% 41% 16% • 11%
43	R0	85	8% 44% 47% 6% •
43	Y0	85	39% 49% 8% •
44	R1	98	6% 58% 32% 7% • •
44	Y1	98	11% 54% 36% 7% • •
45	R2	72	61% 28% 7% •
45	Y2	72	42% 39% 14% • •
46	R3	60	3% 70% 23% 5% •
46	Y3	60	2% 58% 30% 10% •
47	R4	71	17% 35% 42% 17% 6%
47	Y4	71	7% 28% 34% 31% 7%
48	R5	60	3% 43% 43% 10% • •
48	Y5	60	13% 42% 43% 12% • •
49	R6	54	81% 19% 41% 30% • 9%
49	Y6	54	78% 30% 39% 19% • 9%
50	R7	49	4% 61% 31% 8%
50	Y7	49	8% 63% 29% 8%
51	R8	65	9% 48% 38% 12% •
51	Y8	65	8% 38% 42% 15% • •
52	R9	37	100% 62% 32% 5%
52	Y9	37	100% 59% 38% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	QV	77	
53	XV	77	
54	QX	25	
54	XX	25	
55	QY	17	
55	XY	17	
56	Z6	3	
56	Z8	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	RA	3002	-	-	-	X
58	MG	RA	3067	-	-	-	X
58	MG	RA	3212	-	-	-	X
58	MG	RA	3227	-	-	-	X
58	MG	Y0	101	-	-	-	X
58	MG	YA	3018	-	-	-	X
58	MG	YA	3214	-	-	-	X

2 Entry composition ⓘ

There are 59 unique types of molecules in this entry. The entry contains 291730 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 32247	C 14353	N 5981	O 10414	P 1499	0	0	0
1	XA	1500	Total 32249	C 14354	N 5984	O 10412	P 1499	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- 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			

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total 734	C 459	N 147	O 126	S 2	0	0	0
15	XO	88	Total 734	C 459	N 147	O 126	S 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 23S rRNA.

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

- Molecule 23 is a RNA chain called 5S rRNA.

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

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

Continued on next page...

Continued from previous page...

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

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

- Molecule 32 is a protein called 50S ribosomal protein L15.

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

- Molecule 33 is a protein called 50S ribosomal protein L16.

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

- Molecule 34 is a protein called 50S ribosomal protein L17.

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

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

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

- Molecule 41 is a protein called 50S ribosomal protein L24.

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

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

Continued on next page...

Continued from previous page...

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

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

- Molecule 44 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	R1	97	763	481	150	131	1	0	0	0
44	Y1	97	763	481	150	131	1	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L29.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L31.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a RNA chain called P-site tRNA fMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
53	QV	77	1644	732	297	538	77	0	0	0
53	XV	77	1644	732	297	538	77	0	0	0

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
54	QX	8	173	77	33	55	8	0	0	0
54	XX	8	173	77	33	55	8	0	0	0

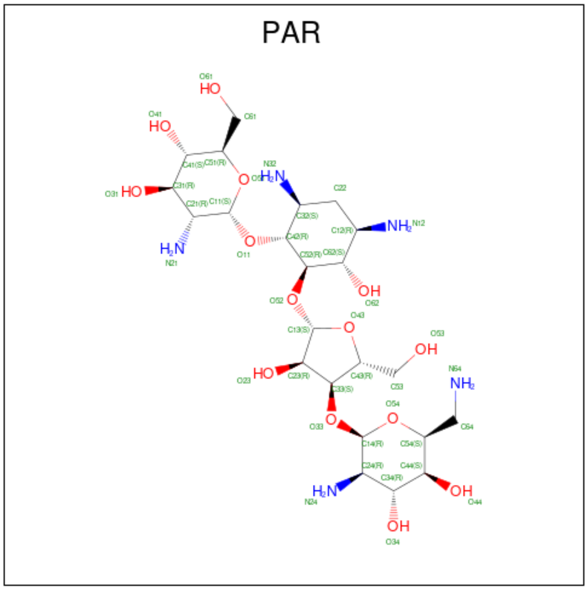
- Molecule 55 is a RNA chain called A site ASL of tRNA-Proline CGG (unmodified).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
55	QY	8	174	77	33	56	8	0	0	0
55	XY	8	174	77	33	56	8	0	0	0

- Molecule 56 is a RNA chain called tRNA acceptor end mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
56	Z6	3	74	40	13	19	2	0	0	0
56	Z8	3	74	40	13	19	2	0	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 C N O 42 23 5 14	0	0
57	XA	1	Total C N O 42 23 5 14	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	QA	76	Total Mg 76 76	0	0
58	QF	1	Total Mg 1 1	0	0
58	QM	1	Total Mg 1 1	0	0
58	RA	247	Total Mg 247 247	0	0
58	RB	2	Total Mg 2 2	0	0
58	RD	1	Total Mg 1 1	0	0
58	RE	2	Total Mg 2 2	0	0
58	RF	1	Total Mg 1 1	0	0
58	RP	2	Total Mg 2 2	0	0
58	R0	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	R5	1	Total Mg 1 1	0	0
58	R8	2	Total Mg 2 2	0	0
58	XA	82	Total Mg 82 82	0	0
58	XB	1	Total Mg 1 1	0	0
58	XM	1	Total Mg 1 1	0	0
58	YA	265	Total Mg 265 265	0	0
58	YB	3	Total Mg 3 3	0	0
58	YD	2	Total Mg 2 2	0	0
58	YP	2	Total Mg 2 2	0	0
58	YQ	1	Total Mg 1 1	0	0
58	YX	1	Total Mg 1 1	0	0
58	Y0	1	Total Mg 1 1	0	0
58	Y5	1	Total Mg 1 1	0	0
58	QV	1	Total Mg 1 1	0	0
58	XV	2	Total Mg 2 2	0	0

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

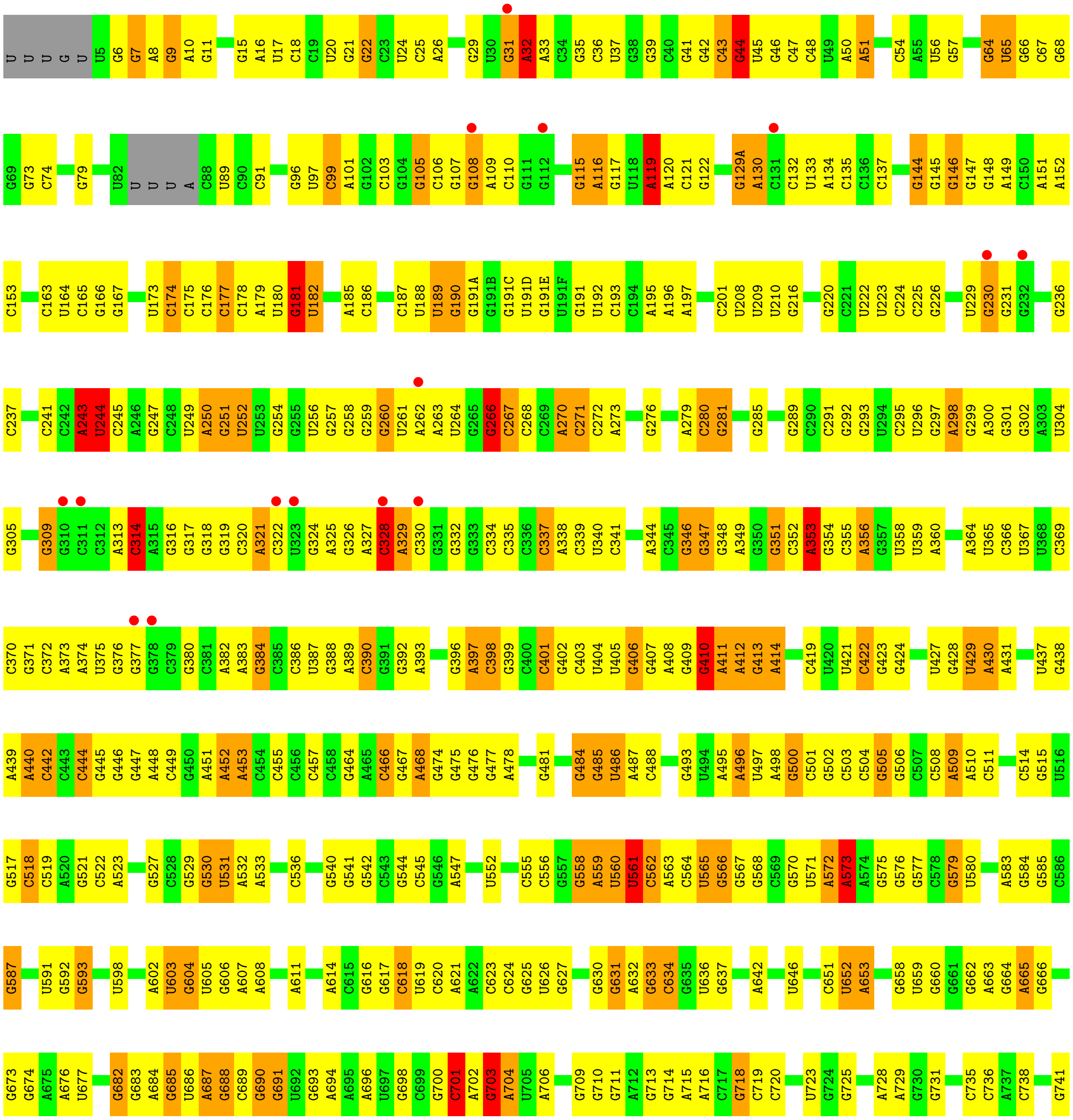
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	QD	1	Total Zn 1 1	0	0
59	QN	1	Total Zn 1 1	0	0
59	XD	1	Total Zn 1 1	0	0
59	XN	1	Total Zn 1 1	0	0

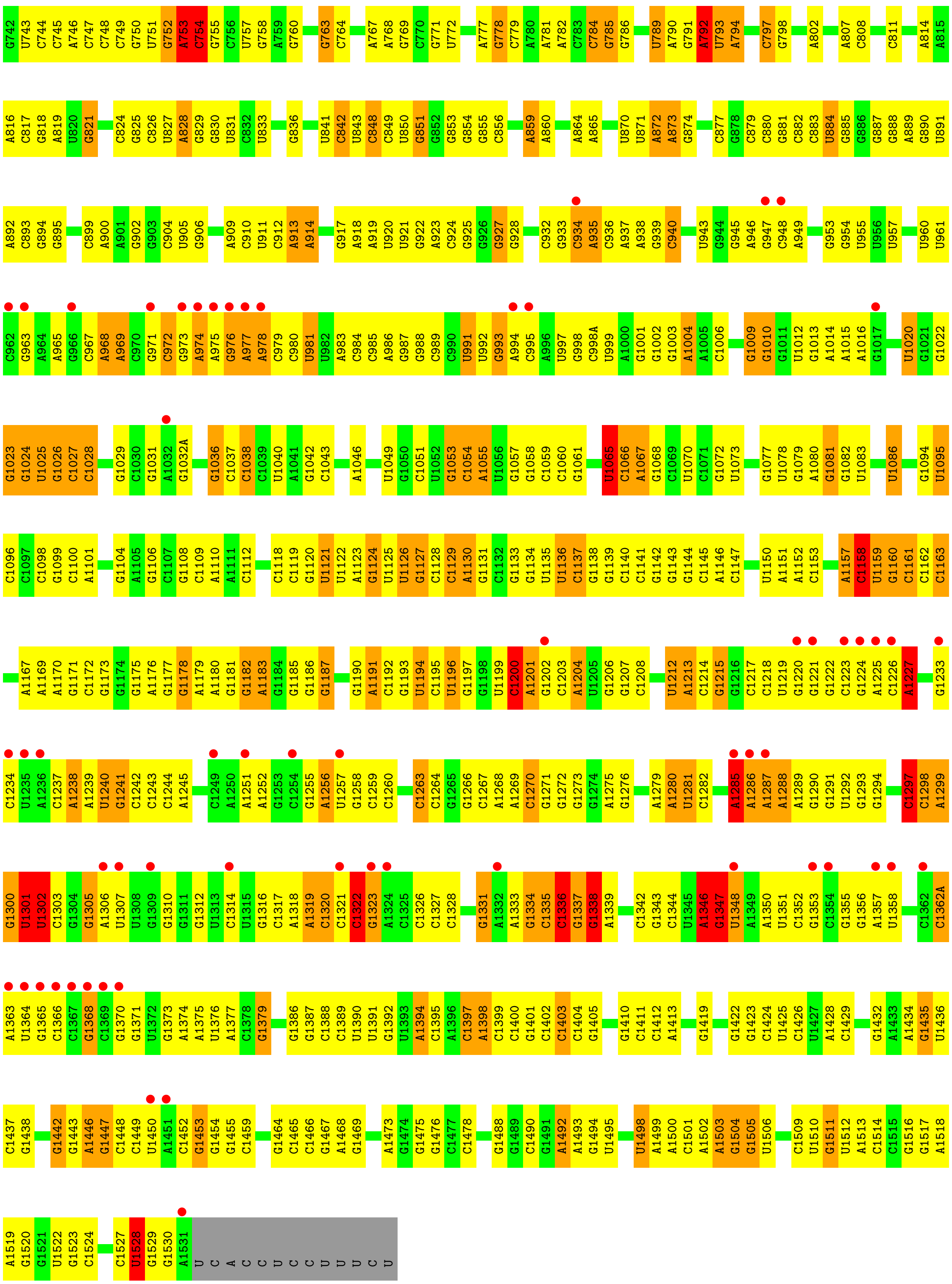
3 Residue-property plots ⓘ

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

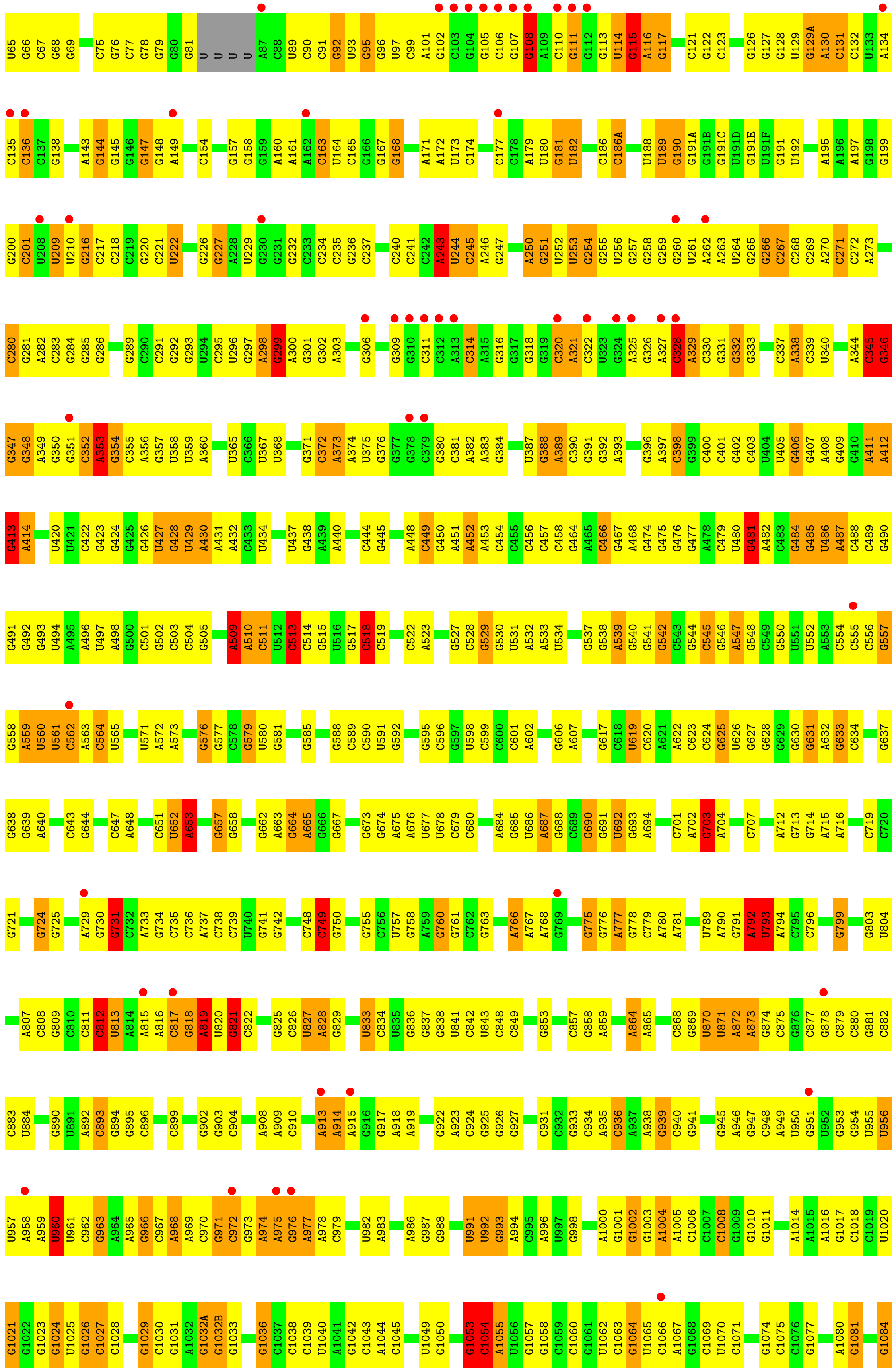
- Molecule 1: 16S rRNA

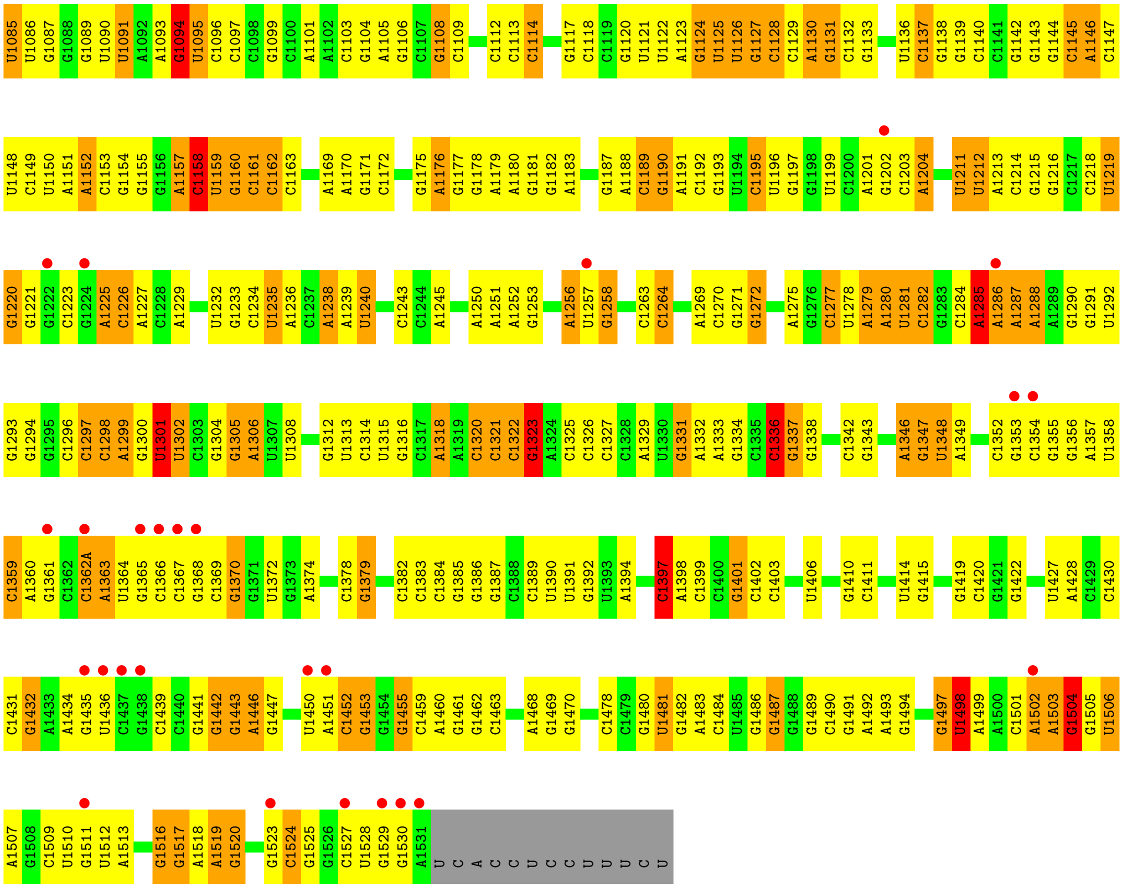
Chain QA:





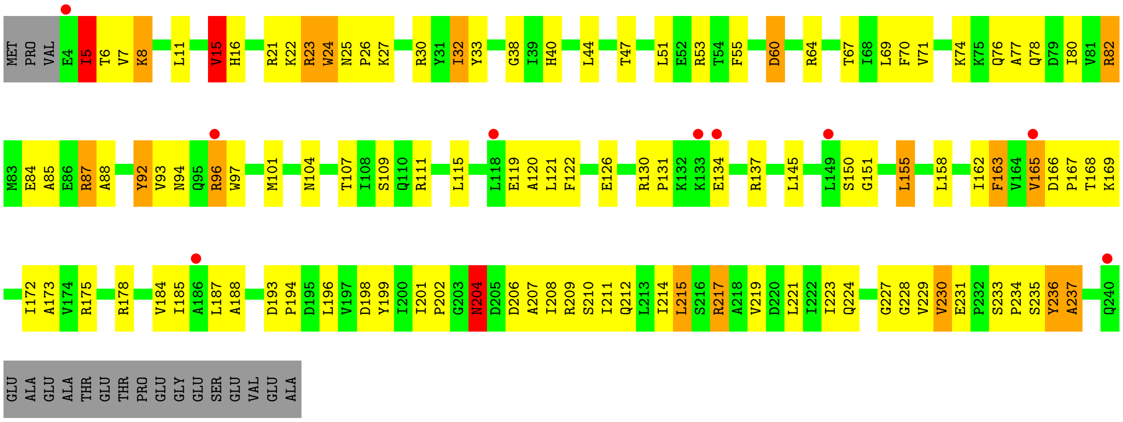
- Molecule 1: 16S rRNA


U65 G66 C67 G68 G69 C75 G76 C77 G78 G79 C80 G81 U U U U A87 C88 U89 C90 C91 G92 U93 G95 G96 U97 C99 A101 G102 C103 G104 G105 C106 G107 G108 A109 C110 G111 G112 G113 U114 G115 A116 G117 C121 G122 C123 G126 G127 G128 U129 G129A A130 C131 C132 U133 A134
C135 C136 C137 G138 A143 G144 G145 G146 G147 G148 A149 C154 G157 G158 G159 A160 A161 A162 C163 U164 C165 G166 G167 G168 A171 A172 U173 C174 C177 C178 A179 U180 G181 U182 C186 C186A U188 U189 G190 G191A G191B G191C U191D G191E U191F G191 U192 A195 A196 A197 G198 G199
G200 C201 U208 U209 U210 G216 C217 C218 C219 G220 C221 U222 G226 G227 A228 U229 G230 G231 G232 C233 C234 C235 G236 C237 C240 C241 C242 A243 U244 C245 A246 G247 A250 G251 U252 U253 G254 G255 U256 G257 G258 G259 G260 U261 A262 A263 U264 G265 G266 C267 C268 C269 A270 C271 C272 A273
C280 G281 A282 C283 G284 G285 G286 G289 C290 C291 G292 G293 U294 C295 U296 G297 A298 G299 A300 C301 G302 A303 G306 G309 G310 C311 C312 A313 C314 A315 G316 G317 G318 G319 C320 A321 C322 U323 G324 A325 G326 A327 C328 A329 C330 G331 G332 G333 C337 A338 C339 U340 A344 C345 G346
G347 G348 A349 G350 G351 C352 A353 G354 C355 A356 G357 U358 U359 A360 U365 C366 U367 U368 G371 C372 A373 A374 U375 G376 G377 G378 C379 G380 C381 A382 A383 G384 U387 G388 A389 G390 G391 G392 A393 G396 A397 C398 G399 C400 C401 G402 C403 U404 U405 G406 G407 A408 G409 G410 A411 A412
G413 A414 U420 U421 C422 G423 G424 G425 G426 U427 G428 U429 A430 A431 A432 C433 U434 U437 G438 A439 A440 C444 G445 A448 C449 G450 A451 A452 A453 C454 C455 C456 C457 C458 G464 A465 C466 G467 A468 G474 G475 G476 G477 A478 C479 U480 G481 A482 C483 G484 G485 U486 A487 C488 C489 G490
G491 G492 G493 U494 A495 A496 U497 A498 G500 C501 G502 C503 C504 G505 A509 A510 C511 U512 C513 C514 G515 U516 G517 C518 C519 C522 A523 G527 C528 G529 G530 U531 A532 A533 U534 G537 G538 A539 G540 G541 G542 C543 G544 C545 G546 A547 G548 C549 G550 U551 U552 A553 C554 G555 C556 G557
G558 A559 U560 U561 C562 A563 C564 U565 U571 A572 A573 G576 G577 C578 G579 U580 G581 G585 G588 C589 C590 U591 G592 G595 C596 G597 U598 C599 C600 C601 A602 G606 A607 G617 C618 U619 C620 A621 A622 C623 C624 G625 U626 G627 G628 G629 G630 G631 A632 G633 C634 G637
G638 G639 A640 C643 G644 C647 A648 C651 U652 A653 G657 G658 G662 A663 G664 A665 G666 G667 G673 G674 A675 A676 U677 U678 C679 C680 A684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 C701 A702 G703 A704 C707 A712 G713 G714 A715 A716 C719 C720
G721 G724 G725 A729 C730 G731 C732 A733 G734 C735 C736 A737 G738 C739 U740 G741 G742 C748 C749 G750 G755 C756 U757 G758 A759 G760 G761 C762 G763 A766 A767 A768 G769 G775 G776 A777 G778 C779 A780 A781 U789 A790 G791 A792 U793 A794 C795 C796 G799 G803 U804
A807 C808 G809 C810 C811 C812 U813 A814 A815 A816 C817 G818 A819 U820 G821 C822 G825 C826 U827 A828 G829 U833 C834 U835 G836 G837 G838 U841 C842 U843 C848 C849 G853 C857 G858 A859 A864 A865 C868 G869 U870 U871 A872 A873 G874 C875 G876 C877 G878 C879 G880 G881 C882
C883 U884 G890 U891 A892 G893 G894 G895 C896 C899 G902 G903 C904 A908 A909 C910 A913 A914 A915 G916 G917 A918 A919 G922 A923 C924 G925 G926 G927 C931 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G945 A946 G947 C948 A949 U950 G951 U952 G953 G954 U955 U956
U957 A958 A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 U982 A983 A986 G987 G988 U991 U992 G993 A994 C995 A996 U997 G998 A1000 G1001 G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 G1011 A1014 A1015 A1016 G1017 C1018 C1019 U1020
G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 G1029 C1030 G1031 A1032 G1032A G1032B G1033 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 U1049 G1050 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061 U1062 C1063 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1074 C1075 C1076 G1077 A1080 G1081 G1084



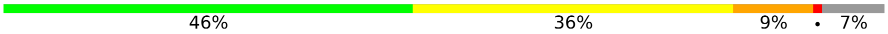
- Molecule 2: 30S ribosomal protein S2

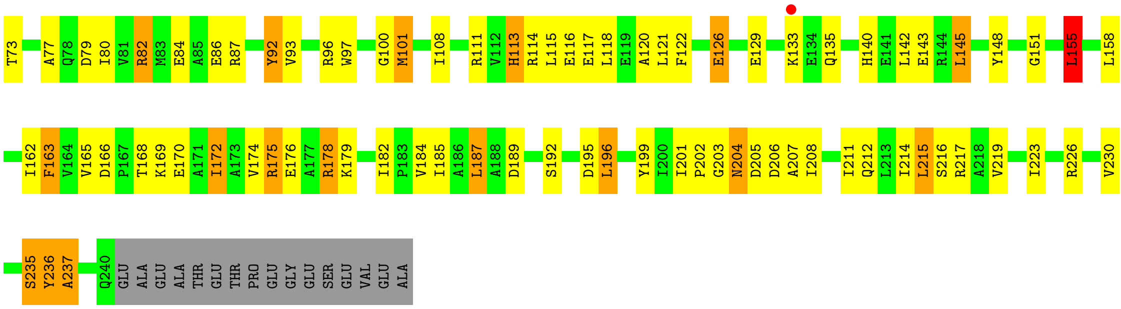
Chain QB:



- Molecule 2: 30S ribosomal protein S2

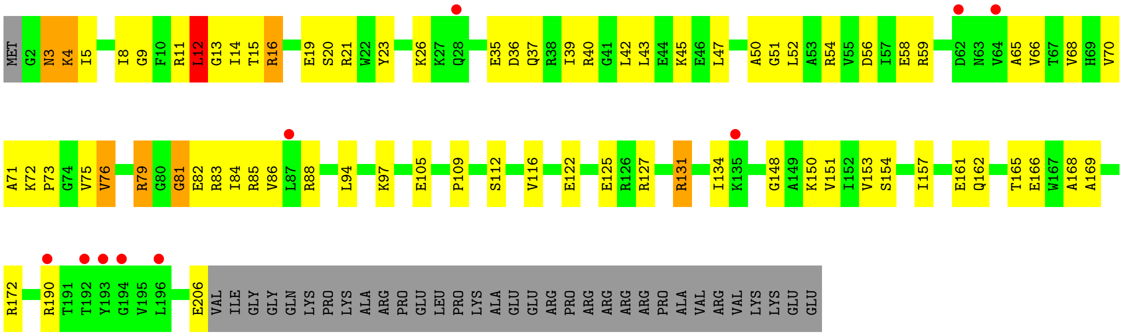
Chain XB:





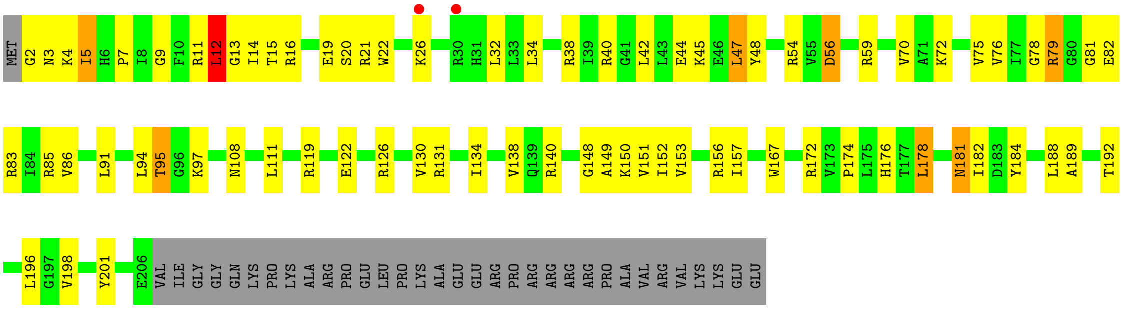
- Molecule 3: 30S ribosomal protein S3

Chain QC:



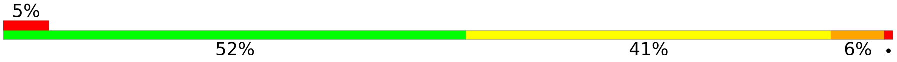
- Molecule 3: 30S ribosomal protein S3

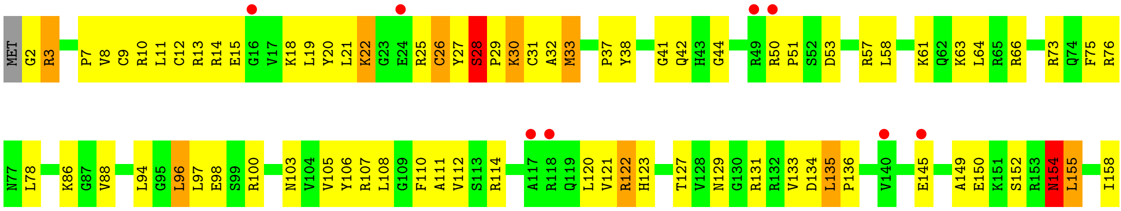
Chain XC:

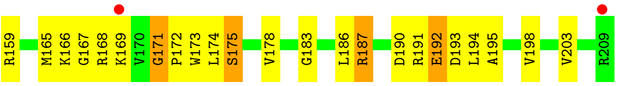


- Molecule 4: 30S ribosomal protein S4

Chain QD:

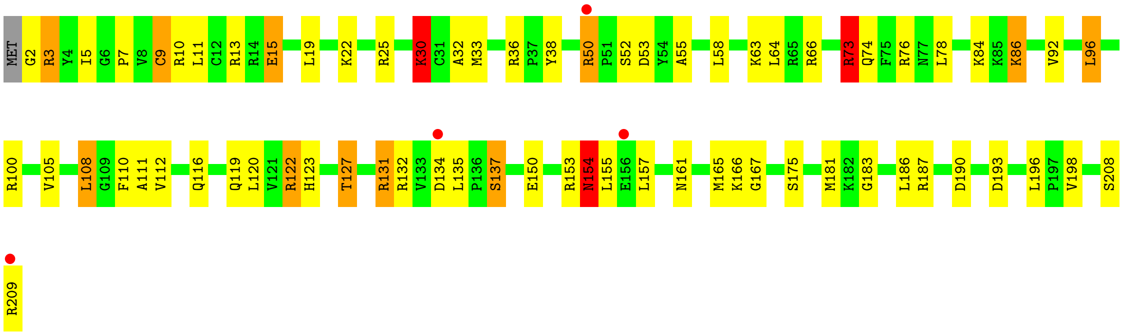






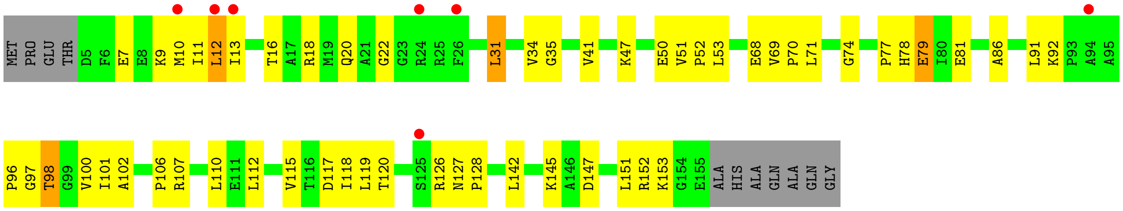
- Molecule 4: 30S ribosomal protein S4

Chain XD:



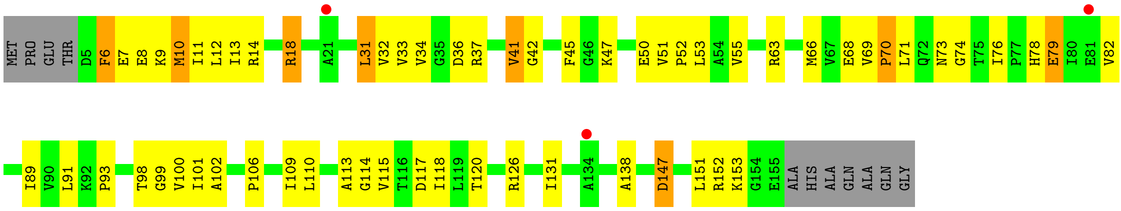
- Molecule 5: 30S ribosomal protein S5

Chain QE:



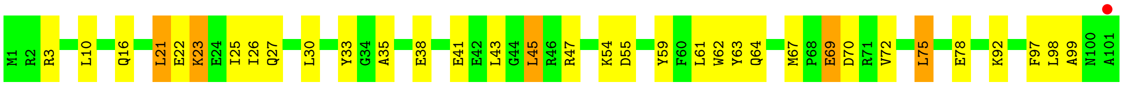
- Molecule 5: 30S ribosomal protein S5

Chain XE:



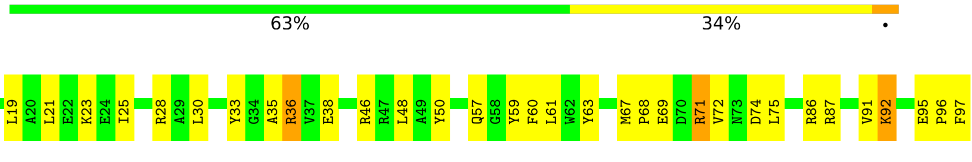
- Molecule 6: 30S ribosomal protein S6

Chain QF:



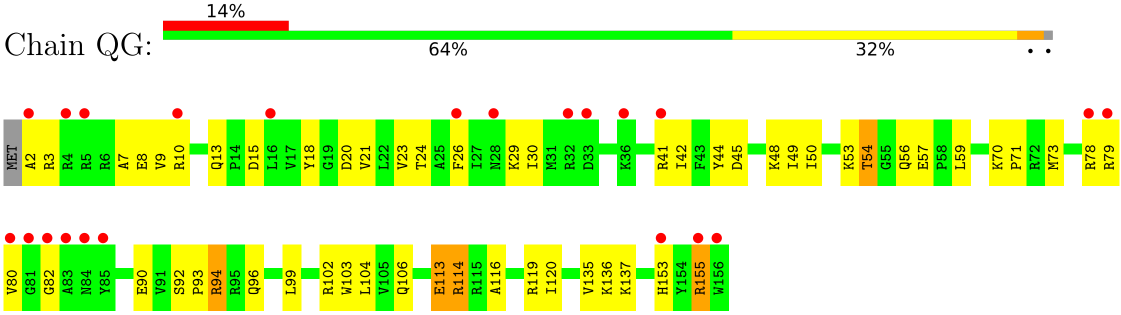
- Molecule 6: 30S ribosomal protein S6

Chain XF:



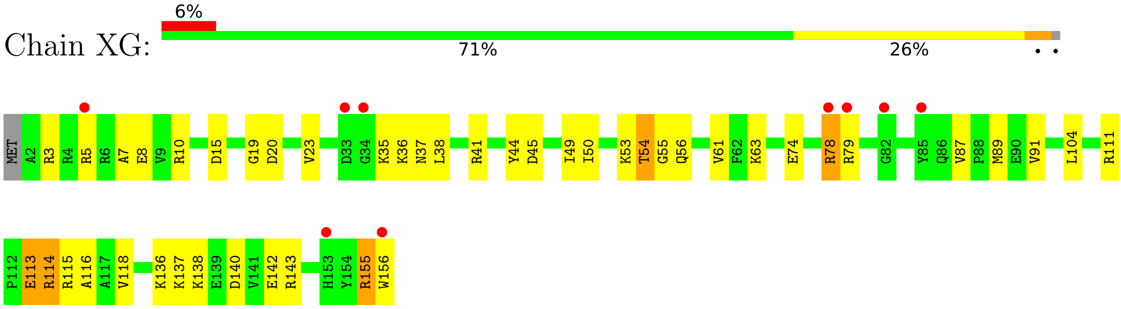
- Molecule 7: 30S ribosomal protein S7

Chain QG:



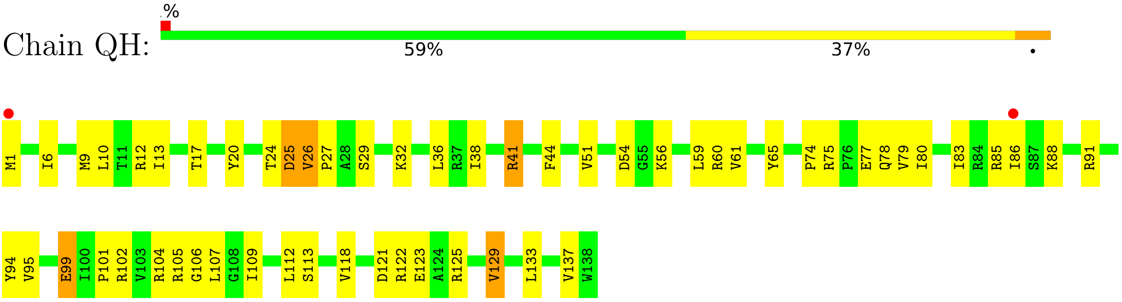
- Molecule 7: 30S ribosomal protein S7

Chain XG:



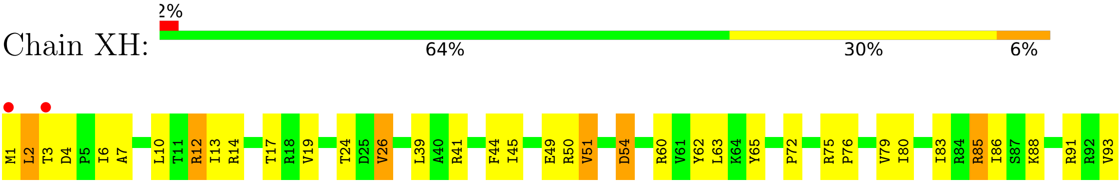
- Molecule 8: 30S ribosomal protein S8

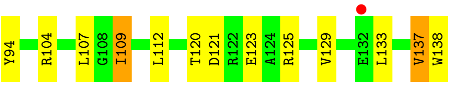
Chain QH:



- Molecule 8: 30S ribosomal protein S8

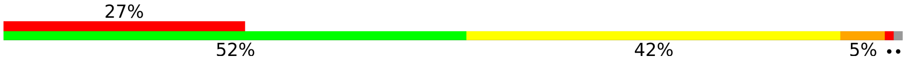
Chain XH:

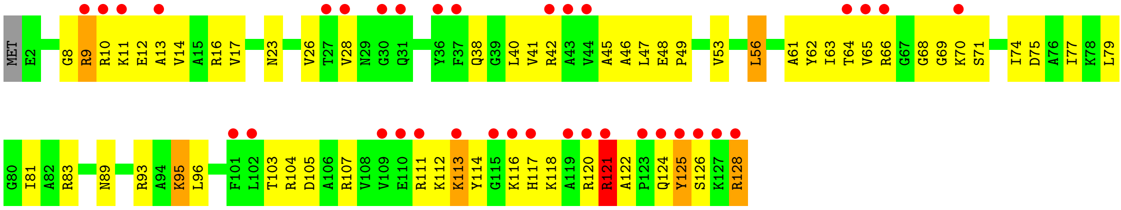




- Molecule 9: 30S ribosomal protein S9

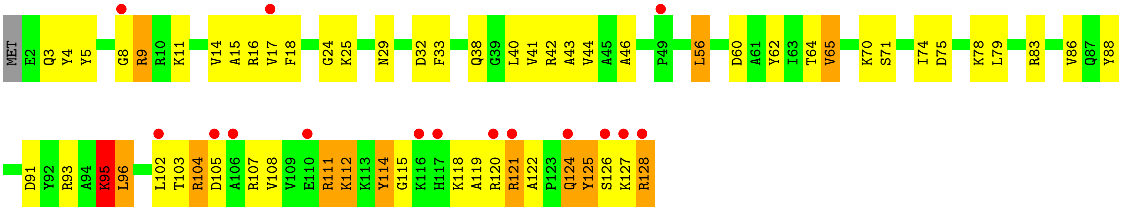
Chain QI:





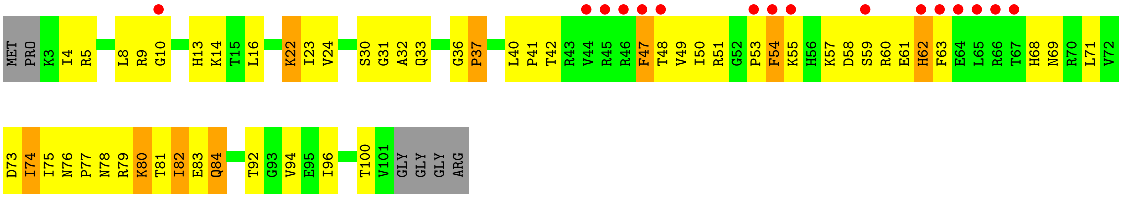
- Molecule 9: 30S ribosomal protein S9

Chain XI:



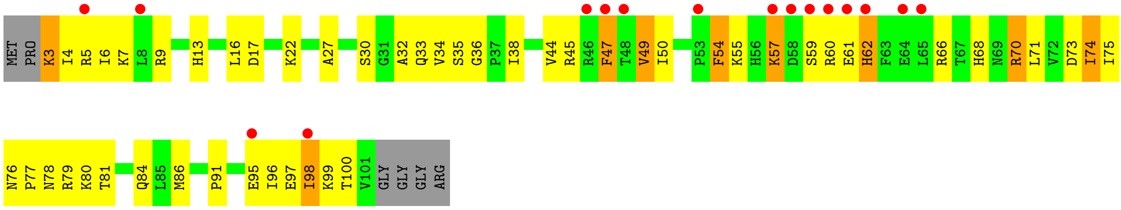
- Molecule 10: 30S ribosomal protein S10

Chain QJ:



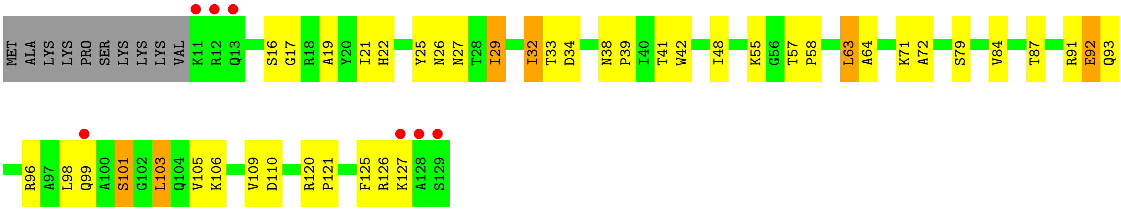
- Molecule 10: 30S ribosomal protein S10

Chain XJ:



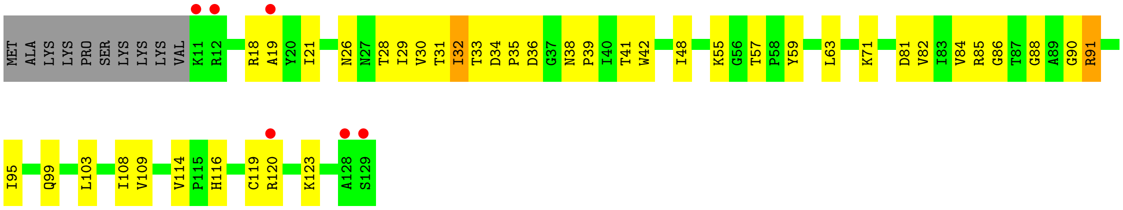
- Molecule 11: 30S ribosomal protein S11

Chain QK:



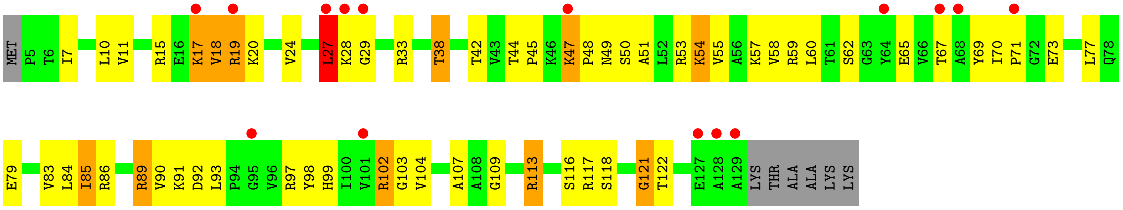
- Molecule 11: 30S ribosomal protein S11

Chain XK:



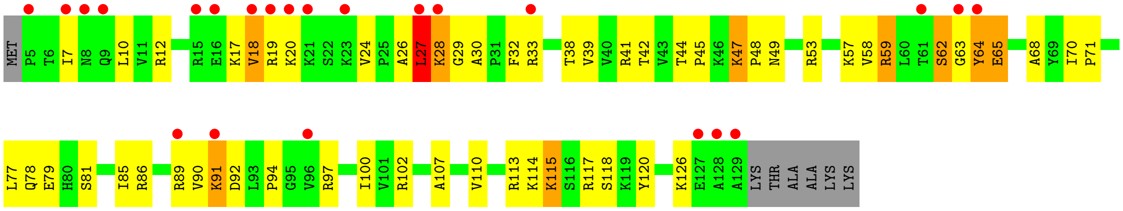
- Molecule 12: 30S ribosomal protein S12

Chain QL:



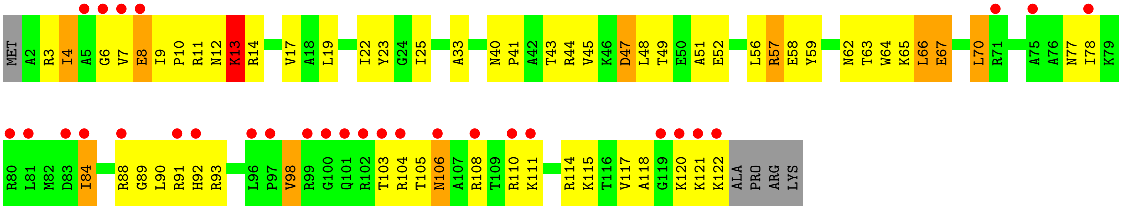
- Molecule 12: 30S ribosomal protein S12

Chain XL:



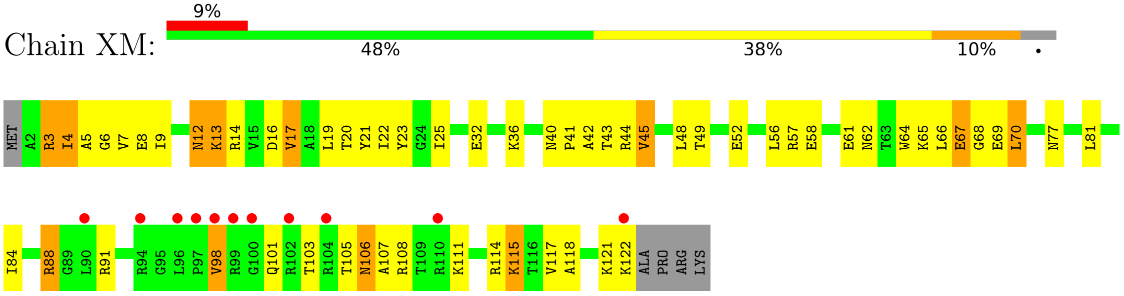
- Molecule 13: 30S ribosomal protein S13

Chain QM:



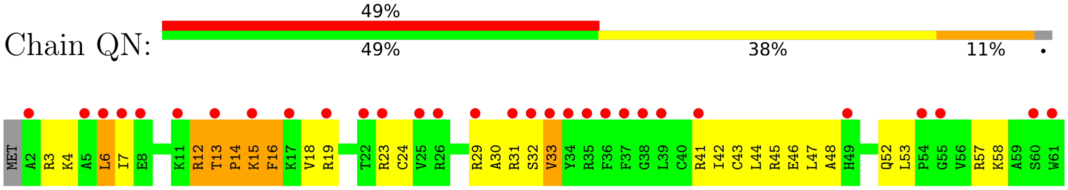
- Molecule 13: 30S ribosomal protein S13

Chain XM:



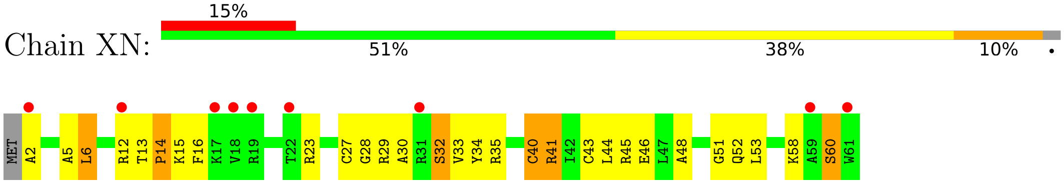
- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:



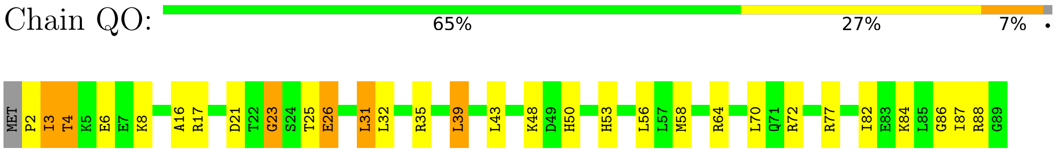
- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:



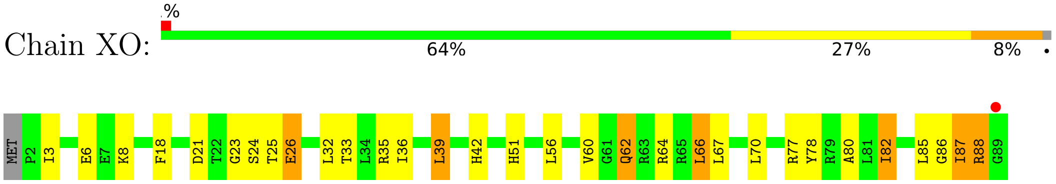
- Molecule 15: 30S ribosomal protein S15

Chain QO:



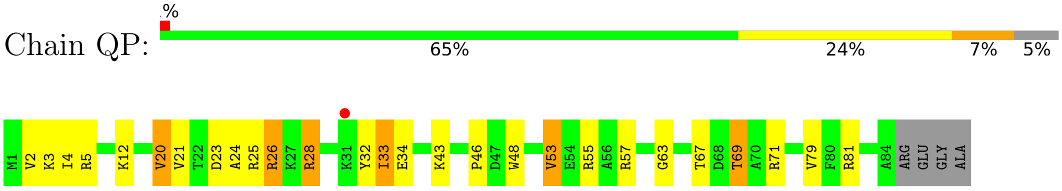
- Molecule 15: 30S ribosomal protein S15

Chain XO:



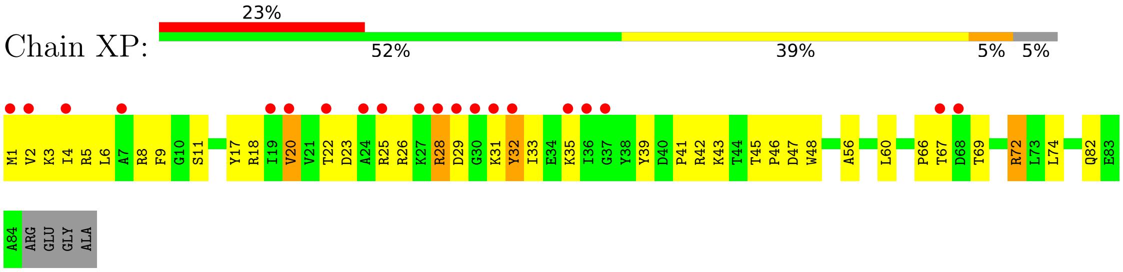
- Molecule 16: 30S ribosomal protein S16

Chain QP:



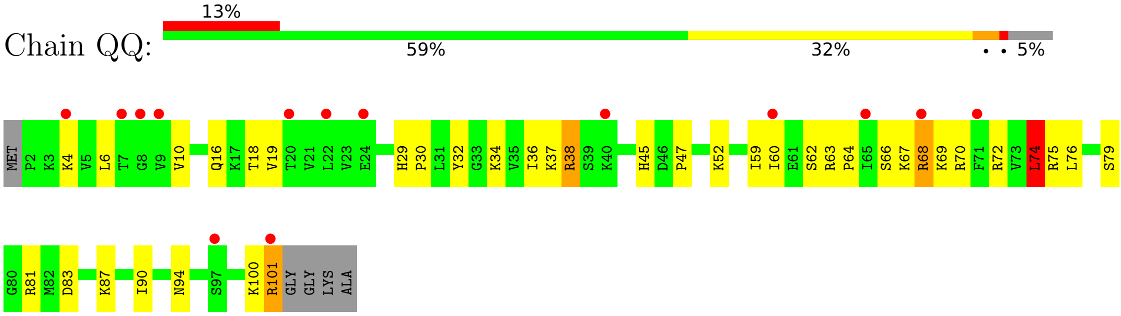
- Molecule 16: 30S ribosomal protein S16

Chain XP:



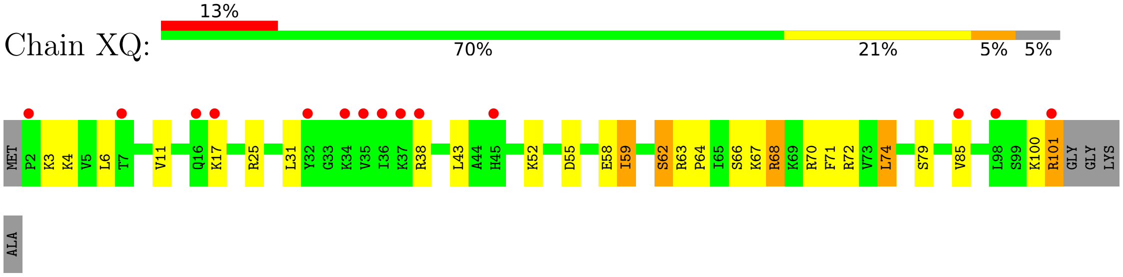
- Molecule 17: 30S ribosomal protein S17

Chain QQ:



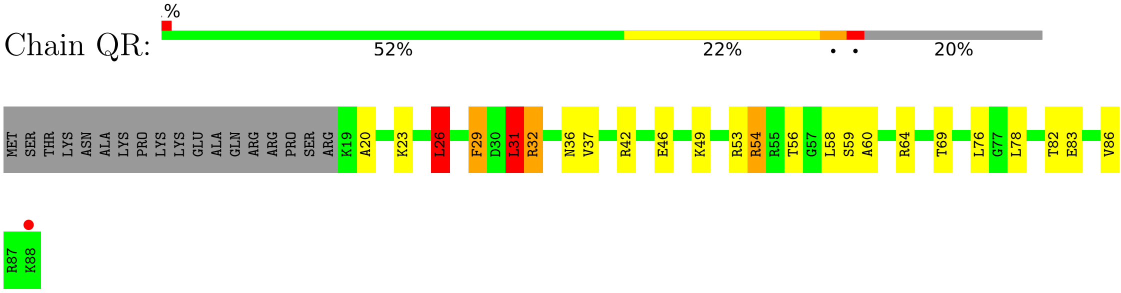
- Molecule 17: 30S ribosomal protein S17

Chain XQ:



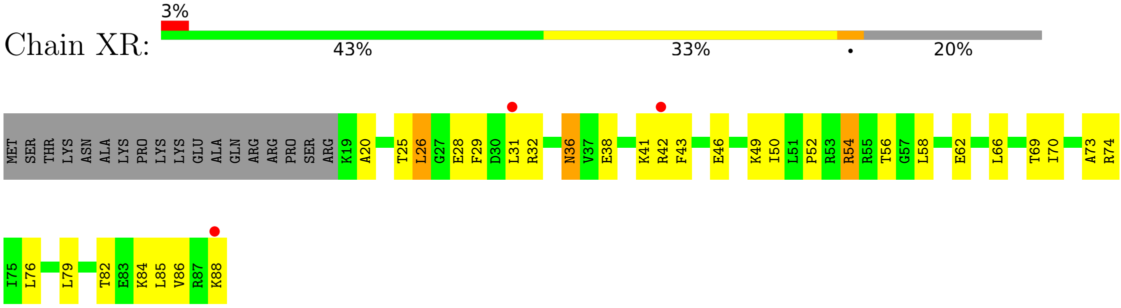
- Molecule 18: 30S ribosomal protein S18

Chain QR:



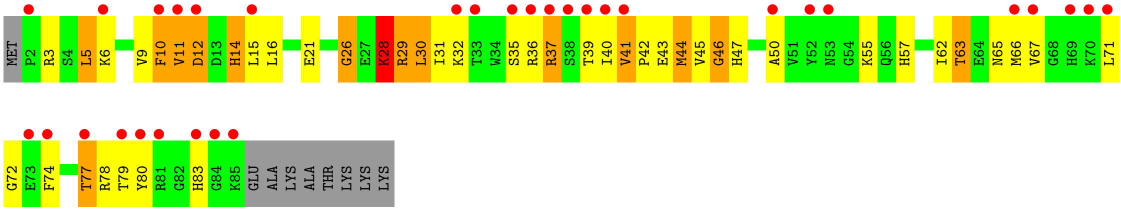
- Molecule 18: 30S ribosomal protein S18

Chain XR:



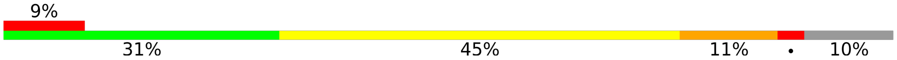
- Molecule 19: 30S ribosomal protein S19

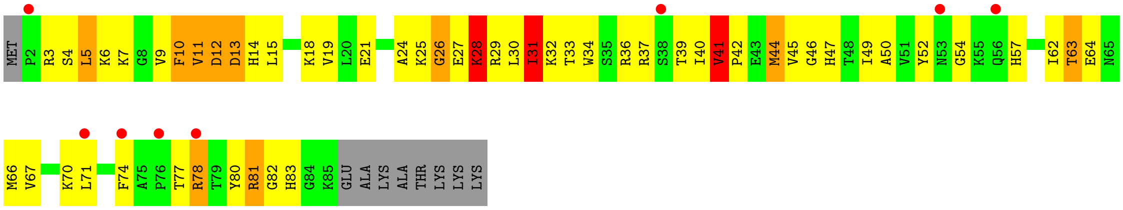
Chain QS:



- Molecule 19: 30S ribosomal protein S19

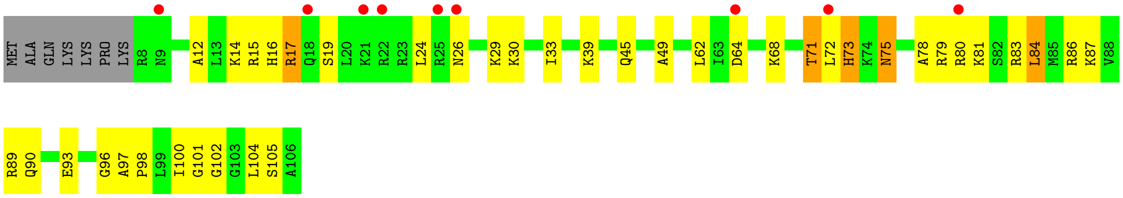
Chain XS:





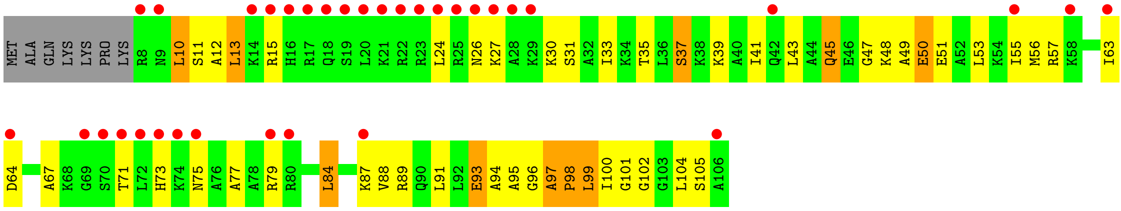
- Molecule 20: 30S ribosomal protein S20

Chain QT:



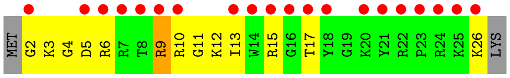
- Molecule 20: 30S ribosomal protein S20

Chain XT:



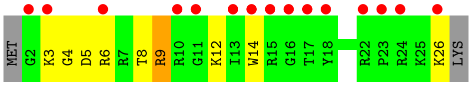
- Molecule 21: 30S ribosomal protein Thx

Chain QU:



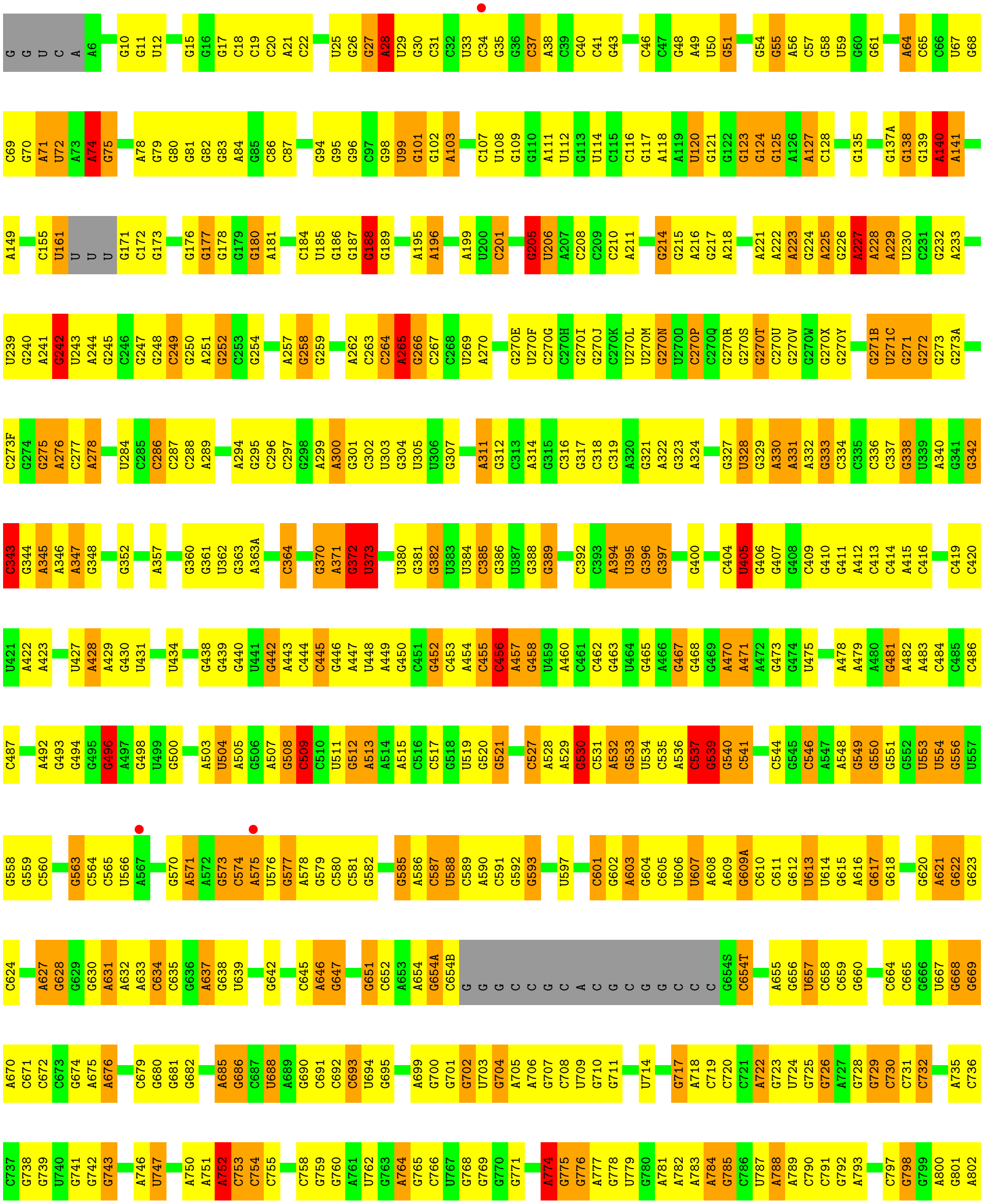
- Molecule 21: 30S ribosomal protein Thx

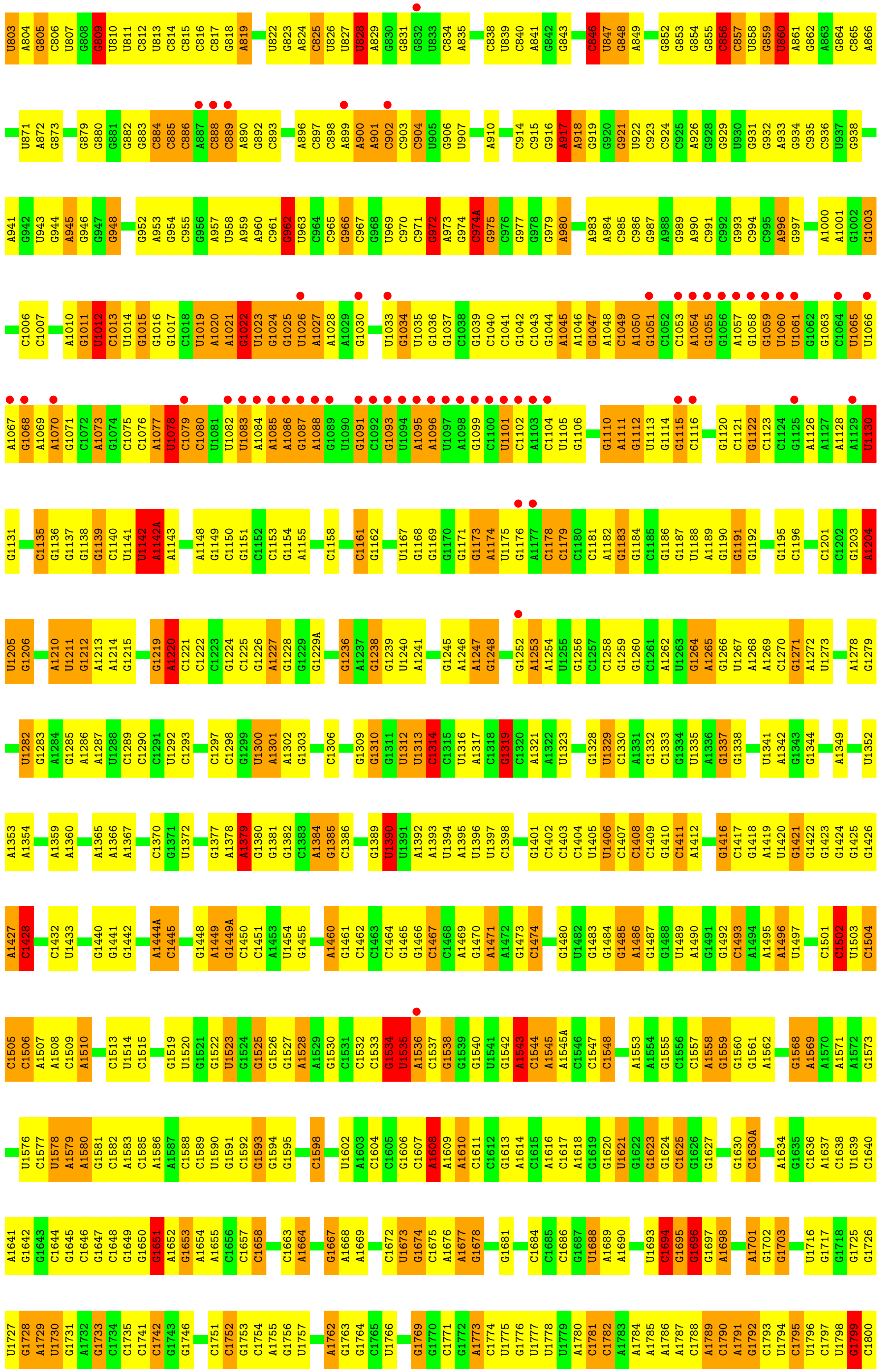
Chain XU:

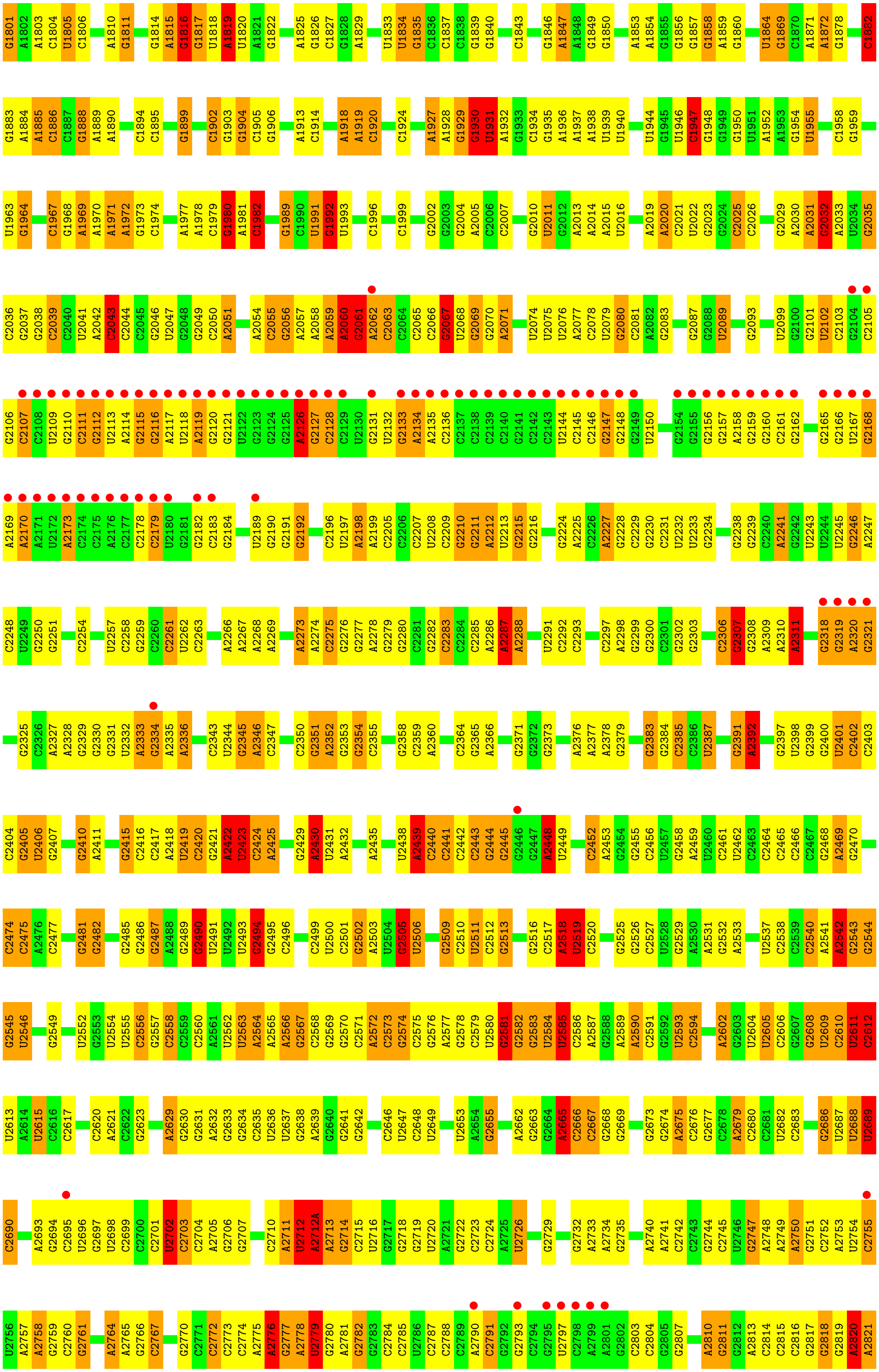


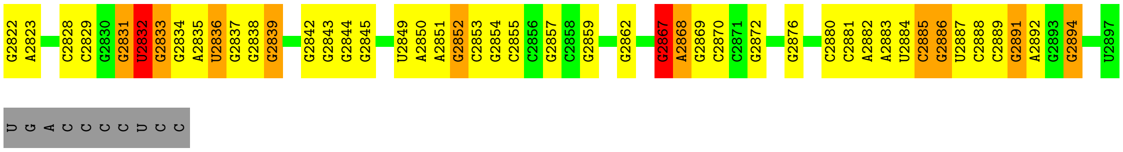
- Molecule 22: 23S rRNA

Chain RA:



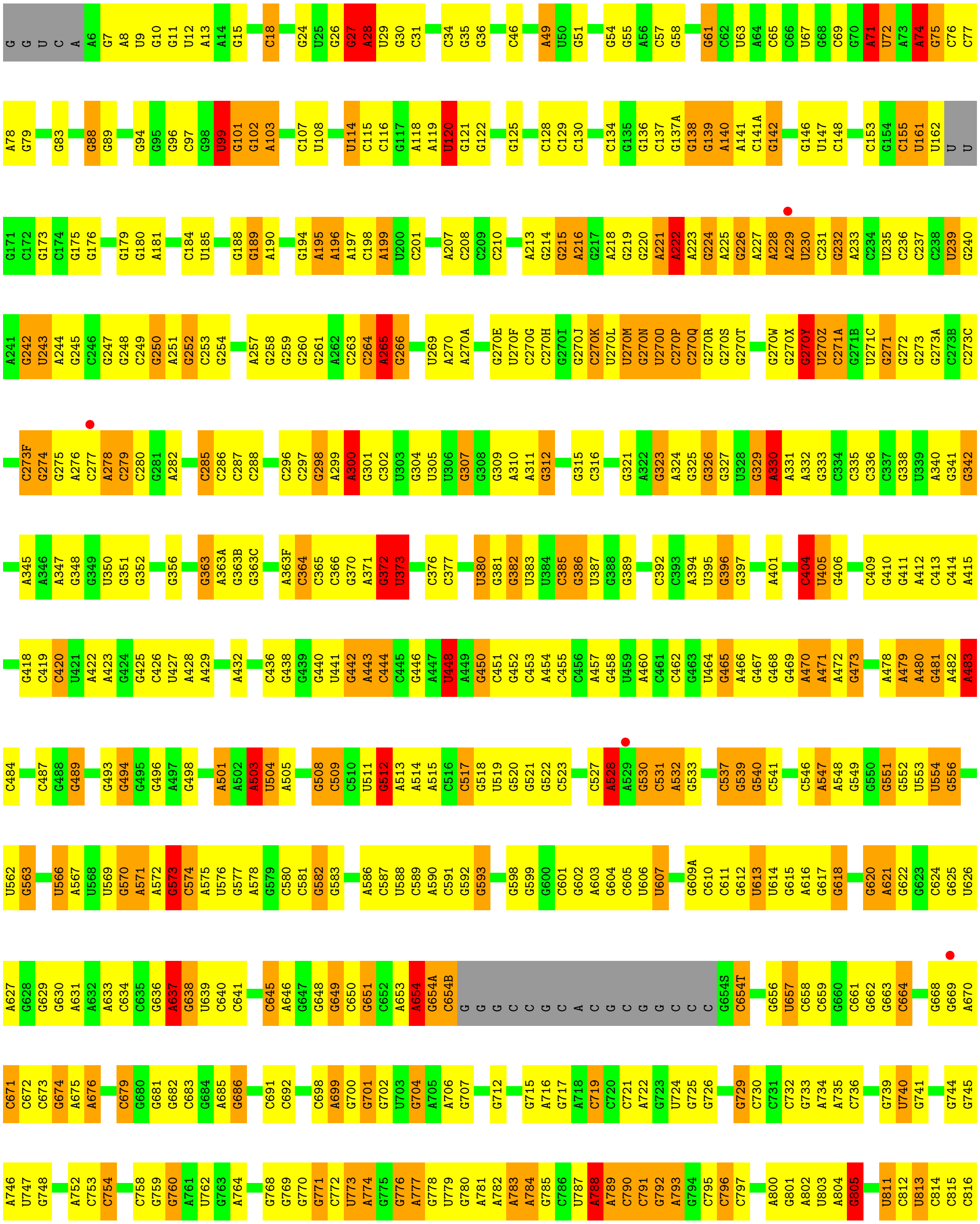

U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813 C814 C815 C816 C817 G818 A819 U822 G823 A824 C825 U826 U827 U828 A829 G830 G831 G832 U833 C834 A835 C838 U839 C840 A841 G842 G843 C846 U847 G848 A849 G852 G853 G854 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865 A866
U871 A872 G873 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 A896 C897 C898 A899 A900 A901 C902 C903 C904 U905 G906 U907 A910 C914 C915 G916 A917 A918 G919 G920 G921 U922 C923 C924 C925 A926 G928 G929 U930 G931 G932 A933 G934 C935 C936 U937 G938
A941 G942 U943 G944 A945 G946 G947 G948 G952 A953 G954 C955 G956 A957 U958 A959 A960 C961 G962 U963 C964 C965 G966 C967 G968 U969 C970 C971 G972 A973 G974 C974A G975 C976 G977 G978 G979 A980 A983 A984 C985 C986 G987 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 A1000 A1001 G1002 G1003
C1006 C1007 A1010 G1011 U1012 C1013 U1014 G1015 C1016 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 U1033 G1034 U1035 G1036 G1037 C1038 G1039 C1040 C1041 G1042 C1043 G1044 A1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066
A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1120 C1121 G1122 C1123 C1124 G1125 A1126 A1127 A1128 A1129 U1130
G1131 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A A1143 A1148 G1149 C1150 G1151 C1152 C1153 G1154 A1155 C1158 C1161 G1162 U1167 G1168 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1184 C1185 G1186 G1187 U1188 G1189 C1190 G1191 G1192 G1195 C1196 C1201 G1202 G1203 A1204
U1205 G1206 A1210 U1211 G1212 A1213 A1214 G1215 G1219 A1220 C1221 C1222 C1223 G1224 C1225 G1226 A1227 G1228 G1229 G1229A G1236 A1237 G1238 G1239 U1240 A1241 G1245 A1246 A1247 G1248 G1252 A1253 A1254 U1255 G1256 C1257 C1258 G1259 G1260 C1261 A1262 U1263 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1278 G1279
U1282 G1283 A1284 G1285 A1286 A1287 U1288 C1289 C1290 C1291 U1292 C1293 C1297 C1298 G1299 U1300 A1301 A1302 G1303 C1306 G1309 G1310 G1311 U1312 U1313 C1314 C1315 U1316 A1317 C1318 G1319 C1320 A1321 A1322 U1323 G1328 U1329 C1330 A1331 G1332 C1333 G1334 U1335 A1336 G1337 G1338 U1341 A1342 G1343 G1344 A1349 U1352
A1353 A1354 A1359 A1360 A1365 A1366 A1367 C1370 G1371 U1372 G1377 A1378 A1379 G1380 G1381 G1382 C1383 A1384 G1385 C1386 G1389 U1390 U1391 A1392 A1393 U1394 A1395 U1396 U1397 C1398 G1401 C1402 C1403 C1404 U1405 U1406 C1407 G1408 C1409 G1410 C1411 A1412 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 G1425 G1426
A1427 C1428 C1432 U1433 G1440 G1441 G1442 A1444A C1445 G1448 A1449 G1449A C1450 C1451 A1453 U1454 G1455 A1460 G1461 C1462 C1463 C1464 G1465 G1466 C1467 C1468 A1469 G1470 A1471 A1472 G1473 C1474 G1480 U1482 G1483 G1484 G1485 A1486 G1487 G1488 U1489 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1501 C1502 U1503 C1504
C1505 C1506 A1507 A1508 C1509 A1510 C1513 U1514 C1515 G1519 U1520 G1521 G1522 U1523 G1524 G1525 G1526 G1527 A1528 A1529 G1530 C1531 C1532 C1533 G1534 U1535 A1536 C1537 G1538 G1539 G1540 U1541 G1542 A1543 C1544 A1545 A1545A C1546 C1547 C1548 A1553 U1554 G1555 C1556 C1557 A1558 G1559 G1560 C1561 A1562 G1568 A1569 A1570 A1571 A1572 G1573
U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 C1585 A1586 A1587 C1588 C1589 U1590 G1591 C1592 G1593 G1594 G1595 C1598 U1602 A1603 C1604 C1605 G1606 C1607 A1608 A1609 A1610 C1611 C1612 G1613 A1614 C1615 A1616 C1617 A1618 G1619 G1620 U1621 G1622 G1623 G1624 C1625 G1626 G1627 G1630 C1630A A1634 G1635 C1636 A1637 C1638 U1639 C1640
A1641 G1642 G1643 C1644 G1645 C1646 G1647 C1648 G1649 G1650 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1658 C1663 A1664 G1667 A1668 A1669 C1672 U1673 G1674 C1675 A1676 A1677 G1678 G1681 C1684 C1685 C1686 G1687 U1688 A1689 A1690 U1693 C1694 G1695 G1696 G1697 A1698 A1701 G1702 G1703 U1716 G1717 G1718 G1725 G1726
U1727 G1728 A1729 U1730 G1731 A1732 G1733 C1734 C1735 C1741 C1742 G1743 G1746 C1751 C1752 G1753 C1754 A1755 G1756 U1757 A1762 G1763 G1764 C1765 U1766 G1769 G1770 C1771 G1772 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800

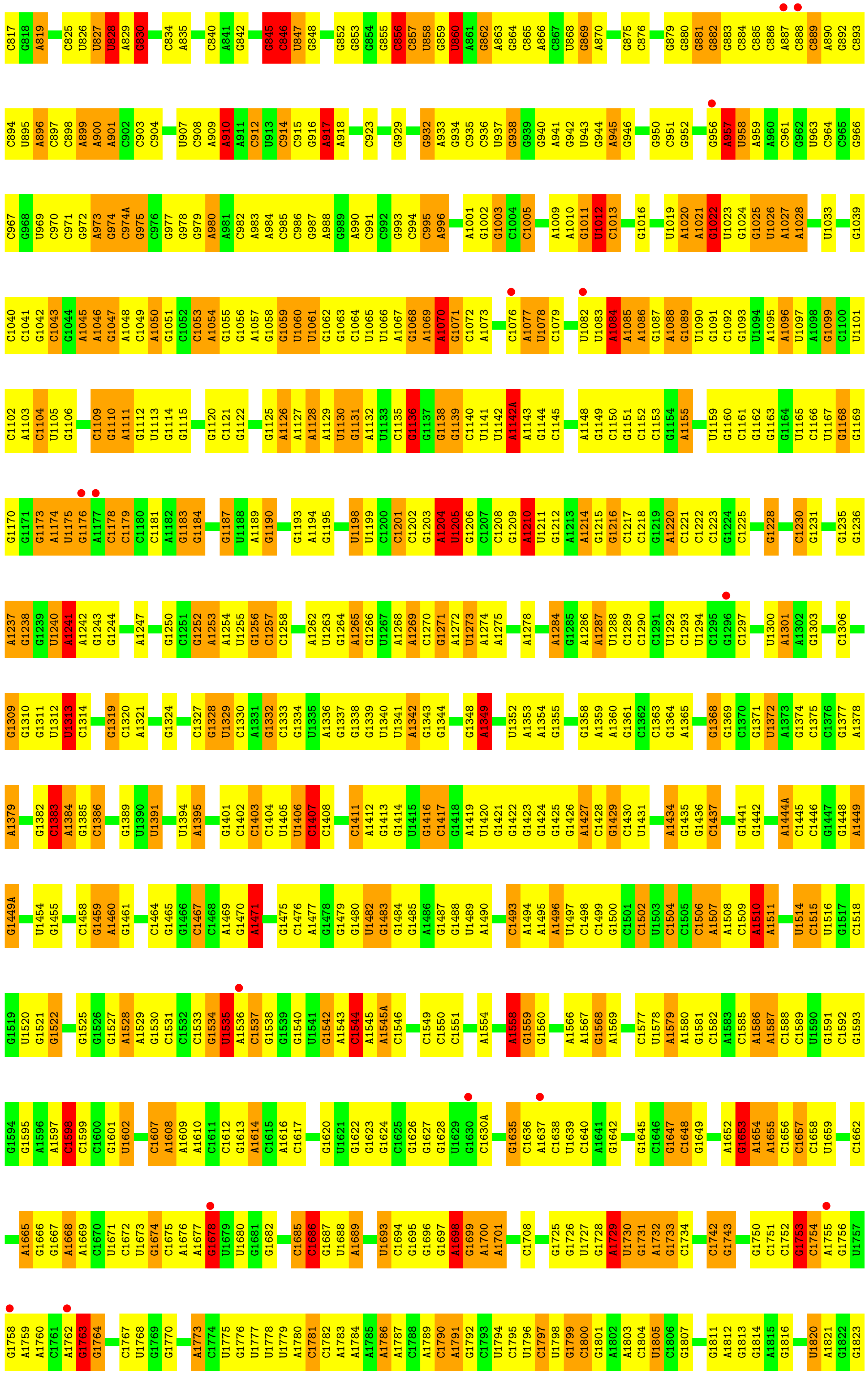

G1801 A1802 A1803 C1804 U1805 C1806 A1810 G1811 G1814 A1815 G1816 G1817 U1818 A1819 U1820 A1821 G1822 A1825 G1826 C1827 G1828 A1829 U1833 U1834 G1835 C1836 C1837 C1838 G1839 G1840 C1843 G1846 A1847 A1848 G1849 G1850 A1853 A1854 G1855 G1856 G1857 G1858 A1859 G1860 U1864 G1869 C1870 A1871 A1872 G1878 C1882
G1883 A1884 A1885 C1886 C1887 G1888 A1889 A1890 C1894 C1895 G1899 C1902 G1903 G1904 C1905 G1906 A1913 C1914 A1918 A1919 C1920 C1924 A1927 A1928 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 U1940 U1944 G1945 U1946 C1947 G1948 G1949 G1950 U1951 A1952 A1953 G1954 U1955 C1958 G1959
U1963 G1964 C1967 G1968 A1969 A1970 A1971 A1972 G1973 C1974 A1977 A1978 C1979 G1980 A1981 C1982 G1989 C1990 U1991 G1992 U1993 C1996 C1999 G2002 G2003 G2004 A2005 C2006 C2007 G2010 U2011 G2012 A2013 A2014 A2015 U2016 A2019 A2020 C2021 U2022 G2023 G2024 C2025 C2026 G2029 A2030 A2031 G2032 A2033 U2034 G2035
C2036 G2037 G2038 C2039 C2040 U2041 A2042 C2043 C2044 C2045 G2046 U2047 G2048 G2049 C2050 A2051 A2054 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 G2070 A2071 U2074 U2075 U2076 A2077 C2078 U2079 G2080 C2081 A2082 G2083 G2087 G2088 U2089 G2093 U2099 G2100 G2101 U2102 C2103 G2104 C2105
G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 G2165 G2166 U2167 G2168
A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 U2189 G2190 G2191 G2192 C2196 U2197 A2198 A2199 C2205 C2206 C2207 U2208 C2209 G2210 G2211 A2212 U2213 G2215 G2216 G2224 A2225 C2226 A2227 G2228 C2229 G2230 C2231 U2232 U2233 G2234 G2238 G2239 C2240 A2241 G2242 U2243 U2244 U2245 G2246 A2247
C2248 U2249 G2250 G2251 C2254 U2257 C2258 G2259 C2260 C2261 U2262 C2263 A2266 A2267 A2268 A2269 A2273 A2274 C2275 G2276 G2277 A2278 G2279 G2280 C2281 G2282 C2283 C2284 C2285 A2286 A2287 A2288 U2291 C2292 C2293 C2297 A2298 G2299 G2300 C2301 G2302 G2303 C2306 G2307 G2308 A2309 A2310 A2311 G2318 G2319 A2320 G2321
G2325 C2326 A2327 A2328 G2329 G2330 G2331 U2332 A2333 G2334 A2335 A2336 C2343 U2344 G2345 A2346 C2347 C2350 G2351 A2352 G2353 G2354 C2355 G2358 C2359 A2360 C2364 G2365 A2366 G2371 G2372 G2373 A2376 A2377 A2378 G2379 G2383 G2384 C2385 C2386 U2387 G2391 A2392 G2397 U2398 G2399 G2400 U2401 C2402 C2403
C2404 G2405 U2406 G2407 G2410 A2411 G2415 C2416 C2417 A2418 U2419 C2420 G2421 A2422 U2423 C2424 A2425 G2429 A2430 U2431 A2432 A2435 U2438 A2439 C2440 C2441 C2442 C2443 G2444 G2445 G2446 G2447 A2448 U2449 C2452 A2453 G2454 G2455 C2456 U2457 G2458 A2459 U2460 C2461 U2462 C2463 C2464 C2465 C2466 C2467 G2468 A2469 G2470
C2474 C2475 A2476 C2477 G2481 G2482 G2485 G2486 G2487 A2488 G2489 G2490 U2491 U2492 U2493 G2494 G2495 C2496 C2499 U2500 C2501 G2502 A2503 U2504 G2505 U2506 G2509 C2510 U2511 C2512 G2513 G2516 C2517 A2518 U2519 C2520 G2525 G2526 C2527 U2528 G2529 A2530 A2531 G2532 A2533 U2537 C2538 C2539 C2540 A2541 A2542 G2543 G2544
G2545 U2546 G2549 U2552 G2553 U2554 U2555 C2556 G2557 C2558 C2559 C2560 A2561 U2562 U2563 A2564 A2565 A2566 G2567 C2568 G2569 G2570 C2571 A2572 C2573 G2574 C2575 G2576 A2577 G2578 C2579 U2580 G2581 G2582 G2583 U2584 U2585 C2586 A2587 G2588 A2589 A2590 C2591 G2592 U2593 C2594 A2602 G2603 U2604 U2605 C2606 G2607 G2608 U2609 C2610 U2611 C2612
U2613 A2614 U2615 C2616 C2617 C2620 A2621 C2622 G2623 A2629 G2630 G2631 A2632 G2633 G2634 C2635 U2636 U2637 G2638 A2639 G2640 G2641 G2642 C2646 U2647 C2648 U2649 U2653 A2654 G2655 A2662 G2663 G2664 A2665 C2666 C2667 G2668 G2669 G2673 G2674 A2675 C2676 G2677 C2678 A2679 C2680 C2681 U2682 C2683 G2686 U2687 U2688 U2689
C2690 A2693 G2694 C2695 U2696 G2697 U2698 C2699 C2700 C2701 U2702 C2703 C2704 A2705 G2706 G2707 C2710 A2711 U2712 A2712A A2713 G2714 C2715 U2716 G2717 G2718 G2719 U2720 A2721 G2722 C2723 C2724 A2725 U2726 G2729 G2732 A2733 A2734 G2735 A2740 A2741 C2742 C2743 G2744 C2745 U2746 G2747 A2748 A2749 A2750 G2751 C2752 A2753 U2754 C2755
U2756 A2757 A2758 G2759 C2760 G2761 A2764 A2765 G2766 C2767 G2770 C2771 C2772 C2773 C2774 A2775 A2776 G2777 A2778 U2779 G2780 A2781 G2782 G2783 C2784 C2785 U2786 C2787 C2788 C2789 A2790 C2791 G2792 G2793 C2794 G2795 U2797 C2798 A2799 A2801 G2802 C2803 C2804 G2805 G2807 A2810 G2811 G2812 A2813 C2814 C2815 C2816 G2817 G2818 G2819 A2820 A2821

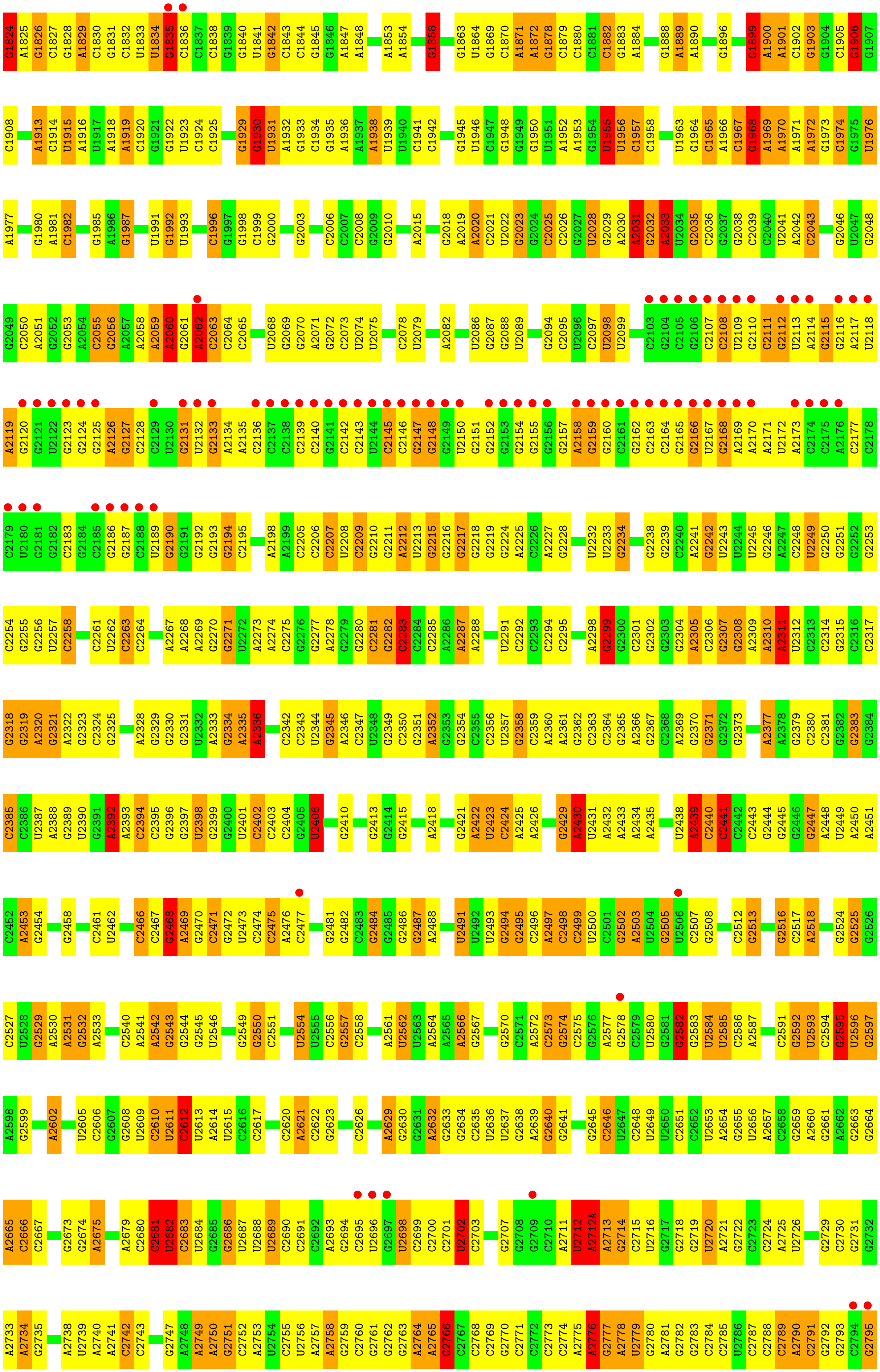


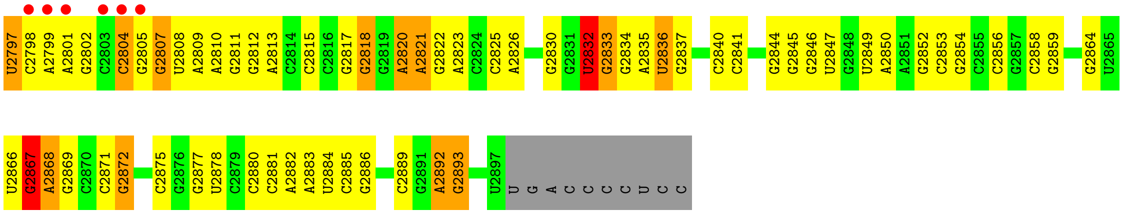
- Molecule 22: 23S rRNA

Chain YA:



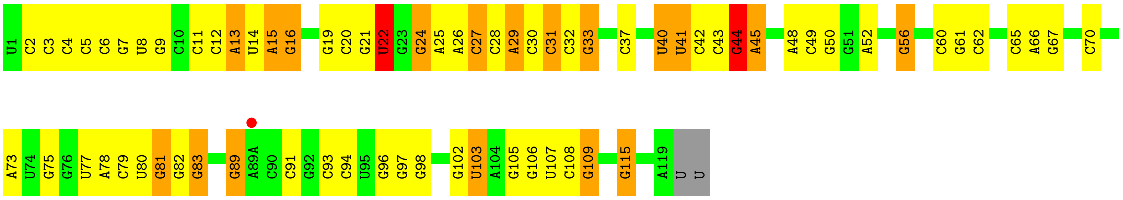

C817 G818 A819 C825 U826 U827 U828 A829 G830 C834 A835 C840 A841 G842 G845 C846 U847 G848 G852 G853 G854 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865 A866 C867 U868 G869 A870 G875 C876 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 G889 A890 G892 C893
C894 U895 A896 C897 C898 A899 A900 A901 C902 C903 C904 U907 C908 A909 A910 A911 C912 U913 C914 C915 G916 A917 A918 C923 G929 G932 A933 G934 C935 C936 U937 G938 G939 G940 A941 G942 U943 G944 A945 G946 G950 C951 G952 G956 A957 U958 A959 A960 C961 G962 U963 C964 C965 G966
C967 G968 U969 C970 C971 G972 A973 G974 C974A G975 C976 G977 G978 G979 A980 A981 C982 A983 A984 C985 C986 G987 A988 G989 A990 C991 G992 G993 C994 C995 A996 A1001 G1002 G1003 C1004 C1005 A1009 A1010 G1011 U1012 C1013 G1016 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 U1033 G1039
C1040 C1041 G1042 C1043 G1044 A1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 C1076 A1077 U1078 C1079 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101
C1102 A1103 C1104 U1105 G1106 C1109 G1110 A1111 G1112 U1113 G1114 G1115 G1120 C1121 G1122 G1125 A1126 A1127 A1128 A1129 U1130 G1131 A1132 U1133 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A A1143 G1144 C1145 A1148 G1149 C1150 G1151 C1152 C1153 G1154 A1155 U1159 G1160 C1161 G1162 G1163 G1164 U1165 C1166 U1167 G1168 G1169
G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1184 G1187 U1188 A1189 G1190 G1193 A1194 G1195 U1198 U1199 C1200 C1201 C1202 G1203 A1204 U1205 G1206 C1207 C1208 G1209 A1210 U1211 G1212 A1213 A1214 G1215 G1216 C1217 C1218 G1219 A1220 C1221 C1222 C1223 G1224 C1225 G1228 C1230 G1231 G1235 G1236
A1237 G1238 G1239 U1240 A1241 A1242 G1243 G1244 A1247 G1250 G1251 G1252 A1253 A1254 U1255 G1256 C1257 C1258 A1262 U1263 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1278 A1284 G1285 A1286 A1287 U1288 C1289 C1290 G1291 U1292 C1293 U1294 C1295 G1296 C1297 U1300 A1301 A1302 G1303 C1306
G1309 G1310 G1311 U1312 U1313 C1314 G1319 C1320 A1321 G1324 C1327 G1328 U1329 C1330 A1331 G1332 C1333 G1334 U1335 A1336 G1337 G1338 G1339 U1340 U1341 A1342 G1343 G1344 G1348 A1349 U1352 A1353 A1354 G1355 G1358 A1359 A1360 G1361 C1362 C1363 G1364 A1365 G1368 G1369 C1370 G1371 U1372 A1373 G1374 C1375 C1376 G1377 A1378
A1379 G1382 C1383 A1384 G1385 C1386 G1389 U1390 U1391 U1394 A1395 G1401 C1402 C1403 C1404 U1405 U1406 C1407 C1408 C1411 A1412 G1413 G1414 U1415 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 G1425 G1426 A1427 C1428 G1429 C1430 U1431 A1434 G1435 G1436 C1437 G1441 G1442 A1444A C1445 C1446 G1447 G1448 A1449
G1449A U1454 G1455 C1458 G1459 A1460 G1461 C1464 G1465 G1466 C1467 C1468 A1469 G1470 A1471 G1475 C1476 A1477 G1478 G1479 G1480 U1482 G1483 G1484 G1485 A1486 G1487 G1488 U1489 A1490 C1493 A1494 A1495 A1496 U1497 C1498 C1499 G1500 C1501 C1502 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1510 A1511 U1514 C1515 U1516 G1517 C1518
G1519 U1520 G1521 G1522 G1525 G1526 G1527 A1528 A1529 G1530 C1531 C1532 C1533 G1534 U1535 A1536 C1537 G1538 G1539 G1540 U1541 G1542 A1543 C1544 A1545 A1545A C1546 C1549 C1550 C1551 A1554 A1558 G1559 G1560 A1566 A1567 G1568 A1569 C1577 U1578 A1579 A1580 G1581 C1582 A1583 C1585 A1586 A1587 C1588 C1589 U1590 G1591 C1592 G1593
G1594 G1595 A1596 A1597 C1598 C1599 C1600 G1601 U1602 C1607 A1608 A1609 A1610 C1611 C1612 G1613 A1614 C1615 A1616 C1617 G1620 U1621 G1622 G1623 G1624 C1625 G1626 G1627 G1628 U1629 G1630 C1630A G1635 C1636 A1637 C1638 U1639 C1640 A1641 G1642 G1645 C1646 G1647 C1648 G1649 A1652 G1653 A1654 A1655 C1656 C1657 C1658 U1659 C1662
A1665 G1666 G1667 A1668 A1669 C1670 U1671 C1672 U1673 G1674 C1675 A1676 A1677 G1678 U1679 U1680 G1681 G1682 C1685 C1686 G1687 U1688 A1689 U1693 C1694 G1695 G1696 G1697 A1698 G1699 A1700 A1701 C1708 G1725 G1726 U1727 G1728 A1729 U1730 G1731 A1732 G1733 C1734 C1742 G1743 G1750 C1751 C1752 G1753 C1754 A1755 G1756 U1757
G1758 A1759 A1760 C1761 A1762 G1763 G1764 C1767 U1768 G1769 G1770 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 U1805 C1806 G1807 G1811 A1812 G1813 G1814 A1815 G1816 U1820 A1821 G1822 G1823


G1824 A1825 G1826 C1827 G1828 A1829 C1830 G1831 C1832 U1833 U1834 G1835 C1836 C1837 C1838 G1839 G1840 U1841 G1842 C1843 C1844 G1845 G1846 A1847 A1848 A1853 A1854 G1858 G1863 U1864 G1869 C1870 A1871 A1872 G1878 C1879 C1880 C1881 C1882 G1883 A1884 G1888 A1889 A1890 G1896 G1899 A1900 A1901 C1902 G1903 G1904 C1905 G1906 G1907
C1908 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1922 U1923 C1924 C1925 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 G1945 U1946 C1947 G1948 G1949 G1950 U1951 A1952 A1953 G1954 U1955 U1956 C1957 C1958 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1973 C1974 G1975 U1976
A1977 G1980 A1981 C1982 G1985 A1986 G1987 U1991 G1992 U1993 C1996 G1997 G1998 C1999 G2000 G2003 C2006 C2007 C2008 G2009 G2010 A2015 G2018 A2019 A2020 C2021 U2022 G2023 G2024 C2025 C2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 C2039 C2040 U2041 A2042 C2043 G2046 U2047 G2048
G2049 C2050 A2051 G2052 G2053 A2054 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 C2063 C2064 C2065 U2068 G2069 G2070 A2071 C2072 C2073 U2074 U2075 C2078 U2079 A2082 U2086 G2087 G2088 U2089 G2094 C2095 U2096 C2097 G2098 U2099 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118
A2119 G2120 G2121 U2122 G2123 G2124 C2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 C2152 G2153 C2154 G2155 G2156 C2157 A2158 G2159 G2160 G2161 C2162 C2163 C2164 C2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178
C2179 U2180 G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 G2193 G2194 C2195 A2198 A2199 C2205 C2206 C2207 U2208 C2209 G2210 G2211 A2212 U2213 G2215 G2216 G2217 G2218 G2219 G2224 A2225 C2226 A2227 G2228 U2232 U2233 G2234 G2238 G2239 C2240 A2241 G2242 U2243 U2244 U2245 G2246 A2247 C2248 U2249 G2250 G2251 G2252 G2253
C2254 G2255 G2256 U2257 C2258 C2261 U2262 C2263 C2264 A2267 A2268 A2269 G2270 G2271 U2272 A2273 A2274 C2275 G2276 G2277 A2278 G2279 C2280 C2281 G2282 C2283 C2284 C2285 A2286 A2287 A2288 U2291 C2292 C2293 C2294 C2295 A2298 G2299 G2300 C2301 G2302 G2303 G2304 A2305 C2306 G2307 G2308 A2309 A2310 A2311 U2312 C2313 C2314 G2315 C2316 C2317
G2318 G2319 A2320 G2321 A2322 G2323 C2324 G2325 A2328 G2329 G2330 G2331 U2332 A2333 G2334 A2335 A2336 C2342 C2343 U2344 G2345 A2346 C2347 U2348 G2349 C2350 G2351 A2352 G2353 C2354 C2355 C2356 U2357 G2358 C2359 A2360 A2361 G2362 C2363 C2364 G2365 A2366 G2367 C2368 A2369 G2370 G2371 G2372 G2373 A2377 A2378 C2379 C2380 C2381 G2382 G2383 G2384
C2385 C2386 U2387 A2388 G2389 U2390 G2391 A2392 A2393 C2394 C2395 G2396 G2397 U2398 G2399 G2400 U2401 C2402 C2403 C2404 G2405 U2406 G2410 G2413 G2414 G2415 A2418 G2421 A2422 U2423 C2424 A2425 A2426 G2429 A2430 U2431 A2432 A2433 A2434 A2435 U2438 A2439 C2440 C2441 C2442 C2443 G2444 C2445 G2446 G2447 A2448 U2449 A2450 A2451
C2452 A2453 G2454 G2458 C2461 U2462 C2466 C2467 G2468 A2469 G2470 C2471 G2472 U2473 C2474 C2475 A2476 C2477 G2481 G2482 C2483 G2484 G2485 G2486 G2487 A2488 U2491 U2492 U2493 G2494 G2495 C2496 A2497 G2498 C2499 U2500 C2501 G2502 A2503 U2504 G2505 U2506 C2507 G2508 C2512 G2513 G2516 C2517 A2518 G2524 G2525 G2526
C2527 U2528 G2529 C2530 A2531 G2532 A2533 C2540 A2541 A2542 G2543 G2544 G2545 U2546 G2549 G2550 C2551 U2554 U2555 C2556 G2557 C2558 A2561 U2562 U2563 A2564 A2565 A2566 G2567 G2570 C2571 A2572 C2573 G2574 C2575 G2576 A2577 G2578 C2579 U2580 G2581 G2582 G2583 U2584 U2585 C2586 A2587 C2591 G2592 U2593 C2594 G2595 U2596 G2597
A2598 G2599 A2602 U2605 C2606 G2607 G2608 U2609 C2610 U2611 C2612 U2613 A2614 U2615 C2616 C2617 C2620 A2621 C2622 G2623 C2626 A2629 G2630 G2631 A2632 G2633 G2634 C2635 U2636 C2637 G2638 A2639 G2640 G2641 G2645 C2646 U2647 C2648 U2649 U2650 C2651 C2652 U2653 A2654 G2655 U2656 A2657 C2658 G2659 A2660 G2661 A2662 G2663 G2664
A2665 C2666 C2667 G2673 G2674 A2675 A2679 C2680 C2681 U2682 C2683 U2684 G2685 G2686 U2687 U2688 U2689 C2690 C2691 C2692 A2693 G2694 C2695 U2696 G2697 U2698 C2699 C2700 C2701 U2702 C2703 G2707 G2708 G2709 C2710 A2711 U2712 A2712A A2713 G2714 C2715 U2716 G2717 G2718 G2719 U2720 A2721 G2722 C2723 C2724 A2725 U2726 G2729 C2730 G2731 G2732
A2733 A2734 G2735 A2738 U2739 A2740 A2741 C2742 C2743 G2747 A2748 A2749 A2750 G2751 C2752 A2753 U2754 C2755 U2756 A2757 A2758 G2759 C2760 G2761 G2762 G2763 A2764 A2765 G2766 C2767 C2768 C2769 C2770 C2771 C2772 C2773 C2774 A2775 A2776 G2777 A2778 U2779 G2780 A2781 G2782 C2783 C2784 C2785 U2786 C2787 C2788 C2789 A2790 C2791 G2792 G2793 C2794 G2795



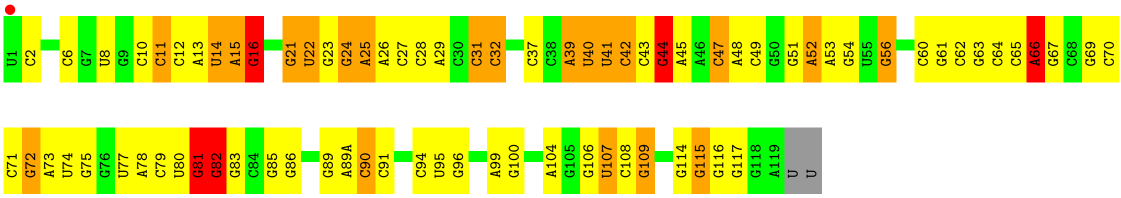
- Molecule 23: 5S rRNA

Chain RB:



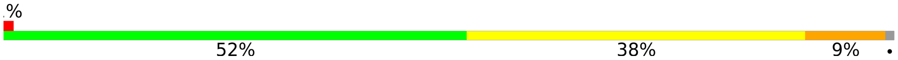
- Molecule 23: 5S rRNA

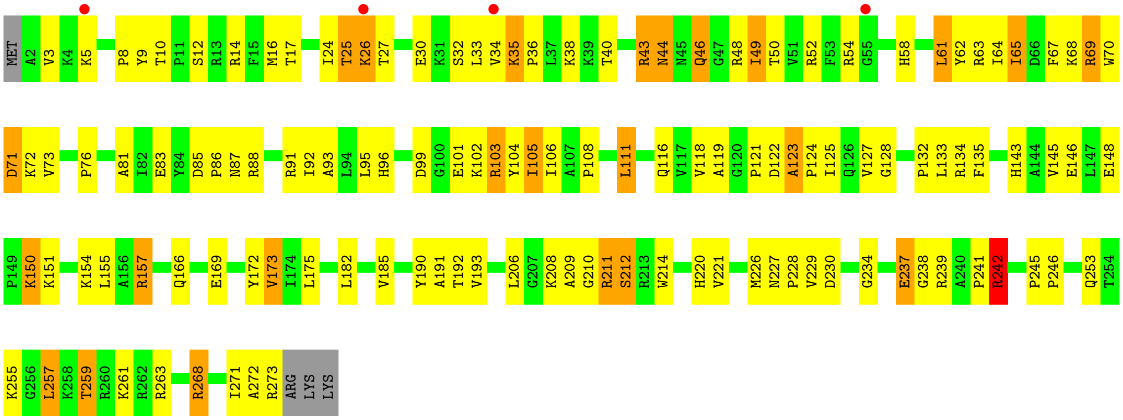
Chain YB:



- Molecule 24: 50S ribosomal protein L2

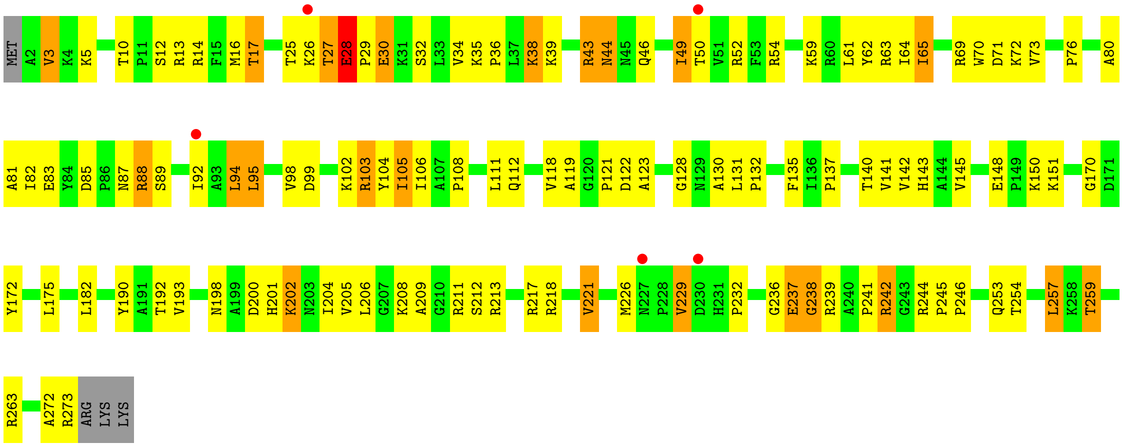
Chain RD:





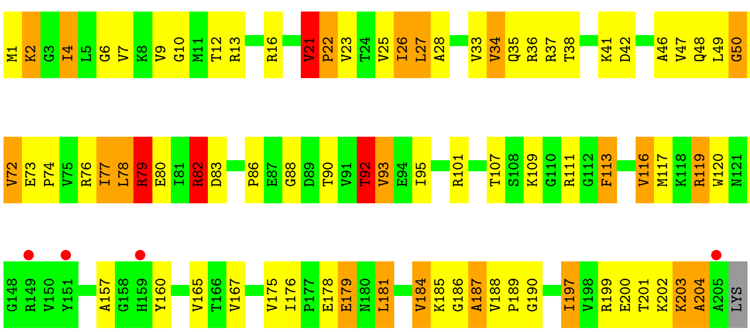
- Molecule 24: 50S ribosomal protein L2

Chain YD:



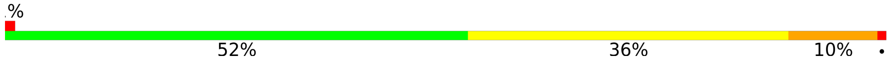
- Molecule 25: 50S ribosomal protein L3

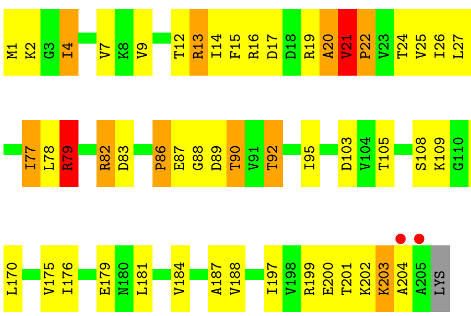
Chain RE:



- Molecule 25: 50S ribosomal protein L3

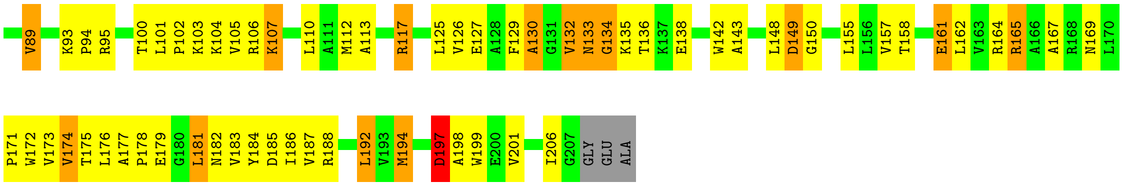
Chain YE:





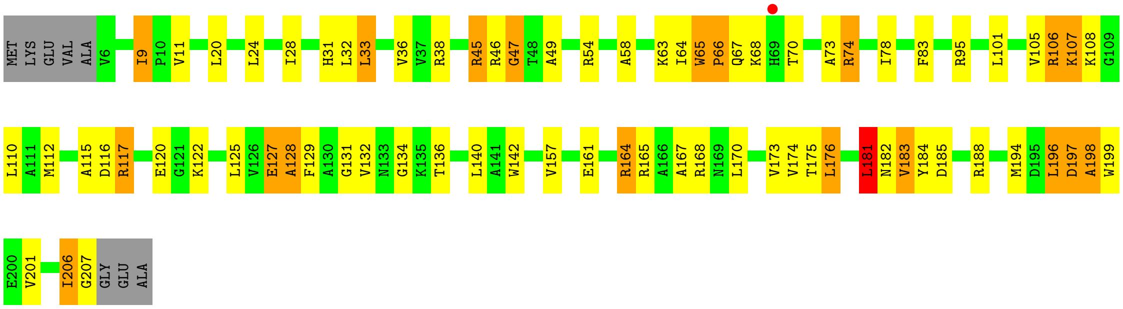
- Molecule 26: 50S ribosomal protein L4

Chain RF:



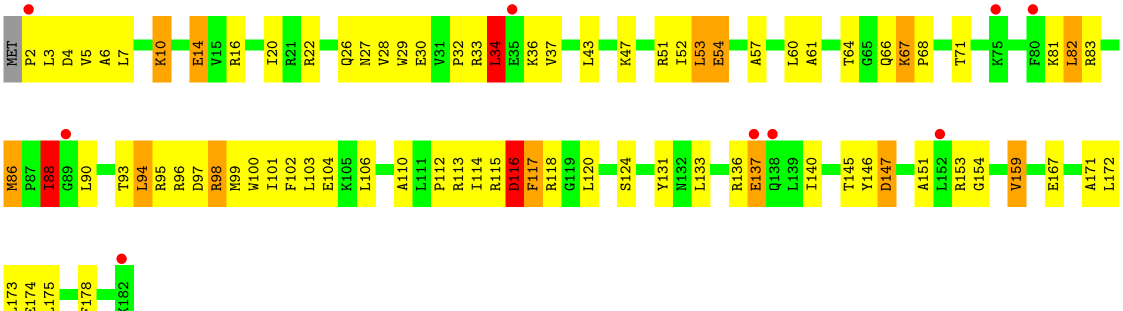
- Molecule 26: 50S ribosomal protein L4

Chain YF:



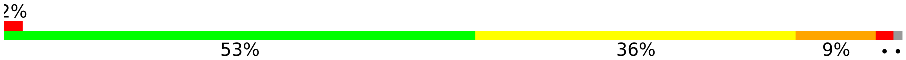
- Molecule 27: 50S ribosomal protein L5

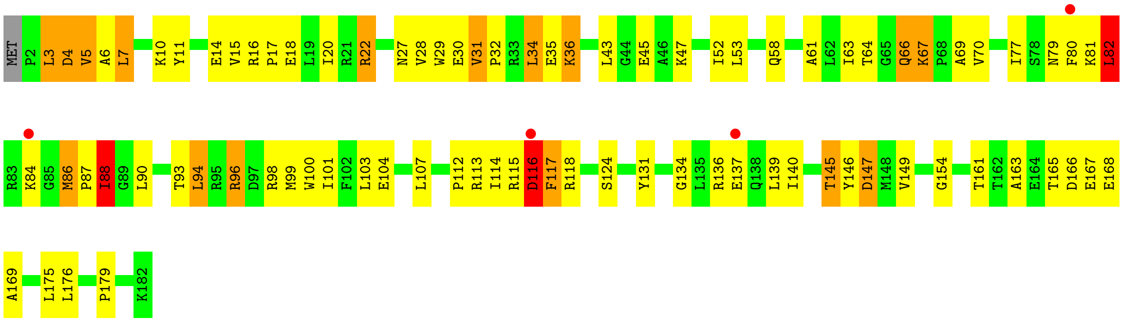
Chain RG:



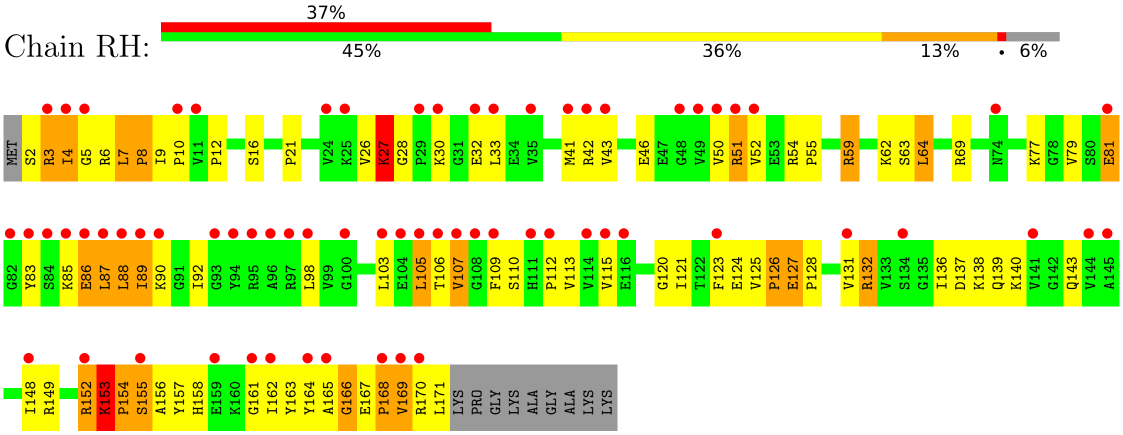
- Molecule 27: 50S ribosomal protein L5

Chain YG:

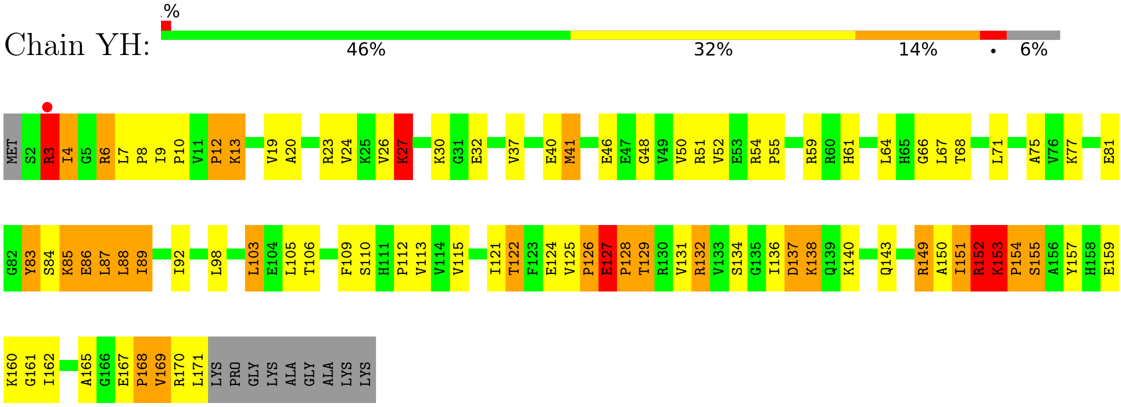




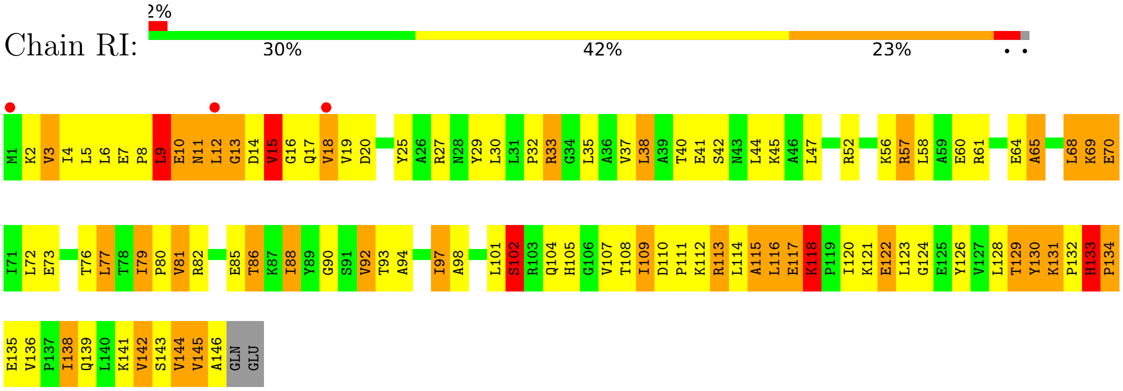
- Molecule 28: 50S ribosomal protein L6



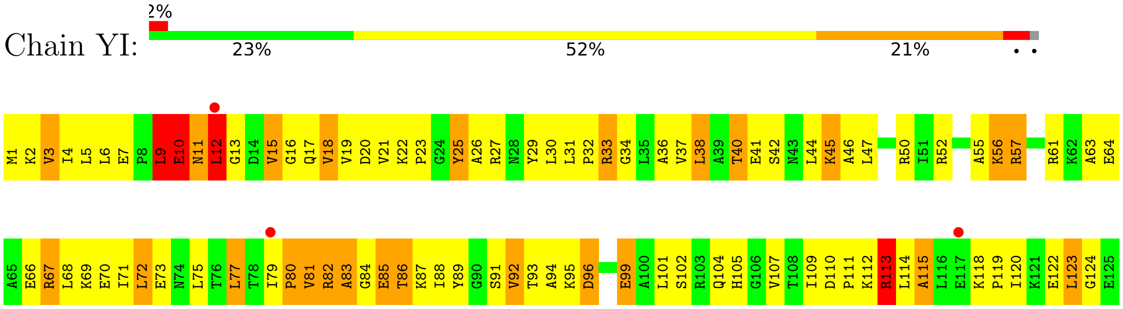
- Molecule 28: 50S ribosomal protein L6

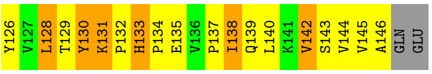


- Molecule 29: 50S ribosomal protein L9



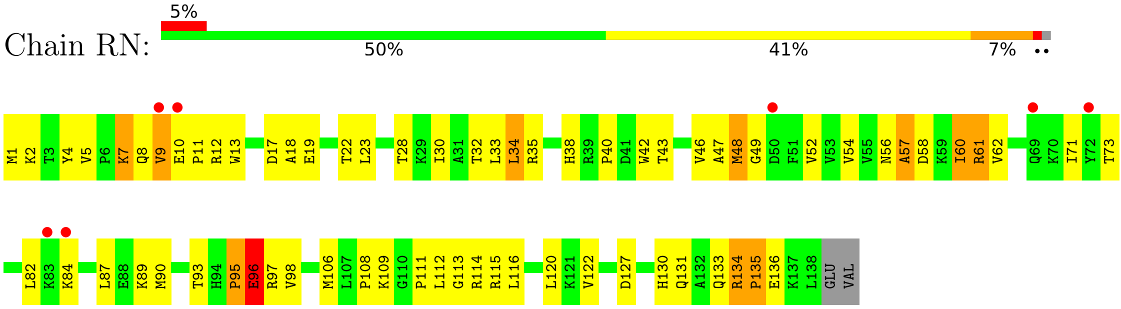
- Molecule 29: 50S ribosomal protein L9





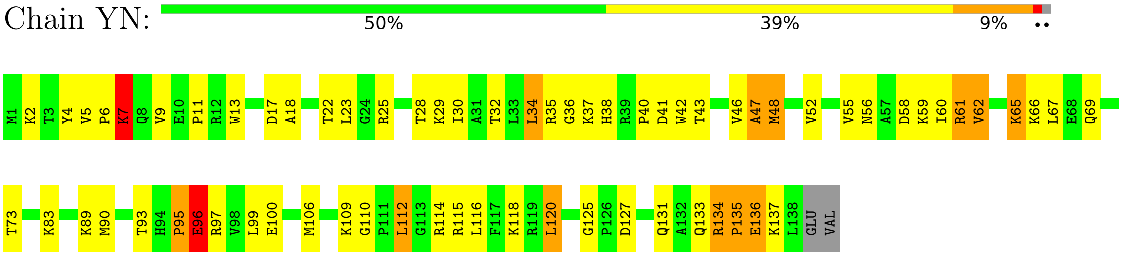
- Molecule 30: 50S ribosomal protein L13

Chain RN:



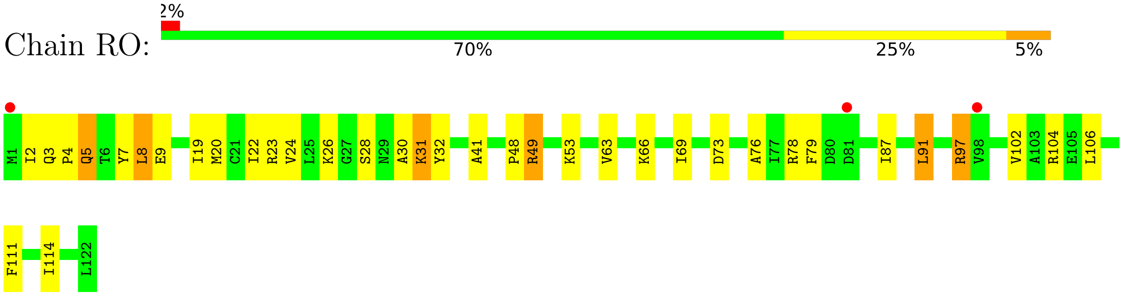
- Molecule 30: 50S ribosomal protein L13

Chain YN:



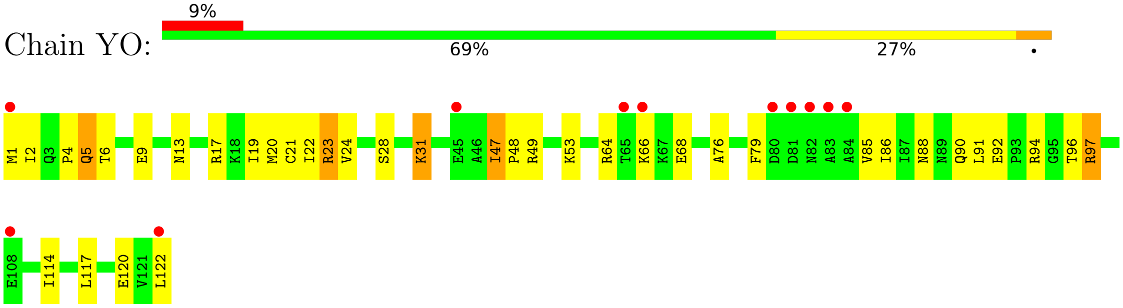
- Molecule 31: 50S ribosomal protein L14

Chain RO:



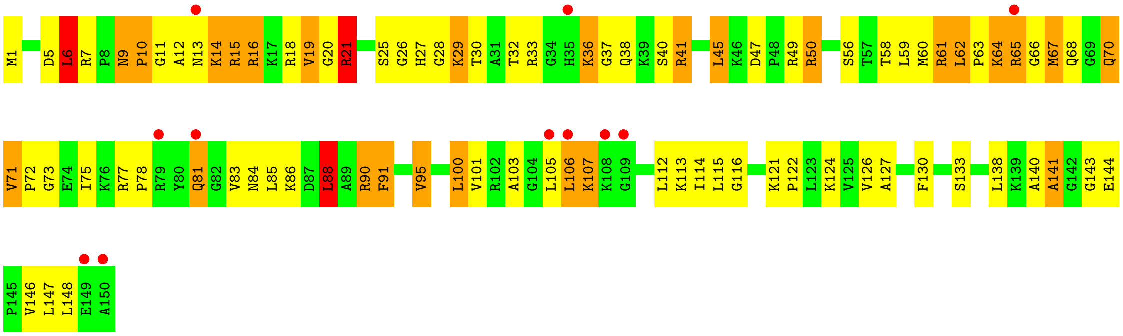
- Molecule 31: 50S ribosomal protein L14

Chain YO:



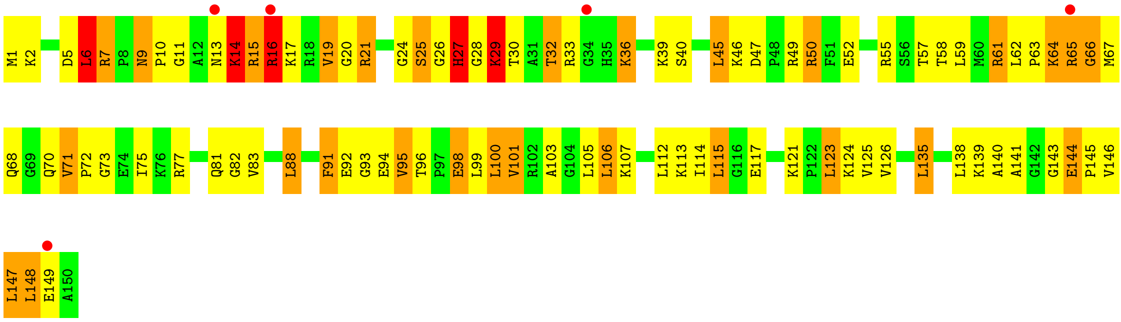
- Molecule 32: 50S ribosomal protein L15

Chain RP:



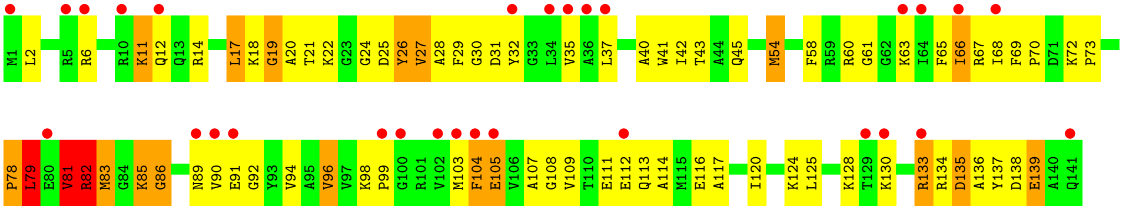
- Molecule 32: 50S ribosomal protein L15

Chain YP:



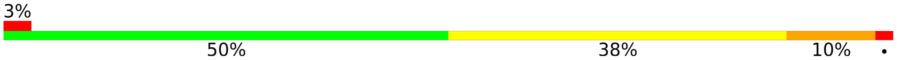
- Molecule 33: 50S ribosomal protein L16

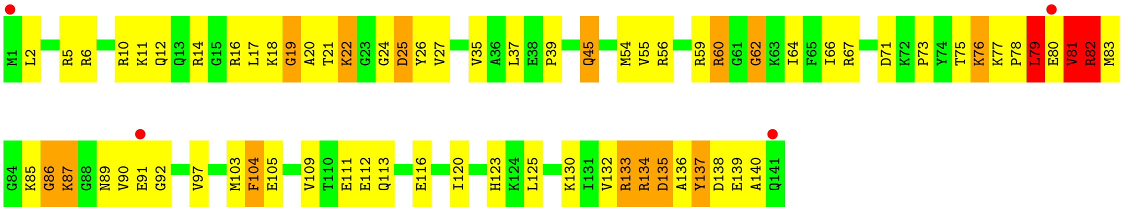
Chain RQ:



- Molecule 33: 50S ribosomal protein L16

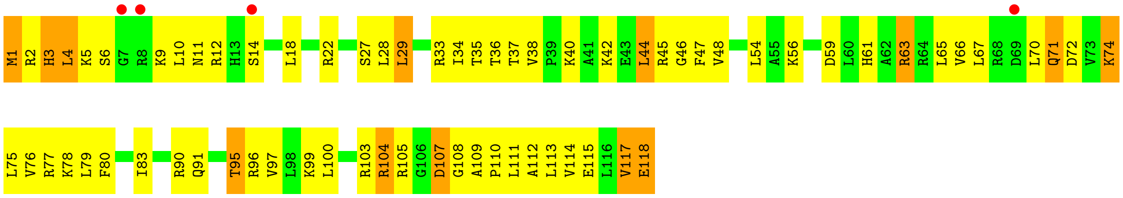
Chain YQ:





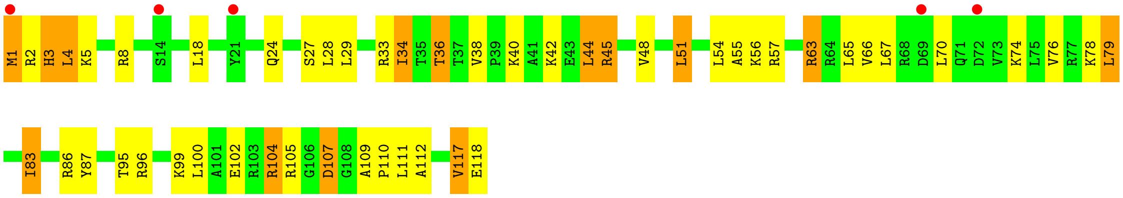
- Molecule 34: 50S ribosomal protein L17

Chain RR:



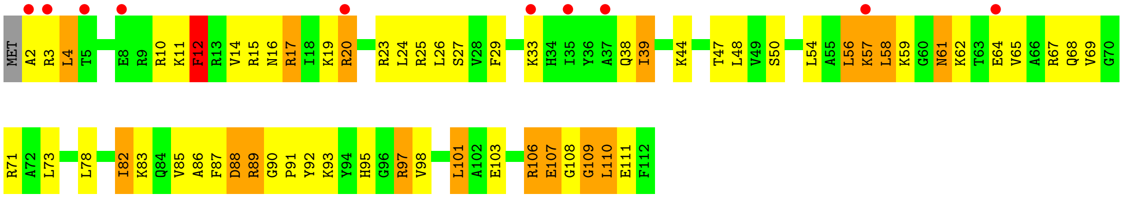
- Molecule 34: 50S ribosomal protein L17

Chain YR:



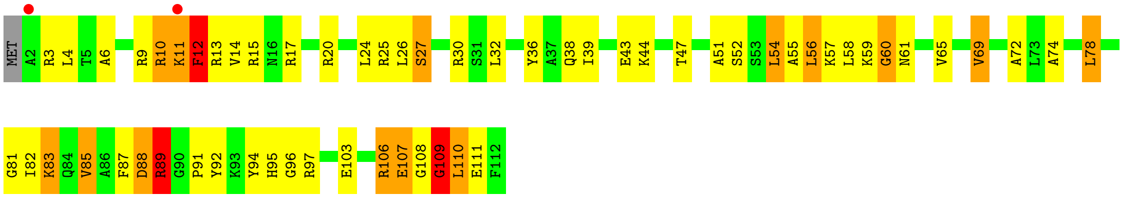
- Molecule 35: 50S ribosomal protein L18

Chain RS:



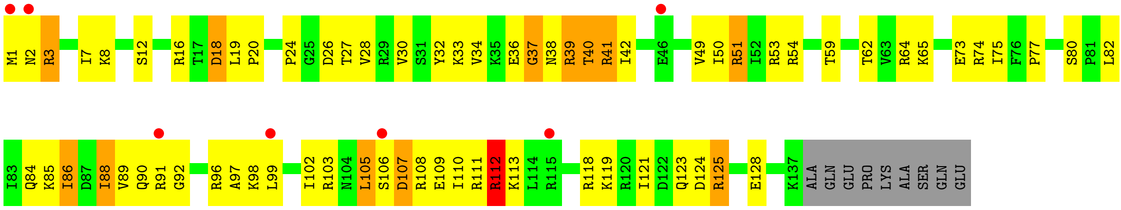
- Molecule 35: 50S ribosomal protein L18

Chain YS:

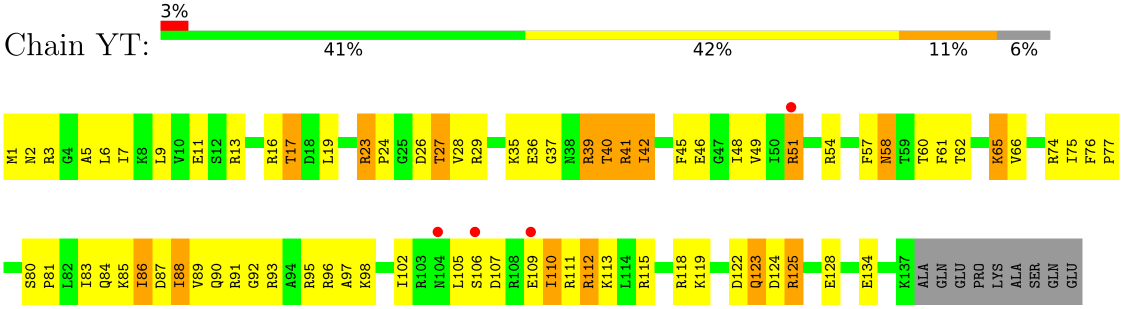


- Molecule 36: 50S ribosomal protein L19

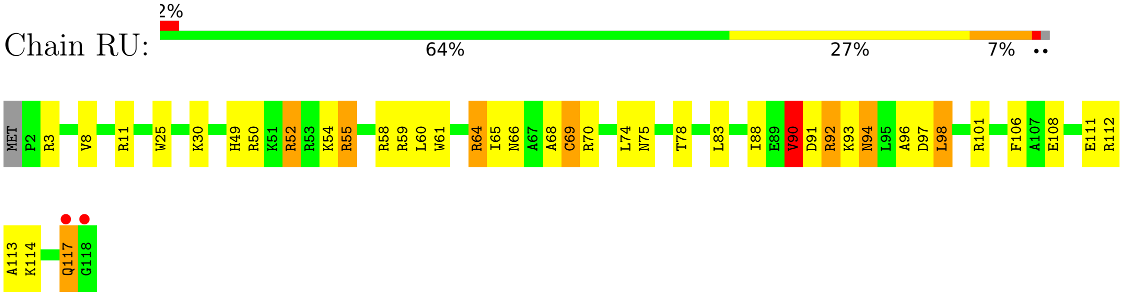
Chain RT:



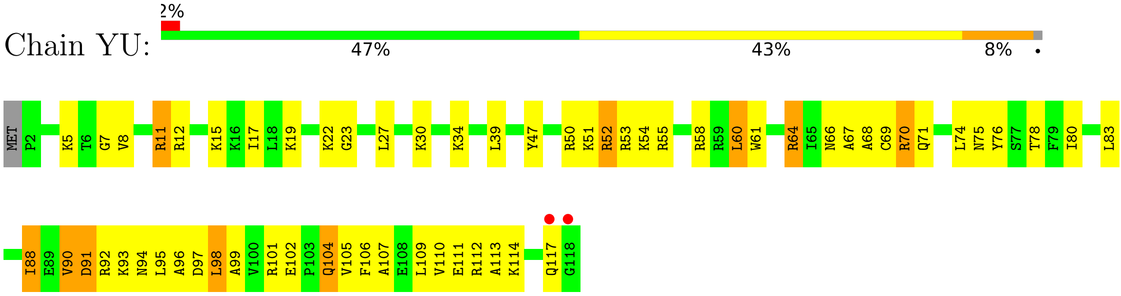
- Molecule 36: 50S ribosomal protein L19



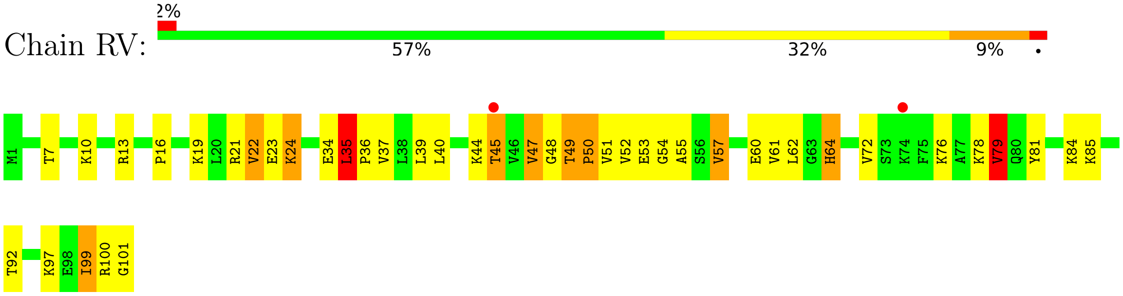
- Molecule 37: 50S ribosomal protein L20



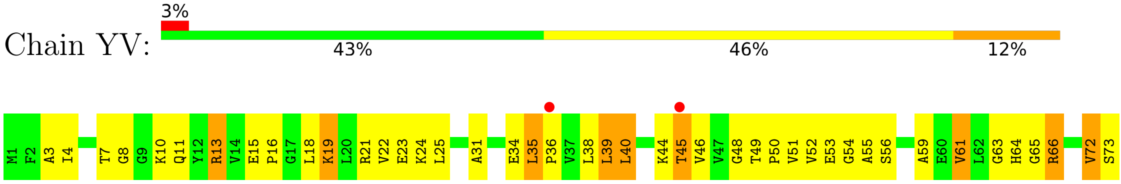
- Molecule 37: 50S ribosomal protein L20

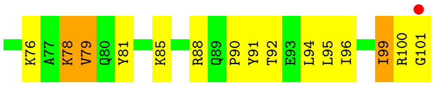


- Molecule 38: 50S ribosomal protein L21



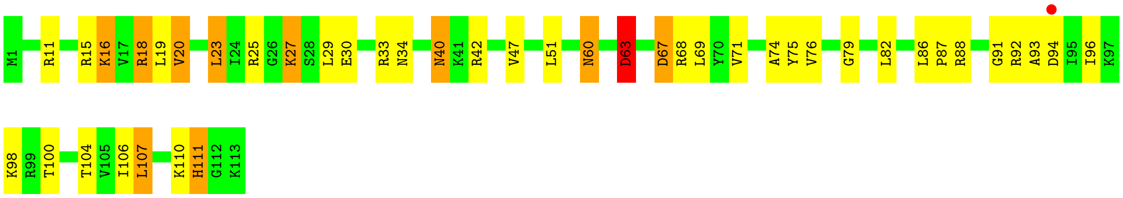
- Molecule 38: 50S ribosomal protein L21





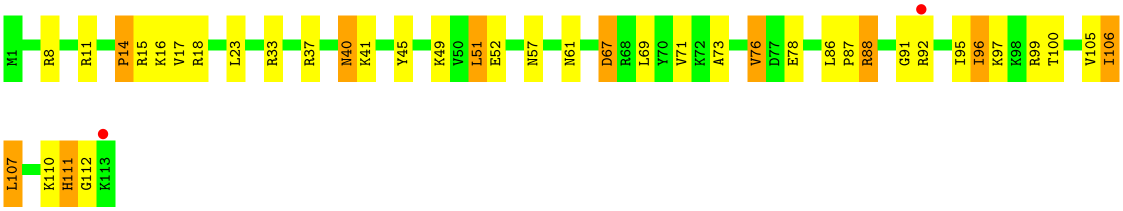
- Molecule 39: 50S ribosomal protein L22

Chain RW:



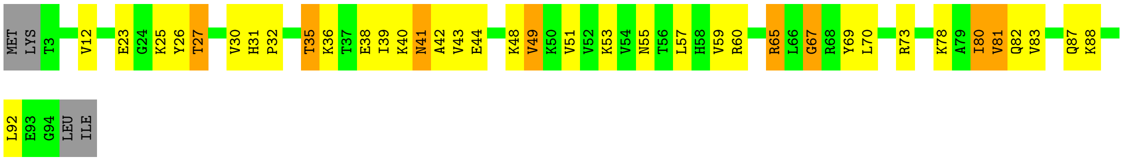
- Molecule 39: 50S ribosomal protein L22

Chain YW:



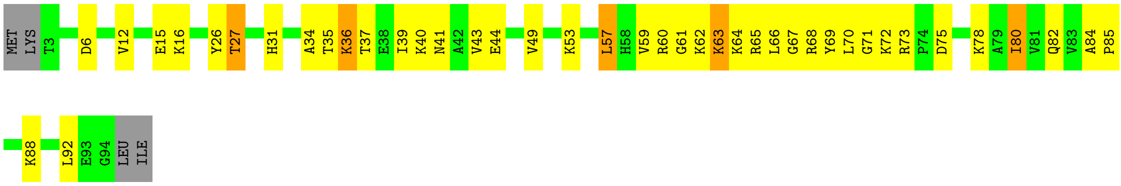
- Molecule 40: 50S ribosomal protein L23

Chain RX:



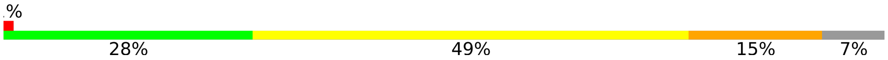
- Molecule 40: 50S ribosomal protein L23

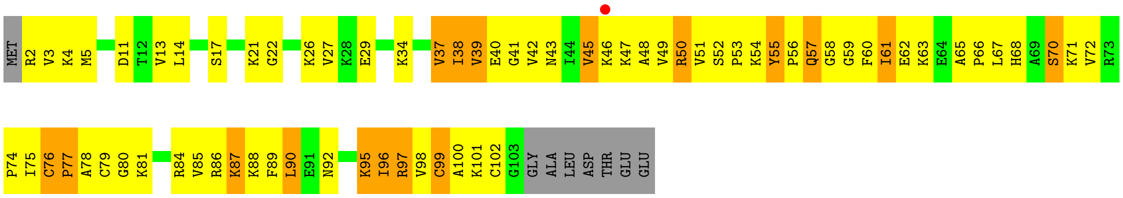
Chain YX:



- Molecule 41: 50S ribosomal protein L24

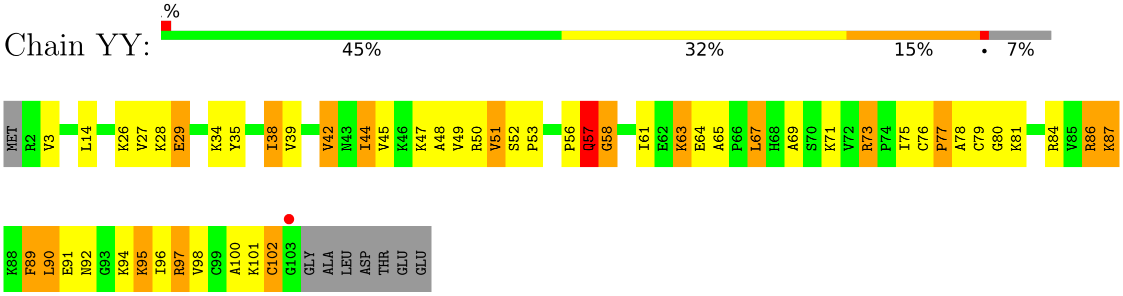
Chain RY:





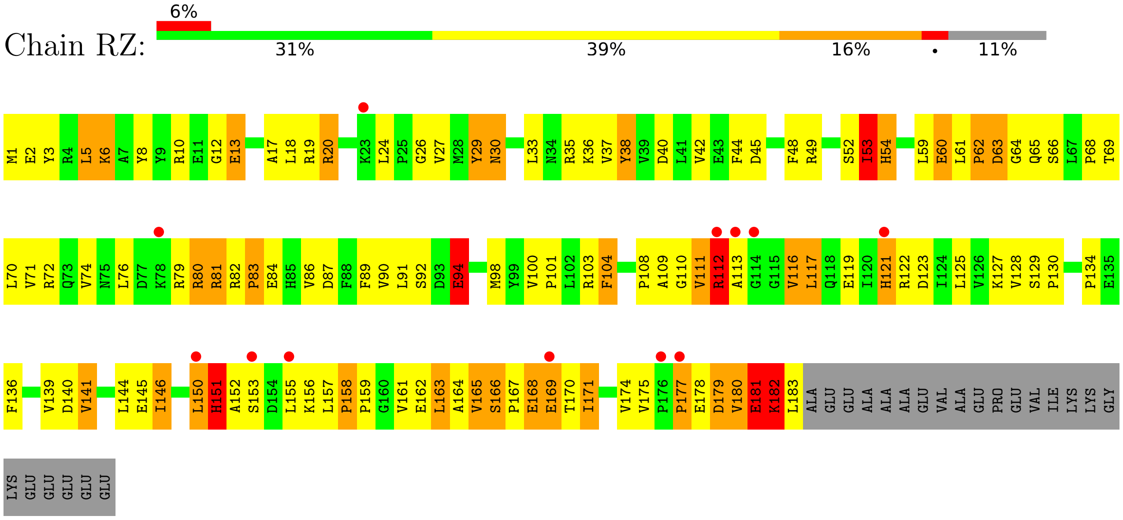
- Molecule 41: 50S ribosomal protein L24

Chain YY:



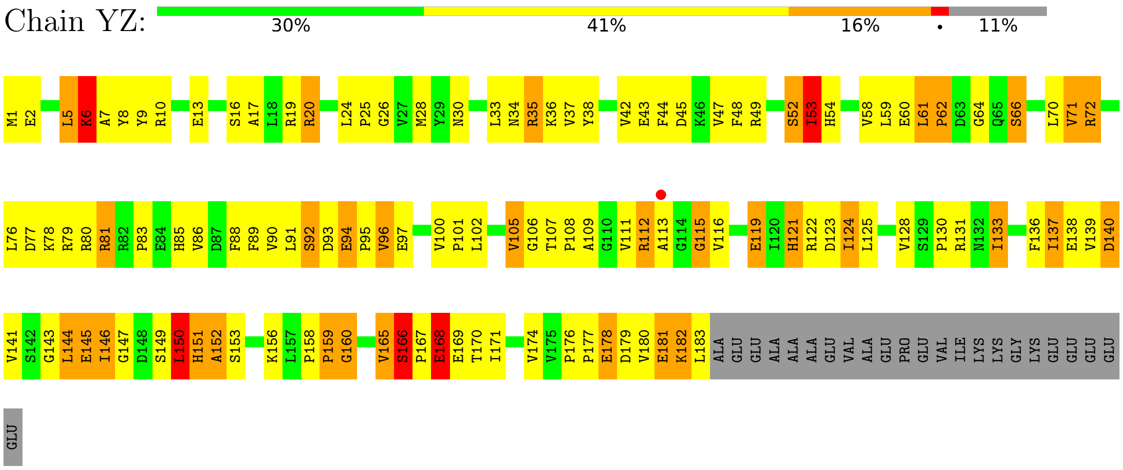
- Molecule 42: 50S ribosomal protein L25

Chain RZ:

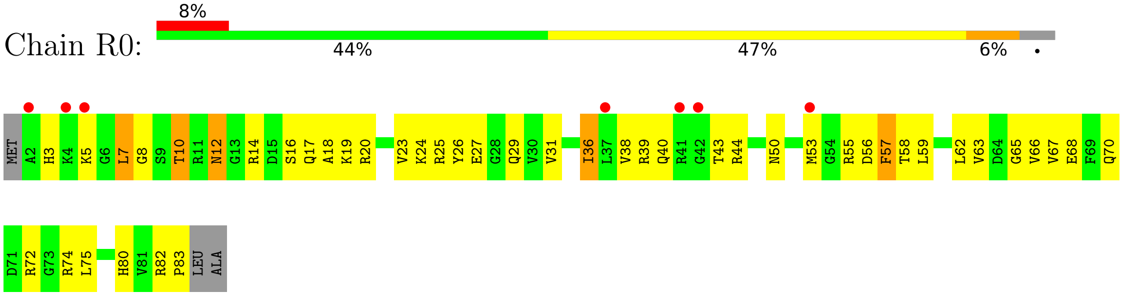


- Molecule 42: 50S ribosomal protein L25

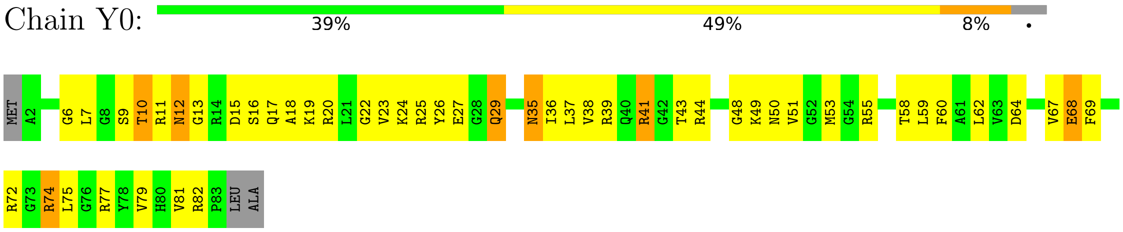
Chain YZ:



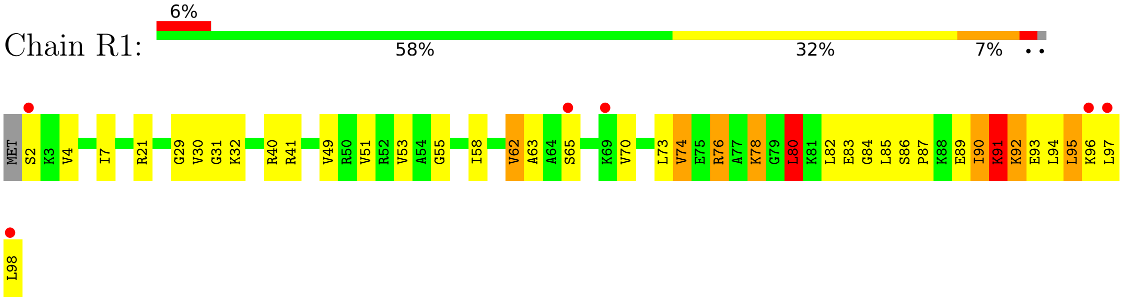
- Molecule 43: 50S ribosomal protein L27



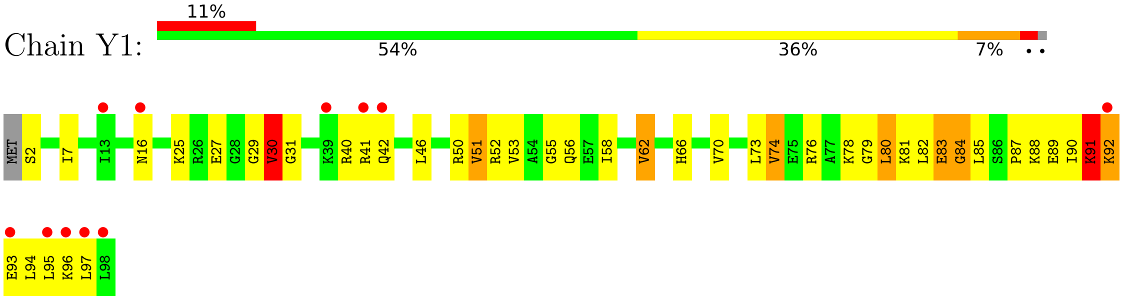
- Molecule 43: 50S ribosomal protein L27



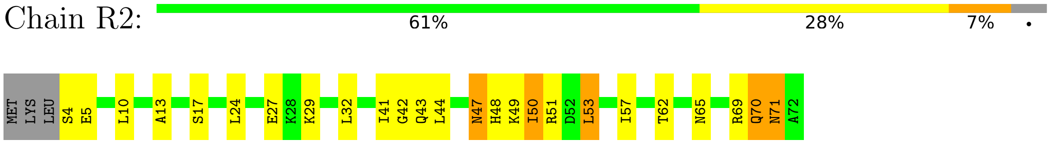
- Molecule 44: 50S ribosomal protein L28



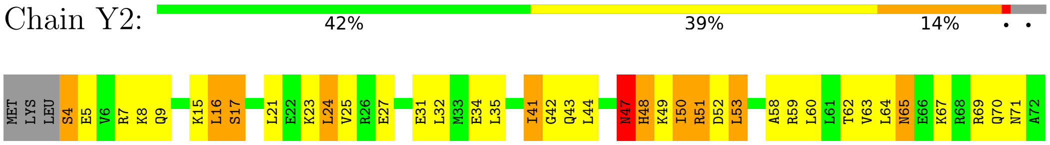
- Molecule 44: 50S ribosomal protein L28



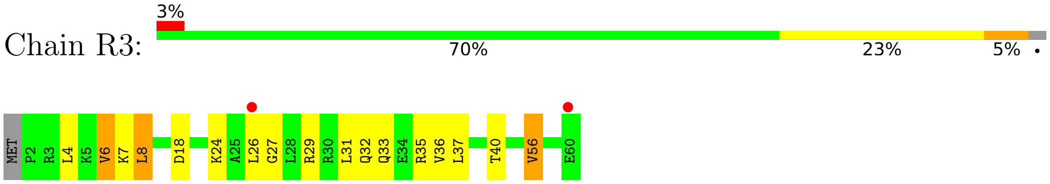
- Molecule 45: 50S ribosomal protein L29



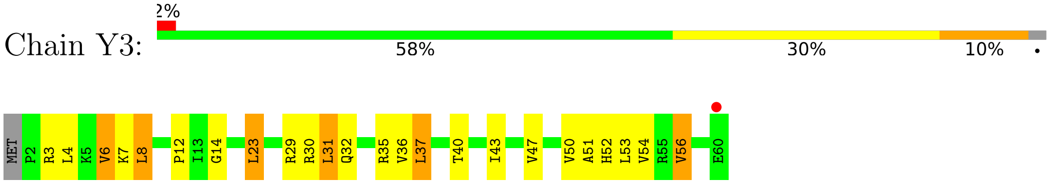
- Molecule 45: 50S ribosomal protein L29



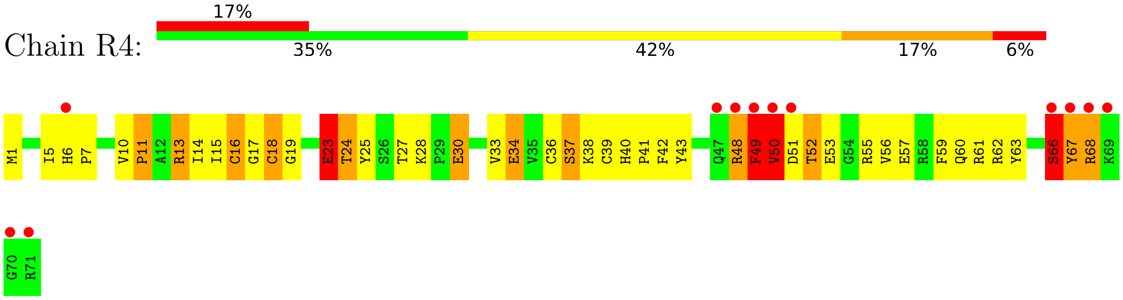
- Molecule 46: 50S ribosomal protein L30



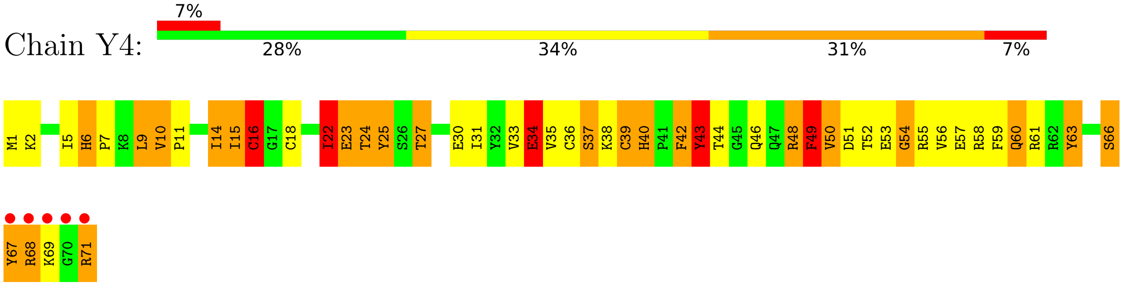
- Molecule 46: 50S ribosomal protein L30



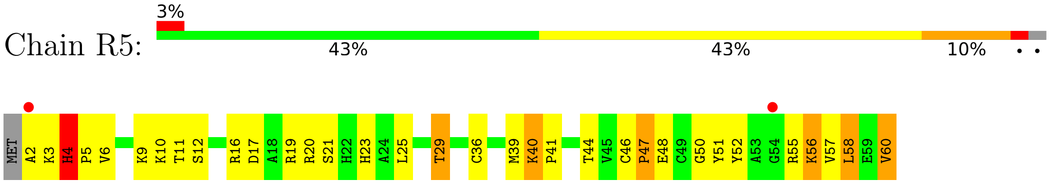
- Molecule 47: 50S ribosomal protein L31



- Molecule 47: 50S ribosomal protein L31

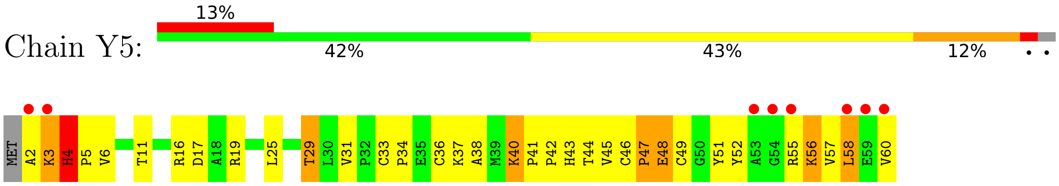


- Molecule 48: 50S ribosomal protein L32



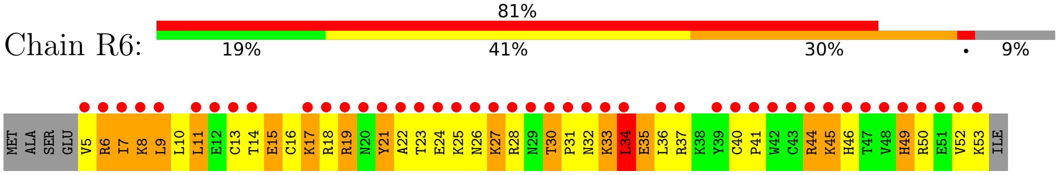
- Molecule 48: 50S ribosomal protein L32

Chain Y5:



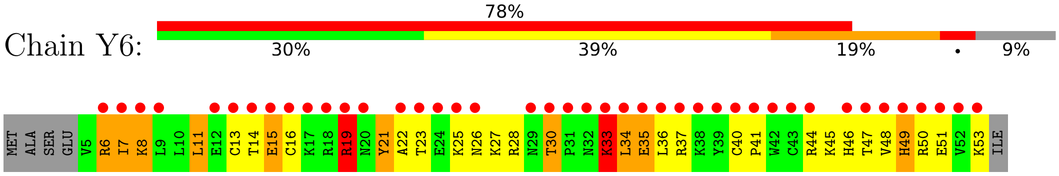
- Molecule 49: 50S ribosomal protein L33

Chain R6:



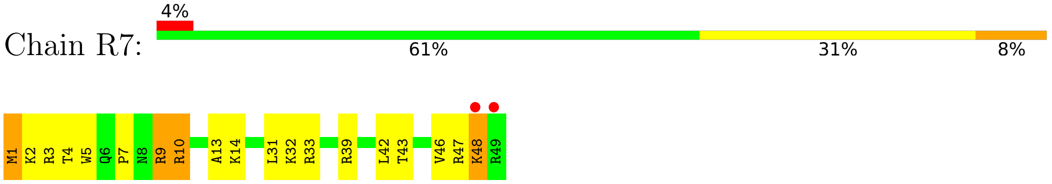
- Molecule 49: 50S ribosomal protein L33

Chain Y6:



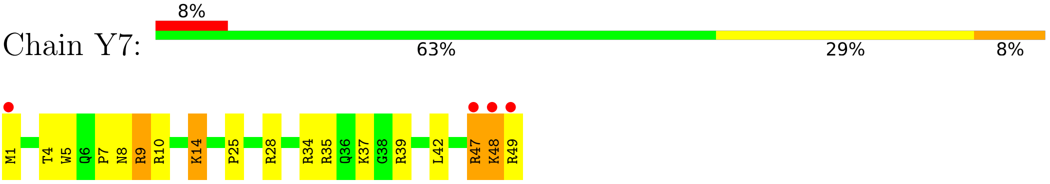
- Molecule 50: 50S ribosomal protein L34

Chain R7:



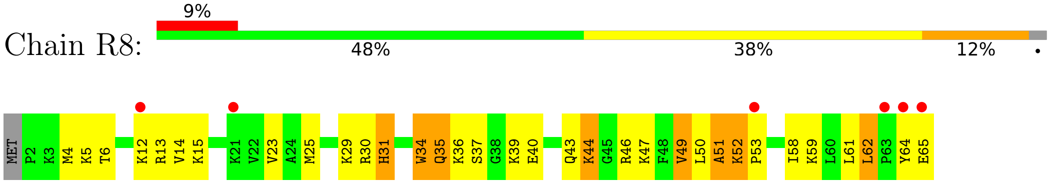
- Molecule 50: 50S ribosomal protein L34

Chain Y7:



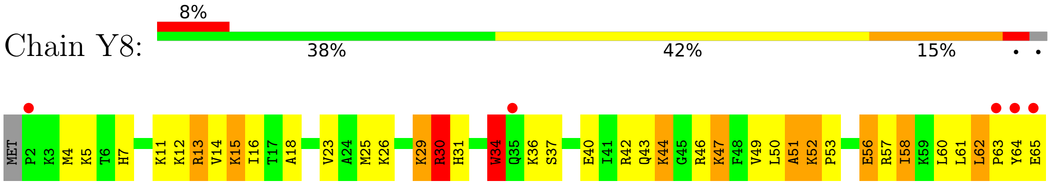
- Molecule 51: 50S ribosomal protein L35

Chain R8:



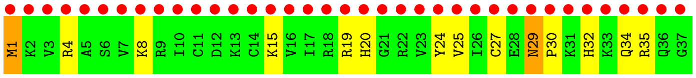
- Molecule 51: 50S ribosomal protein L35

Chain Y8:



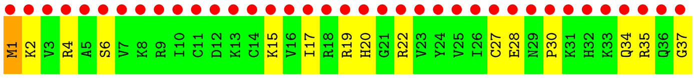
- Molecule 52: 50S ribosomal protein L36

Chain R9:



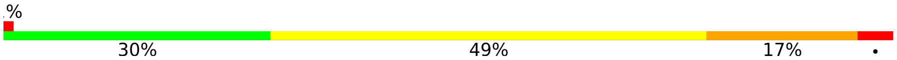
- Molecule 52: 50S ribosomal protein L36

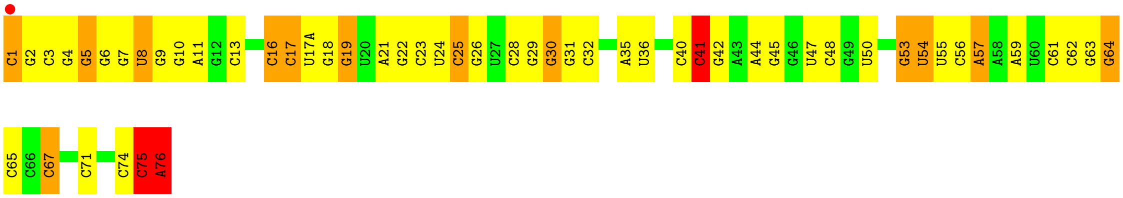
Chain Y9:



- Molecule 53: P-site tRNA fMET

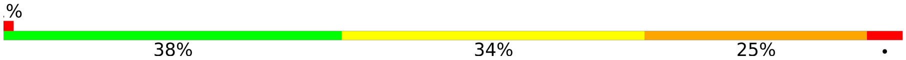
Chain QV:

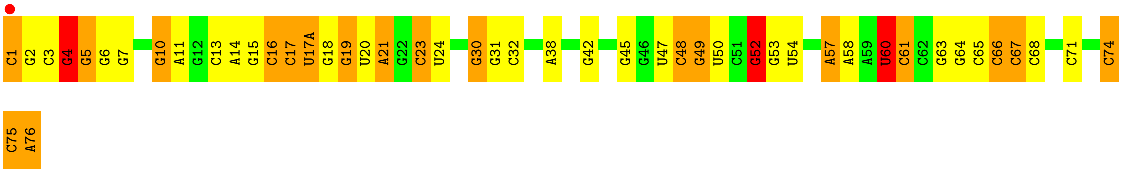




- Molecule 53: P-site tRNA fMET

Chain XV:





- Molecule 54: mRNA

Chain QX:

- Molecule 54: mRNA

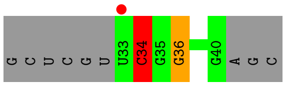
Chain XX:

- Molecule 55: A site ASL of tRNA-Proline CGG (unmodified)

Chain QY:

- Molecule 55: A site ASL of tRNA-Proline CGG (unmodified)

Chain XY:



- Molecule 56: tRNA acceptor end mimic

Chain Z6:

- Molecule 56: tRNA acceptor end mimic

Chain Z8:

4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.82Å 447.39Å 619.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	187.58 – 3.68 189.96 – 3.54	Depositor EDS
% Data completeness (in resolution range)	99.1 (187.58-3.68) 99.2 (189.96-3.54)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 3.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.212 , 0.272 0.214 , 0.272	Depositor DCC
R_{free} test set	31728 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å^2)	83.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 77.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	291730	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	QA	0.59	3/36098 (0.0%)	1.21	155/56341 (0.3%)
1	XA	0.65	1/36101 (0.0%)	1.27	208/56346 (0.4%)
2	QB	0.31	0/1959	0.52	0/2642
2	XB	0.32	0/1959	0.54	0/2642
3	QC	0.31	0/1629	0.53	0/2195
3	XC	0.37	0/1629	0.56	0/2195
4	QD	0.38	0/1733	0.58	1/2318 (0.0%)
4	XD	0.40	0/1733	0.60	0/2318
5	QE	0.35	0/1171	0.56	0/1576
5	XE	0.39	0/1171	0.59	0/1576
6	QF	0.38	0/856	0.54	0/1154
6	XF	0.38	0/856	0.58	0/1154
7	QG	0.33	0/1276	0.50	0/1709
7	XG	0.34	0/1276	0.50	0/1709
8	QH	0.33	0/1136	0.55	0/1527
8	XH	0.38	0/1136	0.58	0/1527
9	QI	0.31	0/1029	0.55	0/1379
9	XI	0.34	0/1029	0.58	0/1379
10	QJ	0.33	0/814	0.54	0/1095
10	XJ	0.35	0/814	0.60	0/1095
11	QK	0.36	0/900	0.57	0/1213
11	XK	0.39	0/900	0.58	0/1213
12	QL	0.37	0/991	0.61	0/1327
12	XL	0.45	0/991	0.74	1/1327 (0.1%)
13	QM	0.32	0/974	0.59	0/1303
13	XM	0.37	0/974	0.63	0/1303
14	QN	0.41	0/501	0.60	0/664
14	XN	0.42	0/501	0.66	0/664
15	QO	0.35	0/745	0.54	0/992
15	XO	0.39	0/745	0.54	0/992
16	QP	0.36	0/721	0.57	0/970
16	XP	0.35	0/721	0.57	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.35	0/847	0.54	0/1131
17	XQ	0.35	0/847	0.54	0/1131
18	QR	0.35	0/579	0.64	1/768 (0.1%)
18	XR	0.37	0/579	0.59	0/768
19	QS	0.33	0/689	0.61	0/926
19	XS	0.38	0/689	0.69	1/926 (0.1%)
20	QT	0.36	0/765	0.64	0/1007
20	XT	0.31	0/765	0.59	0/1007
21	QU	0.31	0/221	0.54	0/288
21	XU	0.31	0/221	0.62	0/288
22	RA	0.72	8/69521 (0.0%)	1.34	555/108529 (0.5%)
22	YA	0.80	28/69543 (0.0%)	1.43	823/108563 (0.8%)
23	RB	0.58	0/2878	1.22	15/4490 (0.3%)
23	YB	0.63	0/2878	1.28	17/4490 (0.4%)
24	RD	0.51	0/2165	0.70	0/2919
24	YD	0.58	0/2165	0.78	1/2919 (0.0%)
25	RE	0.43	0/1601	0.73	3/2160 (0.1%)
25	YE	0.46	0/1601	0.75	2/2160 (0.1%)
26	RF	0.42	0/1620	0.62	0/2194
26	YF	0.48	0/1620	0.71	1/2194 (0.0%)
27	RG	0.31	0/1499	0.57	1/2016 (0.0%)
27	YG	0.40	0/1499	0.60	0/2016
28	RH	0.29	0/1332	0.58	0/1802
28	YH	0.45	0/1332	0.73	0/1802
29	RI	0.52	0/1151	0.79	1/1558 (0.1%)
29	YI	0.55	0/1151	0.80	0/1558
30	RN	0.41	0/1131	0.62	0/1525
30	YN	0.43	0/1131	0.64	0/1525
31	RO	0.41	0/943	0.62	1/1269 (0.1%)
31	YO	0.50	0/943	0.65	0/1269
32	RP	0.44	0/1162	0.81	1/1544 (0.1%)
32	YP	0.49	0/1162	0.90	2/1544 (0.1%)
33	RQ	0.47	0/1143	0.74	2/1527 (0.1%)
33	YQ	0.57	0/1143	0.80	1/1527 (0.1%)
34	RR	0.42	0/982	0.69	0/1312
34	YR	0.44	0/982	0.73	0/1312
35	RS	0.36	0/892	0.65	0/1187
35	YS	0.40	0/892	0.75	1/1187 (0.1%)
36	RT	0.42	0/1155	0.63	0/1542
36	YT	0.44	0/1155	0.67	0/1542
37	RU	0.40	0/982	0.65	0/1306
37	YU	0.50	0/982	0.68	0/1306
38	RV	0.38	0/790	0.61	1/1057 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YV	0.45	0/790	0.73	1/1057 (0.1%)
39	RW	0.49	0/911	0.67	0/1220
39	YW	0.45	0/911	0.68	0/1220
40	RX	0.47	0/739	0.62	0/993
40	YX	0.49	0/739	0.66	0/993
41	RY	0.44	0/798	0.68	0/1064
41	YY	0.46	0/798	0.70	0/1064
42	RZ	0.58	1/1493 (0.1%)	0.77	0/2026
42	YZ	0.56	0/1493	0.79	1/2026 (0.0%)
43	R0	0.65	0/657	0.80	0/874
43	Y0	0.74	1/657 (0.2%)	0.90	1/874 (0.1%)
44	R1	0.44	0/770	0.66	0/1022
44	Y1	0.46	0/770	0.69	0/1022
45	R2	0.39	0/583	0.65	0/771
45	Y2	0.52	0/583	0.73	0/771
46	R3	0.35	0/474	0.57	0/635
46	Y3	0.41	0/474	0.59	0/635
47	R4	0.33	0/594	0.68	0/795
47	Y4	0.37	0/594	0.68	0/795
48	R5	0.44	0/473	0.73	0/639
48	Y5	0.43	0/473	0.77	1/639 (0.2%)
49	R6	0.35	0/431	0.69	0/575
49	Y6	0.37	0/431	0.67	0/575
50	R7	0.49	0/438	0.68	0/575
50	Y7	0.57	0/438	0.71	0/575
51	R8	0.55	0/525	0.79	0/691
51	Y8	0.58	0/525	0.82	0/691
52	R9	0.26	0/310	0.45	0/407
52	Y9	0.32	0/310	0.48	0/407
53	QV	0.85	1/1836 (0.1%)	1.45	24/2859 (0.8%)
53	XV	0.89	1/1836 (0.1%)	1.54	25/2859 (0.9%)
54	QX	0.95	0/193	1.91	7/299 (2.3%)
54	XX	1.12	0/193	1.83	4/299 (1.3%)
55	QY	0.68	0/194	1.53	0/301
55	XY	0.72	0/194	1.25	1/301 (0.3%)
56	Z6	0.74	0/40	1.58	1/60 (1.7%)
56	Z8	0.92	0/40	1.50	0/60
All	All	0.64	44/316105 (0.0%)	1.20	1861/472575 (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
12	QL	0	1
12	XL	0	1
25	RE	0	1
25	YE	0	1
26	YF	0	1
28	RH	0	2
28	YH	0	2
29	RI	0	1
35	YS	0	1
42	YZ	0	2
45	Y2	0	1
47	R4	0	1
51	R8	0	2
51	Y8	0	2
All	All	0	19

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	QV	1	C	OP3-P	-10.81	1.48	1.61
53	XV	1	C	OP3-P	-10.09	1.49	1.61
22	YA	783	A	N9-C4	-8.12	1.32	1.37
22	YA	2542	A	N9-C4	-7.43	1.33	1.37
22	YA	1966	A	N9-C4	-7.42	1.33	1.37

The worst 5 of 1861 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	QV	75	C	O5'-P-OP2	-13.28	93.75	105.70
22	YA	774	A	C2-N3-C4	-12.25	104.47	110.60
22	RA	1931	U	N3-C2-O2	-12.05	113.77	122.20
22	YA	1332	G	C6-C5-N7	-11.94	123.24	130.40
22	YA	450	G	C5-C6-N1	-11.37	105.81	111.50

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	QL	47	LYS	Peptide
25	RE	21	VAL	Peptide
28	RH	127	GLU	Peptide
28	RH	153	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
29	RI	134	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32247	0	16277	775	0
1	XA	32249	0	16279	824	0
2	QB	1924	0	1975	64	0
2	XB	1924	0	1975	83	0
3	QC	1605	0	1668	50	0
3	XC	1605	0	1668	63	0
4	QD	1703	0	1763	68	0
4	XD	1703	0	1764	48	0
5	QE	1155	0	1213	36	0
5	XE	1155	0	1213	43	0
6	QF	843	0	857	20	0
6	XF	843	0	857	23	0
7	QG	1257	0	1296	41	0
7	XG	1257	0	1296	30	0
8	QH	1116	0	1177	40	0
8	XH	1116	0	1177	32	0
9	QI	1010	0	1037	43	0
9	XI	1010	0	1037	60	0
10	QJ	801	0	849	50	0
10	XJ	801	0	849	40	0
11	QK	885	0	904	29	0
11	XK	885	0	904	33	0
12	QL	975	0	1062	43	0
12	XL	975	0	1062	47	0
13	QM	964	0	1034	46	0
13	XM	964	0	1034	62	0
14	QN	492	0	529	27	0
14	XN	492	0	529	23	0
15	QO	734	0	771	23	0
15	XO	734	0	771	22	0
16	QP	705	0	725	21	0
16	XP	705	0	725	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	QQ	834	0	904	26	0
17	XQ	834	0	904	20	0
18	QR	574	0	644	13	0
18	XR	574	0	644	21	0
19	QS	674	0	699	39	0
19	XS	674	0	699	55	0
20	QT	763	0	861	25	0
20	XT	763	0	861	40	0
21	QU	217	0	234	12	0
21	XU	217	0	234	8	0
22	RA	62071	0	31292	1370	0
22	YA	62091	0	31301	1336	1
23	RB	2573	0	1306	57	0
23	YB	2573	0	1306	64	1
24	RD	2115	0	2195	107	0
24	YD	2115	0	2195	106	0
25	RE	1568	0	1634	67	0
25	YE	1568	0	1634	68	0
26	RF	1585	0	1632	76	0
26	YF	1585	0	1632	64	0
27	RG	1474	0	1535	62	0
27	YG	1474	0	1535	69	0
28	RH	1307	0	1382	67	0
28	YH	1307	0	1382	62	0
29	RI	1136	0	1223	84	0
29	YI	1136	0	1223	73	0
30	RN	1104	0	1180	38	0
30	YN	1104	0	1180	51	0
31	RO	933	0	996	23	0
31	YO	933	0	996	25	0
32	RP	1145	0	1227	79	0
32	YP	1145	0	1228	95	0
33	RQ	1122	0	1179	58	0
33	YQ	1122	0	1179	49	0
34	RR	968	0	1033	48	0
34	YR	968	0	1033	37	0
35	RS	882	0	943	45	0
35	YS	882	0	943	43	0
36	RT	1141	0	1202	51	0
36	YT	1141	0	1202	56	0
37	RU	964	0	1022	36	0
37	YU	964	0	1022	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	RV	779	0	852	24	0
38	YV	779	0	852	43	0
39	RW	900	0	964	28	0
39	YW	900	0	964	26	0
40	RX	725	0	778	31	0
40	YX	725	0	778	24	0
41	RY	785	0	878	52	0
41	YY	785	0	878	43	0
42	RZ	1461	0	1493	96	0
42	YZ	1461	0	1493	104	0
43	R0	648	0	671	37	0
43	Y0	648	0	672	41	0
44	R1	763	0	848	32	0
44	Y1	763	0	848	36	0
45	R2	581	0	629	14	0
45	Y2	581	0	629	23	0
46	R3	469	0	518	7	0
46	Y3	469	0	518	15	0
47	R4	581	0	574	30	0
47	Y4	581	0	574	76	0
48	R5	459	0	480	30	0
48	Y5	459	0	480	31	0
49	R6	424	0	450	30	0
49	Y6	424	0	450	29	0
50	R7	430	0	480	17	0
50	Y7	430	0	480	19	0
51	R8	517	0	582	36	0
51	Y8	517	0	582	43	0
52	R9	307	0	338	14	0
52	Y9	307	0	338	17	0
53	QV	1644	0	836	29	0
53	XV	1644	0	836	36	0
54	QX	173	0	88	3	0
54	XX	173	0	88	3	0
55	QY	174	0	88	4	0
55	XY	174	0	88	2	0
56	Z6	74	0	51	0	0
56	Z8	74	0	51	4	0
57	QA	42	0	45	1	0
57	XA	42	0	45	2	0
58	QA	76	0	0	0	0
58	QF	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	QM	1	0	0	0	0
58	QV	1	0	0	0	0
58	R0	1	0	0	0	0
58	R5	1	0	0	0	0
58	R8	2	0	0	0	0
58	RA	247	0	0	0	0
58	RB	2	0	0	0	0
58	RD	1	0	0	0	0
58	RE	2	0	0	0	0
58	RF	1	0	0	0	0
58	RP	2	0	0	0	0
58	XA	82	0	0	0	0
58	XB	1	0	0	0	0
58	XM	1	0	0	0	0
58	XV	2	0	0	0	0
58	Y0	1	0	0	0	0
58	Y5	1	0	0	0	0
58	YA	265	0	0	0	0
58	YB	3	0	0	0	0
58	YD	2	0	0	0	0
58	YP	2	0	0	0	0
58	YQ	1	0	0	0	0
58	YX	1	0	0	0	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
All	All	291730	0	198220	7613	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 16.

The worst 5 of 7613 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)
22:RA:2701:C:H3’	22:RA:2702:U:H5”	1.27	1.07
1:XA:963:G:N3	10:XJ:55:LYS:NZ	2.02	1.07
24:YD:43:ARG:NH1	24:YD:44:ASN:OD1	1.86	1.06
22:YA:2701:C:H3’	22:YA:2702:U:H5”	1.38	1.05
22:YA:1138:G:H21	30:YN:106:MET:HE3	1.22	1.04

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)
22:YA:1593:G:O2'	23:YB:54:G:OP1[1_655]	2.14	0.06

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%)	174 (74%)	44 (19%)	17 (7%)	1	15
2	XB	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	1	18
3	QC	203/239 (85%)	163 (80%)	34 (17%)	6 (3%)	4	32
3	XC	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	10	44
4	QD	206/209 (99%)	176 (85%)	24 (12%)	6 (3%)	4	32
4	XD	206/209 (99%)	177 (86%)	24 (12%)	5 (2%)	6	35
5	QE	149/162 (92%)	136 (91%)	8 (5%)	5 (3%)	3	30
5	XE	149/162 (92%)	133 (89%)	13 (9%)	3 (2%)	7	39
6	QF	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
6	XF	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	QG	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	12	47
7	XG	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	12	47
8	QH	136/138 (99%)	121 (89%)	14 (10%)	1 (1%)	22	59
8	XH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	4	32
9	QI	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	3	26
9	XI	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	4	31
10	QJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	4	31
10	XJ	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	21
11	QK	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	5	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	XK	117/129 (91%)	101 (86%)	14 (12%)	2 (2%)	9	42
12	QL	123/132 (93%)	98 (80%)	18 (15%)	7 (6%)	1	19
12	XL	123/132 (93%)	98 (80%)	15 (12%)	10 (8%)	1	11
13	QM	119/126 (94%)	95 (80%)	15 (13%)	9 (8%)	1	13
13	XM	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	1	13
14	QN	58/61 (95%)	48 (83%)	6 (10%)	4 (7%)	1	15
14	XN	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	0	7
15	QO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	49
15	XO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6	36
16	QP	82/88 (93%)	74 (90%)	7 (8%)	1 (1%)	13	49
16	XP	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	13	49
17	QQ	98/105 (93%)	91 (93%)	5 (5%)	2 (2%)	7	39
17	XQ	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	QR	68/88 (77%)	56 (82%)	9 (13%)	3 (4%)	2	24
18	XR	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	10	44
19	QS	82/93 (88%)	56 (68%)	15 (18%)	11 (13%)	0	4
19	XS	82/93 (88%)	54 (66%)	17 (21%)	11 (13%)	0	4
20	QT	97/106 (92%)	76 (78%)	15 (16%)	6 (6%)	1	18
20	XT	97/106 (92%)	75 (77%)	16 (16%)	6 (6%)	1	18
21	QU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	2	24
21	XU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	24
24	RD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	2	24
24	YD	270/276 (98%)	227 (84%)	34 (13%)	9 (3%)	4	31
25	RE	203/206 (98%)	147 (72%)	36 (18%)	20 (10%)	0	8
25	YE	203/206 (98%)	142 (70%)	41 (20%)	20 (10%)	0	8
26	RF	200/210 (95%)	167 (84%)	20 (10%)	13 (6%)	1	17
26	YF	200/210 (95%)	167 (84%)	25 (12%)	8 (4%)	3	26
27	RG	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1	13
27	YG	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	1	16
28	RH	168/180 (93%)	114 (68%)	33 (20%)	21 (12%)	0	4
28	YH	168/180 (93%)	121 (72%)	23 (14%)	24 (14%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	RI	144/148 (97%)	94 (65%)	31 (22%)	19 (13%)	0	4
29	YI	144/148 (97%)	100 (69%)	23 (16%)	21 (15%)	0	3
30	RN	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	10
30	YN	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	0	7
31	RO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	9	42
31	YO	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	9	42
32	RP	148/150 (99%)	107 (72%)	27 (18%)	14 (10%)	0	9
32	YP	148/150 (99%)	108 (73%)	23 (16%)	17 (12%)	0	5
33	RQ	139/141 (99%)	99 (71%)	22 (16%)	18 (13%)	0	4
33	YQ	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0	3
34	RR	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	2	24
34	YR	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	2	21
35	RS	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	0	8
35	YS	109/112 (97%)	78 (72%)	18 (16%)	13 (12%)	0	5
36	RT	135/146 (92%)	106 (78%)	17 (13%)	12 (9%)	1	10
36	YT	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	1	14
37	RU	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	3	29
37	YU	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3	29
38	RV	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	1	18
38	YV	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	11
39	RW	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	3	29
39	YW	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	8	41
40	RX	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	6	37
40	YX	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	6	37
41	RY	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	3
41	YY	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	0	5
42	RZ	181/206 (88%)	118 (65%)	35 (19%)	28 (16%)	0	3
42	YZ	181/206 (88%)	113 (62%)	46 (25%)	22 (12%)	0	5
43	R0	80/85 (94%)	61 (76%)	15 (19%)	4 (5%)	2	22
43	Y0	80/85 (94%)	66 (82%)	13 (16%)	1 (1%)	12	47
44	R1	95/98 (97%)	75 (79%)	11 (12%)	9 (10%)	0	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	Y1	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	18
45	R2	67/72 (93%)	53 (79%)	9 (13%)	5 (8%)	1	13
45	Y2	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	1	10
46	R3	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3	29
46	Y3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	8	41
47	R4	69/71 (97%)	35 (51%)	18 (26%)	16 (23%)	0	0
47	Y4	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	0
48	R5	57/60 (95%)	44 (77%)	11 (19%)	2 (4%)	3	29
48	Y5	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	3	29
49	R6	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	0
49	Y6	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	2
50	R7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	7	38
50	Y7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	7	38
51	R8	62/65 (95%)	51 (82%)	6 (10%)	5 (8%)	1	11
51	Y8	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	1	17
52	R9	35/37 (95%)	35 (100%)	0	0	100	100
52	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11470/12128 (95%)	9180 (80%)	1546 (14%)	744 (6%)	1	17

5 of 744 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	236	TYR
3	QC	12	LEU
3	QC	190	ARG
4	QD	28	SER
13	QM	67	GLU

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%)	172 (84%)	33 (16%)	2	15
2	XB	205/220 (93%)	180 (88%)	25 (12%)	5	24
3	QC	159/188 (85%)	145 (91%)	14 (9%)	10	38
3	XC	159/188 (85%)	146 (92%)	13 (8%)	11	41
4	QD	180/181 (99%)	157 (87%)	23 (13%)	4	22
4	XD	180/181 (99%)	154 (86%)	26 (14%)	3	19
5	QE	116/123 (94%)	104 (90%)	12 (10%)	7	31
5	XE	116/123 (94%)	104 (90%)	12 (10%)	7	31
6	QF	90/90 (100%)	78 (87%)	12 (13%)	4	21
6	XF	90/90 (100%)	82 (91%)	8 (9%)	9	37
7	QG	126/127 (99%)	114 (90%)	12 (10%)	8	34
7	XG	126/127 (99%)	114 (90%)	12 (10%)	8	34
8	QH	119/119 (100%)	109 (92%)	10 (8%)	11	40
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	29
9	QI	98/99 (99%)	81 (83%)	17 (17%)	2	12
9	XI	98/99 (99%)	80 (82%)	18 (18%)	1	10
10	QJ	89/92 (97%)	77 (86%)	12 (14%)	4	21
10	XJ	89/92 (97%)	74 (83%)	15 (17%)	2	13
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	32
11	XK	90/99 (91%)	82 (91%)	8 (9%)	9	37
12	QL	104/109 (95%)	87 (84%)	17 (16%)	2	15
12	XL	104/109 (95%)	93 (89%)	11 (11%)	6	30
13	QM	97/101 (96%)	73 (75%)	24 (25%)	0	5
13	XM	97/101 (96%)	78 (80%)	19 (20%)	1	9
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	10
14	XN	49/50 (98%)	42 (86%)	7 (14%)	3	19
15	QO	79/80 (99%)	72 (91%)	7 (9%)	9	37
15	XO	79/80 (99%)	69 (87%)	10 (13%)	4	23
16	QP	72/74 (97%)	63 (88%)	9 (12%)	4	23
16	XP	72/74 (97%)	63 (88%)	9 (12%)	4	23
17	QQ	95/97 (98%)	87 (92%)	8 (8%)	11	40
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	QR	61/77 (79%)	50 (82%)	11 (18%)	1	11
18	XR	61/77 (79%)	52 (85%)	9 (15%)	3	18
19	QS	73/80 (91%)	59 (81%)	14 (19%)	1	9
19	XS	73/80 (91%)	57 (78%)	16 (22%)	1	6
20	QT	76/82 (93%)	67 (88%)	9 (12%)	5	26
20	XT	76/82 (93%)	66 (87%)	10 (13%)	4	21
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	55
24	RD	214/218 (98%)	174 (81%)	40 (19%)	1	10
24	YD	214/218 (98%)	181 (85%)	33 (15%)	2	17
25	RE	165/166 (99%)	126 (76%)	39 (24%)	1	5
25	YE	165/166 (99%)	137 (83%)	28 (17%)	2	13
26	RF	161/166 (97%)	132 (82%)	29 (18%)	1	11
26	YF	161/166 (97%)	137 (85%)	24 (15%)	3	18
27	RG	155/156 (99%)	134 (86%)	21 (14%)	4	21
27	YG	155/156 (99%)	133 (86%)	22 (14%)	3	19
28	RH	142/148 (96%)	120 (84%)	22 (16%)	2	17
28	YH	142/148 (96%)	117 (82%)	25 (18%)	2	12
29	RI	122/124 (98%)	86 (70%)	36 (30%)	0	2
29	YI	122/124 (98%)	85 (70%)	37 (30%)	0	2
30	RN	117/119 (98%)	97 (83%)	20 (17%)	2	13
30	YN	117/119 (98%)	96 (82%)	21 (18%)	2	11
31	RO	100/100 (100%)	90 (90%)	10 (10%)	7	32
31	YO	100/100 (100%)	88 (88%)	12 (12%)	5	25
32	RP	116/116 (100%)	85 (73%)	31 (27%)	0	3
32	YP	116/116 (100%)	82 (71%)	34 (29%)	0	2
33	RQ	111/111 (100%)	95 (86%)	16 (14%)	3	19
33	YQ	111/111 (100%)	92 (83%)	19 (17%)	2	13
34	RR	101/101 (100%)	83 (82%)	18 (18%)	2	11
34	YR	101/101 (100%)	81 (80%)	20 (20%)	1	8
35	RS	87/88 (99%)	69 (79%)	18 (21%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	YS	87/88 (99%)	68 (78%)	19 (22%)	1 7
36	RT	120/127 (94%)	102 (85%)	18 (15%)	3 17
36	YT	120/127 (94%)	98 (82%)	22 (18%)	1 10
37	RU	93/94 (99%)	78 (84%)	15 (16%)	2 15
37	YU	93/94 (99%)	77 (83%)	16 (17%)	2 13
38	RV	82/82 (100%)	66 (80%)	16 (20%)	1 9
38	YV	82/82 (100%)	67 (82%)	15 (18%)	1 10
39	RW	92/92 (100%)	73 (79%)	19 (21%)	1 7
39	YW	92/92 (100%)	76 (83%)	16 (17%)	2 12
40	RX	74/78 (95%)	64 (86%)	10 (14%)	4 21
40	YX	74/78 (95%)	60 (81%)	14 (19%)	1 9
41	RY	85/91 (93%)	63 (74%)	22 (26%)	0 4
41	YY	85/91 (93%)	64 (75%)	21 (25%)	0 5
42	RZ	162/179 (90%)	131 (81%)	31 (19%)	1 9
42	YZ	162/179 (90%)	121 (75%)	41 (25%)	0 4
43	R0	65/67 (97%)	56 (86%)	9 (14%)	3 20
43	Y0	65/67 (97%)	53 (82%)	12 (18%)	1 10
44	R1	82/83 (99%)	73 (89%)	9 (11%)	6 29
44	Y1	82/83 (99%)	70 (85%)	12 (15%)	3 18
45	R2	64/67 (96%)	57 (89%)	7 (11%)	6 29
45	Y2	64/67 (96%)	47 (73%)	17 (27%)	0 3
46	R3	51/52 (98%)	45 (88%)	6 (12%)	5 26
46	Y3	51/52 (98%)	43 (84%)	8 (16%)	2 16
47	R4	63/63 (100%)	45 (71%)	18 (29%)	0 2
47	Y4	63/63 (100%)	43 (68%)	20 (32%)	0 1
48	R5	51/52 (98%)	37 (72%)	14 (28%)	0 3
48	Y5	51/52 (98%)	37 (72%)	14 (28%)	0 3
49	R6	48/52 (92%)	35 (73%)	13 (27%)	0 3
49	Y6	48/52 (92%)	38 (79%)	10 (21%)	1 7
50	R7	42/42 (100%)	34 (81%)	8 (19%)	1 9
50	Y7	42/42 (100%)	35 (83%)	7 (17%)	2 14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	R8	54/55 (98%)	44 (82%)	10 (18%)	1	10
51	Y8	54/55 (98%)	41 (76%)	13 (24%)	0	5
52	R9	34/34 (100%)	32 (94%)	2 (6%)	19	51
52	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	51
All	All	9702/10066 (96%)	8111 (84%)	1591 (16%)	2	15

5 of 1591 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	XJ	74	ILE
28	YH	6	ARG
13	XM	19	LEU
10	XJ	70	ARG
24	YD	28	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
52	R9	32	HIS
2	XB	212	GLN
36	YT	58	ASN
10	XJ	78	ASN
19	QS	47	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1522 (98%)	341 (22%)	49 (3%)
1	XA	1498/1522 (98%)	352 (23%)	40 (2%)
22	RA	2879/2916 (98%)	747 (25%)	65 (2%)
22	YA	2880/2916 (98%)	734 (25%)	57 (1%)
23	RB	119/122 (97%)	29 (24%)	2 (1%)
23	YB	119/122 (97%)	32 (26%)	1 (0%)
53	QV	76/77 (98%)	22 (28%)	1 (1%)
53	XV	76/77 (98%)	24 (31%)	3 (3%)
54	QX	7/25 (28%)	4 (57%)	1 (14%)
54	XX	7/25 (28%)	3 (42%)	1 (14%)
55	QY	7/17 (41%)	3 (42%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	XY	7/17 (41%)	2 (28%)	0
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9175/9364 (97%)	2293 (24%)	220 (2%)

5 of 2293 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	7	G
1	QA	9	G
1	QA	22	G
1	QA	32	A
1	QA	39	G

5 of 220 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	RB	66	A
1	XA	992	U
54	XX	3	G
22	YA	1955	U
1	XA	89	U

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	PPU	Z6	76	22,56	32,40,41	1.02	1 (3%)	33,57,60	2.06	10 (30%)
56	PPU	Z8	76	22,56	32,40,41	1.04	3 (9%)	33,57,60	1.67	8 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PPU	Z6	76	22,56	-	3/21/43/44	0/4/4/4
56	PPU	Z8	76	22,56	-	1/21/43/44	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	C2'-C3'	-2.48	1.49	1.53
56	Z6	76	PPU	C5-C4	2.41	1.47	1.40
56	Z8	76	PPU	C5-C4	2.15	1.46	1.40
56	Z8	76	PPU	C4-N3	-2.11	1.32	1.35

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Z6	76	PPU	C3'-N3'-C	-5.98	114.20	123.21
56	Z6	76	PPU	N1-C6-N6	4.60	121.89	117.06
56	Z8	76	PPU	N1-C6-N6	4.54	121.83	117.06
56	Z6	76	PPU	C10-N6-C6	-3.29	109.56	119.51
56	Z6	76	PPU	CM-OC-CZ	3.24	124.55	117.51

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	Z6	76	PPU	CE1-CZ-OC-CM
56	Z6	76	PPU	CE2-CZ-OC-CM
56	Z8	76	PPU	C5-C6-N6-C9
56	Z6	76	PPU	C5-C6-N6-C9

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z8	76	PPU	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 706 ligands modelled in this entry, 704 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	PAR	QA	1601	-	45,45,45	1.47	7 (15%)	64,67,67	1.38	9 (14%)
57	PAR	XA	1601	-	45,45,45	1.50	6 (13%)	64,67,67	1.34	5 (7%)

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	QA	1601	-	-	8/18/94/94	0/4/4/4
57	PAR	XA	1601	-	-	6/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	QA	1601	PAR	C64-C54	5.14	1.59	1.52
57	XA	1601	PAR	C64-C54	4.91	1.58	1.52
57	QA	1601	PAR	C52-C42	3.16	1.58	1.52
57	QA	1601	PAR	O54-C14	2.86	1.49	1.41
57	XA	1601	PAR	O54-C14	2.85	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	XA	1601	PAR	O33-C14-C24	4.73	116.37	108.22
57	XA	1601	PAR	C14-O54-C54	4.30	122.13	113.69
57	QA	1601	PAR	O52-C13-C23	3.82	115.89	107.96
57	QA	1601	PAR	C14-O54-C54	3.79	121.13	113.69
57	QA	1601	PAR	O33-C14-C24	3.76	114.69	108.22

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	QA	1601	PAR	C44-C54-C64-N64
57	QA	1601	PAR	O54-C54-C64-N64
57	QA	1601	PAR	O51-C51-C61-O61
57	XA	1601	PAR	O51-C51-C61-O61
57	QA	1601	PAR	C41-C51-C61-O61

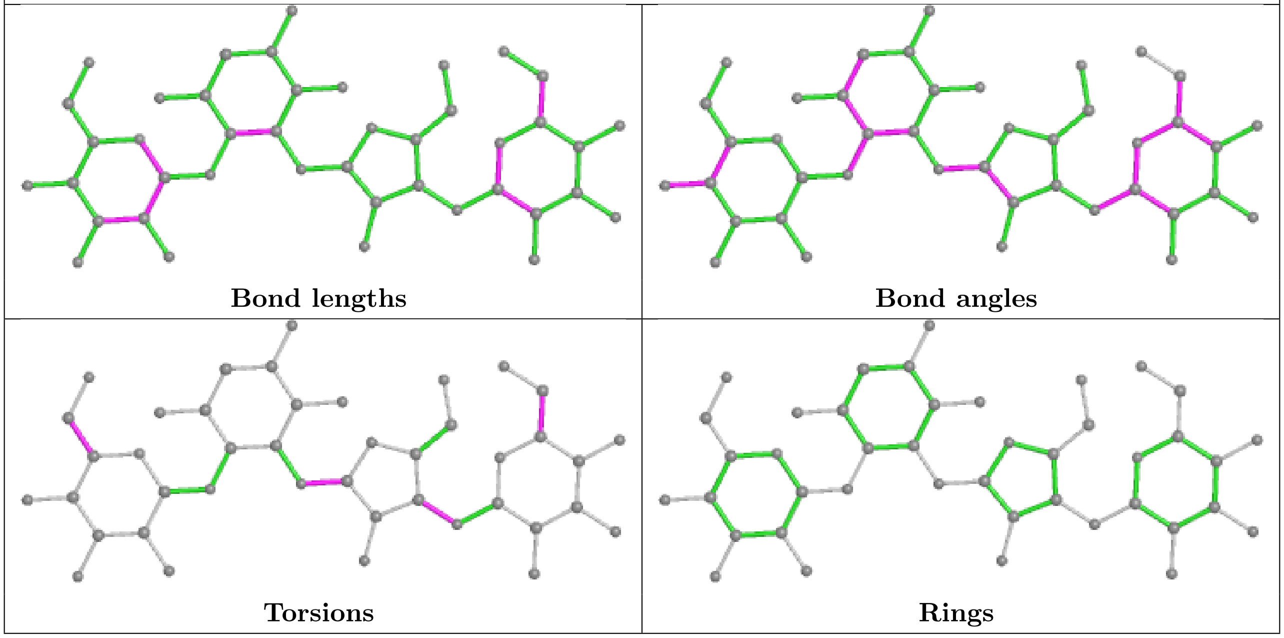
There are no ring outliers.

2 monomers are involved in 3 short contacts:

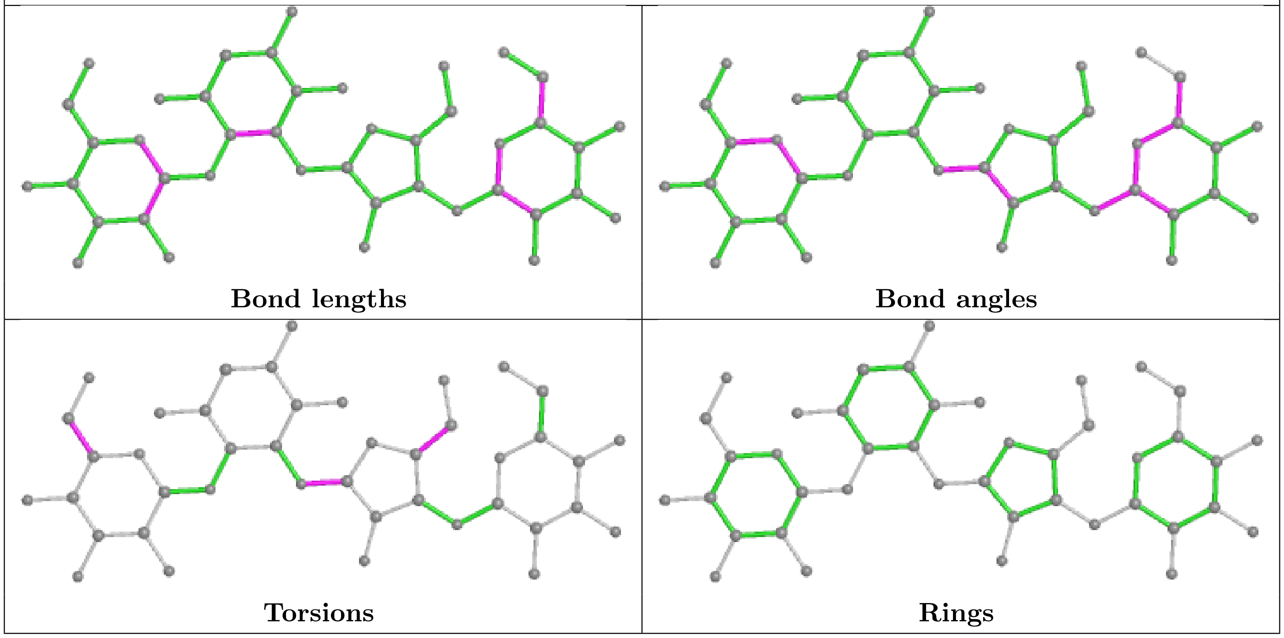
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	QA	1601	PAR	1	0
57	XA	1601	PAR	2	0

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 QA 1601



Ligand PAR XA 1601



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 ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	QA	1500/1522 (98%)	0.42	75 (5%) 28 20	28, 70, 146, 264	0
1	XA	1500/1522 (98%)	0.54	83 (5%) 25 17	18, 64, 151, 247	0
2	QB	237/256 (92%)	0.13	9 (3%) 40 28	48, 115, 166, 191	0
2	XB	237/256 (92%)	-0.23	1 (0%) 92 88	35, 98, 150, 194	0
3	QC	205/239 (85%)	0.52	10 (4%) 29 21	45, 105, 149, 166	0
3	XC	205/239 (85%)	0.15	2 (0%) 82 72	35, 78, 130, 168	0
4	QD	208/209 (99%)	0.46	10 (4%) 30 21	27, 79, 119, 169	0
4	XD	208/209 (99%)	0.30	4 (1%) 66 54	34, 75, 127, 151	0
5	QE	151/162 (93%)	0.45	7 (4%) 32 22	37, 88, 135, 167	0
5	XE	151/162 (93%)	0.29	3 (1%) 65 52	29, 65, 115, 148	0
6	QF	101/101 (100%)	-0.20	1 (0%) 82 72	21, 76, 112, 185	0
6	XF	101/101 (100%)	0.21	0 100 100	32, 72, 115, 153	0
7	QG	155/156 (99%)	0.57	22 (14%) 2 2	46, 96, 152, 185	0
7	XG	155/156 (99%)	0.31	9 (5%) 23 15	40, 87, 145, 167	0
8	QH	138/138 (100%)	0.29	2 (1%) 75 63	41, 90, 125, 153	0
8	XH	138/138 (100%)	0.27	3 (2%) 62 48	33, 72, 108, 149	0
9	QI	127/128 (99%)	1.38	35 (27%) 0 0	67, 109, 148, 172	0
9	XI	127/128 (99%)	0.65	15 (11%) 4 4	28, 99, 147, 164	0
10	QJ	99/105 (94%)	0.96	16 (16%) 1 1	59, 114, 165, 205	0
10	XJ	99/105 (94%)	0.90	16 (16%) 1 1	41, 103, 147, 171	0
11	QK	119/129 (92%)	0.54	7 (5%) 22 15	35, 79, 130, 177	0
11	XK	119/129 (92%)	0.68	6 (5%) 28 20	24, 71, 125, 182	0
12	QL	125/132 (94%)	1.06	15 (12%) 4 3	30, 70, 120, 182	0
12	XL	125/132 (94%)	0.91	23 (18%) 1 1	15, 58, 120, 182	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	QM	121/126 (96%)	1.20	30 (24%)	0	0	36, 106, 144, 196	0
13	XM	121/126 (96%)	0.53	11 (9%)	9	6	38, 88, 137, 187	0
14	QN	60/61 (98%)	2.07	30 (50%)	0	0	58, 97, 124, 142	0
14	XN	60/61 (98%)	1.09	9 (15%)	2	1	34, 75, 109, 125	0
15	QO	88/89 (98%)	0.01	0	100	100	30, 79, 123, 154	0
15	XO	88/89 (98%)	0.25	1 (1%)	80	70	28, 73, 108, 124	0
16	QP	84/88 (95%)	0.44	1 (1%)	79	68	35, 69, 107, 152	0
16	XP	84/88 (95%)	1.14	20 (23%)	0	0	34, 74, 129, 163	0
17	QQ	100/105 (95%)	1.01	14 (14%)	2	2	24, 83, 122, 140	0
17	XQ	100/105 (95%)	0.98	14 (14%)	2	2	39, 78, 113, 165	0
18	QR	70/88 (79%)	0.06	1 (1%)	75	63	26, 78, 137, 167	0
18	XR	70/88 (79%)	0.31	3 (4%)	35	25	24, 70, 120, 147	0
19	QS	84/93 (90%)	1.71	32 (38%)	0	0	68, 111, 151, 176	0
19	XS	84/93 (90%)	0.60	8 (9%)	8	5	32, 97, 148, 177	0
20	QT	99/106 (93%)	0.91	9 (9%)	9	6	34, 79, 133, 144	0
20	XT	99/106 (93%)	1.63	34 (34%)	0	0	44, 88, 140, 174	0
21	QU	25/27 (92%)	3.33	20 (80%)	0	0	36, 102, 144, 147	0
21	XU	25/27 (92%)	2.34	15 (60%)	0	0	67, 92, 119, 132	0
22	RA	2882/2916 (98%)	0.47	145 (5%)	28	20	14, 51, 198, 261	0
22	YA	2883/2916 (98%)	0.42	106 (3%)	41	29	8, 43, 187, 292	0
23	RB	120/122 (98%)	-0.05	1 (0%)	86	77	53, 81, 118, 144	0
23	YB	120/122 (98%)	-0.03	1 (0%)	86	77	36, 67, 98, 136	0
24	RD	272/276 (98%)	0.34	4 (1%)	73	62	9, 50, 100, 155	0
24	YD	272/276 (98%)	0.60	5 (1%)	68	56	2, 42, 86, 187	0
25	RE	205/206 (99%)	0.37	7 (3%)	45	33	17, 61, 126, 193	0
25	YE	205/206 (99%)	0.19	2 (0%)	82	72	3, 56, 124, 170	0
26	RF	202/210 (96%)	-0.04	0	100	100	9, 61, 124, 182	0
26	YF	202/210 (96%)	0.01	1 (0%)	91	85	10, 53, 113, 148	0
27	RG	181/182 (99%)	0.49	9 (4%)	28	20	42, 97, 145, 178	0
27	YG	181/182 (99%)	0.12	4 (2%)	62	48	40, 80, 130, 201	0
28	RH	170/180 (94%)	1.84	67 (39%)	0	0	67, 134, 177, 201	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	YH	170/180 (94%)	-0.05	1 (0%) 89 83	24, 76, 126, 177	0
29	RI	146/148 (98%)	0.05	3 (2%) 63 50	24, 87, 130, 181	0
29	YI	146/148 (98%)	-0.04	3 (2%) 63 50	19, 86, 127, 152	0
30	RN	138/140 (98%)	0.44	7 (5%) 28 19	29, 68, 121, 174	0
30	YN	138/140 (98%)	0.11	0 100 100	13, 56, 111, 173	0
31	RO	122/122 (100%)	0.53	3 (2%) 57 43	11, 55, 102, 158	0
31	YO	122/122 (100%)	0.90	11 (9%) 9 6	9, 51, 88, 123	0
32	RP	150/150 (100%)	0.63	11 (7%) 15 10	13, 69, 133, 176	0
32	YP	150/150 (100%)	0.41	5 (3%) 46 34	12, 61, 122, 182	0
33	RQ	141/141 (100%)	1.22	29 (20%) 1 0	29, 71, 124, 164	0
33	YQ	141/141 (100%)	0.43	4 (2%) 53 39	16, 56, 115, 152	0
34	RR	118/118 (100%)	0.43	4 (3%) 45 33	3, 55, 102, 136	0
34	YR	118/118 (100%)	0.77	5 (4%) 36 25	27, 57, 95, 140	0
35	RS	111/112 (99%)	0.66	10 (9%) 9 6	34, 80, 124, 162	0
35	YS	111/112 (99%)	0.17	2 (1%) 68 56	27, 72, 113, 138	0
36	RT	137/146 (93%)	0.53	7 (5%) 28 19	27, 67, 143, 169	0
36	YT	137/146 (93%)	0.53	4 (2%) 51 38	19, 65, 135, 172	0
37	RU	117/118 (99%)	0.21	2 (1%) 70 58	12, 62, 111, 167	0
37	YU	117/118 (99%)	0.36	2 (1%) 70 58	13, 45, 111, 172	0
38	RV	101/101 (100%)	0.03	2 (1%) 65 52	16, 78, 131, 186	0
38	YV	101/101 (100%)	0.34	3 (2%) 50 36	21, 68, 139, 214	0
39	RW	113/113 (100%)	0.29	1 (0%) 84 75	15, 47, 106, 158	0
39	YW	113/113 (100%)	0.27	2 (1%) 68 56	16, 46, 106, 168	0
40	RX	92/96 (95%)	0.34	0 100 100	17, 56, 103, 130	0
40	YX	92/96 (95%)	0.10	0 100 100	9, 42, 86, 138	0
41	RY	102/110 (92%)	0.41	1 (0%) 82 72	28, 86, 142, 176	0
41	YY	102/110 (92%)	0.09	1 (0%) 82 72	30, 73, 138, 185	0
42	RZ	183/206 (88%)	0.42	12 (6%) 18 11	45, 92, 141, 160	0
42	YZ	183/206 (88%)	-0.18	1 (0%) 91 85	21, 82, 136, 178	0
43	R0	82/85 (96%)	0.97	7 (8%) 10 8	9, 51, 88, 102	0
43	Y0	82/85 (96%)	0.34	0 100 100	20, 48, 73, 92	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	R1	97/98 (98%)	0.82	6 (6%) 20 13	13, 60, 144, 182	0
44	Y1	97/98 (98%)	1.05	11 (11%) 5 4	7, 53, 136, 172	0
45	R2	69/72 (95%)	-0.06	0 100 100	36, 77, 136, 164	0
45	Y2	69/72 (95%)	-0.06	0 100 100	18, 57, 116, 159	0
46	R3	59/60 (98%)	0.80	2 (3%) 45 33	33, 76, 118, 142	0
46	Y3	59/60 (98%)	0.03	1 (1%) 70 58	19, 57, 109, 169	0
47	R4	71/71 (100%)	0.87	12 (16%) 1 1	61, 142, 196, 236	0
47	Y4	71/71 (100%)	0.14	5 (7%) 16 10	58, 131, 182, 223	0
48	R5	59/60 (98%)	0.42	2 (3%) 45 33	12, 66, 149, 160	0
48	Y5	59/60 (98%)	0.85	8 (13%) 3 2	17, 64, 166, 185	0
49	R6	49/54 (90%)	4.49	44 (89%) 0 0	101, 159, 184, 200	0
49	Y6	49/54 (90%)	3.64	42 (85%) 0 0	95, 152, 182, 209	0
50	R7	49/49 (100%)	0.39	2 (4%) 37 26	11, 41, 95, 153	0
50	Y7	49/49 (100%)	0.42	4 (8%) 11 8	6, 33, 78, 135	0
51	R8	64/65 (98%)	0.83	6 (9%) 8 5	18, 59, 121, 163	0
51	Y8	64/65 (98%)	0.74	5 (7%) 13 9	16, 52, 108, 164	0
52	R9	37/37 (100%)	8.37	37 (100%) 0 0	92, 141, 184, 204	0
52	Y9	37/37 (100%)	5.96	37 (100%) 0 0	102, 132, 168, 182	0
53	QV	77/77 (100%)	-0.12	1 (1%) 77 66	35, 82, 137, 160	0
53	XV	77/77 (100%)	-0.07	1 (1%) 77 66	11, 71, 111, 159	0
54	QX	8/25 (32%)	0.84	0 100 100	44, 56, 107, 137	0
54	XX	8/25 (32%)	1.20	2 (25%) 0 0	37, 46, 104, 148	0
55	QY	8/17 (47%)	1.51	2 (25%) 0 0	62, 74, 124, 144	0
55	XY	8/17 (47%)	0.50	1 (12%) 3 3	54, 71, 109, 122	0
56	Z6	2/3 (66%)	0.82	0 100 100	45, 45, 45, 52	0
56	Z8	2/3 (66%)	1.45	0 100 100	30, 30, 30, 32	0
All	All	20861/21492 (97%)	0.50	1352 (6%) 18 12	2, 66, 150, 292	0

The worst 5 of 1352 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	R9	11	CYS	18.9
52	R9	37	GLY	15.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	R9	14	CYS	14.9
52	Y9	1	MET	14.0
52	R9	36	GLN	14.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	PPU	Z6	76	37/38	0.96	0.40	37,37,37,37	0
56	PPU	Z8	76	37/38	0.96	0.41	30,30,30,30	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	RA	3227	1/1	0.32	0.47	60,60,60,60	0
58	MG	RA	3212	1/1	0.57	0.75	73,73,73,73	0
58	MG	XM	201	1/1	0.58	0.35	98,98,98,98	0
58	MG	RA	3221	1/1	0.60	0.23	30,30,30,30	0
58	MG	QA	1667	1/1	0.66	0.24	35,35,35,35	0
58	MG	YA	3214	1/1	0.66	0.68	50,50,50,50	0
58	MG	YA	3170	1/1	0.67	0.33	33,33,33,33	0
58	MG	RA	3157	1/1	0.67	0.38	37,37,37,37	0
58	MG	RA	3234	1/1	0.68	0.33	69,69,69,69	0
58	MG	YA	3205	1/1	0.70	0.37	62,62,62,62	0
58	MG	RA	3204	1/1	0.71	0.24	50,50,50,50	0
58	MG	QA	1621	1/1	0.73	0.21	38,38,38,38	0
58	MG	RA	3182	1/1	0.73	0.39	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	RA	3144	1/1	0.73	0.33	32,32,32,32	0
58	MG	RA	3209	1/1	0.73	0.25	47,47,47,47	0
58	MG	RA	3225	1/1	0.74	0.39	33,33,33,33	0
58	MG	YA	3263	1/1	0.74	0.26	40,40,40,40	0
58	MG	YA	3174	1/1	0.75	0.12	10,10,10,10	0
58	MG	RA	3143	1/1	0.76	0.14	5,5,5,5	0
58	MG	QA	1604	1/1	0.76	0.25	5,5,5,5	0
58	MG	YA	3182	1/1	0.76	0.24	3,3,3,3	0
58	MG	RA	3002	1/1	0.76	0.46	30,30,30,30	0
58	MG	RA	3138	1/1	0.76	0.28	38,38,38,38	0
58	MG	YA	3169	1/1	0.76	0.15	16,16,16,16	0
58	MG	XA	1679	1/1	0.77	0.18	18,18,18,18	0
58	MG	RA	3171	1/1	0.77	0.29	31,31,31,31	0
58	MG	YA	3144	1/1	0.77	0.15	6,6,6,6	0
58	MG	RA	3013	1/1	0.77	0.27	29,29,29,29	0
58	MG	RA	3067	1/1	0.77	0.94	74,74,74,74	0
58	MG	YA	3126	1/1	0.78	0.15	0,0,0,0	0
58	MG	YA	3130	1/1	0.78	0.25	21,21,21,21	0
58	MG	YA	3203	1/1	0.78	0.18	18,18,18,18	0
58	MG	RA	3247	1/1	0.78	0.30	9,9,9,9	0
58	MG	RA	3196	1/1	0.78	0.26	63,63,63,63	0
58	MG	RA	3164	1/1	0.78	0.30	45,45,45,45	0
58	MG	YA	3018	1/1	0.79	0.77	74,74,74,74	0
58	MG	RA	3233	1/1	0.79	0.22	42,42,42,42	0
58	MG	XA	1680	1/1	0.79	0.31	45,45,45,45	0
58	MG	YA	3254	1/1	0.79	0.29	16,16,16,16	0
58	MG	XA	1650	1/1	0.79	0.21	14,14,14,14	0
58	MG	Y0	101	1/1	0.79	0.42	74,74,74,74	0
58	MG	YA	3116	1/1	0.80	0.22	14,14,14,14	0
58	MG	RA	3126	1/1	0.80	0.22	16,16,16,16	0
58	MG	QA	1603	1/1	0.81	0.23	11,11,11,11	0
58	MG	RA	3056	1/1	0.81	0.54	74,74,74,74	0
58	MG	YA	3164	1/1	0.81	0.39	44,44,44,44	0
58	MG	RA	3006	1/1	0.81	0.41	10,10,10,10	0
58	MG	YA	3222	1/1	0.81	0.19	13,13,13,13	0
58	MG	YA	3228	1/1	0.81	0.14	9,9,9,9	0
58	MG	RA	3229	1/1	0.81	0.24	23,23,23,23	0
58	MG	RA	3232	1/1	0.81	0.11	15,15,15,15	0
58	MG	YA	3179	1/1	0.81	0.23	26,26,26,26	0
58	MG	XA	1635	1/1	0.82	0.17	26,26,26,26	0
58	MG	XA	1667	1/1	0.83	0.21	34,34,34,34	0
58	MG	RA	3004	1/1	0.83	0.43	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	YA	3132	1/1	0.83	0.17	7,7,7,7	0
58	MG	RA	3105	1/1	0.83	0.15	14,14,14,14	0
58	MG	YA	3151	1/1	0.83	0.21	3,3,3,3	0
58	MG	XA	1632	1/1	0.83	0.14	9,9,9,9	0
58	MG	YA	3165	1/1	0.83	0.22	1,1,1,1	0
58	MG	YA	3236	1/1	0.83	0.22	18,18,18,18	0
58	MG	RA	3201	1/1	0.83	0.25	34,34,34,34	0
58	MG	YA	3080	1/1	0.83	0.56	74,74,74,74	0
58	MG	QA	1677	1/1	0.83	0.19	47,47,47,47	0
58	MG	YA	3218	1/1	0.84	0.82	59,59,59,59	0
58	MG	RA	3203	1/1	0.84	0.18	15,15,15,15	0
58	MG	YA	3155	1/1	0.84	0.25	45,45,45,45	0
58	MG	YA	3233	1/1	0.84	0.22	34,34,34,34	0
58	MG	RA	3183	1/1	0.84	0.29	11,11,11,11	0
58	MG	YA	3250	1/1	0.84	0.33	15,15,15,15	0
58	MG	XA	1630	1/1	0.84	0.16	15,15,15,15	0
58	MG	YA	3259	1/1	0.84	0.28	5,5,5,5	0
58	MG	YA	3133	1/1	0.84	0.25	32,32,32,32	0
58	MG	XA	1681	1/1	0.84	0.20	31,31,31,31	0
58	MG	YA	3234	1/1	0.85	0.21	17,17,17,17	0
58	MG	YA	3207	1/1	0.85	0.34	55,55,55,55	0
58	MG	YA	3246	1/1	0.85	0.22	0,0,0,0	0
58	MG	YA	3249	1/1	0.85	0.33	20,20,20,20	0
58	MG	RA	3220	1/1	0.85	0.15	13,13,13,13	0
58	MG	RA	3161	1/1	0.85	0.23	10,10,10,10	0
58	MG	YA	3099	1/1	0.85	0.58	74,74,74,74	0
58	MG	XA	1602	1/1	0.85	0.23	15,15,15,15	0
58	MG	YD	301	1/1	0.85	0.46	74,74,74,74	0
58	MG	RA	3228	1/1	0.85	0.16	13,13,13,13	0
58	MG	RA	3177	1/1	0.86	0.35	15,15,15,15	0
58	MG	YA	3162	1/1	0.86	0.35	11,11,11,11	0
58	MG	RA	3130	1/1	0.86	0.20	15,15,15,15	0
58	MG	XA	1651	1/1	0.86	0.28	33,33,33,33	0
58	MG	YA	3105	1/1	0.86	0.19	19,19,19,19	0
58	MG	XA	1656	1/1	0.86	0.20	17,17,17,17	0
58	MG	YA	3118	1/1	0.86	0.35	8,8,8,8	0
58	MG	YA	3248	1/1	0.86	0.20	8,8,8,8	0
58	MG	XA	1658	1/1	0.86	0.14	3,3,3,3	0
58	MG	RA	3205	1/1	0.86	0.46	17,17,17,17	0
58	MG	YA	3183	1/1	0.86	0.12	19,19,19,19	0
58	MG	RA	3074	1/1	0.86	0.20	6,6,6,6	0
58	MG	XA	1628	1/1	0.86	0.14	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	QA	1672	1/1	0.86	0.32	19,19,19,19	0
58	MG	RA	3005	1/1	0.86	0.22	24,24,24,24	0
58	MG	RA	3199	1/1	0.87	0.78	63,63,63,63	0
58	MG	QA	1645	1/1	0.87	0.29	4,4,4,4	0
58	MG	YA	3208	1/1	0.87	0.41	35,35,35,35	0
58	MG	YA	3145	1/1	0.87	0.20	20,20,20,20	0
58	MG	YA	3216	1/1	0.87	0.34	55,55,55,55	0
58	MG	YA	3217	1/1	0.87	0.13	18,18,18,18	0
58	MG	QA	1671	1/1	0.87	0.16	6,6,6,6	0
58	MG	YA	3014	1/1	0.87	0.46	74,74,74,74	0
58	MG	QA	1653	1/1	0.87	0.17	0,0,0,0	0
58	MG	XA	1646	1/1	0.87	0.14	21,21,21,21	0
58	MG	QA	1675	1/1	0.87	0.26	32,32,32,32	0
58	MG	QA	1664	1/1	0.87	0.16	56,56,56,56	0
58	MG	YA	3245	1/1	0.87	0.18	33,33,33,33	0
58	MG	RA	3158	1/1	0.87	0.22	15,15,15,15	0
58	MG	RA	3243	1/1	0.87	0.26	1,1,1,1	0
58	MG	YA	3120	1/1	0.87	0.29	46,46,46,46	0
58	MG	YA	3181	1/1	0.87	0.26	0,0,0,0	0
58	MG	RA	3188	1/1	0.87	0.48	48,48,48,48	0
58	MG	XA	1672	1/1	0.87	0.19	16,16,16,16	0
58	MG	YA	3184	1/1	0.87	0.20	23,23,23,23	0
58	MG	YA	3191	1/1	0.87	0.28	9,9,9,9	0
58	MG	RA	3159	1/1	0.87	0.12	23,23,23,23	0
58	MG	XA	1636	1/1	0.88	0.18	8,8,8,8	0
58	MG	YA	3223	1/1	0.88	0.21	34,34,34,34	0
58	MG	YA	3041	1/1	0.88	0.56	74,74,74,74	0
58	MG	RA	3216	1/1	0.88	0.28	2,2,2,2	0
58	MG	RA	3193	1/1	0.88	0.23	47,47,47,47	0
58	MG	YA	3187	1/1	0.88	0.29	41,41,41,41	0
58	MG	YA	3244	1/1	0.88	0.25	0,0,0,0	0
58	MG	YA	3102	1/1	0.88	0.10	8,8,8,8	0
58	MG	YA	3200	1/1	0.88	0.15	6,6,6,6	0
58	MG	YA	3247	1/1	0.88	0.49	34,34,34,34	0
58	MG	YA	3156	1/1	0.88	0.57	29,29,29,29	0
58	MG	RA	3235	1/1	0.88	0.47	74,74,74,74	0
58	MG	QA	1674	1/1	0.88	0.18	8,8,8,8	0
58	MG	XA	1682	1/1	0.88	0.20	35,35,35,35	0
58	MG	XB	301	1/1	0.88	0.17	41,41,41,41	0
58	MG	RA	3172	1/1	0.88	0.24	42,42,42,42	0
58	MG	YB	202	1/1	0.88	0.34	19,19,19,19	0
58	MG	YA	3013	1/1	0.88	0.32	3,3,3,3	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	YQ	201	1/1	0.88	0.11	90,90,90,90	0
58	MG	XA	1663	1/1	0.88	0.21	32,32,32,32	0
58	MG	RA	3223	1/1	0.89	0.32	54,54,54,54	0
58	MG	RA	3014	1/1	0.89	0.19	28,28,28,28	0
58	MG	QA	1643	1/1	0.89	0.23	21,21,21,21	0
58	MG	XA	1639	1/1	0.89	0.21	45,45,45,45	0
58	MG	YA	3163	1/1	0.89	0.29	21,21,21,21	0
58	MG	RA	3202	1/1	0.89	0.30	0,0,0,0	0
58	MG	YA	3226	1/1	0.89	0.14	11,11,11,11	0
58	MG	YA	3075	1/1	0.89	0.15	12,12,12,12	0
58	MG	QA	1632	1/1	0.89	0.17	42,42,42,42	0
58	MG	RA	3073	1/1	0.89	0.21	10,10,10,10	0
58	MG	YA	3173	1/1	0.89	0.25	15,15,15,15	0
58	MG	QA	1640	1/1	0.89	0.27	13,13,13,13	0
58	MG	RA	3207	1/1	0.89	0.20	7,7,7,7	0
58	MG	RA	3148	1/1	0.89	0.39	47,47,47,47	0
58	MG	RA	3154	1/1	0.89	0.20	59,59,59,59	0
58	MG	RA	3214	1/1	0.89	0.26	24,24,24,24	0
58	MG	XA	1676	1/1	0.89	0.34	19,19,19,19	0
58	MG	YA	3127	1/1	0.89	0.30	23,23,23,23	0
58	MG	RF	301	1/1	0.89	0.22	13,13,13,13	0
58	MG	YA	3256	1/1	0.89	0.60	74,74,74,74	0
58	MG	YA	3199	1/1	0.89	0.25	12,12,12,12	0
58	MG	YA	3262	1/1	0.89	0.23	26,26,26,26	0
58	MG	QA	1660	1/1	0.89	0.10	36,36,36,36	0
58	MG	YB	201	1/1	0.89	0.25	33,33,33,33	0
58	MG	XA	1621	1/1	0.89	0.10	19,19,19,19	0
58	MG	RA	3120	1/1	0.89	0.18	4,4,4,4	0
58	MG	YD	302	1/1	0.89	0.21	5,5,5,5	0
58	MG	RA	3124	1/1	0.89	0.16	2,2,2,2	0
58	MG	YA	3150	1/1	0.89	0.30	16,16,16,16	0
58	MG	RA	3136	1/1	0.90	0.20	5,5,5,5	0
58	MG	XA	1642	1/1	0.90	0.16	47,47,47,47	0
58	MG	YA	3158	1/1	0.90	0.36	21,21,21,21	0
58	MG	YA	3161	1/1	0.90	0.26	23,23,23,23	0
58	MG	RA	3238	1/1	0.90	0.24	32,32,32,32	0
58	MG	YA	3072	1/1	0.90	0.21	22,22,22,22	0
58	MG	RA	3242	1/1	0.90	0.32	13,13,13,13	0
58	MG	RA	3094	1/1	0.90	0.28	16,16,16,16	0
58	MG	YA	3081	1/1	0.90	0.29	10,10,10,10	0
58	MG	QA	1658	1/1	0.90	0.16	39,39,39,39	0
58	MG	YA	3235	1/1	0.90	0.21	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	RA	3191	1/1	0.90	0.17	46,46,46,46	0
58	MG	YA	3239	1/1	0.90	0.17	41,41,41,41	0
58	MG	RA	3226	1/1	0.90	0.32	1,1,1,1	0
58	MG	YA	3176	1/1	0.90	0.13	45,45,45,45	0
58	MG	XA	1665	1/1	0.90	0.15	33,33,33,33	0
58	MG	XA	1604	1/1	0.90	0.29	9,9,9,9	0
58	MG	XA	1607	1/1	0.90	0.28	7,7,7,7	0
58	MG	XA	1610	1/1	0.90	0.21	6,6,6,6	0
58	MG	XA	1617	1/1	0.90	0.36	74,74,74,74	0
58	MG	RA	3068	1/1	0.90	0.25	13,13,13,13	0
58	MG	RA	3017	1/1	0.90	0.35	18,18,18,18	0
58	MG	YA	3194	1/1	0.90	0.26	36,36,36,36	0
58	MG	YA	3197	1/1	0.90	1.19	42,42,42,42	0
58	MG	RA	3198	1/1	0.90	0.19	26,26,26,26	0
58	MG	YA	3135	1/1	0.90	0.22	6,6,6,6	0
58	MG	QA	1668	1/1	0.90	0.17	0,0,0,0	0
58	MG	RA	3215	1/1	0.90	0.09	13,13,13,13	0
58	MG	YA	3012	1/1	0.90	0.29	10,10,10,10	0
58	MG	RA	3088	1/1	0.90	0.16	7,7,7,7	0
58	MG	YA	3210	1/1	0.90	0.20	17,17,17,17	0
58	MG	XV	102	1/1	0.90	0.18	2,2,2,2	0
58	MG	QA	1602	1/1	0.91	0.21	6,6,6,6	0
58	MG	YA	3028	1/1	0.91	0.19	15,15,15,15	0
58	MG	YA	3035	1/1	0.91	0.33	12,12,12,12	0
58	MG	YA	3219	1/1	0.91	0.42	22,22,22,22	0
58	MG	YA	3036	1/1	0.91	0.28	11,11,11,11	0
58	MG	RA	3135	1/1	0.91	0.13	12,12,12,12	0
58	MG	YA	3054	1/1	0.91	0.26	14,14,14,14	0
58	MG	YA	3056	1/1	0.91	0.22	5,5,5,5	0
58	MG	YA	3230	1/1	0.91	0.15	42,42,42,42	0
58	MG	YA	3071	1/1	0.91	0.21	1,1,1,1	0
58	MG	XA	1655	1/1	0.91	0.29	68,68,68,68	0
58	MG	QA	1627	1/1	0.91	0.18	30,30,30,30	0
58	MG	QA	1673	1/1	0.91	0.24	9,9,9,9	0
58	MG	RA	3051	1/1	0.91	0.31	1,1,1,1	0
58	MG	YA	3090	1/1	0.91	0.27	26,26,26,26	0
58	MG	XA	1609	1/1	0.91	0.09	51,51,51,51	0
58	MG	RA	3101	1/1	0.91	0.18	18,18,18,18	0
58	MG	XA	1670	1/1	0.91	0.19	27,27,27,27	0
58	MG	YA	3112	1/1	0.91	0.17	13,13,13,13	0
58	MG	RA	3146	1/1	0.91	0.16	25,25,25,25	0
58	MG	XA	1620	1/1	0.91	0.33	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	YA	3251	1/1	0.91	0.57	10,10,10,10	0
58	MG	RA	3208	1/1	0.91	0.16	30,30,30,30	0
58	MG	QF	201	1/1	0.91	0.25	36,36,36,36	0
58	MG	YA	3257	1/1	0.91	0.26	14,14,14,14	0
58	MG	RA	3010	1/1	0.91	0.47	14,14,14,14	0
58	MG	RA	3155	1/1	0.91	0.16	54,54,54,54	0
58	MG	RA	3237	1/1	0.91	0.38	6,6,6,6	0
58	MG	YA	3264	1/1	0.91	0.35	5,5,5,5	0
58	MG	RA	3156	1/1	0.91	0.17	9,9,9,9	0
58	MG	YA	3011	1/1	0.91	0.20	9,9,9,9	0
58	MG	YA	3137	1/1	0.91	0.11	10,10,10,10	0
58	MG	YA	3142	1/1	0.91	0.61	31,31,31,31	0
58	MG	RA	3241	1/1	0.91	0.13	8,8,8,8	0
58	MG	RA	3012	1/1	0.91	0.40	31,31,31,31	0
58	MG	RA	3072	1/1	0.91	0.29	18,18,18,18	0
58	MG	RA	3033	1/1	0.92	0.37	6,6,6,6	0
58	MG	RA	3121	1/1	0.92	0.17	36,36,36,36	0
58	MG	RE	301	1/1	0.92	0.20	9,9,9,9	0
58	MG	XA	1675	1/1	0.92	0.32	14,14,14,14	0
58	MG	YA	3206	1/1	0.92	0.27	52,52,52,52	0
58	MG	RA	3160	1/1	0.92	0.19	19,19,19,19	0
58	MG	XA	1677	1/1	0.92	0.16	2,2,2,2	0
57	PAR	QA	1601	42/42	0.92	0.35	42,42,42,42	0
58	MG	RA	3162	1/1	0.92	0.52	18,18,18,18	0
58	MG	RA	3003	1/1	0.92	0.18	4,4,4,4	0
58	MG	RA	3129	1/1	0.92	0.23	21,21,21,21	0
58	MG	YA	3139	1/1	0.92	0.15	8,8,8,8	0
58	MG	YA	3140	1/1	0.92	0.34	8,8,8,8	0
58	MG	RA	3063	1/1	0.92	0.24	19,19,19,19	0
58	MG	XA	1611	1/1	0.92	0.15	11,11,11,11	0
58	MG	RA	3218	1/1	0.92	0.12	17,17,17,17	0
58	MG	QA	1647	1/1	0.92	0.32	38,38,38,38	0
58	MG	RA	3180	1/1	0.92	0.24	17,17,17,17	0
58	MG	YA	3152	1/1	0.92	0.24	27,27,27,27	0
58	MG	XA	1624	1/1	0.92	0.10	22,22,22,22	0
58	MG	RA	3181	1/1	0.92	0.33	21,21,21,21	0
58	MG	RA	3224	1/1	0.92	0.83	142,142,142,142	0
58	MG	YA	3160	1/1	0.92	0.14	16,16,16,16	0
58	MG	QA	1626	1/1	0.92	0.11	17,17,17,17	0
58	MG	QA	1655	1/1	0.92	0.21	14,14,14,14	0
58	MG	RA	3184	1/1	0.92	0.35	23,23,23,23	0
58	MG	YA	3051	1/1	0.92	0.25	13,13,13,13	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	XA	1637	1/1	0.92	0.16	14,14,14,14	0
58	MG	RA	3140	1/1	0.92	0.32	34,34,34,34	0
58	MG	RA	3141	1/1	0.92	0.59	40,40,40,40	0
58	MG	YA	3171	1/1	0.92	0.22	22,22,22,22	0
58	MG	QA	1612	1/1	0.92	0.29	15,15,15,15	0
58	MG	YA	3255	1/1	0.92	0.38	12,12,12,12	0
58	MG	XA	1647	1/1	0.92	0.12	22,22,22,22	0
58	MG	QA	1616	1/1	0.92	0.15	52,52,52,52	0
58	MG	QA	1617	1/1	0.92	0.18	46,46,46,46	0
58	MG	RA	3092	1/1	0.92	0.32	0,0,0,0	0
58	MG	YA	3093	1/1	0.92	0.27	10,10,10,10	0
58	MG	YA	3096	1/1	0.92	0.20	6,6,6,6	0
58	MG	QA	1618	1/1	0.92	0.09	17,17,17,17	0
58	MG	RA	3001	1/1	0.92	0.27	16,16,16,16	0
58	MG	YA	3188	1/1	0.92	0.13	13,13,13,13	0
58	MG	YA	3190	1/1	0.92	0.15	8,8,8,8	0
58	MG	YP	202	1/1	0.92	0.10	1,1,1,1	0
58	MG	RA	3104	1/1	0.92	0.18	11,11,11,11	0
58	MG	RA	3031	1/1	0.92	0.36	9,9,9,9	0
58	MG	YA	3115	1/1	0.92	0.22	17,17,17,17	0
58	MG	RA	3106	1/1	0.93	0.14	6,6,6,6	0
58	MG	RA	3142	1/1	0.93	0.38	20,20,20,20	0
58	MG	YA	3078	1/1	0.93	0.17	9,9,9,9	0
58	MG	YA	3159	1/1	0.93	0.15	12,12,12,12	0
58	MG	RA	3075	1/1	0.93	0.14	9,9,9,9	0
58	MG	RA	3076	1/1	0.93	0.15	7,7,7,7	0
58	MG	RA	3086	1/1	0.93	0.22	22,22,22,22	0
58	MG	YA	3227	1/1	0.93	0.40	39,39,39,39	0
58	MG	XA	1678	1/1	0.93	0.23	2,2,2,2	0
58	MG	XA	1634	1/1	0.93	0.17	7,7,7,7	0
58	MG	YA	3231	1/1	0.93	0.20	34,34,34,34	0
58	MG	RA	3173	1/1	0.93	0.28	35,35,35,35	0
58	MG	RA	3125	1/1	0.93	0.30	19,19,19,19	0
57	PAR	XA	1601	42/42	0.93	0.30	38,38,38,38	0
58	MG	R0	101	1/1	0.93	0.09	2,2,2,2	0
58	MG	YA	3237	1/1	0.93	0.32	36,36,36,36	0
58	MG	YA	3172	1/1	0.93	0.37	40,40,40,40	0
58	MG	YA	3243	1/1	0.93	0.21	13,13,13,13	0
58	MG	XA	1640	1/1	0.93	0.26	27,27,27,27	0
58	MG	XA	1641	1/1	0.93	0.24	11,11,11,11	0
58	MG	R5	101	1/1	0.93	0.32	11,11,11,11	0
58	MG	QA	1622	1/1	0.93	0.09	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	RA	3036	1/1	0.93	0.48	18,18,18,18	0
58	MG	RA	3095	1/1	0.93	0.25	18,18,18,18	0
58	MG	RA	3231	1/1	0.93	0.17	16,16,16,16	0
58	MG	QA	1676	1/1	0.93	0.14	13,13,13,13	0
58	MG	RA	3185	1/1	0.93	0.22	16,16,16,16	0
58	MG	YA	3040	1/1	0.93	0.17	19,19,19,19	0
58	MG	XA	1613	1/1	0.93	0.12	8,8,8,8	0
58	MG	YA	3049	1/1	0.93	0.39	74,74,74,74	0
58	MG	QA	1670	1/1	0.93	0.34	5,5,5,5	0
58	MG	YA	3195	1/1	0.93	0.19	5,5,5,5	0
58	MG	YA	3141	1/1	0.93	0.13	19,19,19,19	0
58	MG	XA	1664	1/1	0.93	0.19	22,22,22,22	0
58	MG	YA	3055	1/1	0.93	0.28	6,6,6,6	0
58	MG	XA	1619	1/1	0.93	0.24	5,5,5,5	0
58	MG	YA	3146	1/1	0.93	0.23	40,40,40,40	0
58	MG	YA	3058	1/1	0.93	0.17	20,20,20,20	0
58	MG	YA	3060	1/1	0.93	0.24	8,8,8,8	0
58	MG	RA	3062	1/1	0.93	0.36	21,21,21,21	0
58	MG	YA	3153	1/1	0.93	0.11	14,14,14,14	0
58	MG	YA	3154	1/1	0.93	0.44	11,11,11,11	0
58	MG	RA	3022	1/1	0.94	0.20	24,24,24,24	0
58	MG	RA	3190	1/1	0.94	0.07	40,40,40,40	0
58	MG	XA	1671	1/1	0.94	0.38	33,33,33,33	0
58	MG	QA	1636	1/1	0.94	0.18	1,1,1,1	0
58	MG	QA	1639	1/1	0.94	0.22	33,33,33,33	0
58	MG	YA	3192	1/1	0.94	0.30	21,21,21,21	0
58	MG	YA	3193	1/1	0.94	0.08	14,14,14,14	0
58	MG	YA	3103	1/1	0.94	0.25	8,8,8,8	0
58	MG	RA	3127	1/1	0.94	0.16	22,22,22,22	0
58	MG	YA	3106	1/1	0.94	0.15	16,16,16,16	0
58	MG	YA	3198	1/1	0.94	0.27	18,18,18,18	0
58	MG	YA	3108	1/1	0.94	0.30	7,7,7,7	0
58	MG	RA	3230	1/1	0.94	0.20	41,41,41,41	0
58	MG	QA	1629	1/1	0.94	0.20	11,11,11,11	0
58	MG	XA	1626	1/1	0.94	0.13	15,15,15,15	0
58	MG	XA	1627	1/1	0.94	0.17	12,12,12,12	0
58	MG	YA	3119	1/1	0.94	0.24	9,9,9,9	0
58	MG	QA	1641	1/1	0.94	0.14	43,43,43,43	0
58	MG	YA	3124	1/1	0.94	0.23	6,6,6,6	0
58	MG	YA	3211	1/1	0.94	0.50	55,55,55,55	0
58	MG	QA	1642	1/1	0.94	0.18	38,38,38,38	0
58	MG	YA	3215	1/1	0.94	0.13	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	XA	1683	1/1	0.94	0.10	10,10,10,10	0
58	MG	XA	1631	1/1	0.94	0.21	4,4,4,4	0
58	MG	QA	1663	1/1	0.94	0.21	19,19,19,19	0
58	MG	YA	3001	1/1	0.94	0.20	23,23,23,23	0
58	MG	YA	3220	1/1	0.94	0.16	1,1,1,1	0
58	MG	YA	3134	1/1	0.94	0.13	19,19,19,19	0
58	MG	YA	3002	1/1	0.94	0.22	0,0,0,0	0
58	MG	YA	3136	1/1	0.94	0.17	0,0,0,0	0
58	MG	YA	3003	1/1	0.94	0.42	74,74,74,74	0
58	MG	XA	1633	1/1	0.94	0.10	7,7,7,7	0
58	MG	RA	3163	1/1	0.94	0.26	34,34,34,34	0
58	MG	RA	3008	1/1	0.94	0.46	6,6,6,6	0
58	MG	QA	1628	1/1	0.94	0.26	10,10,10,10	0
58	MG	YA	3016	1/1	0.94	0.10	7,7,7,7	0
58	MG	QA	1665	1/1	0.94	0.09	37,37,37,37	0
58	MG	YA	3020	1/1	0.94	0.41	8,8,8,8	0
58	MG	YA	3024	1/1	0.94	0.24	10,10,10,10	0
58	MG	QA	1666	1/1	0.94	0.12	68,68,68,68	0
58	MG	YA	3242	1/1	0.94	0.14	9,9,9,9	0
58	MG	YA	3031	1/1	0.94	0.18	5,5,5,5	0
58	MG	YA	3032	1/1	0.94	0.22	1,1,1,1	0
58	MG	RA	3107	1/1	0.94	0.17	2,2,2,2	0
58	MG	RA	3245	1/1	0.94	0.36	7,7,7,7	0
58	MG	RA	3178	1/1	0.94	0.13	25,25,25,25	0
58	MG	XA	1643	1/1	0.94	0.34	74,74,74,74	0
58	MG	YA	3046	1/1	0.94	0.50	74,74,74,74	0
58	MG	RD	301	1/1	0.94	0.33	12,12,12,12	0
58	MG	RA	3115	1/1	0.94	0.26	21,21,21,21	0
58	MG	YA	3252	1/1	0.94	0.36	1,1,1,1	0
58	MG	YA	3053	1/1	0.94	0.22	8,8,8,8	0
58	MG	XA	1648	1/1	0.94	0.16	19,19,19,19	0
58	MG	QA	1635	1/1	0.94	0.39	76,76,76,76	0
58	MG	RA	3147	1/1	0.94	0.37	32,32,32,32	0
58	MG	XA	1654	1/1	0.94	0.27	54,54,54,54	0
58	MG	YA	3260	1/1	0.94	0.71	74,74,74,74	0
58	MG	YA	3059	1/1	0.94	0.14	11,11,11,11	0
58	MG	QM	201	1/1	0.94	0.06	51,51,51,51	0
58	MG	YA	3070	1/1	0.94	0.20	1,1,1,1	0
58	MG	RA	3149	1/1	0.94	0.25	4,4,4,4	0
58	MG	RA	3122	1/1	0.94	0.15	5,5,5,5	0
58	MG	YA	3074	1/1	0.94	0.12	1,1,1,1	0
58	MG	YA	3178	1/1	0.94	0.26	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	XA	1661	1/1	0.94	0.09	2,2,2,2	0
58	MG	RA	3222	1/1	0.94	0.12	2,2,2,2	0
58	MG	RA	3186	1/1	0.94	0.28	17,17,17,17	0
58	MG	RA	3187	1/1	0.94	0.21	42,42,42,42	0
58	MG	RA	3240	1/1	0.95	0.29	5,5,5,5	0
58	MG	RA	3114	1/1	0.95	0.16	10,10,10,10	0
58	MG	RA	3054	1/1	0.95	0.25	18,18,18,18	0
58	MG	YA	3019	1/1	0.95	0.34	13,13,13,13	0
58	MG	RA	3055	1/1	0.95	0.12	10,10,10,10	0
58	MG	QA	1625	1/1	0.95	0.29	29,29,29,29	0
58	MG	QA	1615	1/1	0.95	0.21	9,9,9,9	0
58	MG	YA	3029	1/1	0.95	0.22	12,12,12,12	0
58	MG	YA	3030	1/1	0.95	0.61	18,18,18,18	0
58	MG	RB	201	1/1	0.95	0.08	16,16,16,16	0
58	MG	QA	1619	1/1	0.95	0.25	12,12,12,12	0
58	MG	RA	3009	1/1	0.95	0.94	74,74,74,74	0
58	MG	RA	3165	1/1	0.95	0.23	30,30,30,30	0
58	MG	QA	1606	1/1	0.95	0.43	10,10,10,10	0
58	MG	RA	3071	1/1	0.95	0.24	11,11,11,11	0
58	MG	QA	1662	1/1	0.95	0.12	0,0,0,0	0
58	MG	YA	3147	1/1	0.95	0.27	9,9,9,9	0
58	MG	YA	3149	1/1	0.95	0.21	16,16,16,16	0
58	MG	YA	3047	1/1	0.95	0.31	3,3,3,3	0
58	MG	XA	1603	1/1	0.95	0.11	1,1,1,1	0
58	MG	RA	3175	1/1	0.95	0.27	14,14,14,14	0
58	MG	XA	1660	1/1	0.95	0.18	22,22,22,22	0
58	MG	XA	1606	1/1	0.95	0.23	3,3,3,3	0
58	MG	XA	1662	1/1	0.95	0.14	12,12,12,12	0
58	MG	QA	1613	1/1	0.95	0.36	8,8,8,8	0
58	MG	YA	3057	1/1	0.95	0.34	11,11,11,11	0
58	MG	RA	3219	1/1	0.95	0.24	8,8,8,8	0
58	MG	QA	1630	1/1	0.95	0.17	7,7,7,7	0
58	MG	RA	3179	1/1	0.95	0.14	4,4,4,4	0
58	MG	YA	3241	1/1	0.95	0.17	18,18,18,18	0
58	MG	YA	3065	1/1	0.95	0.22	31,31,31,31	0
58	MG	XA	1669	1/1	0.95	0.06	55,55,55,55	0
58	MG	QA	1624	1/1	0.95	0.12	26,26,26,26	0
58	MG	XA	1615	1/1	0.95	0.08	19,19,19,19	0
58	MG	RA	3018	1/1	0.95	0.26	5,5,5,5	0
58	MG	XA	1673	1/1	0.95	0.12	6,6,6,6	0
58	MG	XA	1618	1/1	0.95	0.12	0,0,0,0	0
58	MG	RA	3019	1/1	0.95	0.11	8,8,8,8	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	QA	1633	1/1	0.95	0.23	15,15,15,15	0
58	MG	YA	3084	1/1	0.95	0.15	12,12,12,12	0
58	MG	RA	3090	1/1	0.95	0.20	6,6,6,6	0
58	MG	XA	1622	1/1	0.95	0.23	6,6,6,6	0
58	MG	RA	3027	1/1	0.95	0.21	15,15,15,15	0
58	MG	QA	1646	1/1	0.95	0.16	28,28,28,28	0
58	MG	QA	1634	1/1	0.95	0.42	23,23,23,23	0
58	MG	YA	3258	1/1	0.95	0.34	4,4,4,4	0
58	MG	QA	1669	1/1	0.95	0.20	18,18,18,18	0
58	MG	XA	1629	1/1	0.95	0.23	4,4,4,4	0
58	MG	YA	3186	1/1	0.95	0.24	25,25,25,25	0
58	MG	RA	3102	1/1	0.95	0.33	21,21,21,21	0
58	MG	RA	3042	1/1	0.95	0.23	1,1,1,1	0
58	MG	YA	3265	1/1	0.95	0.17	24,24,24,24	0
58	MG	RA	3043	1/1	0.95	0.27	10,10,10,10	0
58	MG	RA	3195	1/1	0.95	0.14	7,7,7,7	0
58	MG	YA	3007	1/1	0.95	0.16	8,8,8,8	0
58	MG	YA	3008	1/1	0.95	0.24	8,8,8,8	0
58	MG	RA	3044	1/1	0.95	0.21	8,8,8,8	0
58	MG	QA	1649	1/1	0.95	0.14	32,32,32,32	0
58	MG	YA	3121	1/1	0.95	0.11	6,6,6,6	0
58	MG	RA	3108	1/1	0.95	0.10	6,6,6,6	0
58	MG	XA	1605	1/1	0.96	0.35	15,15,15,15	0
58	MG	RA	3011	1/1	0.96	0.23	0,0,0,0	0
58	MG	RA	3206	1/1	0.96	0.14	5,5,5,5	0
58	MG	YA	3076	1/1	0.96	0.34	10,10,10,10	0
58	MG	YA	3077	1/1	0.96	0.25	6,6,6,6	0
58	MG	XA	1608	1/1	0.96	0.17	1,1,1,1	0
58	MG	YA	3079	1/1	0.96	0.19	22,22,22,22	0
58	MG	YA	3189	1/1	0.96	0.07	30,30,30,30	0
58	MG	QA	1657	1/1	0.96	0.12	19,19,19,19	0
58	MG	XA	1674	1/1	0.96	0.17	4,4,4,4	0
58	MG	RA	3064	1/1	0.96	0.24	4,4,4,4	0
58	MG	YA	3086	1/1	0.96	0.20	3,3,3,3	0
58	MG	RA	3109	1/1	0.96	0.20	0,0,0,0	0
58	MG	RA	3111	1/1	0.96	0.20	12,12,12,12	0
58	MG	YA	3196	1/1	0.96	0.11	41,41,41,41	0
58	MG	YA	3094	1/1	0.96	0.17	12,12,12,12	0
58	MG	RA	3213	1/1	0.96	0.13	9,9,9,9	0
58	MG	RA	3032	1/1	0.96	0.25	14,14,14,14	0
58	MG	QA	1648	1/1	0.96	0.12	43,43,43,43	0
58	MG	RA	3119	1/1	0.96	0.16	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	RA	3217	1/1	0.96	0.09	8,8,8,8	0
58	MG	RA	3070	1/1	0.96	0.17	4,4,4,4	0
58	MG	RA	3034	1/1	0.96	0.27	6,6,6,6	0
58	MG	XA	1623	1/1	0.96	0.05	28,28,28,28	0
58	MG	YA	3113	1/1	0.96	0.22	17,17,17,17	0
58	MG	RA	3166	1/1	0.96	0.23	5,5,5,5	0
58	MG	YA	3212	1/1	0.96	0.09	10,10,10,10	0
58	MG	RA	3167	1/1	0.96	0.18	1,1,1,1	0
58	MG	YA	3117	1/1	0.96	0.11	28,28,28,28	0
58	MG	RA	3168	1/1	0.96	0.19	3,3,3,3	0
58	MG	YA	3004	1/1	0.96	0.15	11,11,11,11	0
58	MG	YA	3005	1/1	0.96	0.22	26,26,26,26	0
58	MG	RA	3169	1/1	0.96	0.20	13,13,13,13	0
58	MG	QA	1637	1/1	0.96	0.09	17,17,17,17	0
58	MG	RA	3123	1/1	0.96	0.08	10,10,10,10	0
58	MG	RA	3038	1/1	0.96	0.22	4,4,4,4	0
58	MG	YA	3224	1/1	0.96	0.26	18,18,18,18	0
58	MG	RA	3039	1/1	0.96	0.29	7,7,7,7	0
58	MG	RA	3041	1/1	0.96	0.26	9,9,9,9	0
58	MG	YA	3015	1/1	0.96	0.52	74,74,74,74	0
58	MG	RA	3015	1/1	0.96	0.27	0,0,0,0	0
58	MG	RA	3079	1/1	0.96	0.07	25,25,25,25	0
58	MG	RA	3081	1/1	0.96	0.39	18,18,18,18	0
58	MG	RA	3133	1/1	0.96	0.16	7,7,7,7	0
58	MG	YA	3022	1/1	0.96	0.26	7,7,7,7	0
58	MG	RA	3134	1/1	0.96	0.26	17,17,17,17	0
58	MG	YA	3026	1/1	0.96	0.26	5,5,5,5	0
58	MG	RA	3084	1/1	0.96	0.20	14,14,14,14	0
58	MG	YA	3240	1/1	0.96	0.15	12,12,12,12	0
58	MG	YA	3143	1/1	0.96	0.09	0,0,0,0	0
58	MG	RA	3007	1/1	0.96	0.42	8,8,8,8	0
58	MG	RA	3137	1/1	0.96	0.25	14,14,14,14	0
58	MG	QA	1652	1/1	0.96	0.10	13,13,13,13	0
58	MG	RA	3089	1/1	0.96	0.16	6,6,6,6	0
58	MG	YA	3034	1/1	0.96	0.22	7,7,7,7	0
58	MG	RA	3045	1/1	0.96	0.15	2,2,2,2	0
58	MG	RA	3189	1/1	0.96	0.12	14,14,14,14	0
58	MG	XA	1649	1/1	0.96	0.13	17,17,17,17	0
58	MG	RA	3046	1/1	0.96	0.36	24,24,24,24	0
58	MG	YA	3043	1/1	0.96	0.28	5,5,5,5	0
58	MG	YA	3045	1/1	0.96	0.25	5,5,5,5	0
58	MG	QA	1610	1/1	0.96	0.22	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	XA	1653	1/1	0.96	0.37	42,42,42,42	0
58	MG	YA	3048	1/1	0.96	0.15	4,4,4,4	0
58	MG	QA	1644	1/1	0.96	0.11	26,26,26,26	0
58	MG	RA	3097	1/1	0.96	0.21	5,5,5,5	0
58	MG	YA	3052	1/1	0.96	0.16	12,12,12,12	0
58	MG	RA	3100	1/1	0.96	0.13	0,0,0,0	0
58	MG	YA	3261	1/1	0.96	0.49	16,16,16,16	0
58	MG	RA	3197	1/1	0.96	0.18	81,81,81,81	0
58	MG	XA	1659	1/1	0.96	0.12	36,36,36,36	0
58	MG	RA	3025	1/1	0.96	0.23	3,3,3,3	0
58	MG	RA	3026	1/1	0.96	0.24	7,7,7,7	0
58	MG	RA	3150	1/1	0.96	0.23	27,27,27,27	0
58	MG	R8	101	1/1	0.96	0.15	6,6,6,6	0
58	MG	RA	3153	1/1	0.96	0.12	0,0,0,0	0
58	MG	RA	3058	1/1	0.96	0.11	5,5,5,5	0
58	MG	YA	3067	1/1	0.96	0.27	17,17,17,17	0
58	MG	YA	3177	1/1	0.96	0.13	4,4,4,4	0
58	MG	YX	101	1/1	0.96	0.19	47,47,47,47	0
58	MG	XA	1666	1/1	0.96	0.52	85,85,85,85	0
58	MG	RA	3060	1/1	0.96	0.20	15,15,15,15	0
58	MG	YA	3109	1/1	0.97	0.08	10,10,10,10	0
58	MG	YA	3110	1/1	0.97	0.14	4,4,4,4	0
58	MG	RA	3085	1/1	0.97	0.23	7,7,7,7	0
58	MG	RA	3061	1/1	0.97	0.16	0,0,0,0	0
58	MG	YA	3114	1/1	0.97	0.22	6,6,6,6	0
58	MG	YA	3033	1/1	0.97	0.17	12,12,12,12	0
58	MG	XA	1616	1/1	0.97	0.18	5,5,5,5	0
58	MG	RA	3023	1/1	0.97	0.23	9,9,9,9	0
58	MG	RA	3024	1/1	0.97	0.29	11,11,11,11	0
58	MG	YA	3037	1/1	0.97	0.14	16,16,16,16	0
58	MG	YA	3202	1/1	0.97	0.21	38,38,38,38	0
58	MG	YA	3038	1/1	0.97	0.33	16,16,16,16	0
58	MG	YA	3204	1/1	0.97	0.59	42,42,42,42	0
58	MG	YA	3039	1/1	0.97	0.17	20,20,20,20	0
58	MG	YA	3122	1/1	0.97	0.15	9,9,9,9	0
58	MG	YA	3123	1/1	0.97	0.21	1,1,1,1	0
58	MG	QA	1605	1/1	0.97	0.28	6,6,6,6	0
58	MG	YA	3209	1/1	0.97	0.14	7,7,7,7	0
58	MG	YA	3125	1/1	0.97	0.14	11,11,11,11	0
58	MG	RA	3192	1/1	0.97	0.24	17,17,17,17	0
58	MG	YA	3042	1/1	0.97	0.23	15,15,15,15	0
58	MG	YA	3129	1/1	0.97	0.16	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	RA	3066	1/1	0.97	0.16	7,7,7,7	0
58	MG	YA	3044	1/1	0.97	0.24	2,2,2,2	0
58	MG	RA	3093	1/1	0.97	0.24	12,12,12,12	0
58	MG	RA	3049	1/1	0.97	0.23	12,12,12,12	0
58	MG	RA	3050	1/1	0.97	0.18	9,9,9,9	0
58	MG	XA	1625	1/1	0.97	0.11	5,5,5,5	0
58	MG	YA	3221	1/1	0.97	0.08	19,19,19,19	0
58	MG	RA	3069	1/1	0.97	0.17	19,19,19,19	0
58	MG	YA	3050	1/1	0.97	0.23	5,5,5,5	0
58	MG	RA	3236	1/1	0.97	0.37	13,13,13,13	0
58	MG	YA	3225	1/1	0.97	0.14	12,12,12,12	0
58	MG	RA	3099	1/1	0.97	0.31	11,11,11,11	0
58	MG	RA	3131	1/1	0.97	0.30	7,7,7,7	0
58	MG	RA	3132	1/1	0.97	0.20	9,9,9,9	0
58	MG	QA	1620	1/1	0.97	0.10	3,3,3,3	0
58	MG	RA	3052	1/1	0.97	0.17	1,1,1,1	0
58	MG	RA	3053	1/1	0.97	0.10	2,2,2,2	0
58	MG	RA	3244	1/1	0.97	0.17	0,0,0,0	0
58	MG	RA	3103	1/1	0.97	0.28	5,5,5,5	0
58	MG	RA	3246	1/1	0.97	0.17	33,33,33,33	0
58	MG	YA	3062	1/1	0.97	0.20	4,4,4,4	0
58	MG	RA	3170	1/1	0.97	0.09	9,9,9,9	0
58	MG	XA	1638	1/1	0.97	0.15	4,4,4,4	0
58	MG	YA	3068	1/1	0.97	0.19	20,20,20,20	0
58	MG	YA	3069	1/1	0.97	0.26	12,12,12,12	0
58	MG	QA	1654	1/1	0.97	0.14	12,12,12,12	0
58	MG	RA	3028	1/1	0.97	0.30	17,17,17,17	0
58	MG	RA	3210	1/1	0.97	0.22	8,8,8,8	0
58	MG	RA	3211	1/1	0.97	0.20	16,16,16,16	0
58	MG	YA	3006	1/1	0.97	0.16	26,26,26,26	0
58	MG	RA	3029	1/1	0.97	0.23	2,2,2,2	0
58	MG	XA	1645	1/1	0.97	0.18	5,5,5,5	0
58	MG	RA	3057	1/1	0.97	0.14	4,4,4,4	0
58	MG	RA	3176	1/1	0.97	0.06	21,21,21,21	0
58	MG	YA	3166	1/1	0.97	0.12	11,11,11,11	0
58	MG	YA	3167	1/1	0.97	0.12	15,15,15,15	0
58	MG	R8	102	1/1	0.97	0.20	2,2,2,2	0
58	MG	RA	3077	1/1	0.97	0.18	6,6,6,6	0
58	MG	RA	3030	1/1	0.97	0.19	8,8,8,8	0
58	MG	YA	3085	1/1	0.97	0.25	17,17,17,17	0
58	MG	RA	3059	1/1	0.97	0.23	8,8,8,8	0
58	MG	YA	3088	1/1	0.97	0.20	6,6,6,6	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	YA	3175	1/1	0.97	0.25	14,14,14,14	0
58	MG	XA	1652	1/1	0.97	0.07	32,32,32,32	0
58	MG	RA	3145	1/1	0.97	0.17	3,3,3,3	0
58	MG	RA	3112	1/1	0.97	0.18	7,7,7,7	0
58	MG	YA	3095	1/1	0.97	0.20	19,19,19,19	0
58	MG	RA	3113	1/1	0.97	0.13	1,1,1,1	0
58	MG	YA	3097	1/1	0.97	0.14	11,11,11,11	0
58	MG	YB	203	1/1	0.97	0.14	4,4,4,4	0
58	MG	RA	3083	1/1	0.97	0.22	32,32,32,32	0
58	MG	YA	3025	1/1	0.97	0.13	16,16,16,16	0
58	MG	XA	1657	1/1	0.97	0.18	19,19,19,19	0
58	MG	YA	3104	1/1	0.97	0.09	0,0,0,0	0
58	MG	QA	1651	1/1	0.97	0.11	5,5,5,5	0
58	MG	RA	3116	1/1	0.97	0.11	8,8,8,8	0
58	MG	RA	3152	1/1	0.97	0.24	14,14,14,14	0
58	MG	YA	3087	1/1	0.98	0.19	5,5,5,5	0
58	MG	RA	3117	1/1	0.98	0.12	11,11,11,11	0
58	MG	YA	3089	1/1	0.98	0.26	13,13,13,13	0
58	MG	RA	3118	1/1	0.98	0.24	16,16,16,16	0
58	MG	YA	3091	1/1	0.98	0.22	29,29,29,29	0
58	MG	YA	3092	1/1	0.98	0.14	28,28,28,28	0
58	MG	QA	1609	1/1	0.98	0.10	32,32,32,32	0
58	MG	QA	1638	1/1	0.98	0.10	14,14,14,14	0
58	MG	RA	3096	1/1	0.98	0.30	17,17,17,17	0
58	MG	XA	1612	1/1	0.98	0.24	10,10,10,10	0
58	MG	YA	3157	1/1	0.98	0.17	0,0,0,0	0
58	MG	RA	3040	1/1	0.98	0.20	13,13,13,13	0
58	MG	YA	3098	1/1	0.98	0.33	8,8,8,8	0
58	MG	XA	1614	1/1	0.98	0.10	21,21,21,21	0
58	MG	YA	3100	1/1	0.98	0.23	8,8,8,8	0
58	MG	YA	3101	1/1	0.98	0.32	5,5,5,5	0
58	MG	RA	3098	1/1	0.98	0.12	10,10,10,10	0
58	MG	QA	1656	1/1	0.98	0.27	44,44,44,44	0
58	MG	YA	3229	1/1	0.98	0.15	14,14,14,14	0
58	MG	RA	3239	1/1	0.98	0.23	0,0,0,0	0
58	MG	QA	1631	1/1	0.98	0.14	50,50,50,50	0
58	MG	YA	3232	1/1	0.98	0.24	35,35,35,35	0
58	MG	QA	1614	1/1	0.98	0.13	2,2,2,2	0
58	MG	YA	3107	1/1	0.98	0.17	9,9,9,9	0
58	MG	YA	3009	1/1	0.98	0.17	15,15,15,15	0
58	MG	YA	3010	1/1	0.98	0.28	15,15,15,15	0
58	MG	RA	3078	1/1	0.98	0.21	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	RA	3128	1/1	0.98	0.11	9,9,9,9	0
58	MG	QA	1607	1/1	0.98	0.15	22,22,22,22	0
58	MG	QA	1661	1/1	0.98	0.16	50,50,50,50	0
58	MG	RA	3082	1/1	0.98	0.18	10,10,10,10	0
58	MG	QA	1650	1/1	0.98	0.17	53,53,53,53	0
58	MG	YA	3017	1/1	0.98	0.14	11,11,11,11	0
58	MG	YA	3061	1/1	0.98	0.14	15,15,15,15	0
58	MG	RA	3047	1/1	0.98	0.15	19,19,19,19	0
58	MG	YA	3064	1/1	0.98	0.14	4,4,4,4	0
58	MG	RB	202	1/1	0.98	0.13	29,29,29,29	0
58	MG	YA	3066	1/1	0.98	0.31	6,6,6,6	0
58	MG	YA	3185	1/1	0.98	0.28	22,22,22,22	0
58	MG	RA	3065	1/1	0.98	0.19	0,0,0,0	0
58	MG	QA	1611	1/1	0.98	0.11	1,1,1,1	0
58	MG	YA	3253	1/1	0.98	0.14	22,22,22,22	0
58	MG	YA	3023	1/1	0.98	0.29	18,18,18,18	0
58	MG	RE	302	1/1	0.98	0.23	15,15,15,15	0
58	MG	XA	1668	1/1	0.98	0.13	0,0,0,0	0
58	MG	YA	3128	1/1	0.98	0.46	6,6,6,6	0
58	MG	RA	3110	1/1	0.98	0.13	19,19,19,19	0
58	MG	YA	3073	1/1	0.98	0.10	4,4,4,4	0
58	MG	YA	3131	1/1	0.98	0.14	16,16,16,16	0
58	MG	RP	201	1/1	0.98	0.92	118,118,118,118	0
58	MG	RP	202	1/1	0.98	0.43	76,76,76,76	0
58	MG	QA	1608	1/1	0.98	0.06	4,4,4,4	0
58	MG	RA	3194	1/1	0.98	0.25	0,0,0,0	0
58	MG	RA	3020	1/1	0.98	0.20	4,4,4,4	0
58	MG	RA	3139	1/1	0.98	0.19	12,12,12,12	0
58	MG	YA	3201	1/1	0.98	0.13	57,57,57,57	0
58	MG	YA	3138	1/1	0.98	0.18	6,6,6,6	0
58	MG	RA	3021	1/1	0.98	0.22	18,18,18,18	0
58	MG	RA	3091	1/1	0.98	0.28	9,9,9,9	0
58	MG	YP	201	1/1	0.98	1.20	54,54,54,54	0
58	MG	YA	3082	1/1	0.98	0.13	17,17,17,17	0
58	MG	YA	3083	1/1	0.98	0.25	5,5,5,5	0
58	MG	QA	1623	1/1	0.98	0.13	46,46,46,46	0
58	MG	RA	3200	1/1	0.98	0.12	9,9,9,9	0
58	MG	Y5	101	1/1	0.98	0.26	13,13,13,13	0
58	MG	QV	101	1/1	0.98	0.20	22,22,22,22	0
58	MG	XV	101	1/1	0.98	0.12	3,3,3,3	0
58	MG	RA	3037	1/1	0.98	0.88	74,74,74,74	0
59	ZN	XN	101	1/1	0.98	0.12	70,70,70,70	0

Continued on next page...

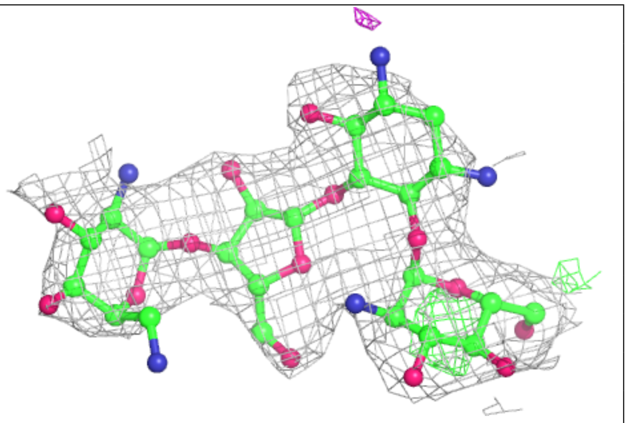
Continued from previous page...

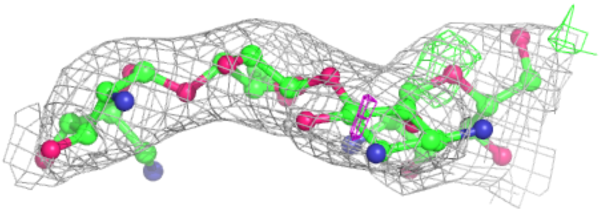
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	QA	1659	1/1	0.99	0.09	42,42,42,42	0
58	MG	RA	3016	1/1	0.99	0.18	8,8,8,8	0
58	MG	YA	3180	1/1	0.99	0.24	19,19,19,19	0
58	MG	YA	3213	1/1	0.99	0.12	31,31,31,31	0
58	MG	YA	3111	1/1	0.99	0.08	26,26,26,26	0
58	MG	YA	3063	1/1	0.99	0.36	12,12,12,12	0
58	MG	RA	3035	1/1	0.99	0.11	2,2,2,2	0
58	MG	YA	3168	1/1	0.99	0.26	3,3,3,3	0
58	MG	RA	3151	1/1	0.99	0.38	3,3,3,3	0
58	MG	YA	3021	1/1	0.99	0.26	8,8,8,8	0
58	MG	RA	3080	1/1	0.99	0.25	10,10,10,10	0
58	MG	YA	3238	1/1	0.99	0.27	76,76,76,76	0
58	MG	XA	1644	1/1	0.99	0.13	4,4,4,4	0
58	MG	RA	3174	1/1	0.99	0.06	17,17,17,17	0
58	MG	RA	3048	1/1	0.99	0.17	2,2,2,2	0
58	MG	RA	3087	1/1	0.99	0.18	10,10,10,10	0
58	MG	YA	3027	1/1	0.99	0.22	21,21,21,21	0
59	ZN	QN	101	1/1	0.99	0.07	86,86,86,86	0
58	MG	YA	3148	1/1	0.99	0.12	15,15,15,15	0
59	ZN	XD	301	1/1	1.00	0.29	10,10,10,10	0
59	ZN	QD	301	1/1	1.00	0.23	27,27,27,27	0

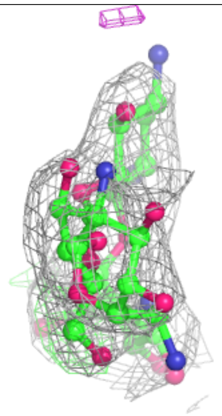
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAR QA 1601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

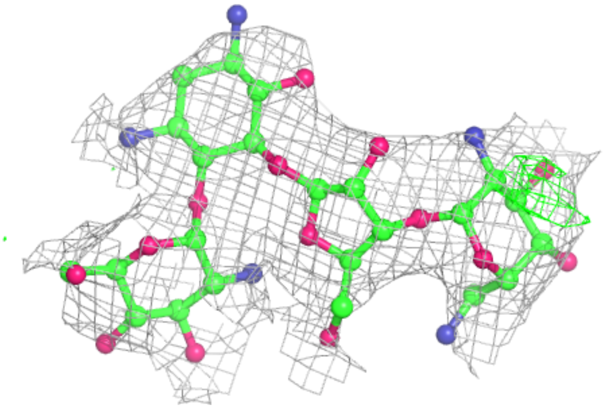


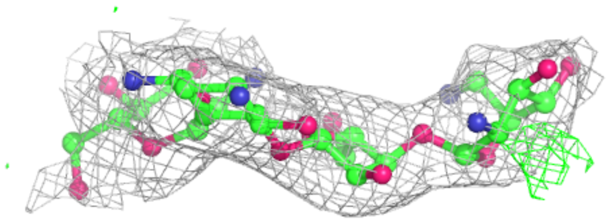


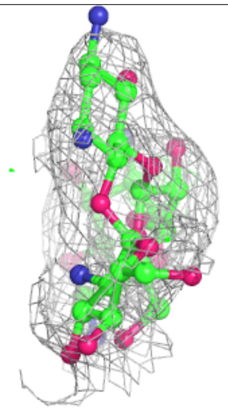


Electron density around PAR XA 1601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers ⓘ

There are no such residues in this entry.