wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2023 – 06:52 PM EDT

PDB ID	:	4L71
Title	:	Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-A on the Ribosome
Authors	:	Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on	:	2013-06-13
Resolution	:	3.90 Å(reported)

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

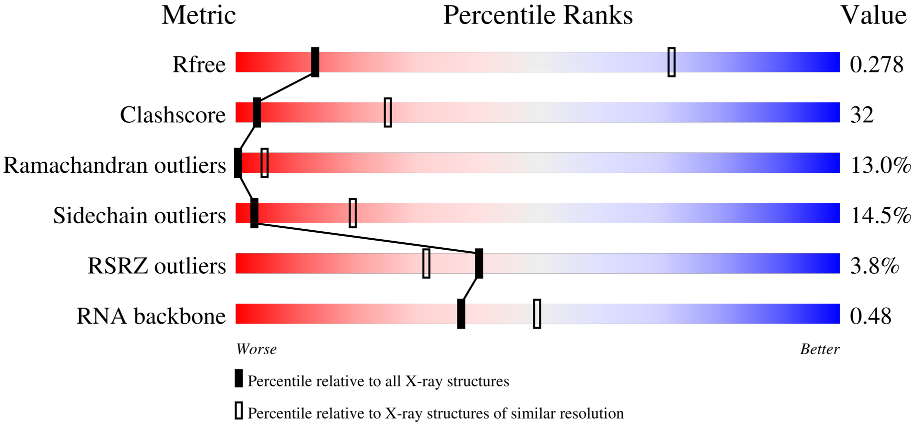
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

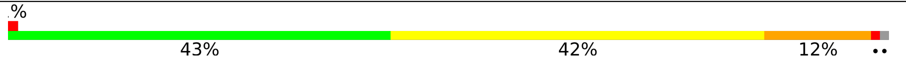
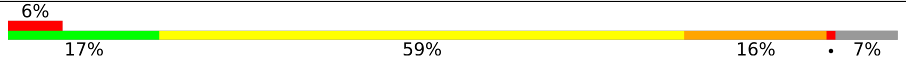
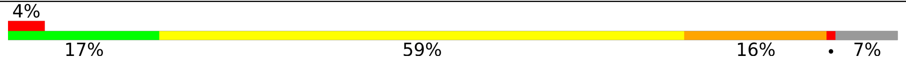
The reported resolution of this entry is 3.90 Å.

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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)
RNA backbone	3102	1040 (4.76-3.00)

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	
1	XA	1522	
2	QB	256	
2	XB	256	

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Mol	Chain	Length	Quality of chain
3	QC	239	2% 23% 52% 10% • 14%
3	XC	239	% 23% 53% 9% • 14%
4	QD	209	% 26% 59% 13% •
4	XD	209	% 26% 60% 12% •
5	QE	162	4% 28% 53% 12% 7%
5	XE	162	% 31% 49% 13% 7%
6	QF	101	% 25% 59% 15% •
6	XF	101	% 25% 58% 16% •
7	QG	156	11% 28% 62% 10% •
7	XG	156	4% 29% 60% 10% •
8	QH	138	2% 28% 59% 12% •
8	XH	138	% 27% 60% 12% •
9	QI	128	10% 22% 64% 12% ••
9	XI	128	2% 20% 64% 15% ••
10	QJ	105	18% 18% 63% 12% • 6%
10	XJ	105	10% 16% 65% 12% • 6%
11	QK	129	11% 32% 50% 9% • 8%
11	XK	129	4% 32% 49% 11% • 8%
12	QL	132	6% 30% 49% 12% • 5%
12	XL	132	2% 29% 48% 14% • 5%
13	QM	126	10% 20% 53% 21% • •
13	XM	126	2% 20% 52% 23% • •
14	QN	61	8% 16% 57% 16% 8% •
14	XN	61	13% 62% 18% 5% •
15	QO	89	7% 33% 55% 11% •

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Mol	Chain	Length	Quality of chain
15	XO	89	% 33% 55% 11% •
16	QP	88	3% 17% 61% 15% • 5%
16	XP	88	2% 20% 57% 16% • 5%
17	QQ	105	7% 41% 43% 11% 5%
17	XQ	105	36% 48% 11% 5%
18	QR	88	10% 22% 45% 11% • 20%
18	XR	88	5% 22% 45% 11% • 20%
19	QS	93	8% 25% 40% 23% • 10%
19	XS	93	2% 25% 39% 23% • 10%
20	QT	106	3% 26% 47% 19% • 7%
20	XT	106	3% 25% 50% 18% • 7%
21	QU	27	33% 30% 44% 19% 7%
21	XU	27	11% 26% 48% 19% 7%
22	RA	2916	3% 42% 42% 13% ••
22	YA	2916	2% 41% 43% 13% ••
23	RB	122	39% 49% 9% ••
23	YB	122	% 41% 43% 13% ••
24	RD	276	30% 52% 15% ••
24	YD	276	30% 51% 14% ••
25	RE	206	2% 23% 48% 24% 5%
25	YE	206	% 23% 48% 24% 5%
26	RF	210	% 34% 48% 13% • •
26	YF	210	% 34% 49% 12% • •
27	RG	182	5% 23% 58% 16% ••
27	YG	182	% 24% 57% 16% ••

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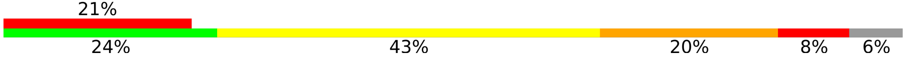
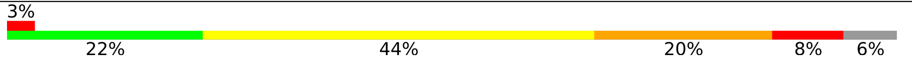
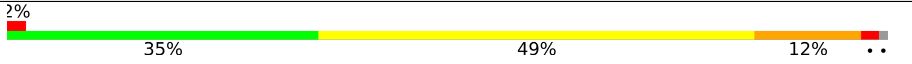
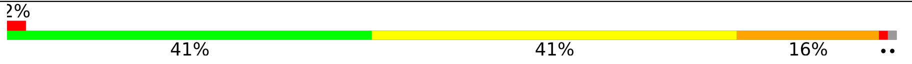
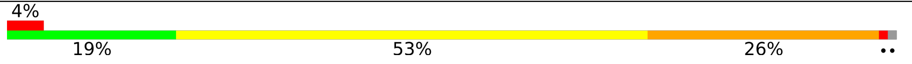
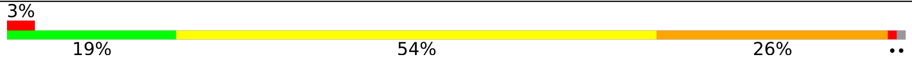
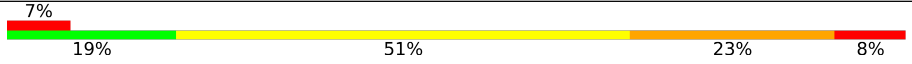
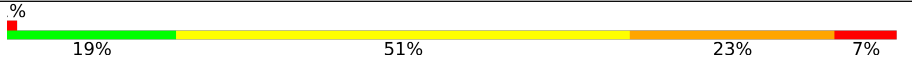
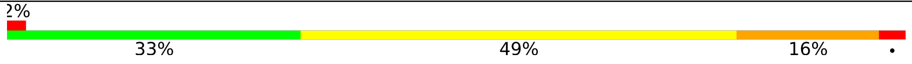
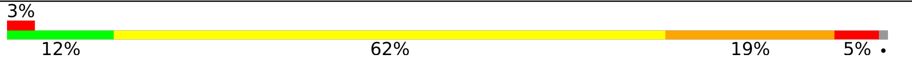
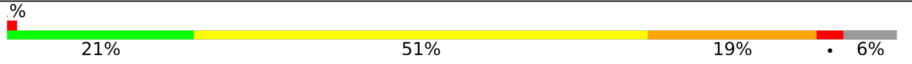
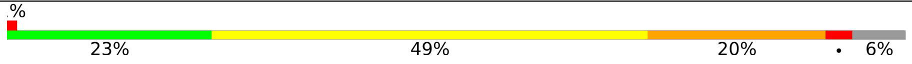
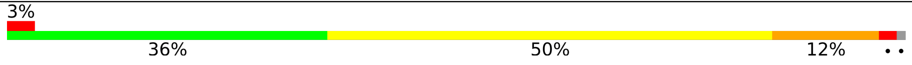
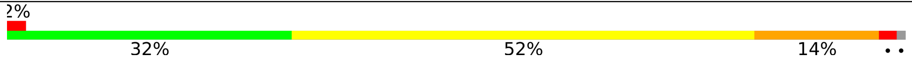
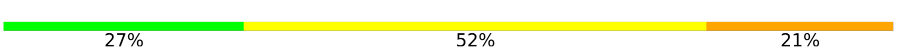
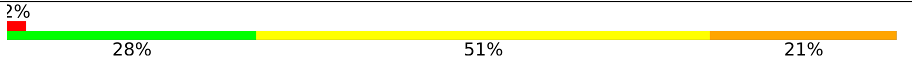
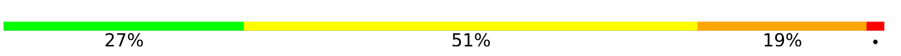
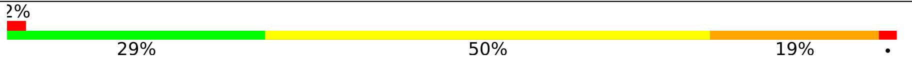
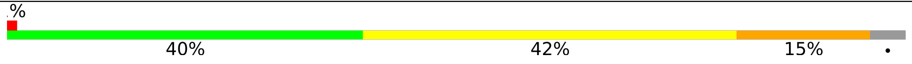
Mol	Chain	Length	Quality of chain
28	RH	180	 21% 24% 43% 20% 8% 6%
28	YH	180	 3% 22% 44% 20% 8% 6%
29	RI	148	 2% 35% 49% 12% • •
29	YI	148	 2% 41% 41% 16% • •
30	RN	140	 4% 19% 53% 26% • •
30	YN	140	 3% 19% 54% 26% • •
31	RO	122	 35% 54% 9% •
31	YO	122	 34% 55% 9% •
32	RP	150	 7% 19% 51% 23% 8%
32	YP	150	 % 19% 51% 23% 7%
33	RQ	141	 2% 33% 49% 16% •
33	YQ	141	 32% 49% 16% •
34	RR	118	 34% 46% 18% •
34	YR	118	 35% 47% 16% •
35	RS	112	 3% 12% 62% 19% 5% •
35	YS	112	 13% 62% 20% • •
36	RT	146	 % 21% 51% 19% • 6%
36	YT	146	 % 23% 49% 20% • 6%
37	RU	118	 3% 36% 50% 12% • •
37	YU	118	 2% 32% 52% 14% • •
38	RV	101	 27% 52% 21%
38	YV	101	 2% 28% 51% 21%
39	RW	113	 27% 51% 19% •
39	YW	113	 2% 29% 50% 19% •
40	RX	96	 % 40% 42% 15% •

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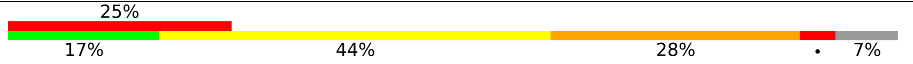
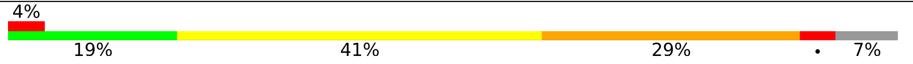
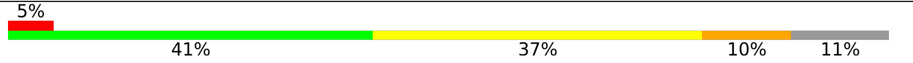
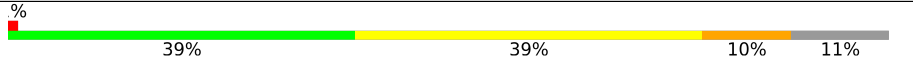
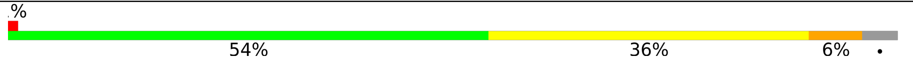
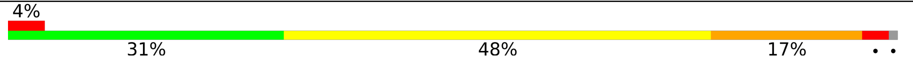
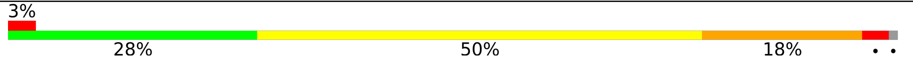
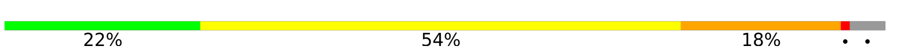
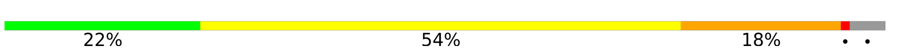
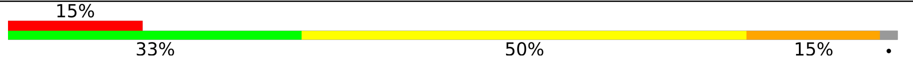
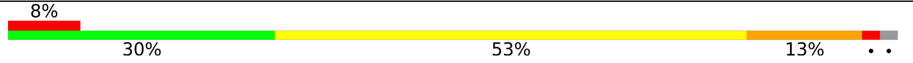
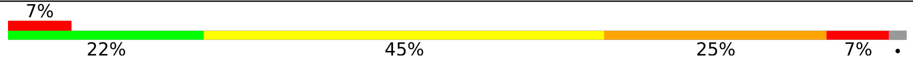
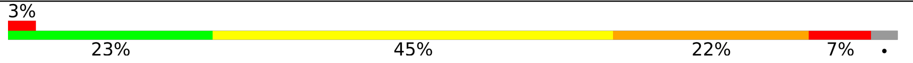
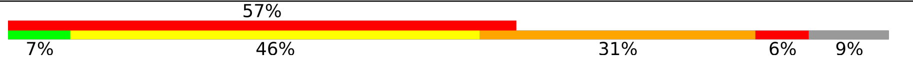
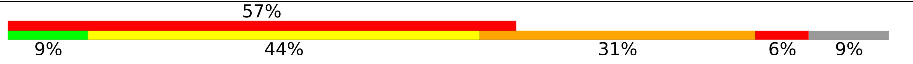
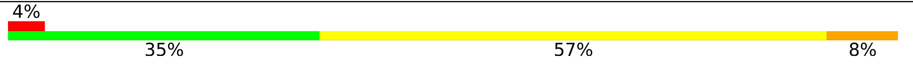
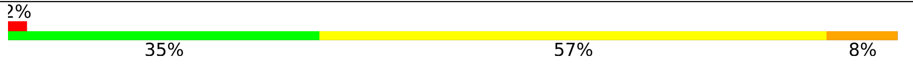
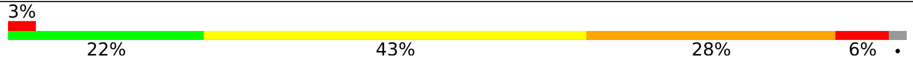
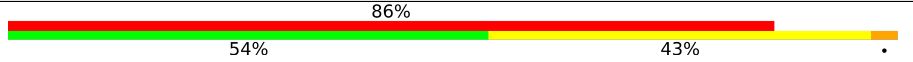
Mol	Chain	Length	Quality of chain
40	YX	96	
41	RY	110	
41	YY	110	
42	RZ	206	
42	YZ	206	
43	R0	85	
43	Y0	85	
44	R1	98	
44	Y1	98	
45	R2	72	
45	Y2	72	
46	R3	60	
46	Y3	60	
47	R4	71	
47	Y4	71	
48	R5	60	
48	Y5	60	
49	R6	54	
49	Y6	54	
50	R7	49	
50	Y7	49	
51	R8	65	
51	Y8	65	
52	R9	37	
52	Y9	37	

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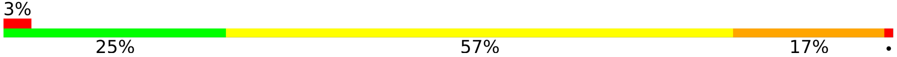
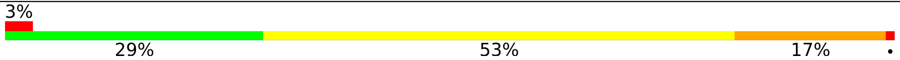
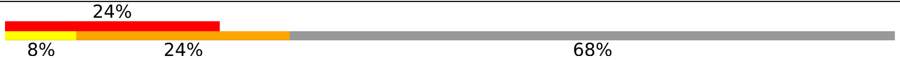
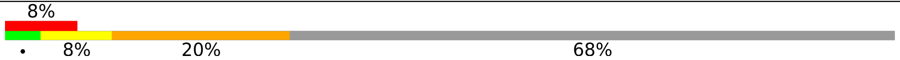
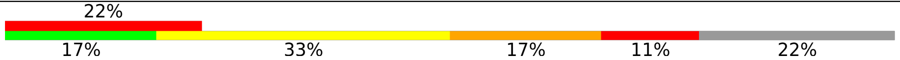
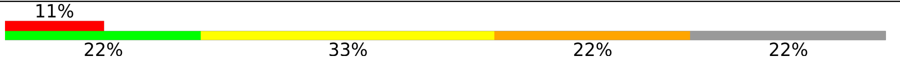
Mol	Chain	Length	Quality of chain
53	QV	77	
53	XV	77	
54	QX	25	
54	XX	25	
55	QY	18	
55	XY	18	
56	Z6	3	
56	Z8	3	

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
57	MG	QA	1602	-	-	-	X
57	MG	QA	1628	-	-	-	X
57	MG	QA	1665	-	-	-	X
57	MG	RA	3004	-	-	-	X
57	MG	RA	3034	-	-	-	X
57	MG	RA	3064	-	-	-	X
57	MG	RA	3065	-	-	-	X
57	MG	RA	3071	-	-	-	X
57	MG	RA	3123	-	-	-	X
57	MG	RA	3127	-	-	-	X
57	MG	RA	3164	-	-	-	X
57	MG	RA	3186	-	-	-	X
57	MG	RA	3205	-	-	-	X
57	MG	RA	3217	-	-	-	X
57	MG	RA	3219	-	-	-	X
57	MG	RA	3230	-	-	-	X
57	MG	XA	1601	-	-	-	X
57	MG	XA	1605	-	-	-	X
57	MG	XA	1635	-	-	-	X
57	MG	XA	1662	-	-	-	X
57	MG	YA	3012	-	-	-	X
57	MG	YA	3043	-	-	-	X
57	MG	YA	3053	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	YA	3079	-	-	-	X
57	MG	YA	3117	-	-	-	X
57	MG	YA	3150	-	-	-	X
57	MG	YA	3151	-	-	-	X
57	MG	YA	3223	-	-	-	X
57	MG	YA	3235	-	-	-	X
57	MG	YA	3245	-	-	-	X
57	MG	YA	3247	-	-	-	X
57	MG	YA	3250	-	-	-	X
57	MG	YA	3259	-	-	-	X
57	MG	YA	3261	-	-	-	X
59	ZN	R9	101	-	-	-	X
59	ZN	Y9	101	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 291950 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 Ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called 23S Ribosomal RNA.

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 Ribosomal RNA.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	YF	202	Total 1585	C 1011	N 297	O 275	S 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 1474	C 942	N 268	O 260	S 4	0	0	0
27	YG	181	Total 1474	C 942	N 268	O 260	S 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 1307	C 829	N 245	O 232	S 1	0	0	0
28	YH	170	Total 1307	C 829	N 245	O 232	S 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 1136	C 726	N 201	O 208	S 1	0	0	0
29	YI	146	Total 1136	C 726	N 201	O 208	S 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 1104	C 712	N 206	O 182	S 4	0	0	0
30	YN	138	Total 1104	C 712	N 206	O 182	S 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 933	C 588	N 171	O 170	S 4	0	0	0
31	YO	122	Total 933	C 588	N 171	O 170	S 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	0	0	0
			1145	712	232	198	3			
32	YP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- 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	0	0	0
			1122	715	212	188	7			
33	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- 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	0	0	0
			968	604	203	160	1			
34	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

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

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

- 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	0	0	0
			1141	710	234	196	1			
36	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RU	117	Total 964	C 610	N 202	O 151	S 1	0	0	0
37	YU	117	Total 964	C 610	N 202	O 151	S 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 779	C 501	N 142	O 135	S 1	0	0	0
38	YV	101	Total 779	C 501	N 142	O 135	S 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 900	C 566	N 177	O 155	S 2	0	0	0
39	YW	113	Total 900	C 566	N 177	O 155	S 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 725	C 471	N 131	O 123	0	0	0
40	YX	92	Total 725	C 471	N 131	O 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 785	C 505	N 150	O 125	S 5	0	0	0
41	YY	102	Total 785	C 505	N 150	O 125	S 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 1461	C 933	N 260	O 265	S 3	0	0	0

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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
			Total	C	N	O	S			
48	R5	59	459	288	90	76	5	0	0	0
48	Y5	58	451	283	89	74	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	R6	49	424	264	87	69	4	0	0	0
49	Y6	49	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
			Total	C	N	O	S			
50	R7	49	430	263	108	57	2	0	0	0
50	Y7	49	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
			Total	C	N	O	S			
51	R8	64	517	331	102	82	2	0	0	0
51	Y8	64	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
			Total	C	N	O	S			
52	R9	37	307	188	68	47	4	0	0	0
52	Y9	37	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
53	QV	77	Total C N O P 1644 732 297 538 77	0	0	0
53	XV	77	Total C N O P 1644 732 297 538 77	0	0	0

- Molecule 54 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
54	QX	8	Total C N O P 169 76 31 54 8	0	0	0
54	XX	8	Total C N O P 169 76 31 54 8	0	0	0

- Molecule 55 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
55	QY	14	Total C N O P 303 135 55 99 14	0	0	0
55	XY	14	Total C N O P 303 135 55 99 14	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
56	Z6	3	Total C N O P 74 40 13 19 2	0	0	0
56	Z8	3	Total C N O P 74 40 13 19 2	0	0	0

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	QA	65	Total Mg 65 65	0	0
57	QF	1	Total Mg 1 1	0	0
57	QH	1	Total Mg 1 1	0	0
57	QM	1	Total Mg 1 1	0	0
57	RA	244	Total Mg 244 244	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	RB	2	Total Mg 2 2	0	0
57	RD	1	Total Mg 1 1	0	0
57	RE	2	Total Mg 2 2	0	0
57	RF	1	Total Mg 1 1	0	0
57	RP	2	Total Mg 2 2	0	0
57	RR	1	Total Mg 1 1	0	0
57	RU	1	Total Mg 1 1	0	0
57	R5	1	Total Mg 1 1	0	0
57	R8	1	Total Mg 1 1	0	0
57	XA	72	Total Mg 72 72	0	0
57	XM	1	Total Mg 1 1	0	0
57	YA	265	Total Mg 265 265	0	0
57	YB	3	Total Mg 3 3	0	0
57	YE	1	Total Mg 1 1	0	0
57	YP	2	Total Mg 2 2	0	0
57	YQ	1	Total Mg 1 1	0	0
57	YX	1	Total Mg 1 1	0	0
57	Y5	1	Total Mg 1 1	0	0
57	Y7	1	Total Mg 1 1	0	0
57	QX	1	Total Mg 1 1	0	0
57	XV	2	Total Mg 2 2	0	0

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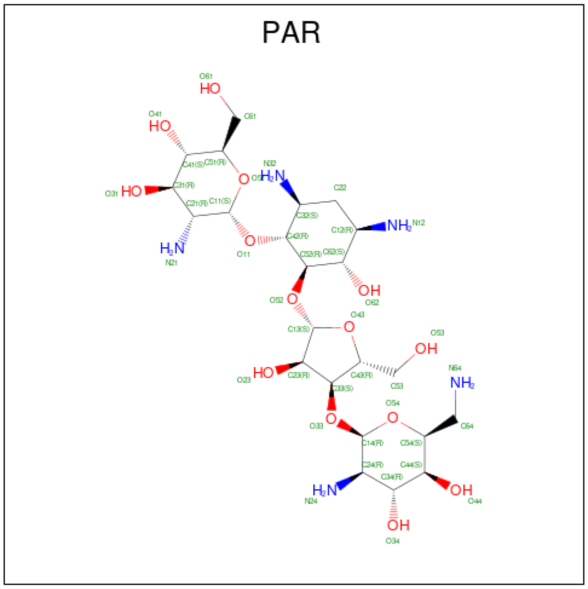
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	XX	1	1	1	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

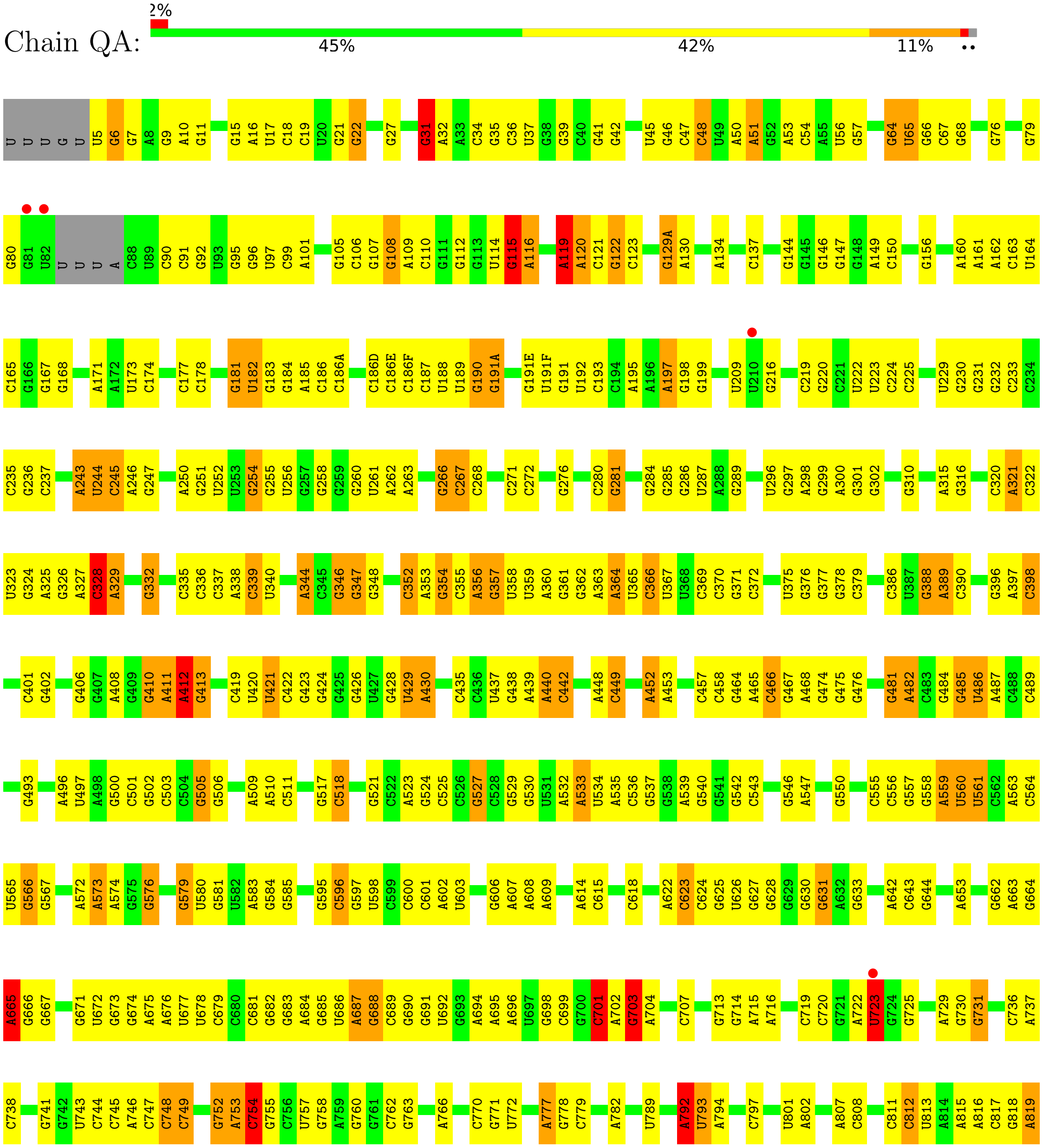
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

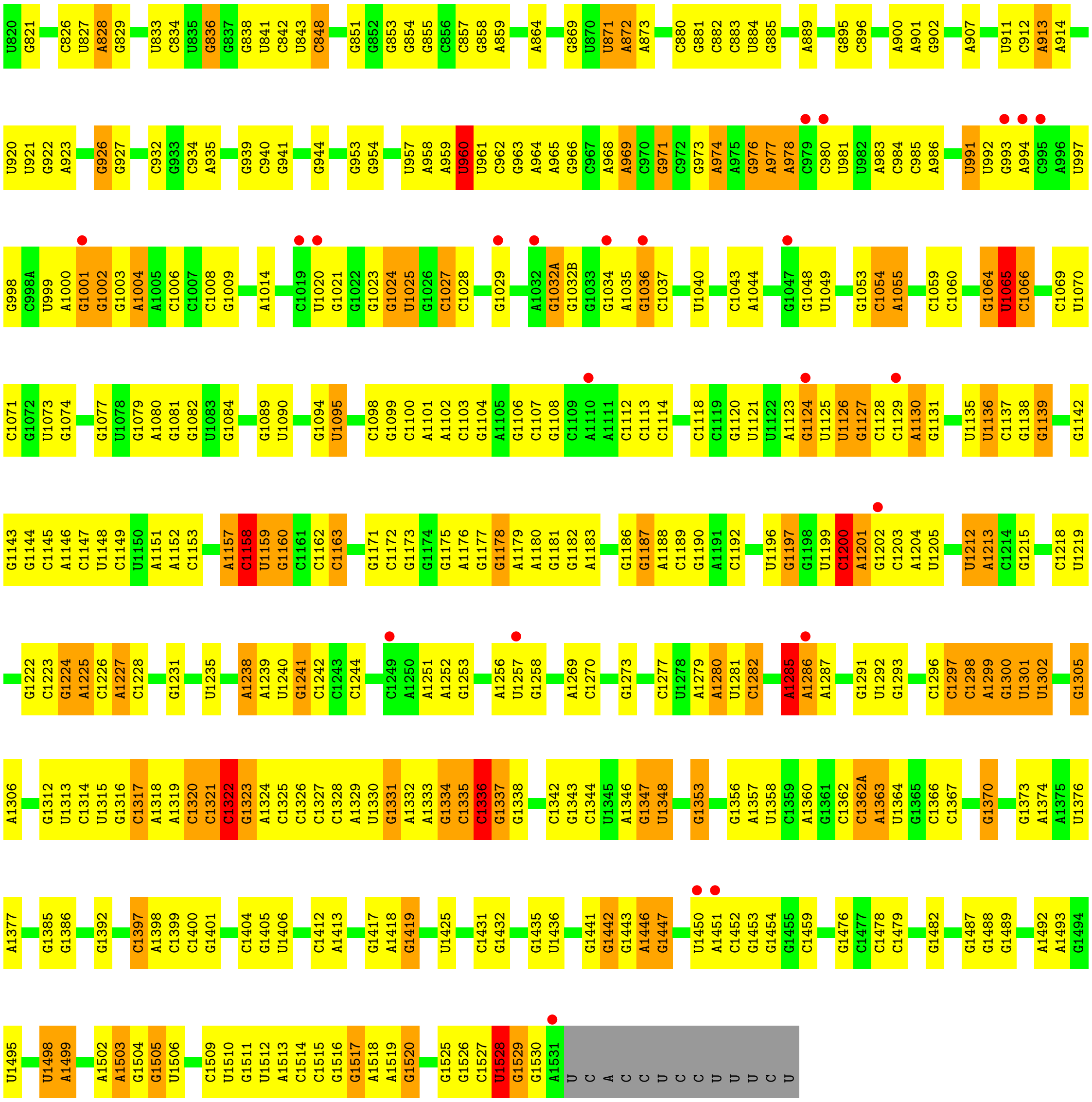
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
59	QD	1	1	1	0	0
59	QN	1	1	1	0	0
59	R9	1	1	1	0	0
59	XD	1	1	1	0	0
59	XN	1	1	1	0	0
59	Y9	1	1	1	0	0

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.

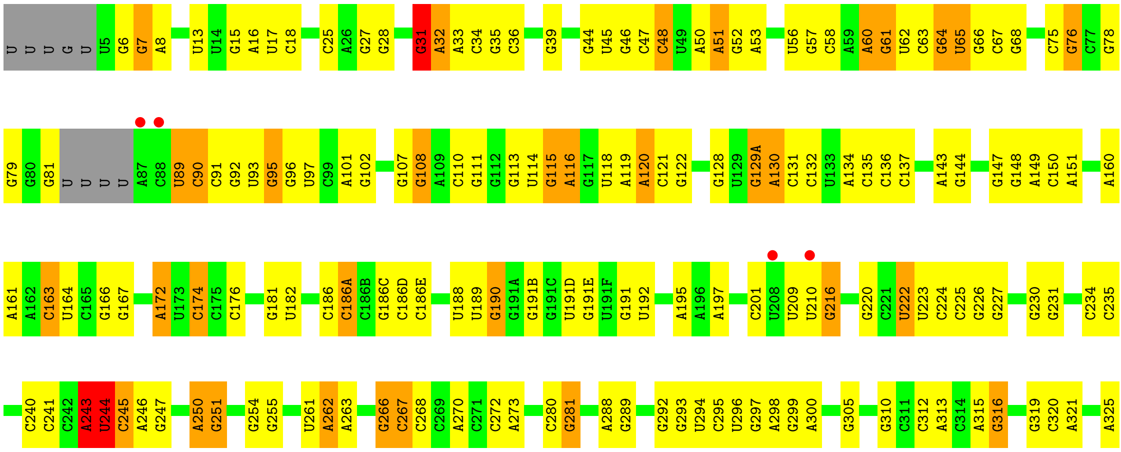
- Molecule 1: 16S Ribosomal RNA

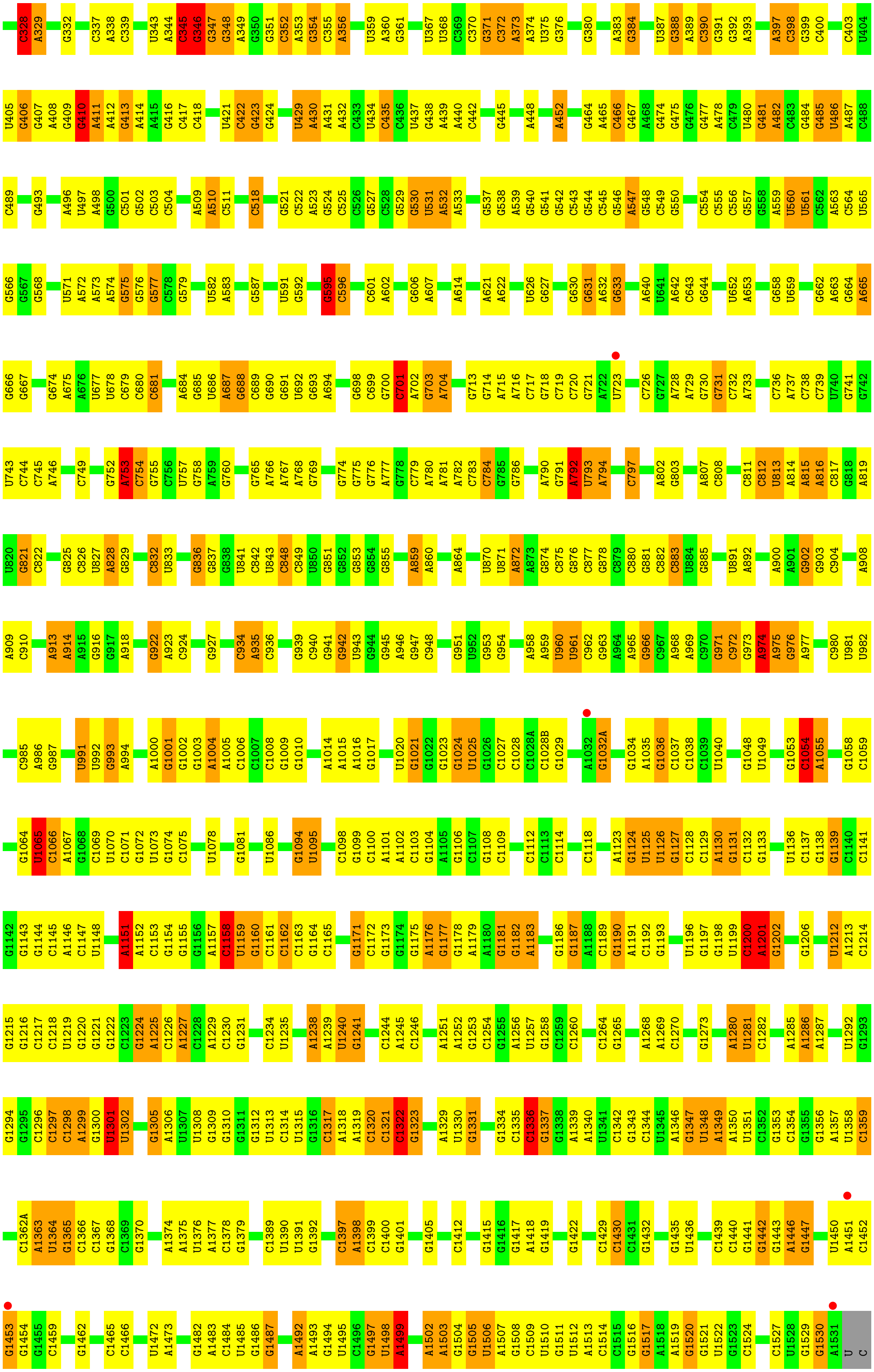




- Molecule 1: 16S Ribosomal RNA

Chain XA:




C328 A329 G332 C337 A338 C339 U343 A344 C345 G346 G347 G348 A349 G350 G351 C352 A353 G354 C355 A356 U359 A360 G361 U367 U368 C369 C370 G371 C372 A373 A374 U375 G376 G380 A383 G384 U387 G388 A389 C390 G391 G392 A393 A397 C398 G399 C400 C403 U404
U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 A415 G416 C417 C418 U421 C422 G423 G424 U429 A430 A431 A432 C433 U434 C435 C436 U437 G438 A439 A440 C442 G445 A448 A452 G464 A465 C466 G467 A468 G474 G475 G476 G477 A478 C479 U480 G481 A482 C483 G484 G485 U486 A487 C488
C489 G493 A496 U497 A498 G500 C501 G502 C503 C504 A509 A510 C511 C518 G521 C522 A523 G524 C525 C526 G527 C528 G529 G530 U531 A532 A533 G537 G538 A539 G540 G541 G542 C543 G544 C545 G546 A547 G548 C549 G550 C554 C555 C556 G557 G558 A559 U560 U561 C562 A563 C564 U565
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G666 G667 G674 A675 A676 U677 U678 C679 C680 G681 A684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 G698 C699 G700 C701 A702 G703 A704 G713 G714 A715 A716 C717 G718 C719 C720 G721 A722 U723 C726 G727 A728 G729 G730 G731 C732 A733 C736 A737 C738 C739 U740 G741 G742
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- Molecule 2: 30S ribosomal protein S2

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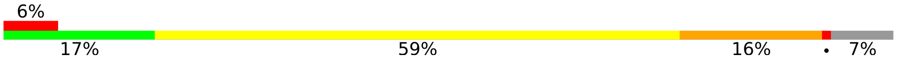

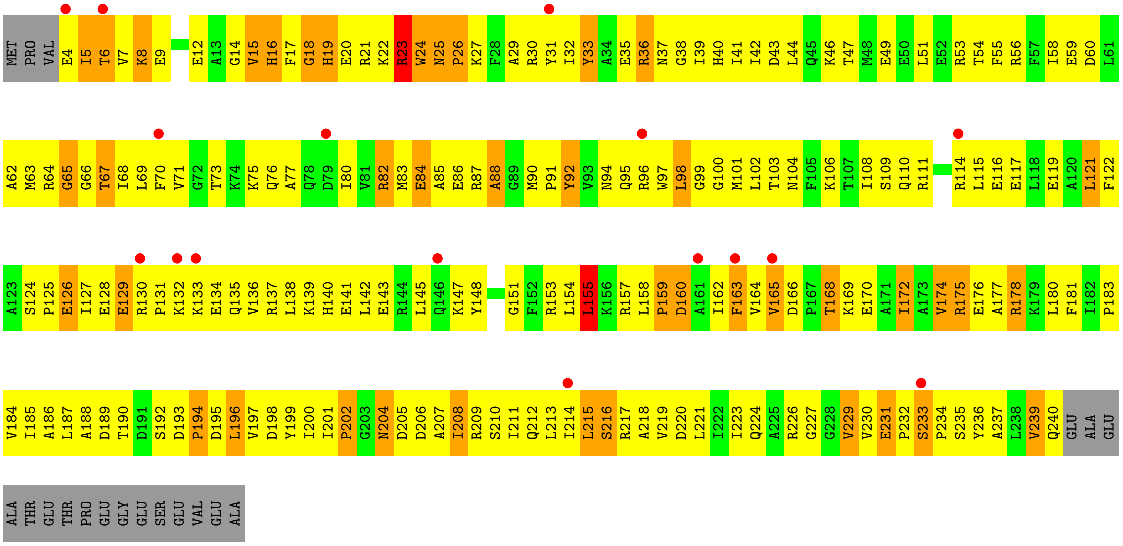

- Molecule 2: 30S ribosomal protein S2

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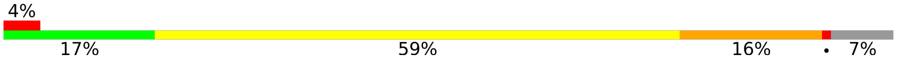
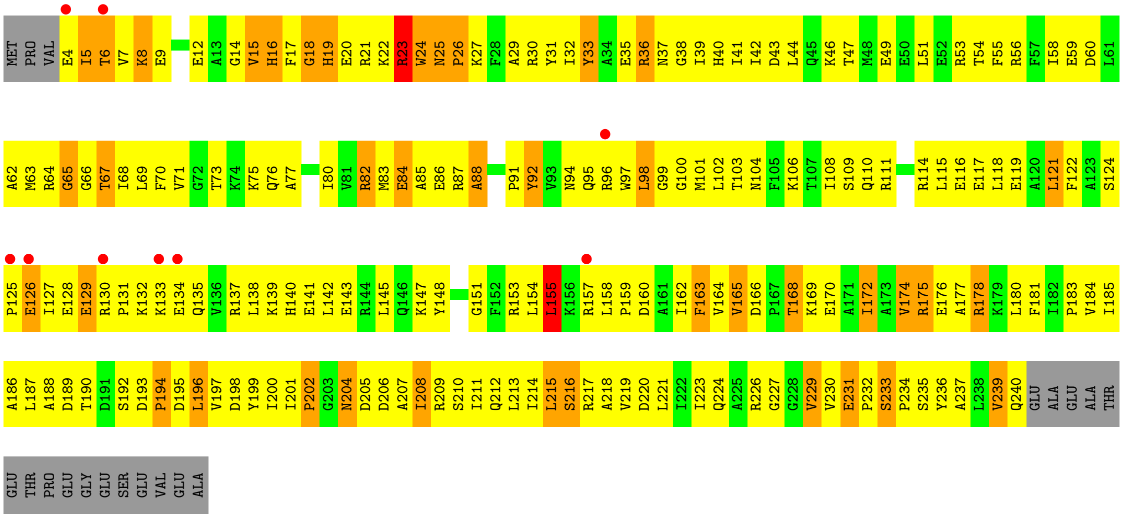
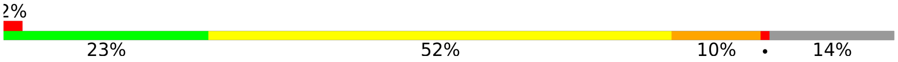
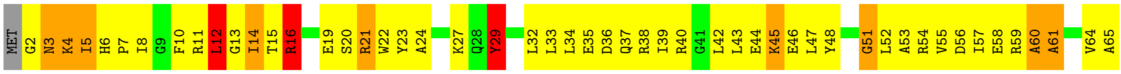


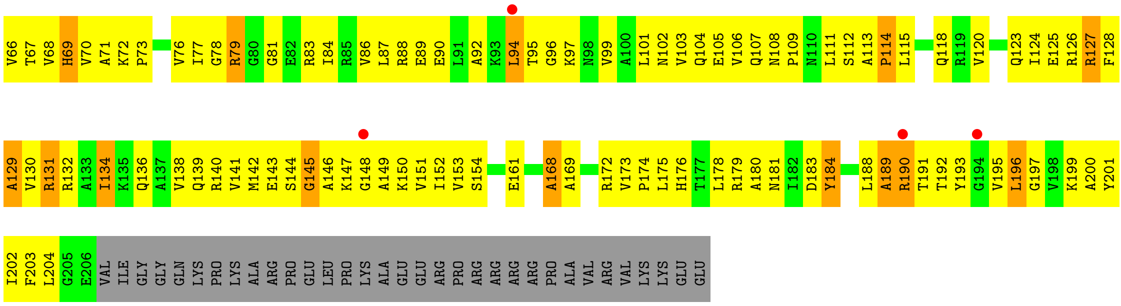


- Molecule 3: 30S ribosomal protein S3

Chain QC:







- Molecule 3: 30S ribosomal protein S3

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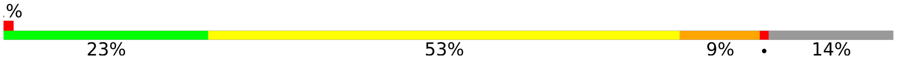

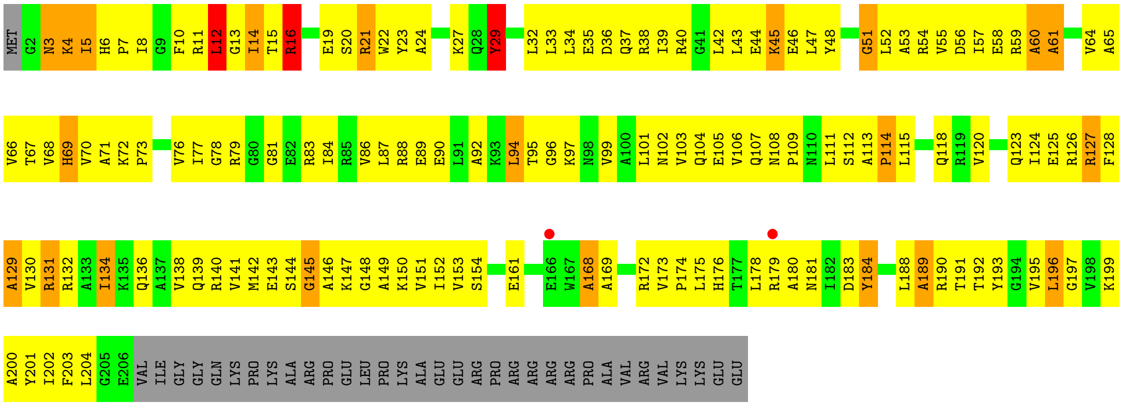

- Molecule 4: 30S ribosomal protein S4

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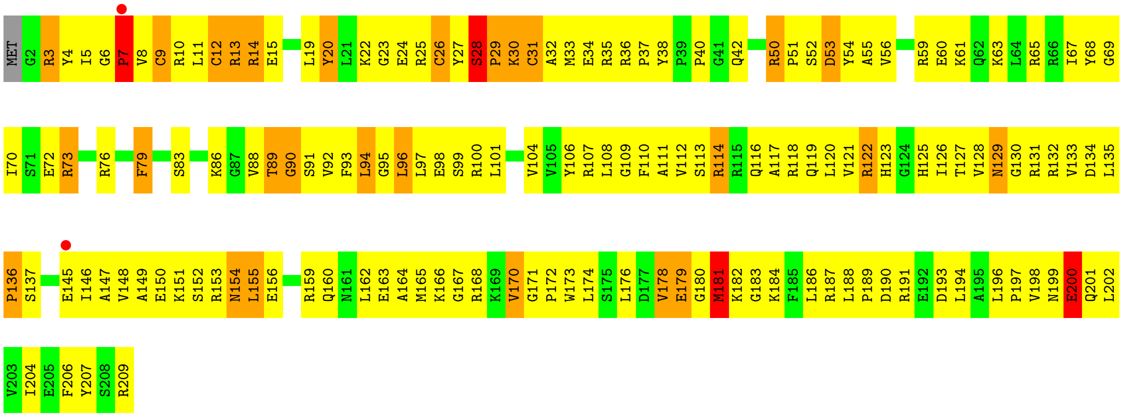

- Molecule 4: 30S ribosomal protein S4

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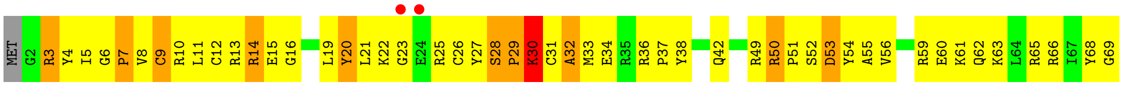

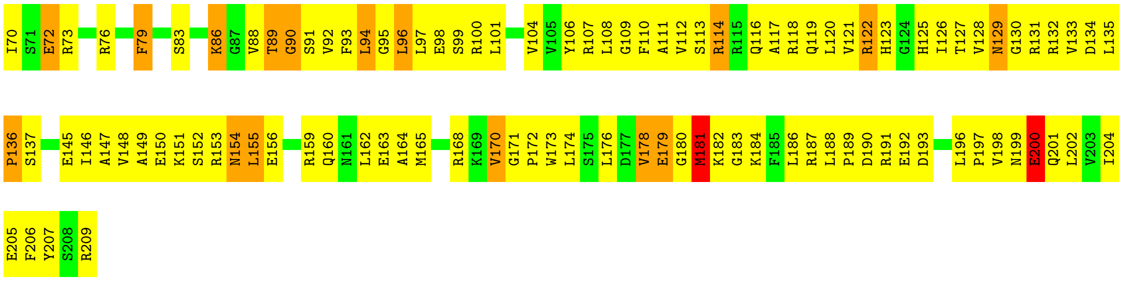

- Molecule 5: 30S ribosomal protein S5

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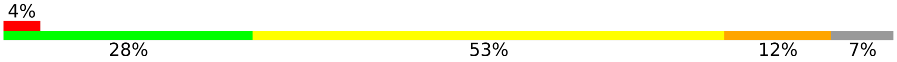

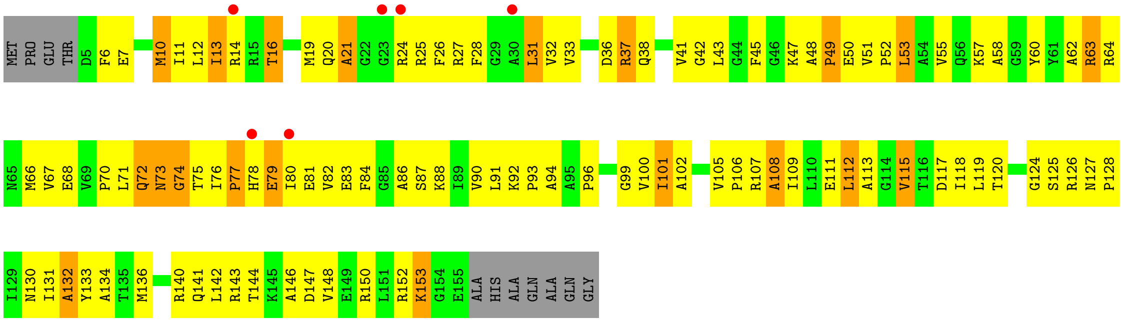

- Molecule 5: 30S ribosomal protein S5

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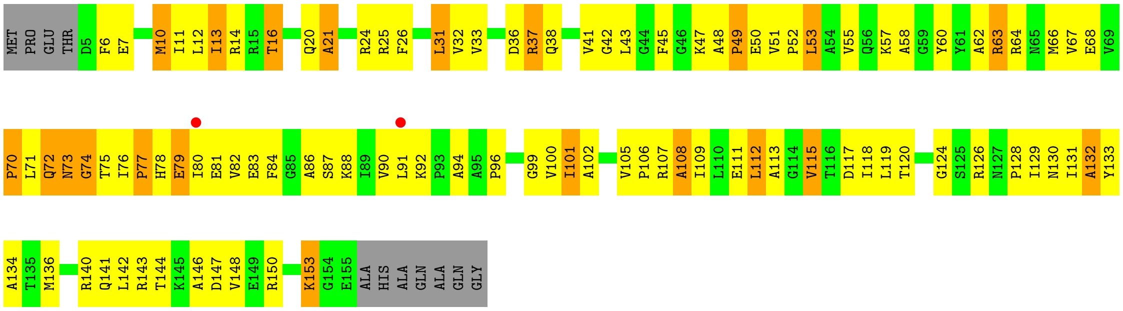
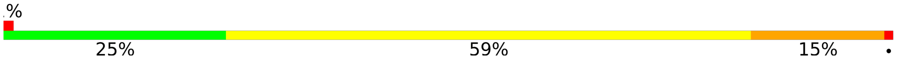
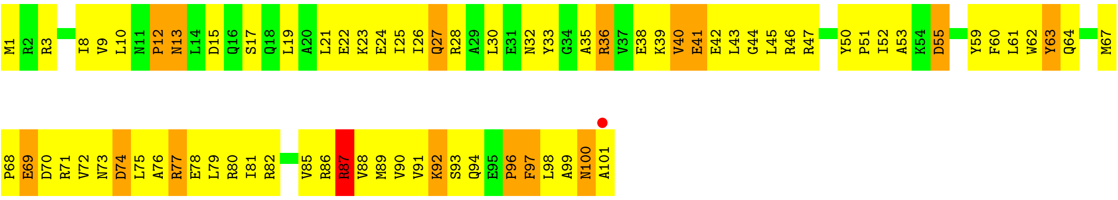


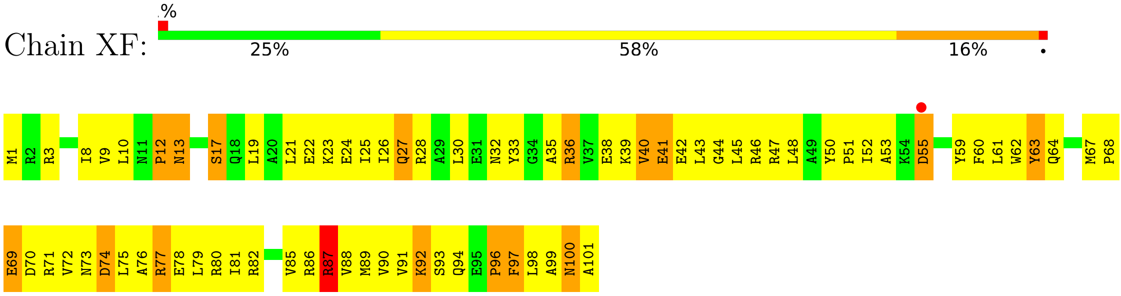
- Molecule 6: 30S ribosomal protein S6

Chain QF:

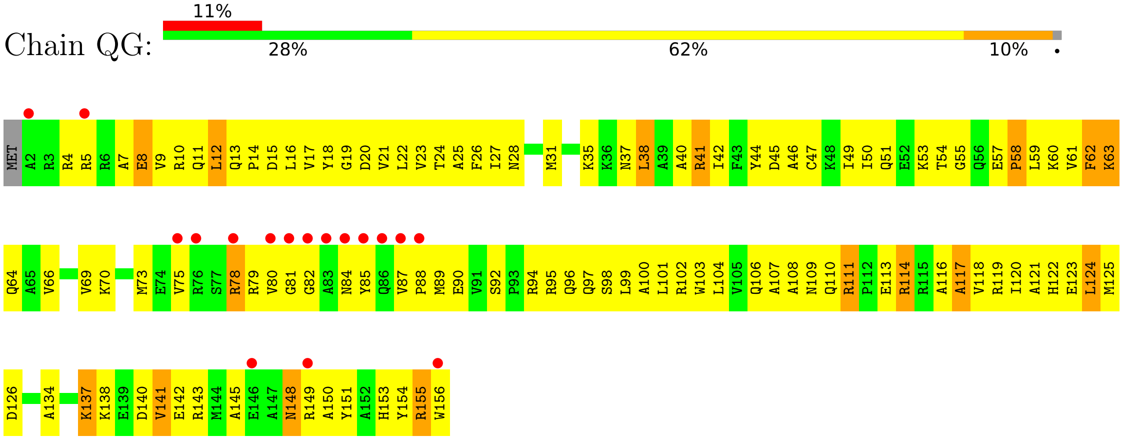




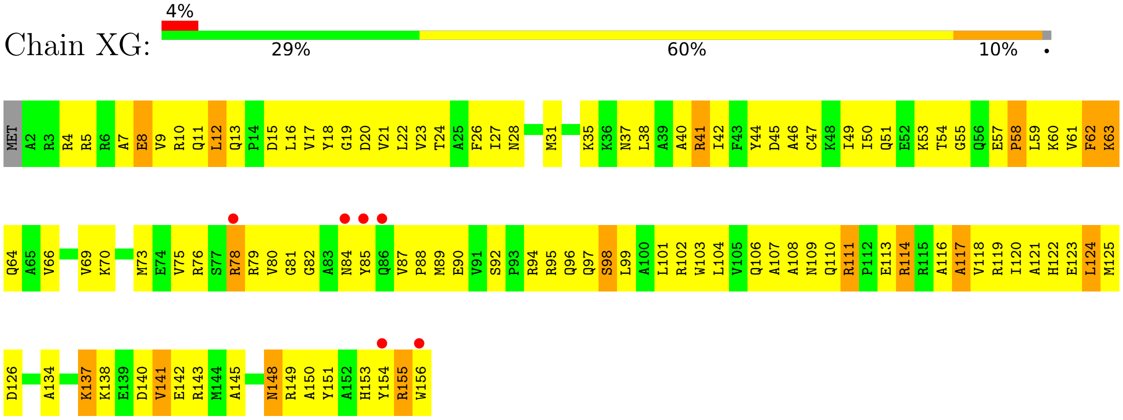
- Molecule 6: 30S ribosomal protein S6



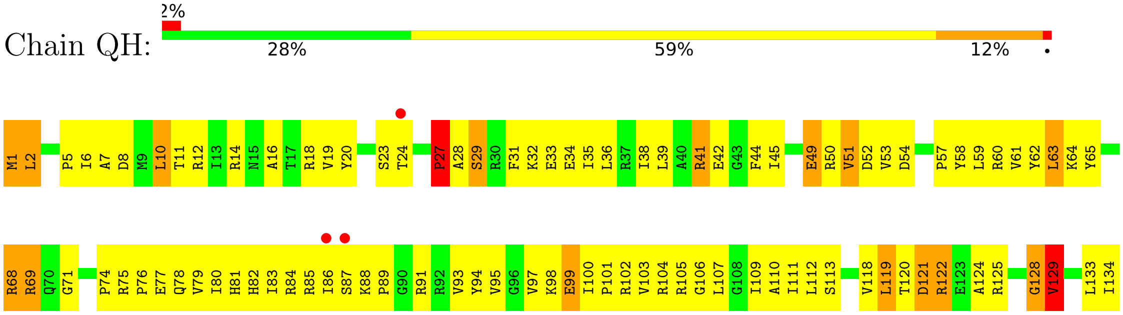
- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8

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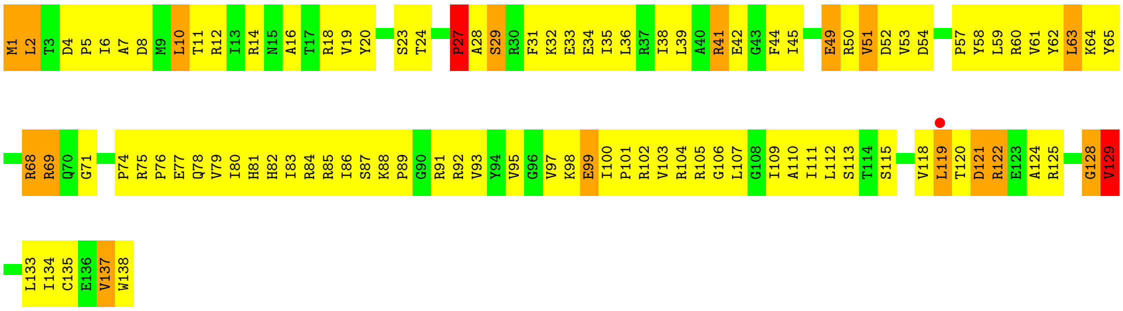
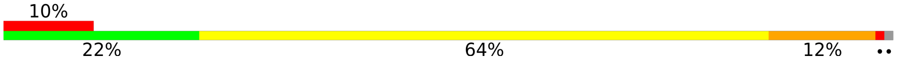
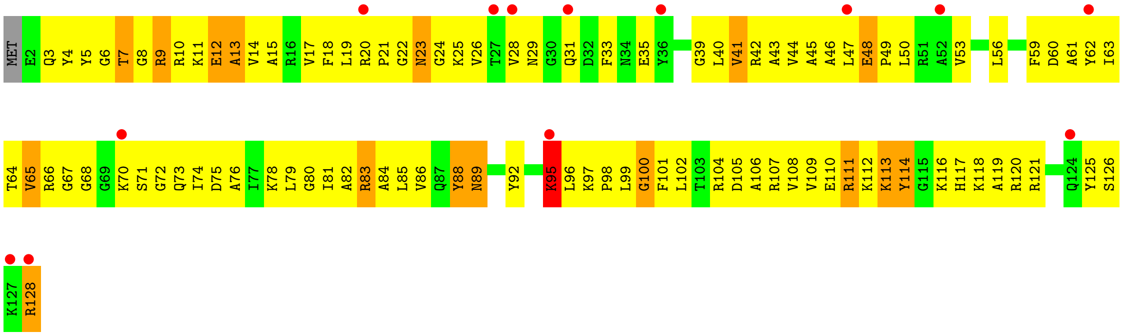


- Molecule 9: 30S ribosomal protein S9

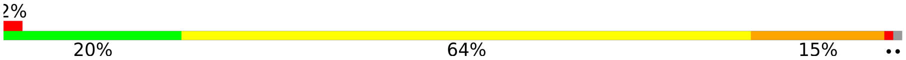
Chain QI:

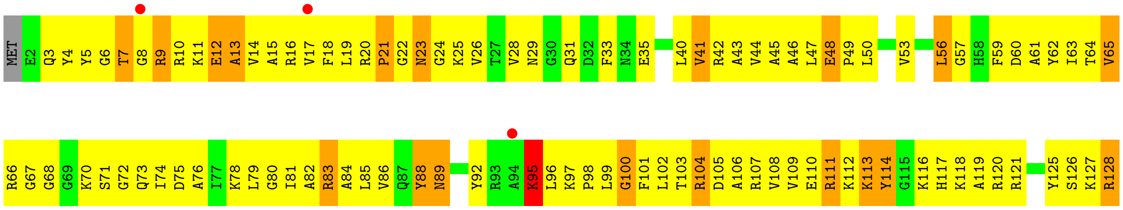




- Molecule 9: 30S ribosomal protein S9

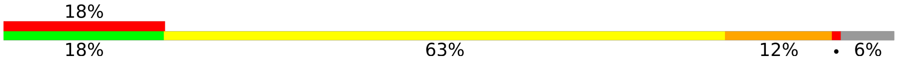
Chain XI:

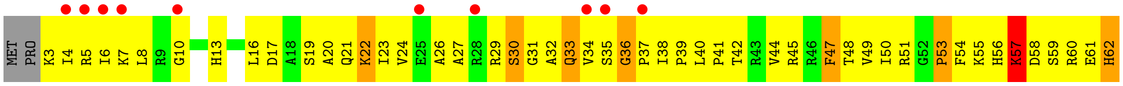


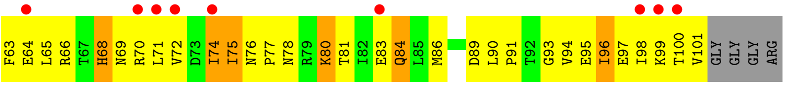


- Molecule 10: 30S ribosomal protein S10

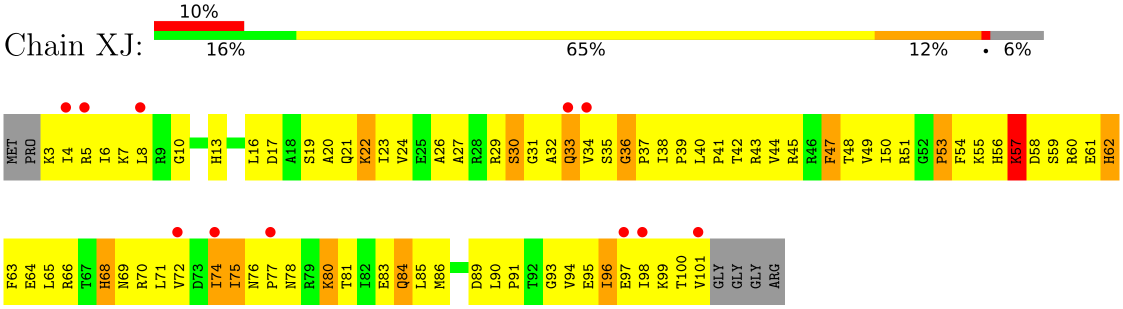
Chain QJ:



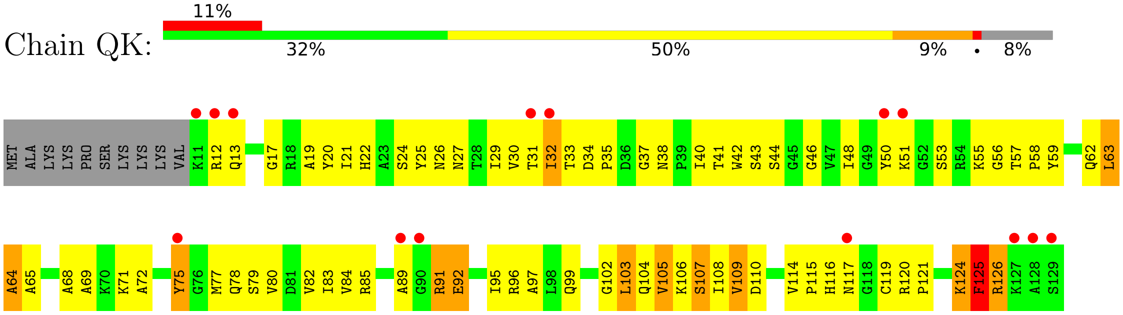




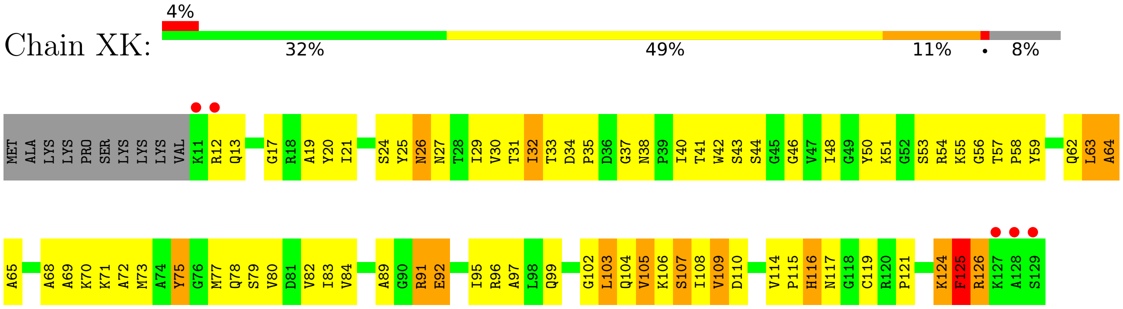
- Molecule 10: 30S ribosomal protein S10



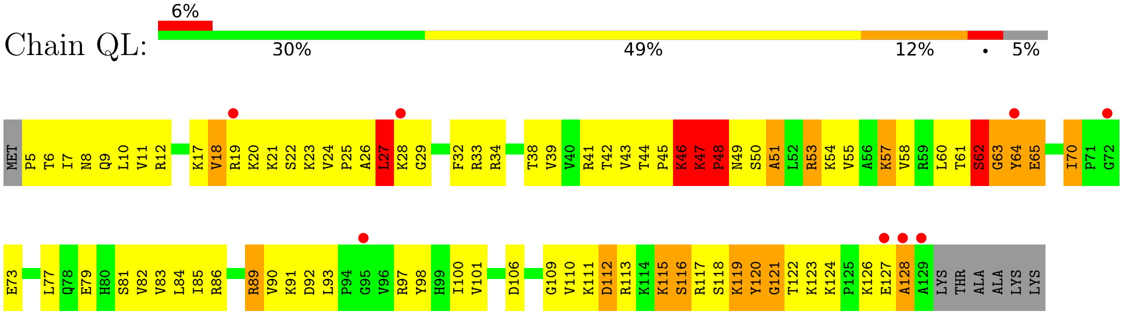
- Molecule 11: 30S ribosomal protein S11



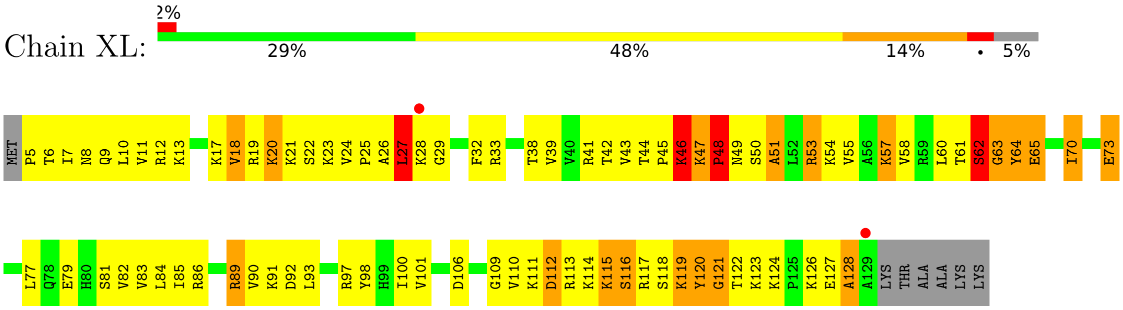
- Molecule 11: 30S ribosomal protein S11



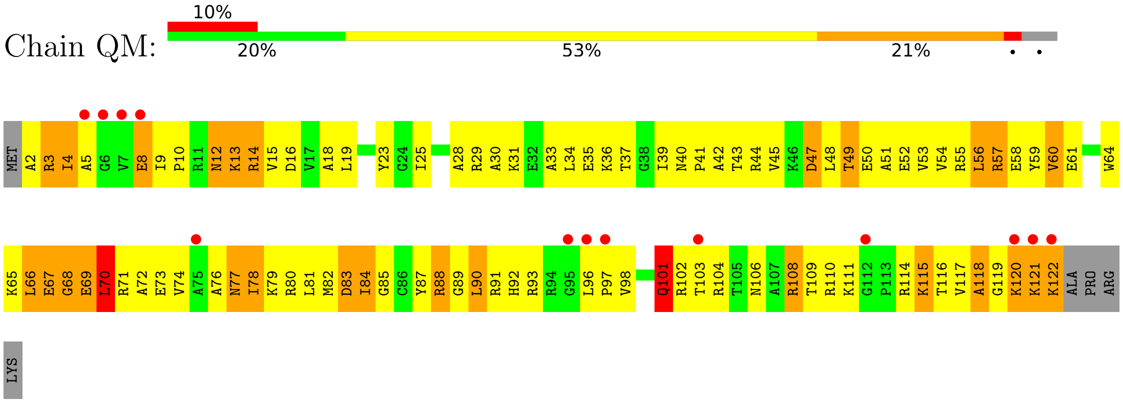
- Molecule 12: 30S ribosomal protein S12



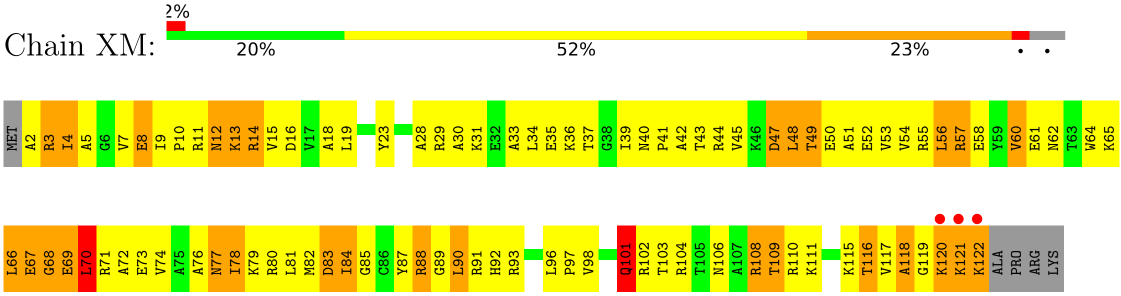
- Molecule 12: 30S ribosomal protein S12



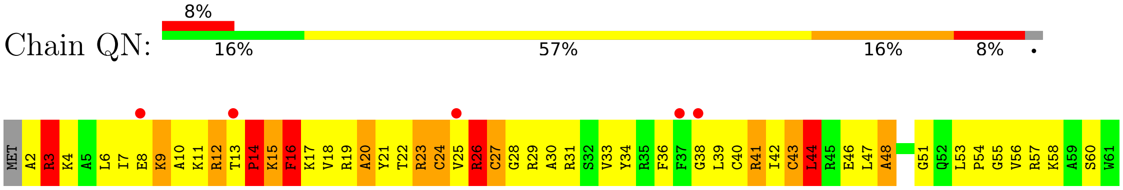
- Molecule 13: 30S ribosomal protein S13



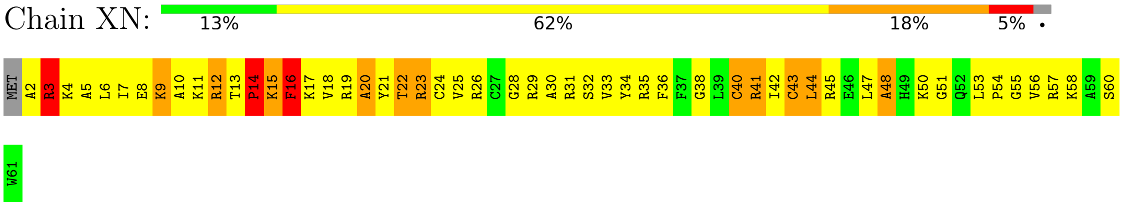
- Molecule 13: 30S ribosomal protein S13



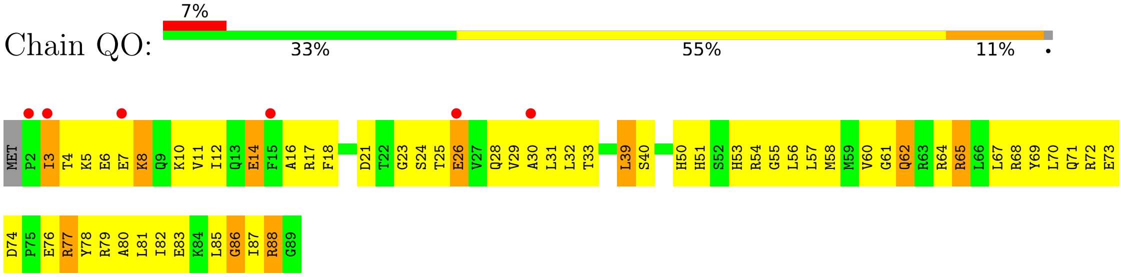
- Molecule 14: 30S ribosomal protein S14 type Z



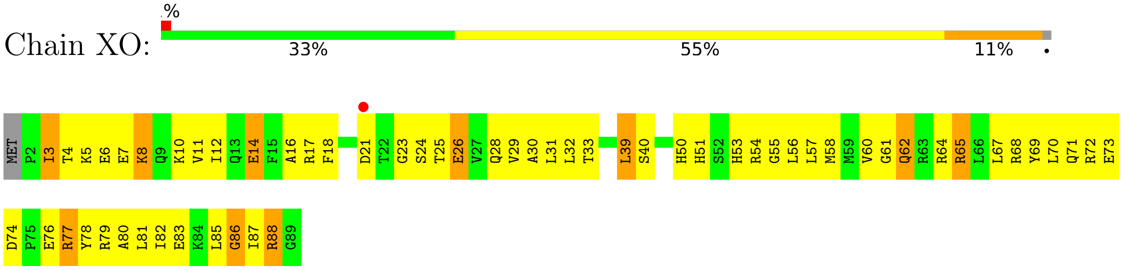
- Molecule 14: 30S ribosomal protein S14 type Z



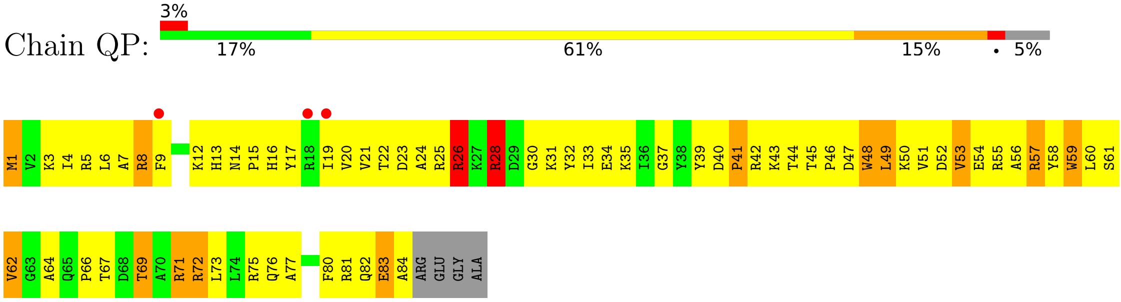
- Molecule 15: 30S ribosomal protein S15



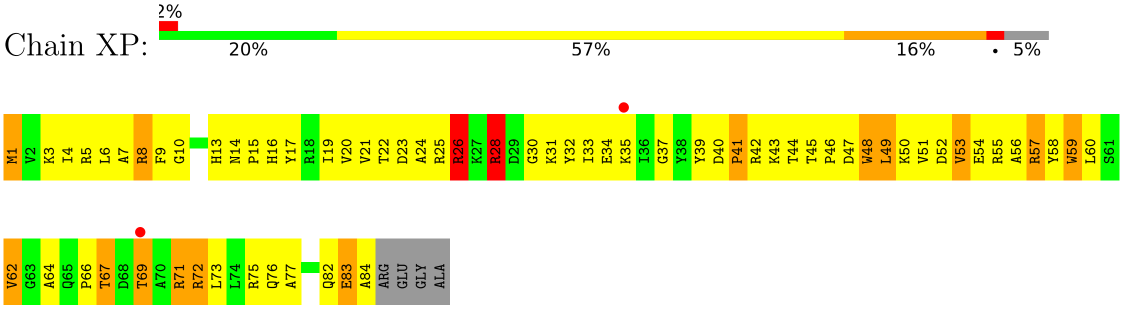
- Molecule 15: 30S ribosomal protein S15



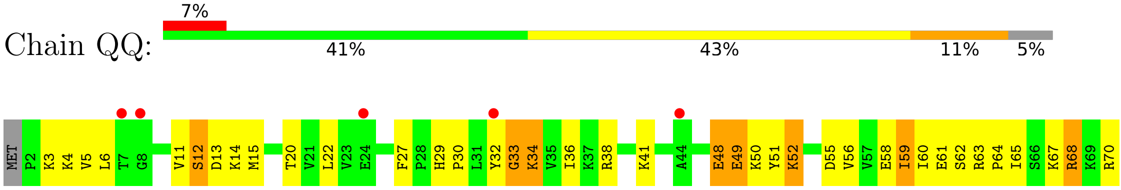
- Molecule 16: 30S ribosomal protein S16

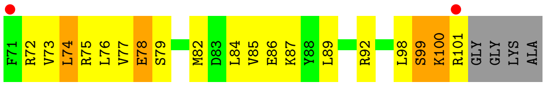


- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17





- Molecule 17: 30S ribosomal protein S17

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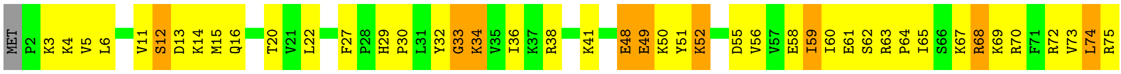
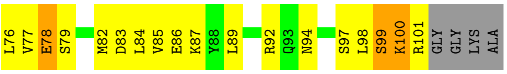
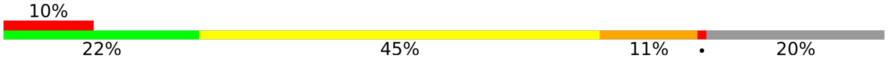
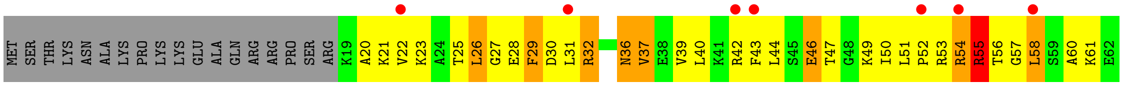




- Molecule 18: 30S ribosomal protein S18

Chain QR:





- Molecule 18: 30S ribosomal protein S18

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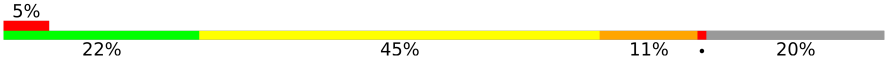
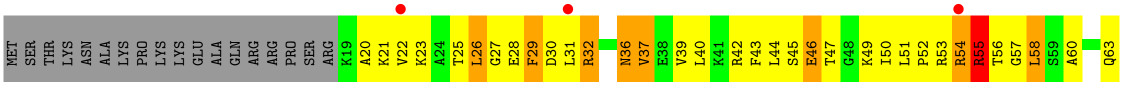
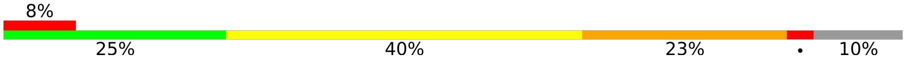
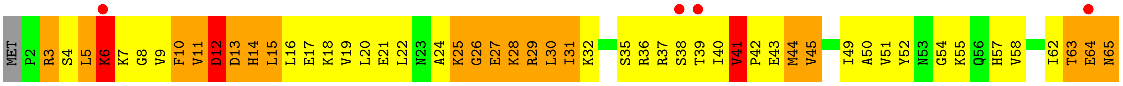


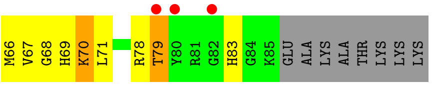


- Molecule 19: 30S ribosomal protein S19

Chain QS:







- Molecule 19: 30S ribosomal protein S19

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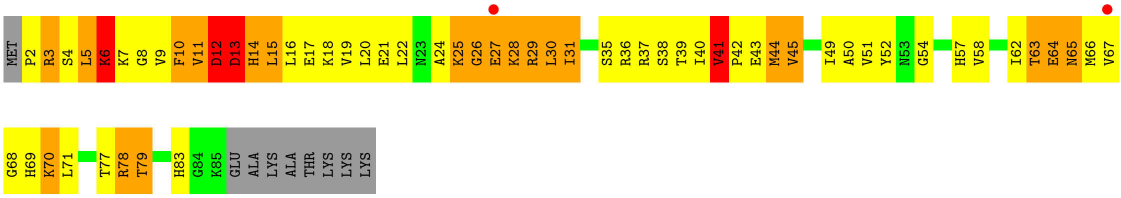
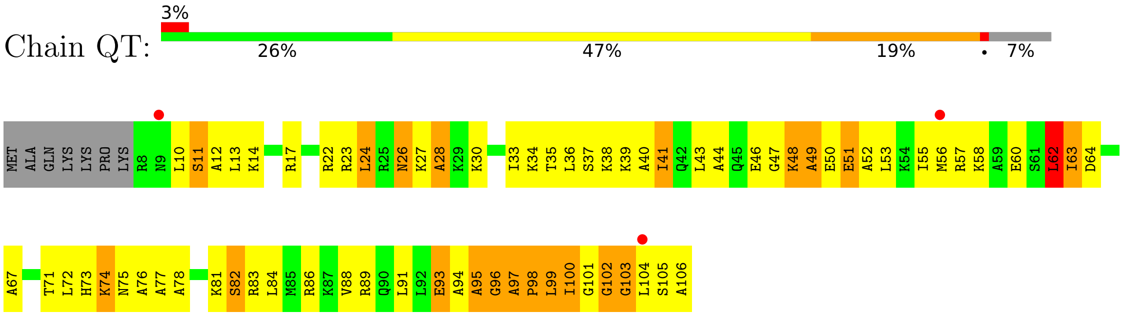
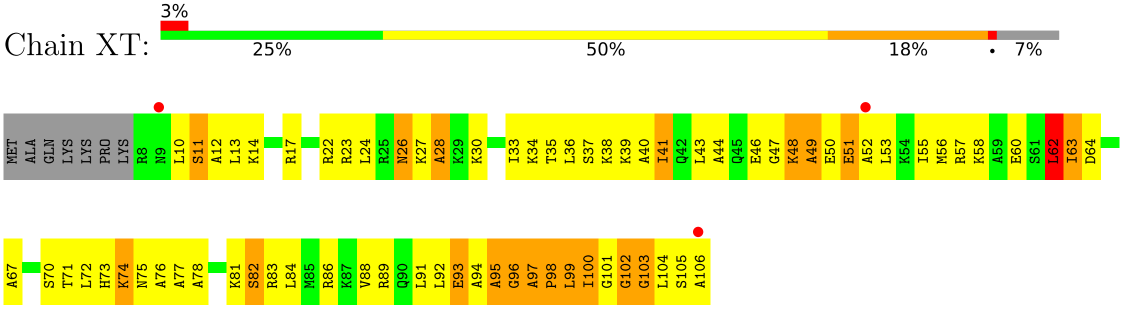


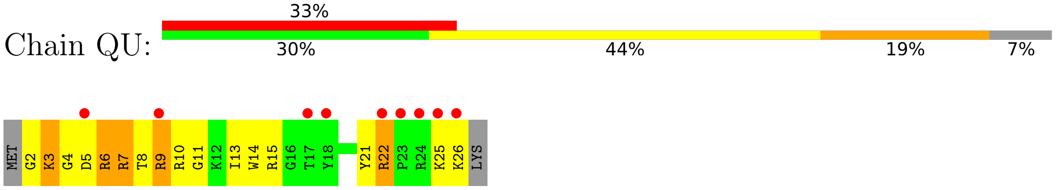
- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



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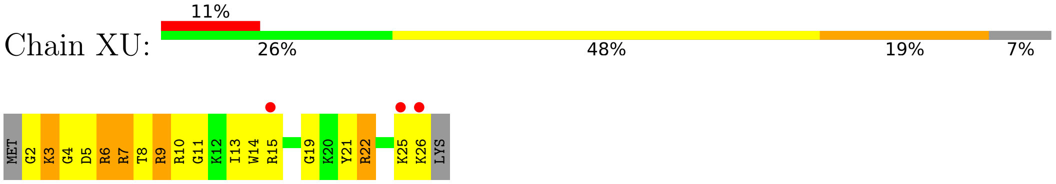
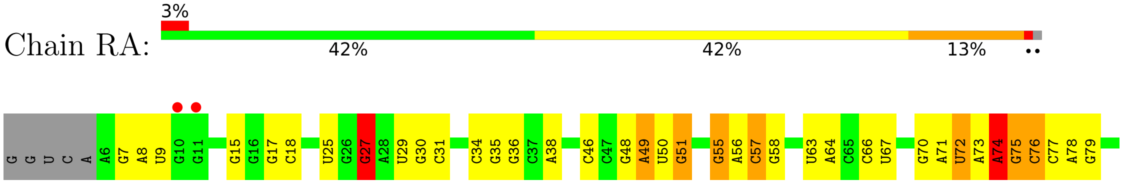
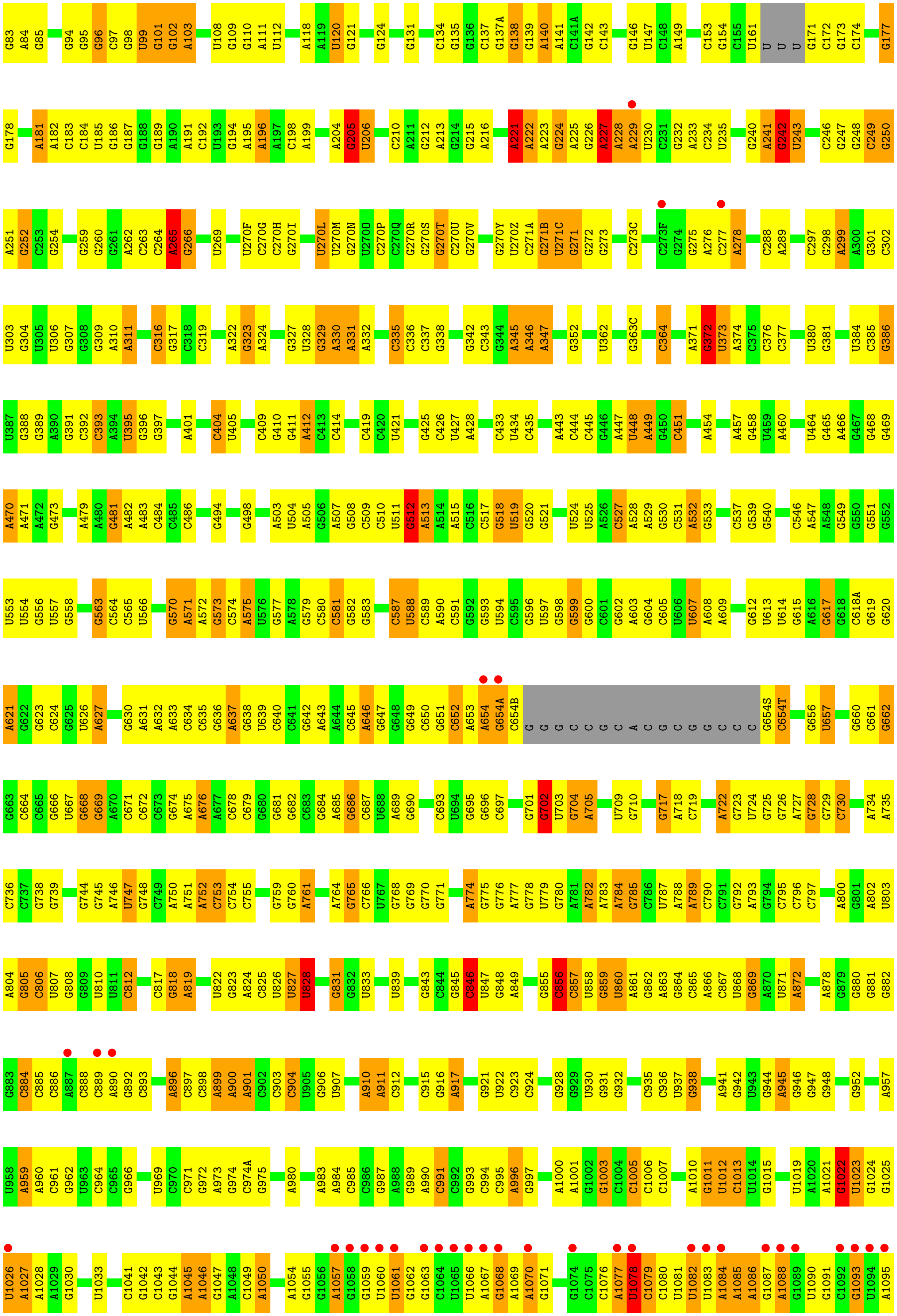


- Molecule 22: 23S Ribosomal RNA

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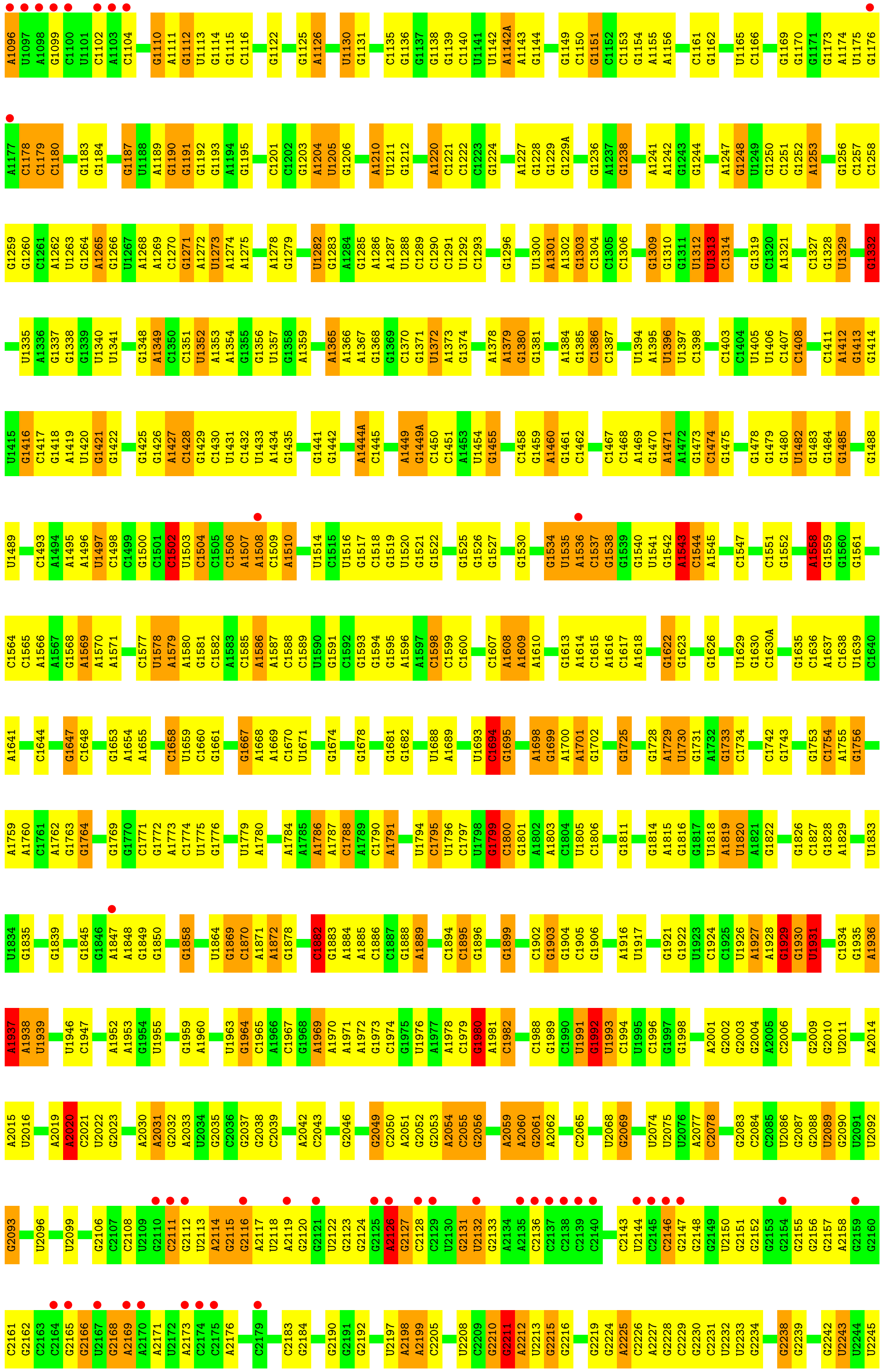
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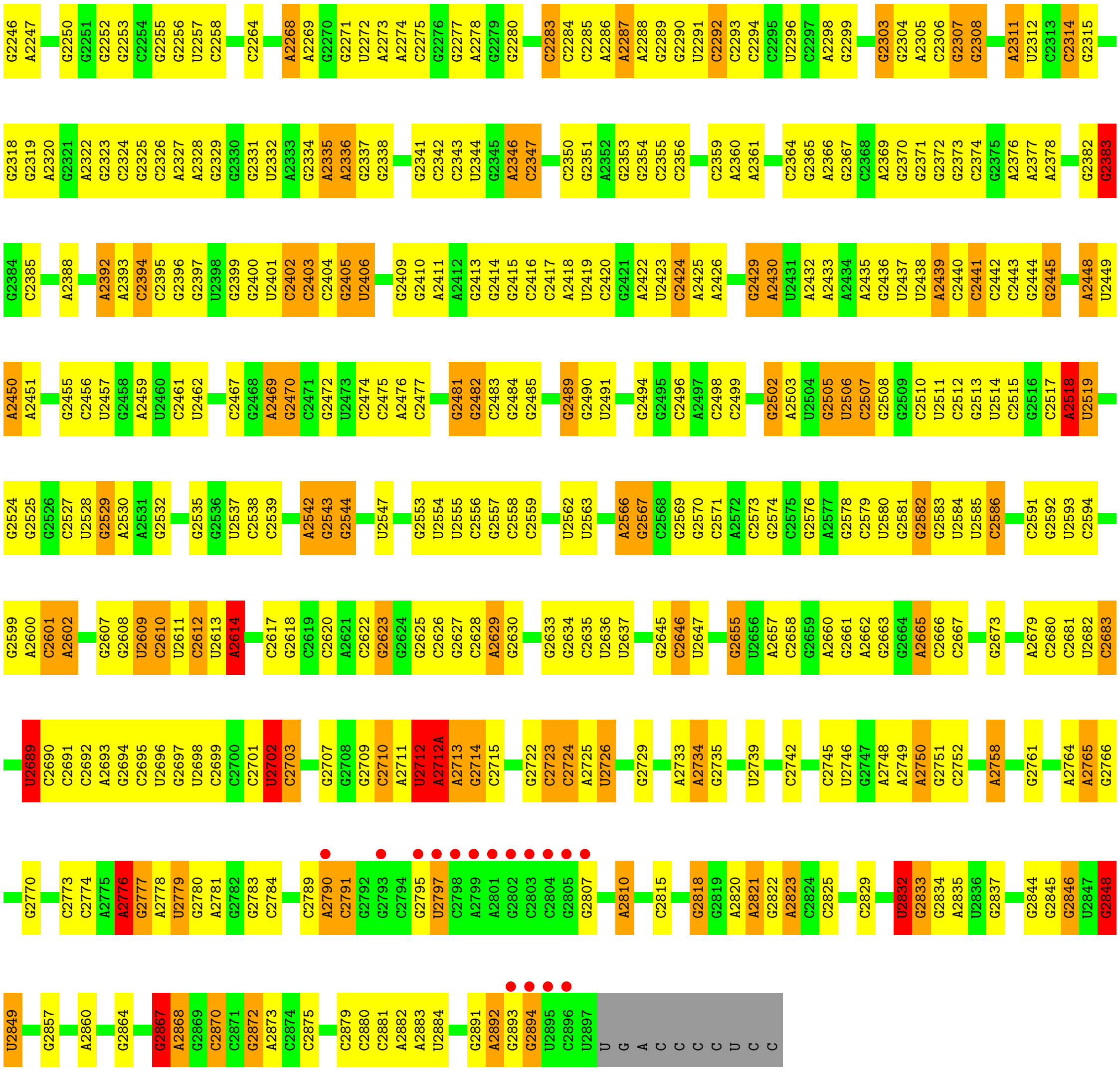

- Molecule 22: 23S Ribosomal RNA

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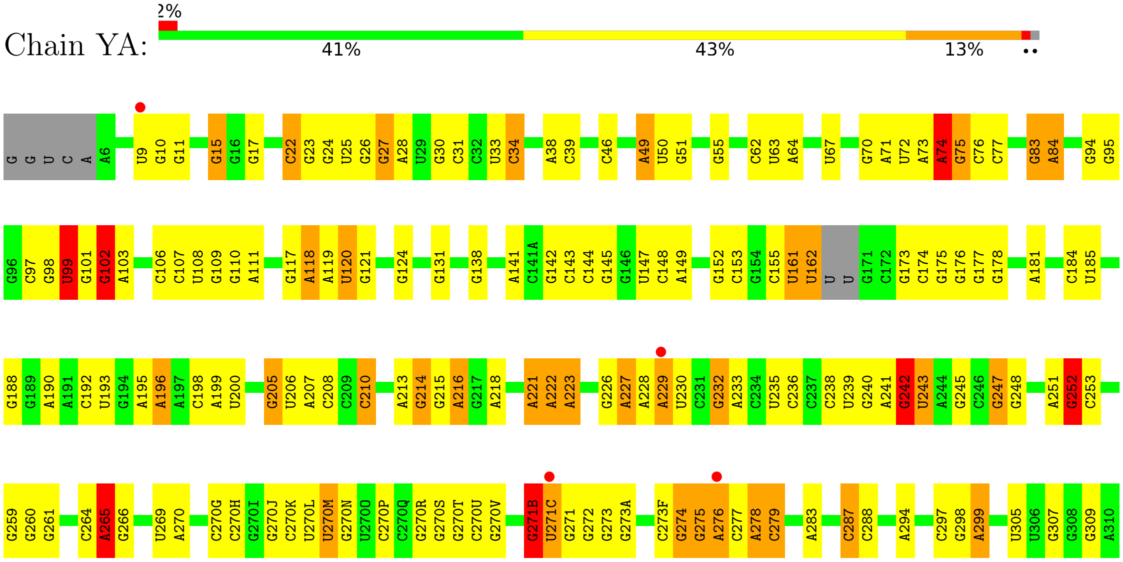

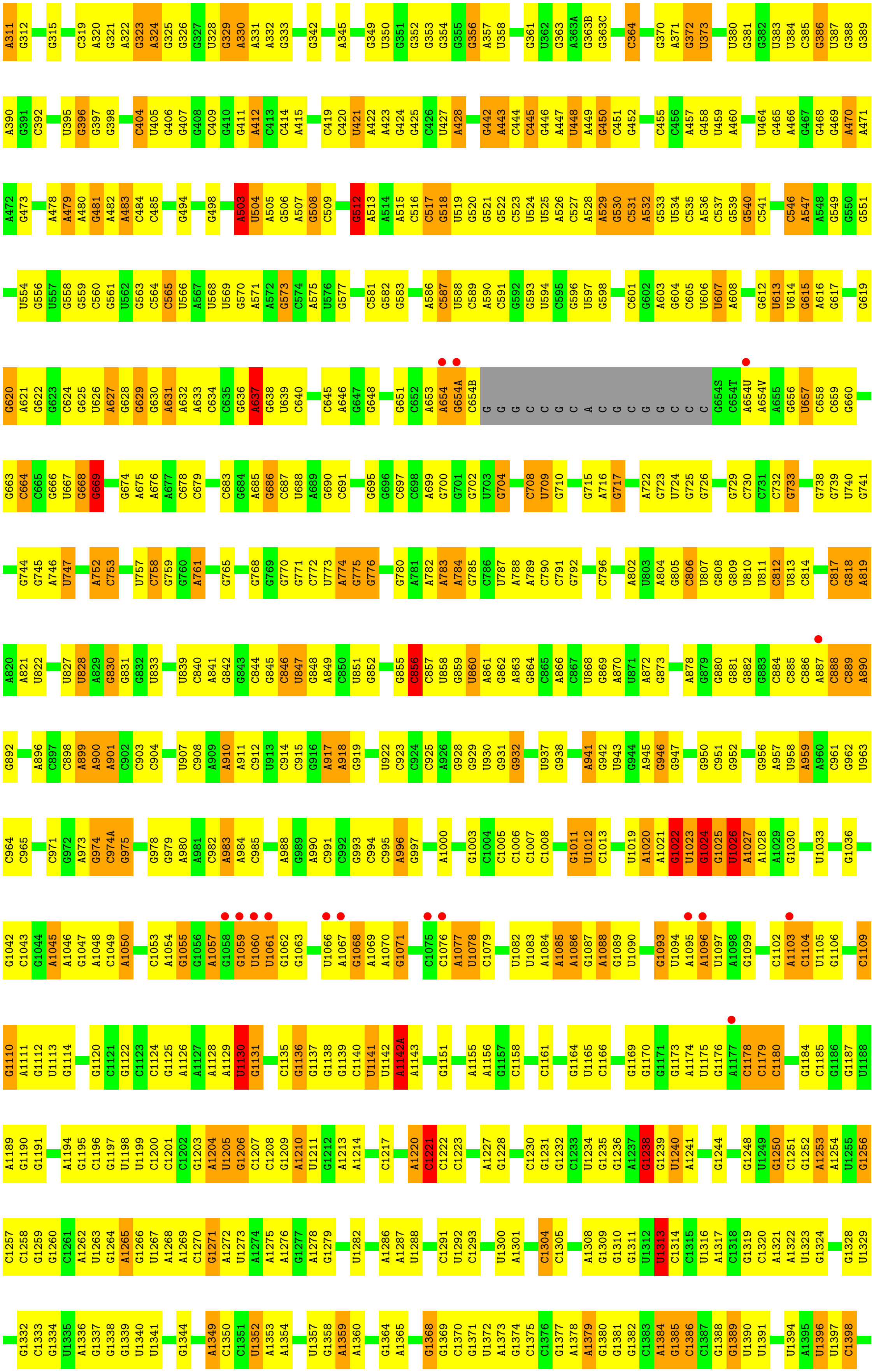
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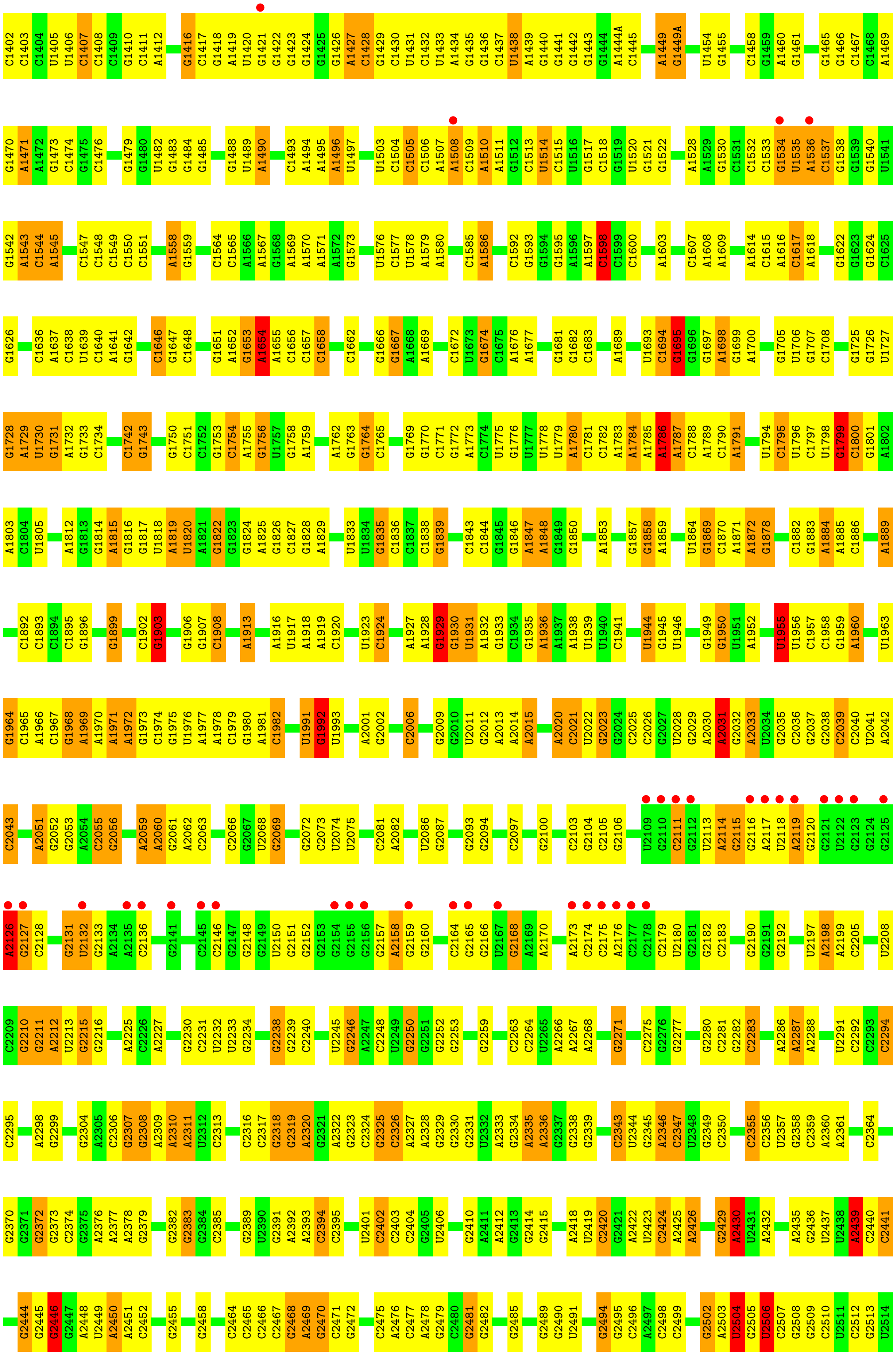
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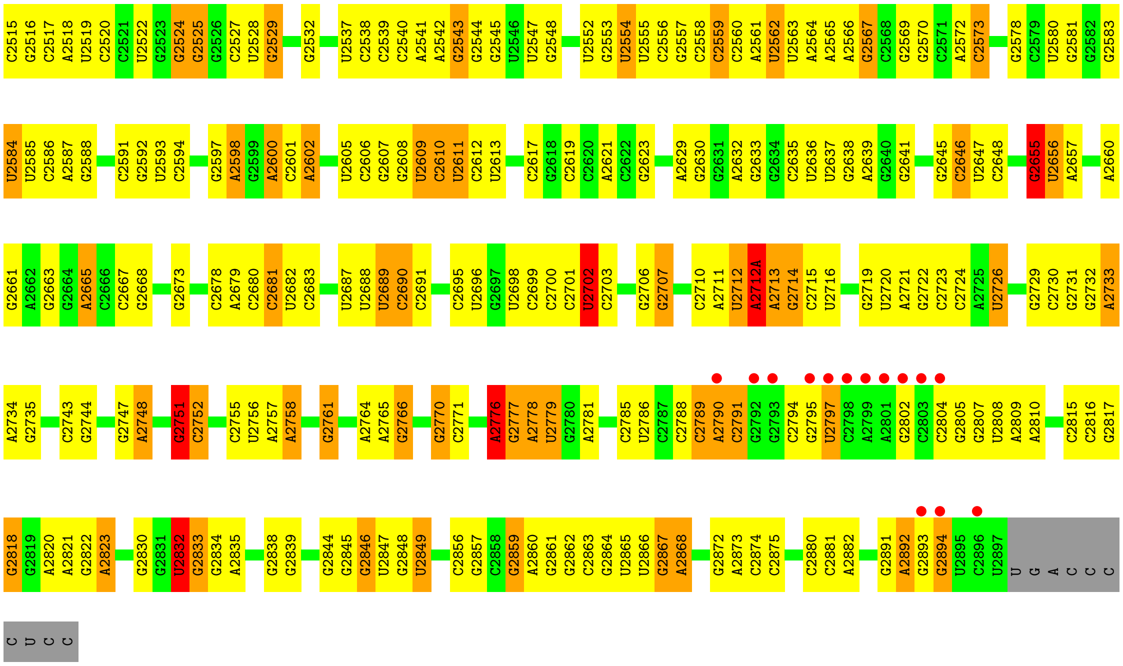
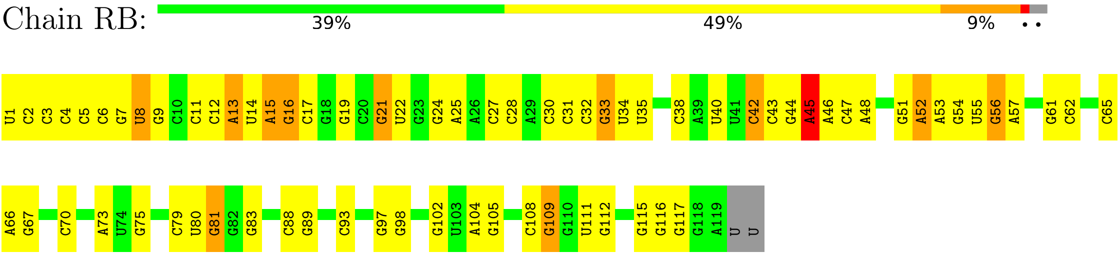
G2444 G2445 G2446 G2447 A2448 U2449 A2450 A2451 C2452 G2455 G2458 C2464 C2465 C2466 C2467 G2468 A2469 G2470 C2471 G2472 C2475 A2476 C2477 A2478 G2479 C2480 G2481 G2482 G2485 G2489 G2490 U2491 G2494 G2495 C2496 A2497 C2498 C2499 G2502 A2503 U2504 G2505 U2506 C2507 G2508 G2509 C2510 U2511 C2512 G2513 U2514



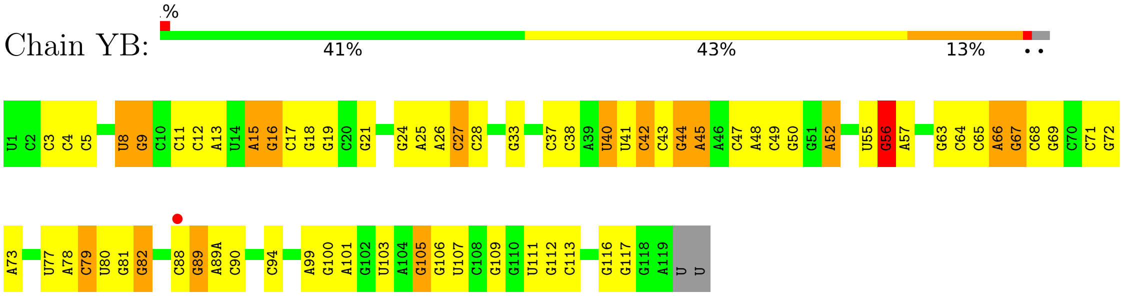
- Molecule 23: 5S Ribosomal RNA

Chain RB:



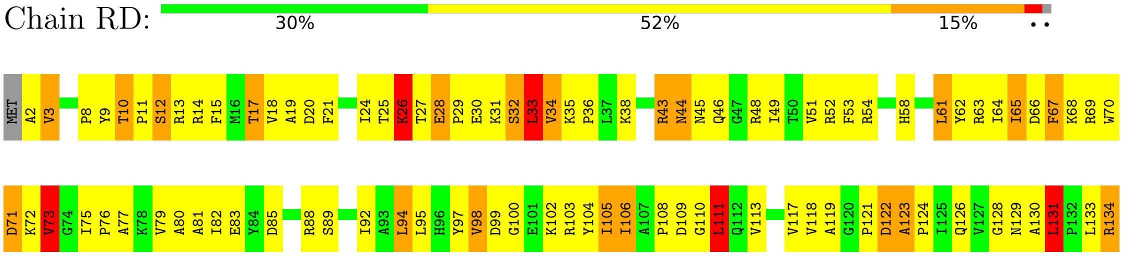
- Molecule 23: 5S Ribosomal RNA

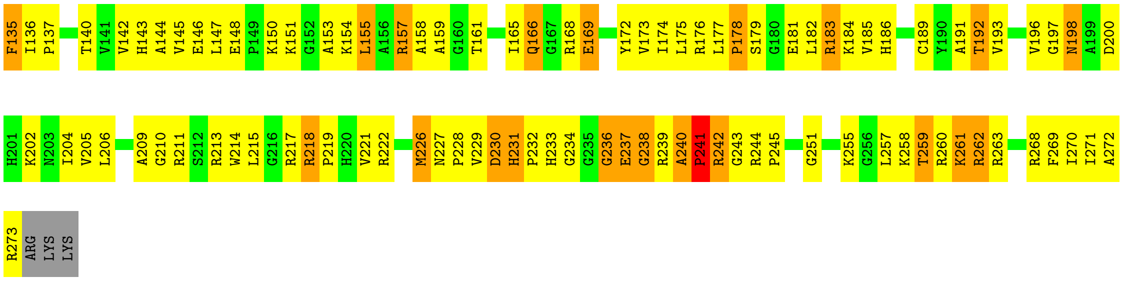
Chain YB:



- Molecule 24: 50S ribosomal protein L2

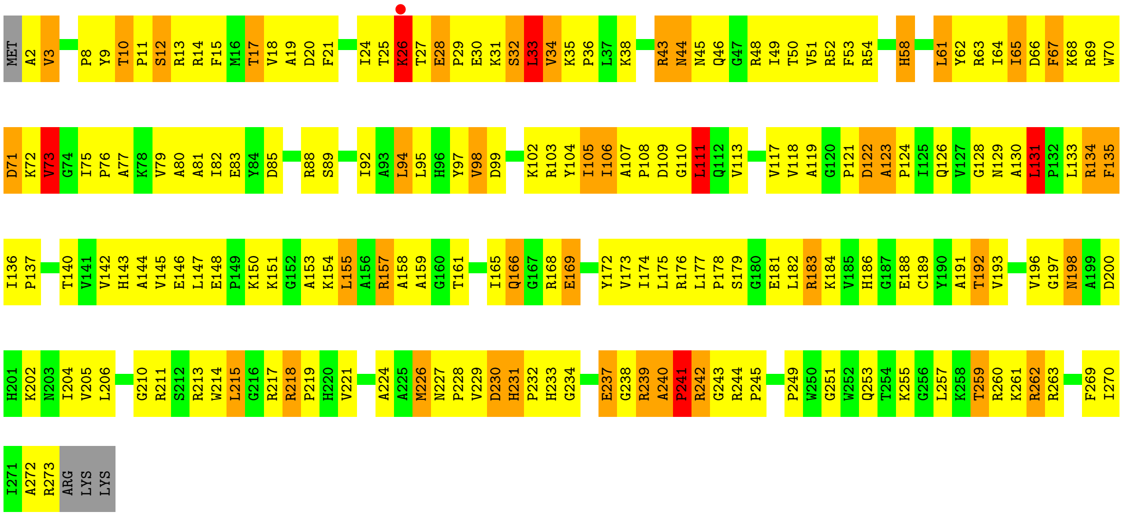
Chain RD:





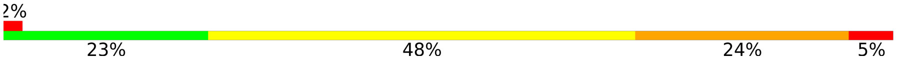
- Molecule 24: 50S ribosomal protein L2

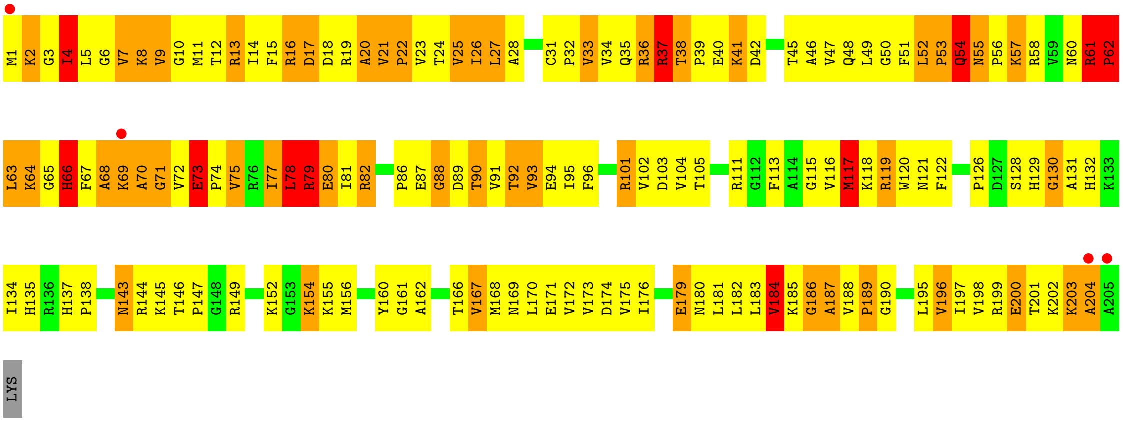
Chain YD:



- Molecule 25: 50S ribosomal protein L3

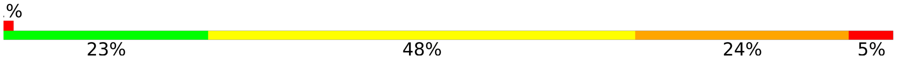
Chain RE:

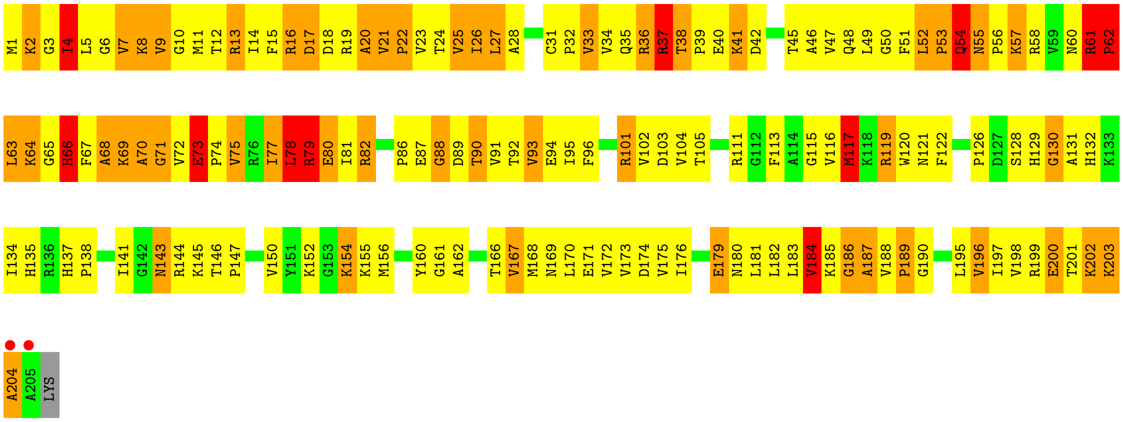




- Molecule 25: 50S ribosomal protein L3

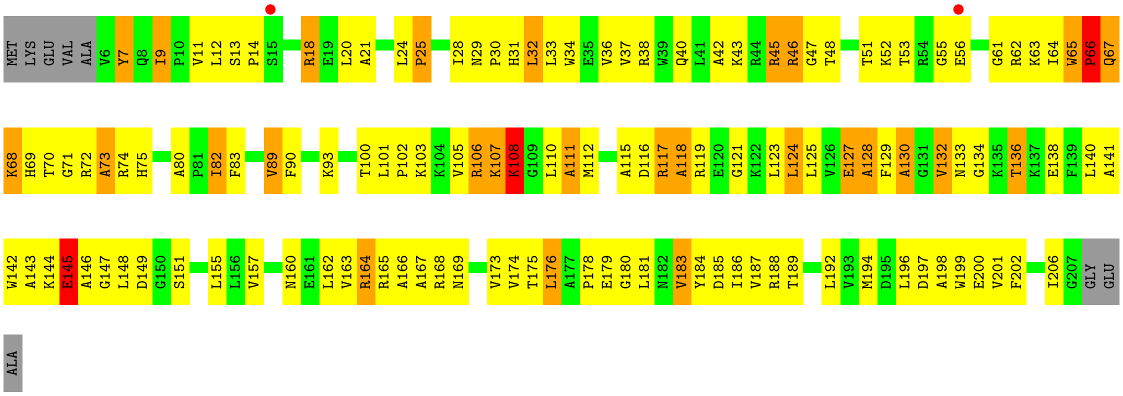
Chain YE:





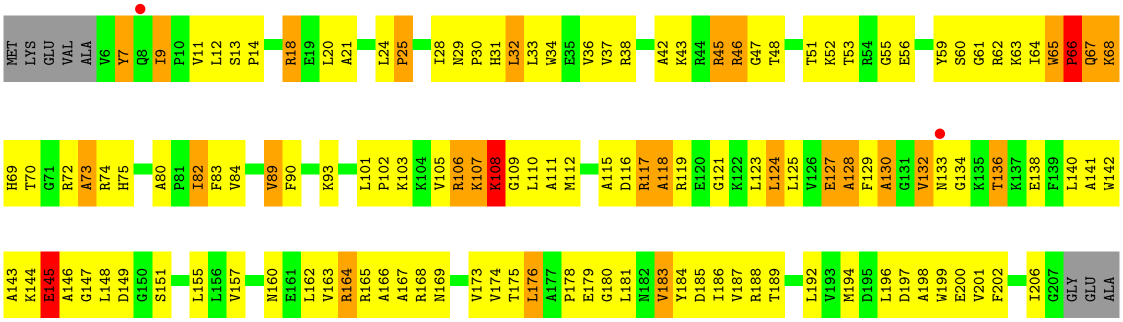
- Molecule 26: 50S ribosomal protein L4

Chain RF:



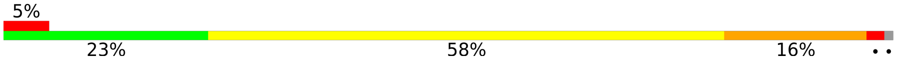
- Molecule 26: 50S ribosomal protein L4

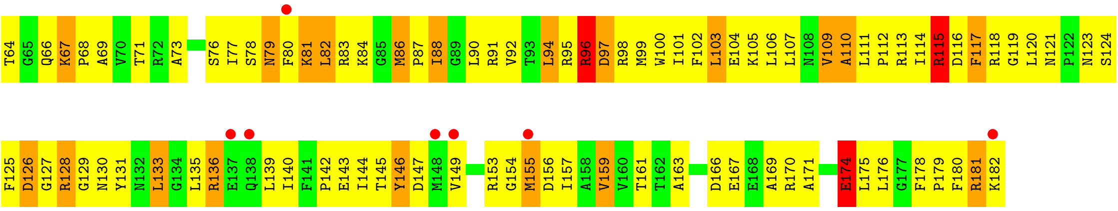
Chain YF:



- Molecule 27: 50S ribosomal protein L5

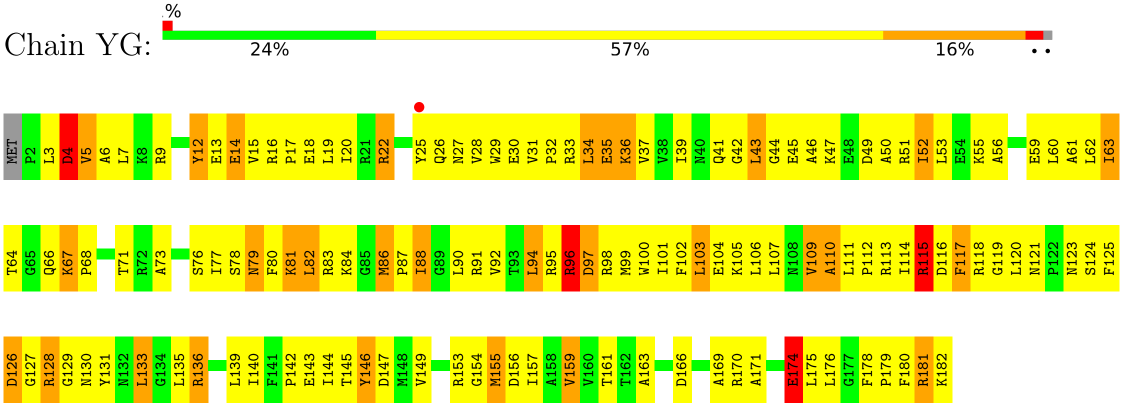
Chain RG:





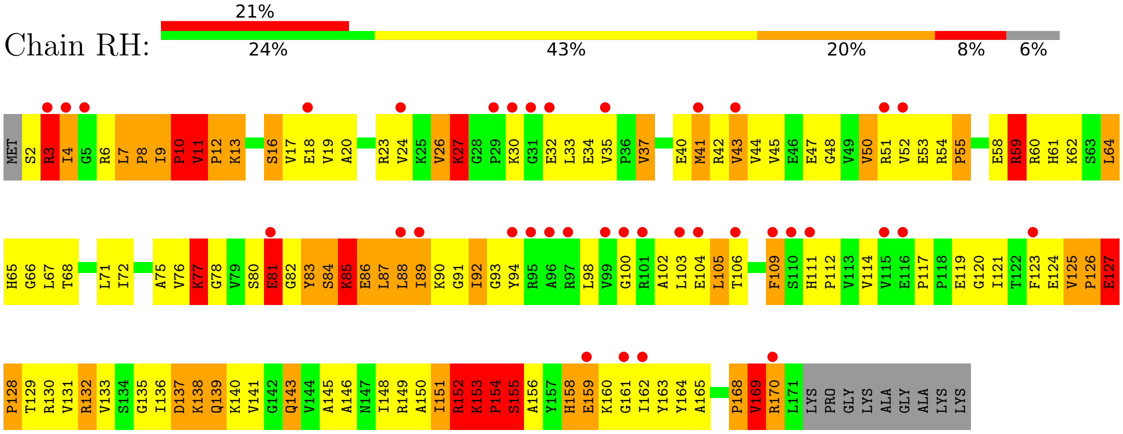
- Molecule 27: 50S ribosomal protein L5

Chain YG:



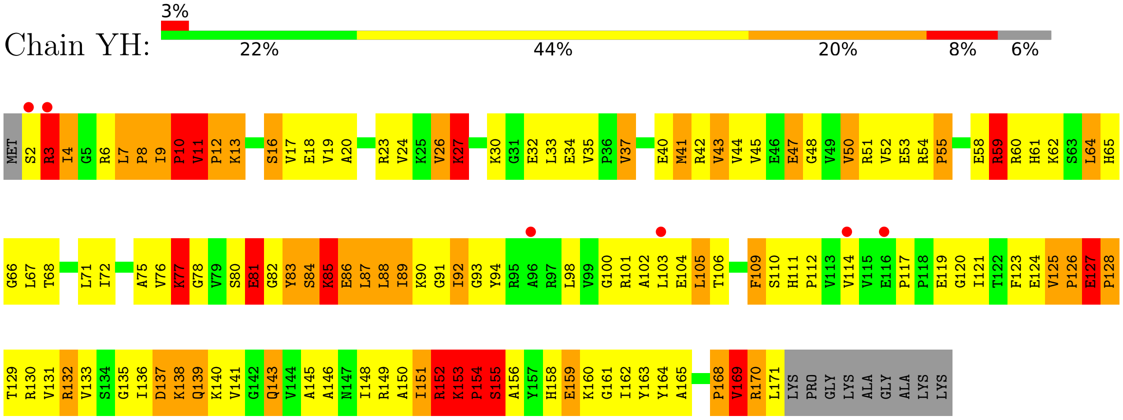
- Molecule 28: 50S ribosomal protein L6

Chain RH:

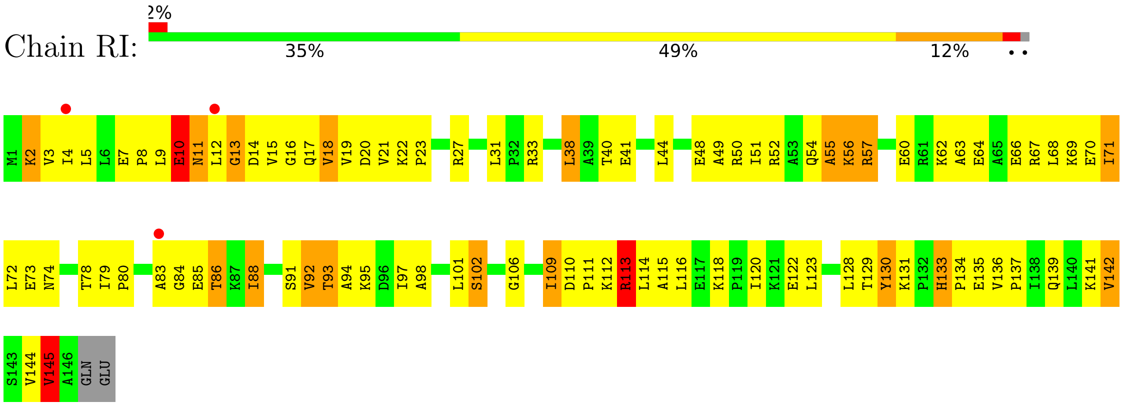


- Molecule 28: 50S ribosomal protein L6

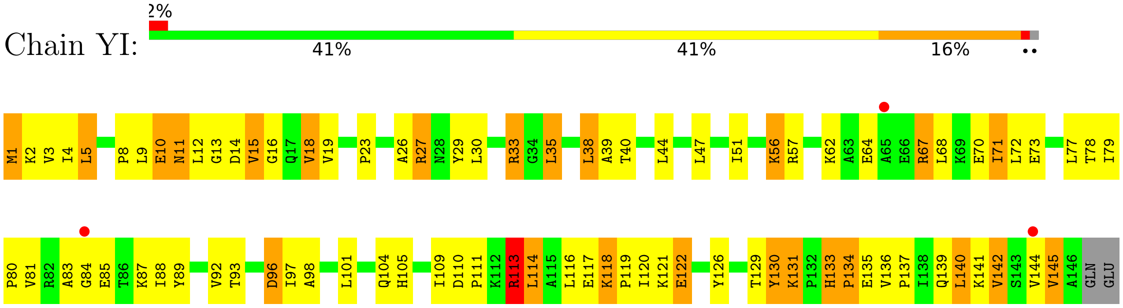
Chain YH:



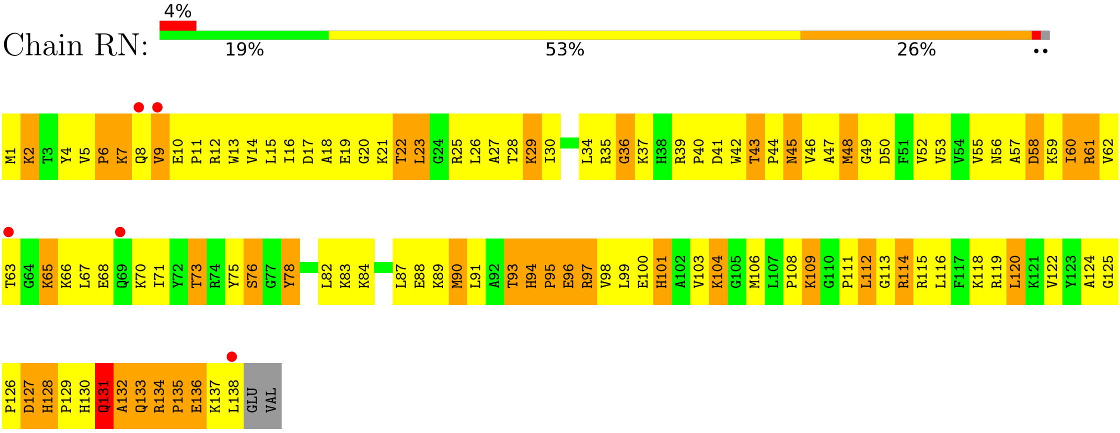
- Molecule 29: 50S ribosomal protein L9



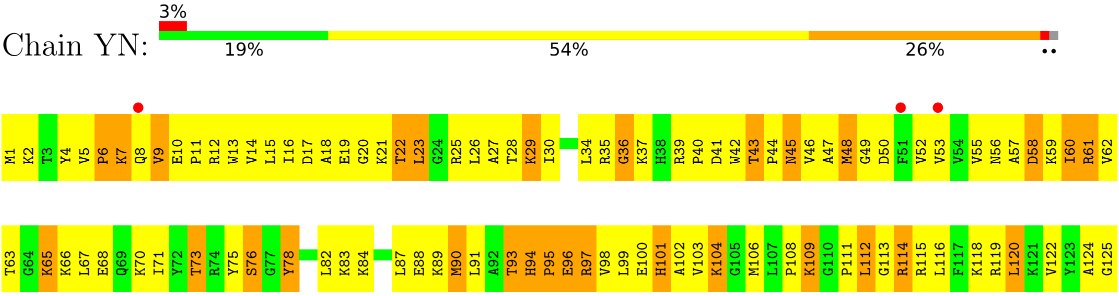
- Molecule 29: 50S ribosomal protein L9

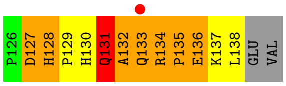


- Molecule 30: 50S ribosomal protein L13



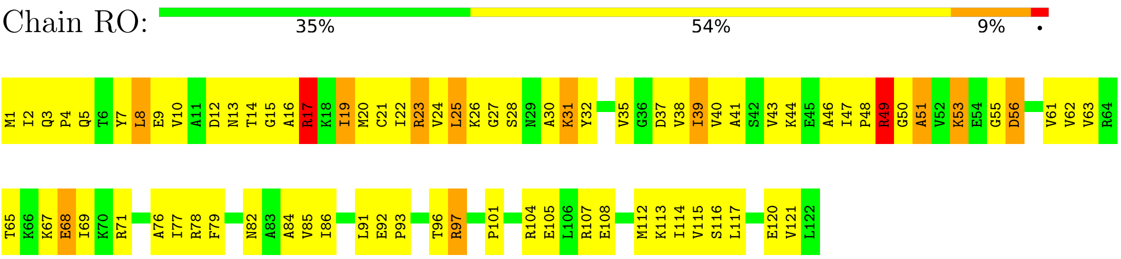
- Molecule 30: 50S ribosomal protein L13





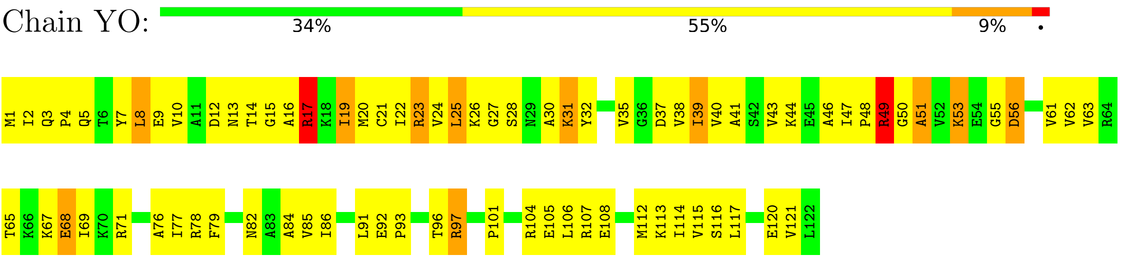
- Molecule 31: 50S ribosomal protein L14

Chain RO:



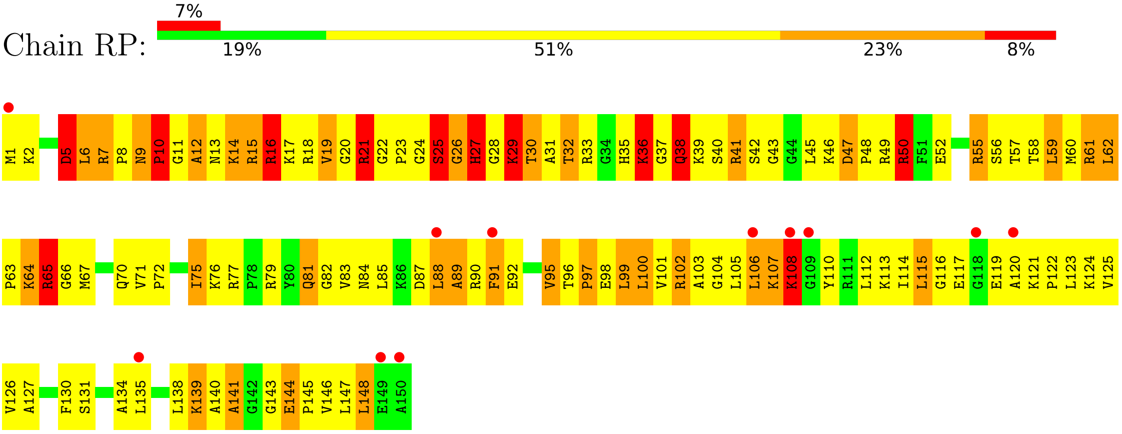
- Molecule 31: 50S ribosomal protein L14

Chain YO:



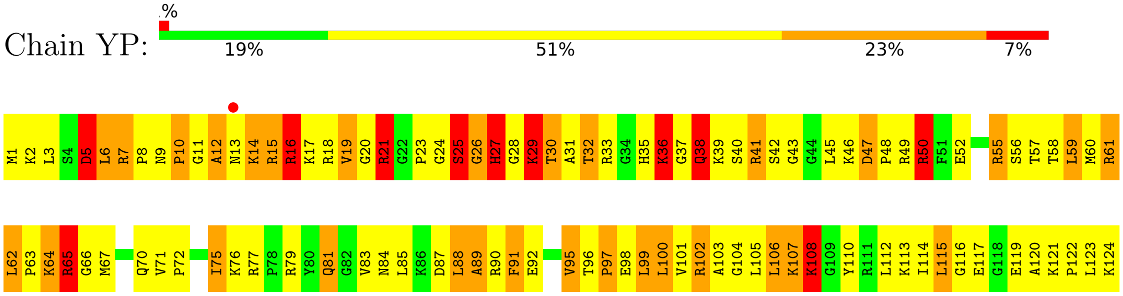
- Molecule 32: 50S ribosomal protein L15

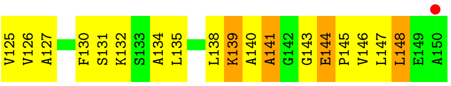
Chain RP:



- Molecule 32: 50S ribosomal protein L15

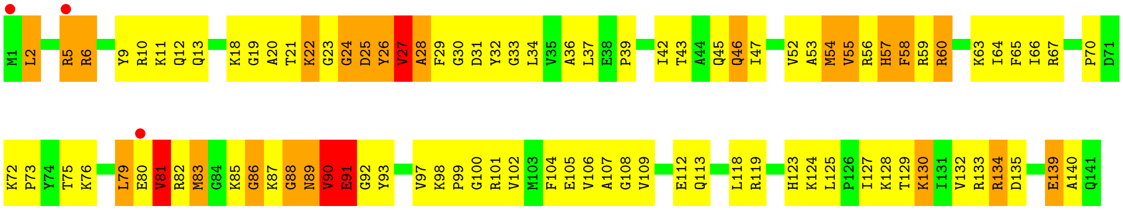
Chain YP:





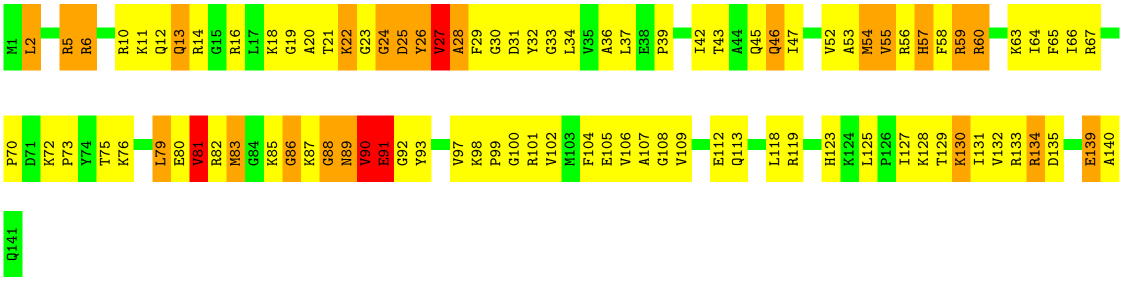
- Molecule 33: 50S ribosomal protein L16

Chain RQ:



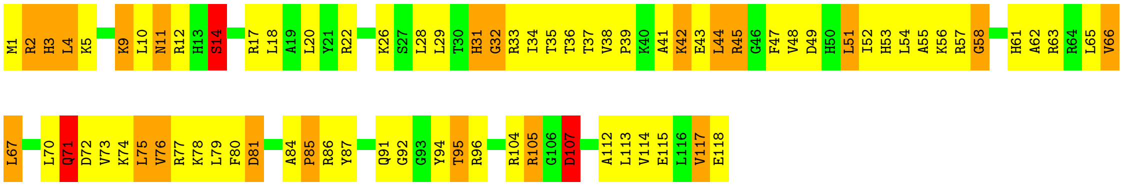
- Molecule 33: 50S ribosomal protein L16

Chain YQ:



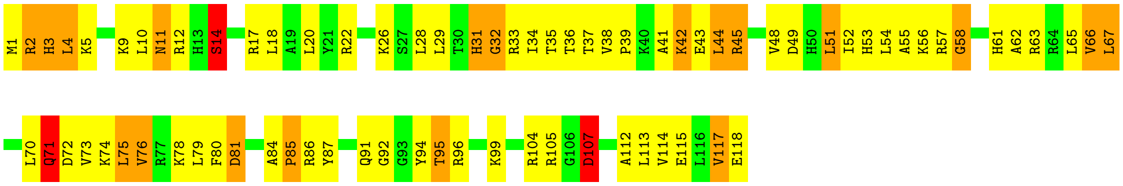
- Molecule 34: 50S ribosomal protein L17

Chain RR:

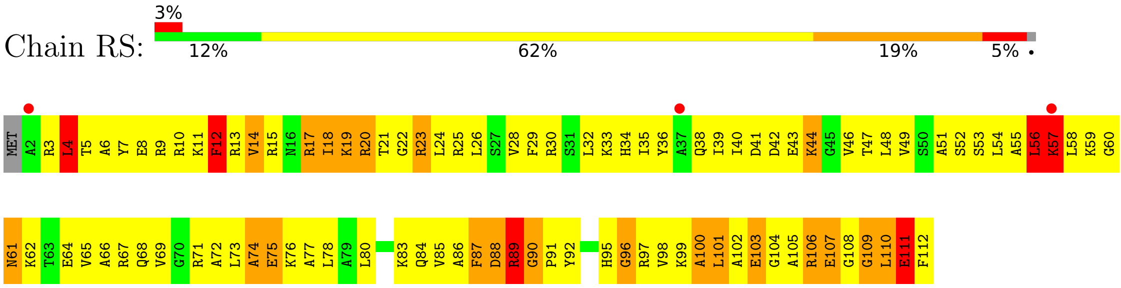


- Molecule 34: 50S ribosomal protein L17

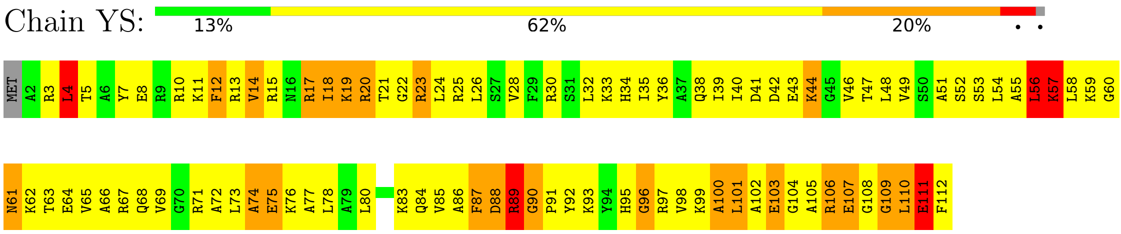
Chain YR:



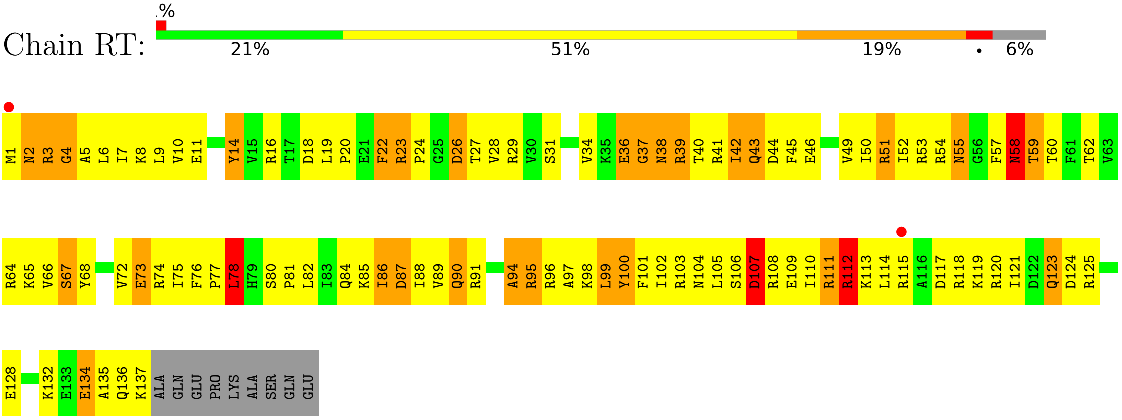
- Molecule 35: 50S ribosomal protein L18



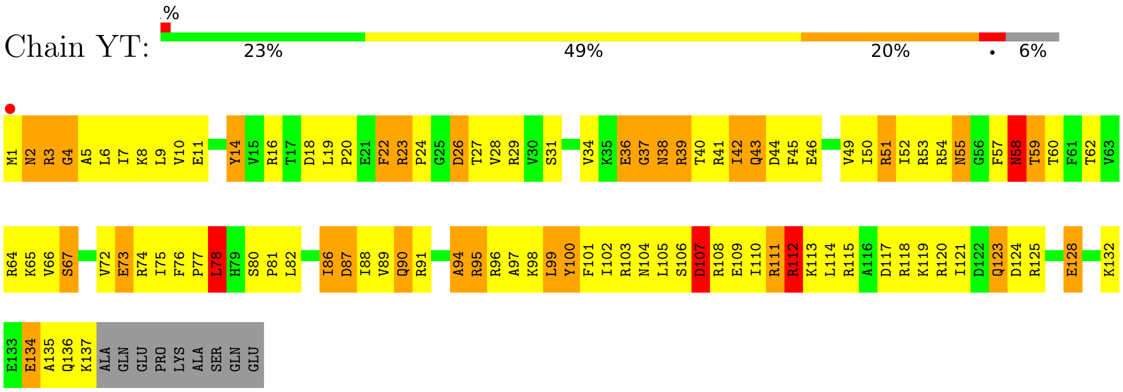
- Molecule 35: 50S ribosomal protein L18



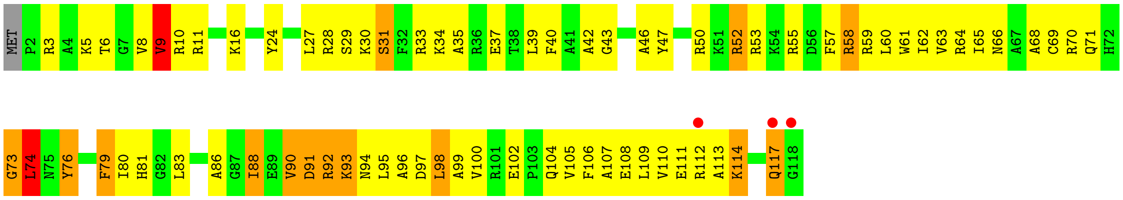
- Molecule 36: 50S ribosomal protein L19



- Molecule 36: 50S ribosomal protein L19

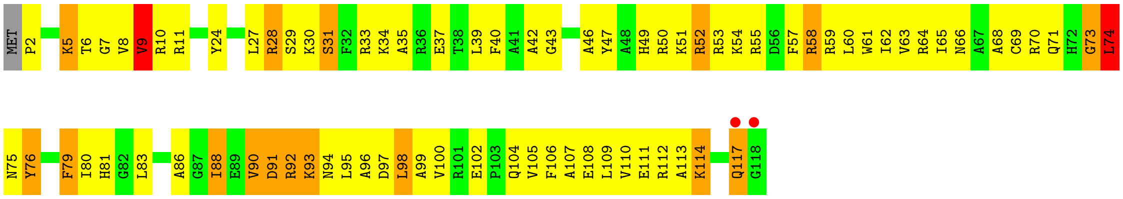


- Molecule 37: 50S ribosomal protein L20



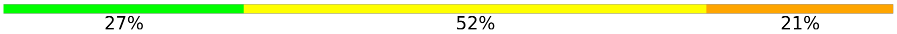
- Molecule 37: 50S ribosomal protein L20

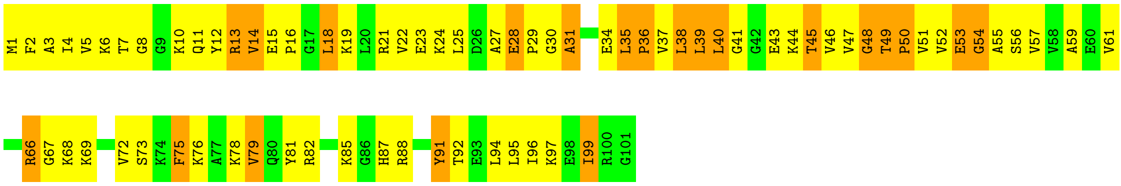
Chain YU:



- Molecule 38: 50S ribosomal protein L21

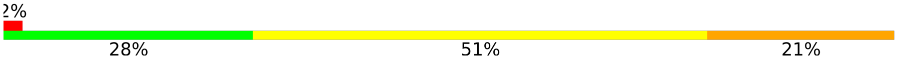
Chain RV:

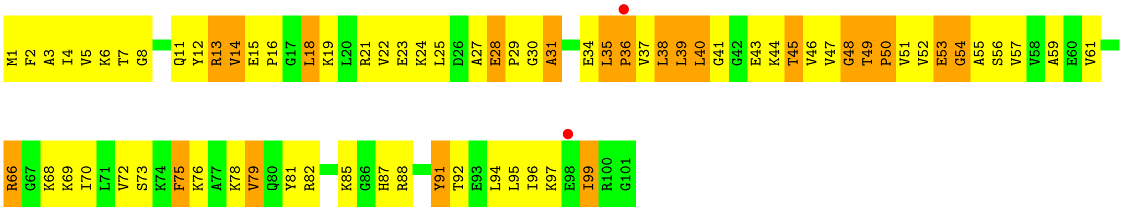




- Molecule 38: 50S ribosomal protein L21

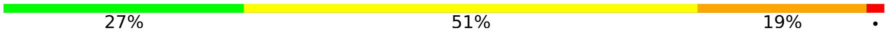
Chain YV:

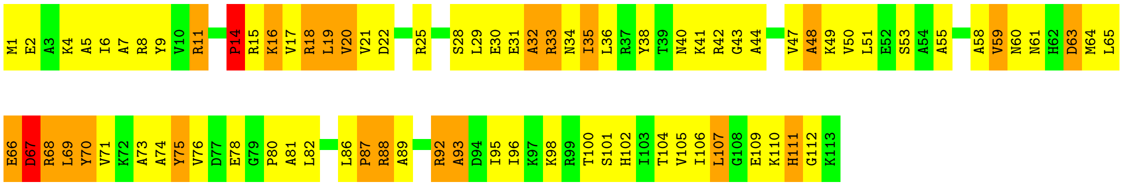




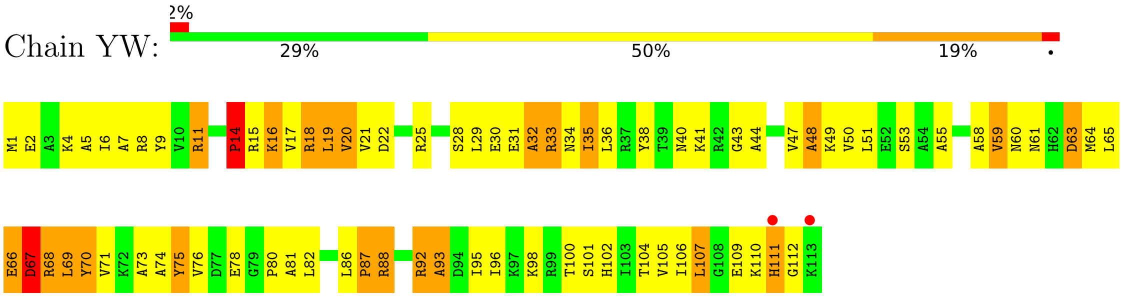
- Molecule 39: 50S ribosomal protein L22

Chain RW:

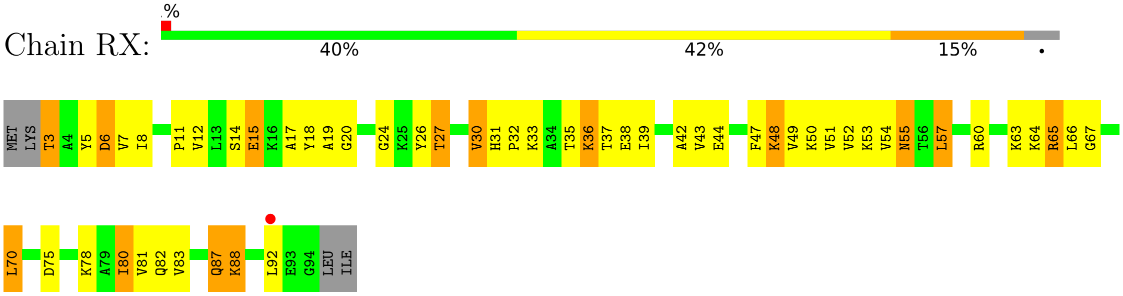




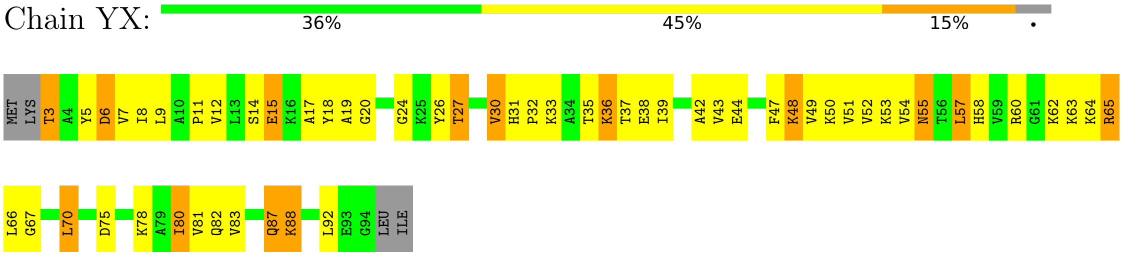
- Molecule 39: 50S ribosomal protein L22



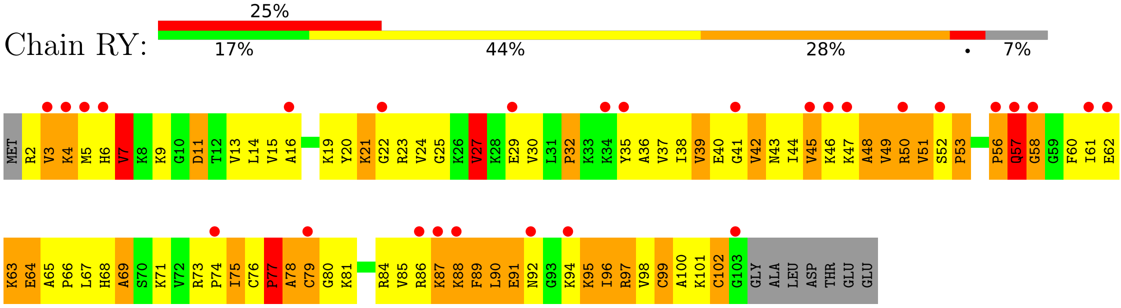
- Molecule 40: 50S ribosomal protein L23



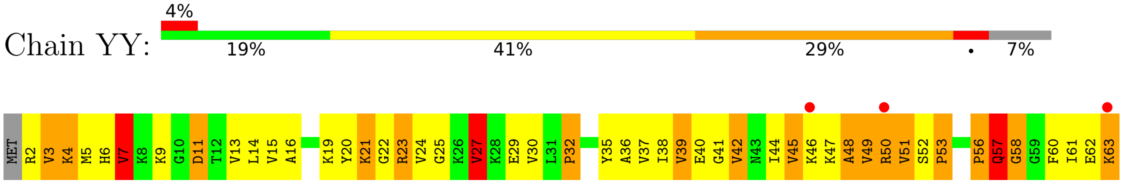
- Molecule 40: 50S ribosomal protein L23

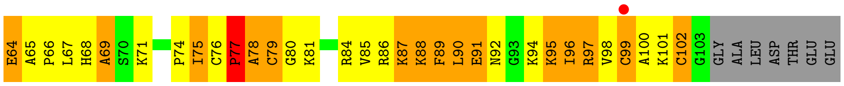


- Molecule 41: 50S ribosomal protein L24



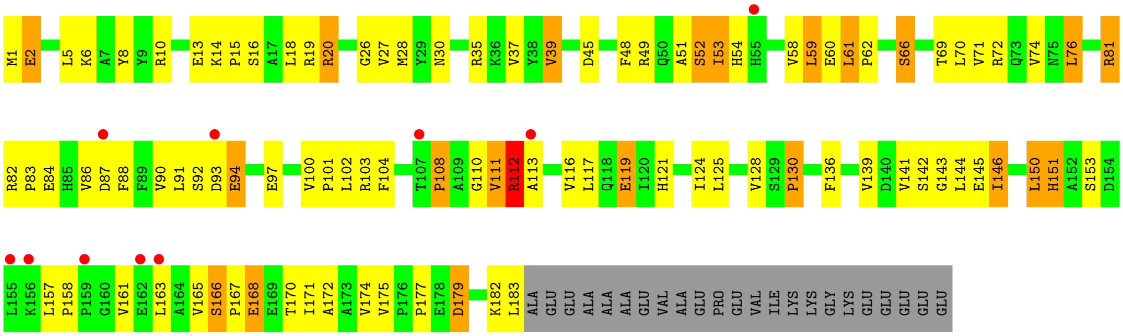
- Molecule 41: 50S ribosomal protein L24





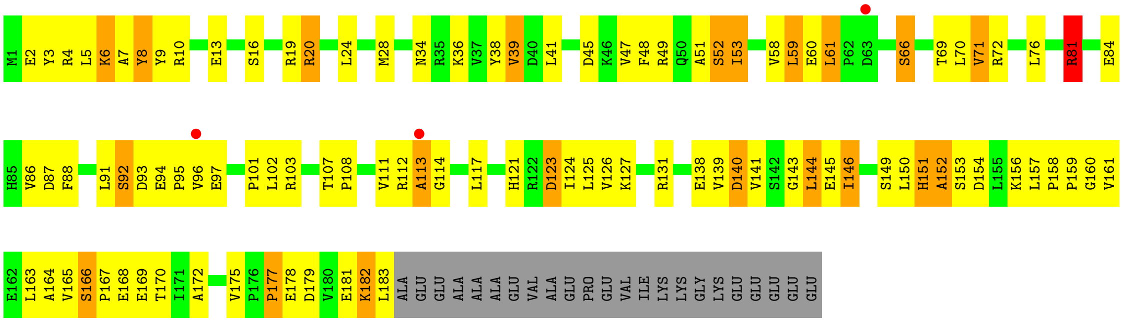
- Molecule 42: 50S ribosomal protein L25

Chain RZ:



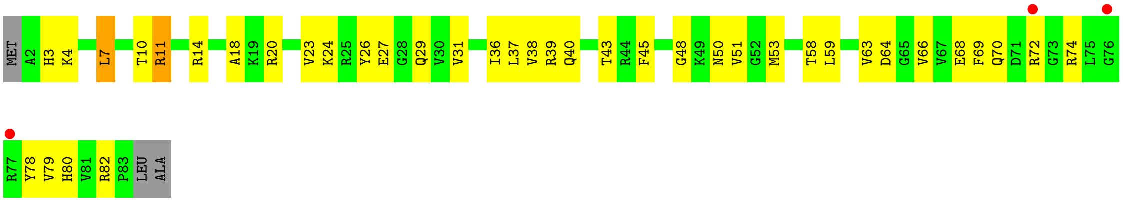
- Molecule 42: 50S ribosomal protein L25

Chain YZ:



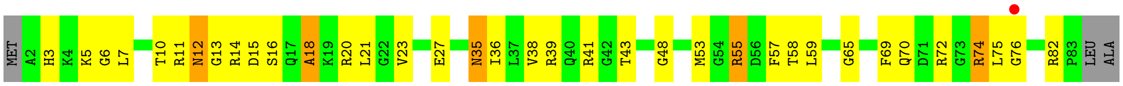
- Molecule 43: 50S ribosomal protein L27

Chain R0:

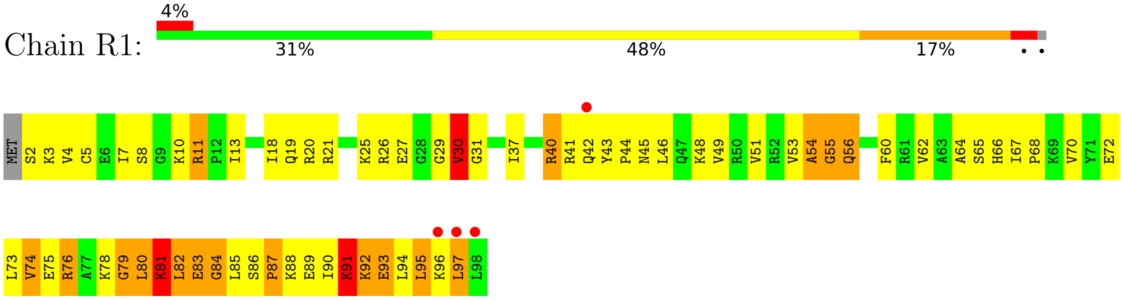


- Molecule 43: 50S ribosomal protein L27

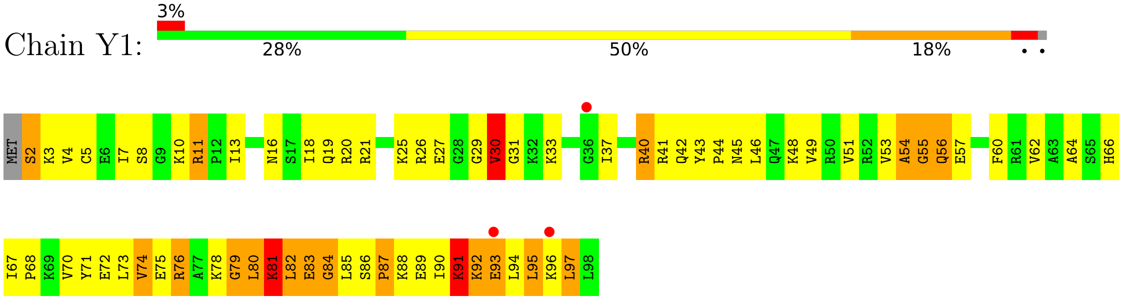
Chain Y0:



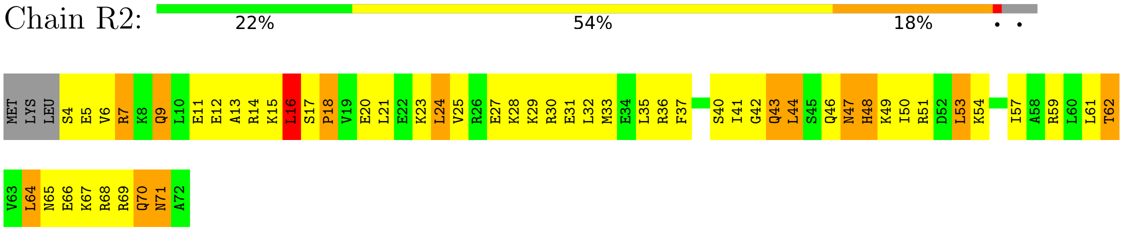
- Molecule 44: 50S ribosomal protein L28



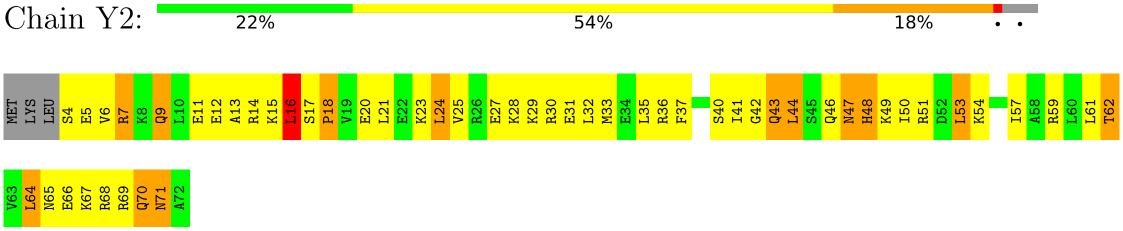
- Molecule 44: 50S ribosomal protein L28



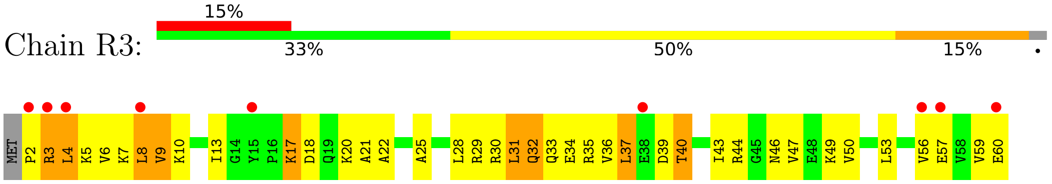
- Molecule 45: 50S ribosomal protein L29



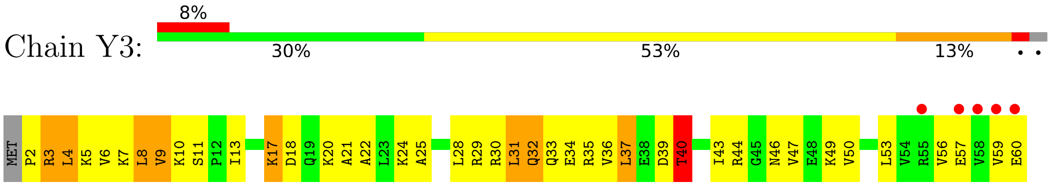
- Molecule 45: 50S ribosomal protein L29



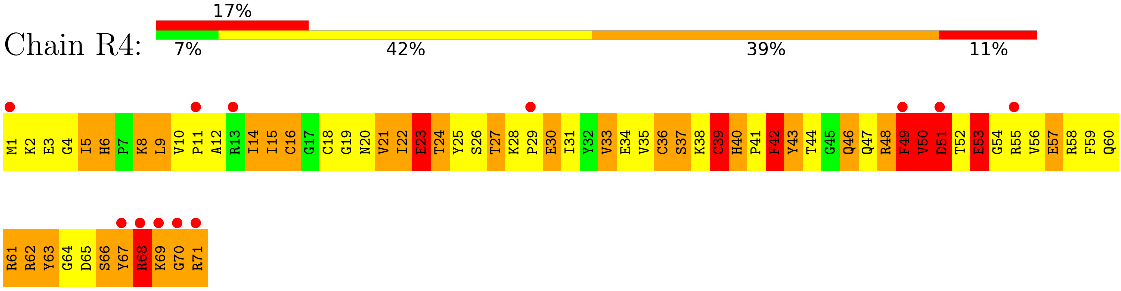
- Molecule 46: 50S ribosomal protein L30



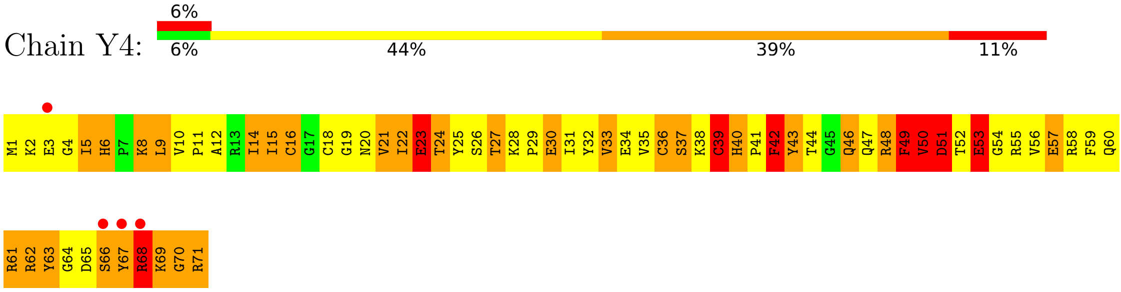
- Molecule 46: 50S ribosomal protein L30



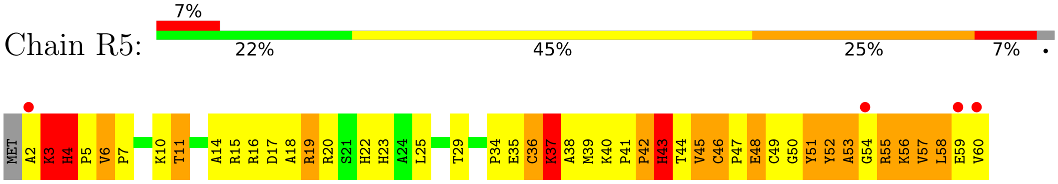
- Molecule 47: 50S ribosomal protein L31



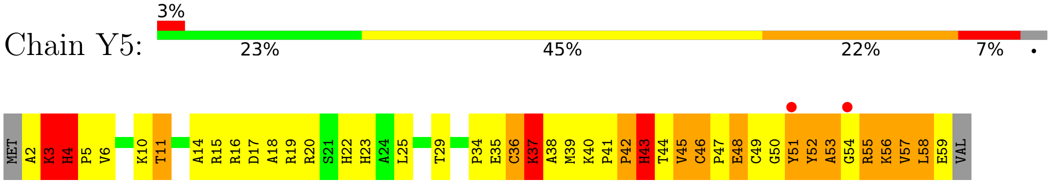
- Molecule 47: 50S ribosomal protein L31



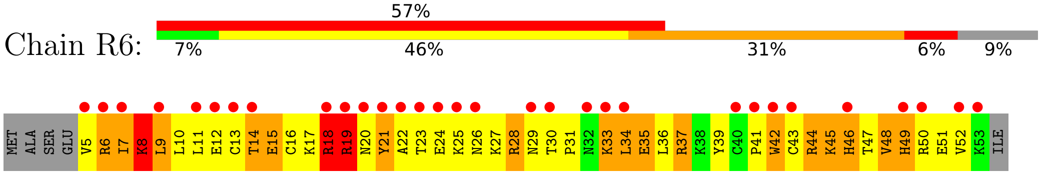
- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32

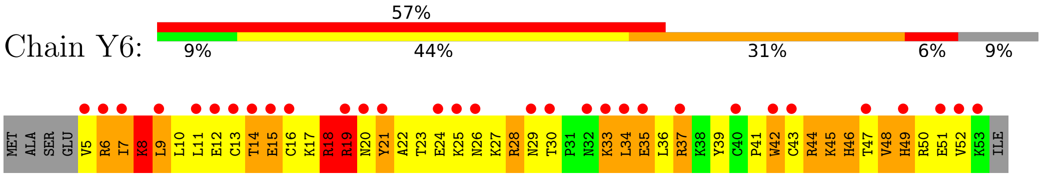


- Molecule 49: 50S ribosomal protein L33



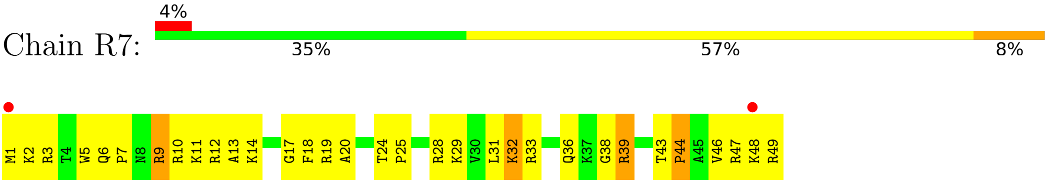
- Molecule 49: 50S ribosomal protein L33

Chain Y6:



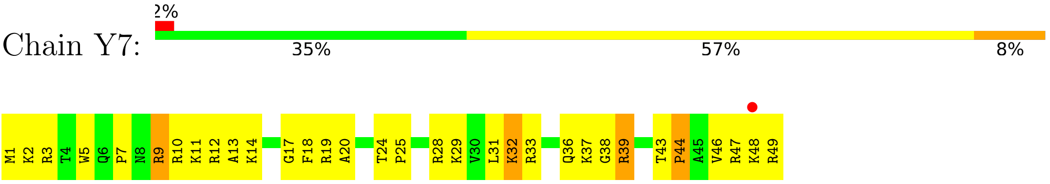
- Molecule 50: 50S ribosomal protein L34

Chain R7:



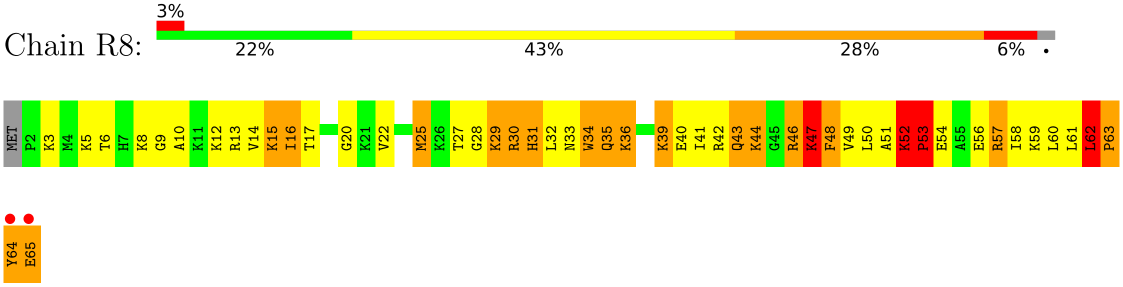
- Molecule 50: 50S ribosomal protein L34

Chain Y7:



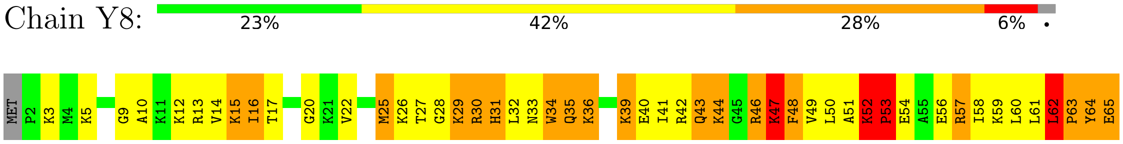
- Molecule 51: 50S ribosomal protein L35

Chain R8:



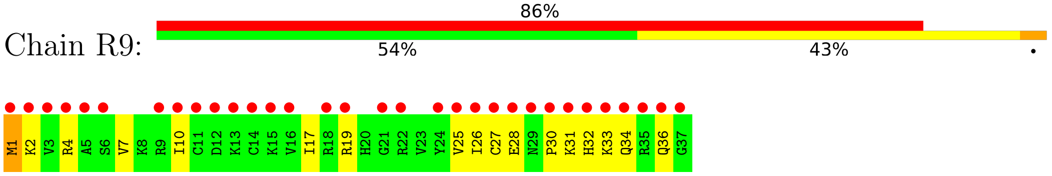
- Molecule 51: 50S ribosomal protein L35

Chain Y8:



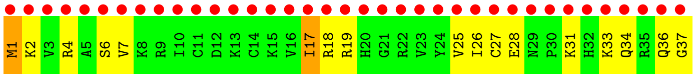
- Molecule 52: 50S ribosomal protein L36

Chain R9:



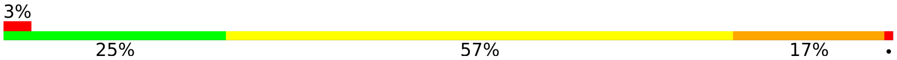
- Molecule 52: 50S ribosomal protein L36

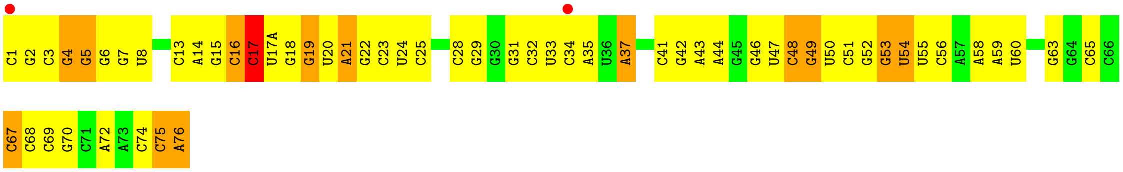
Chain Y9:



- Molecule 53: P-site tRNA fMet

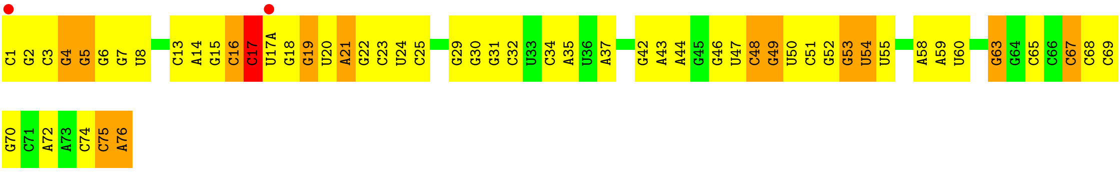
Chain QV:





- Molecule 53: P-site tRNA fMet

Chain XV:



- Molecule 54: A-site ASL SufA6

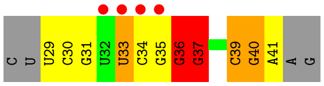
Chain QX:

- Molecule 54: A-site ASL SufA6

Chain XX:

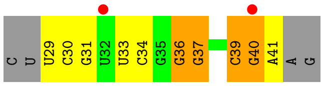
- Molecule 55: messenger RNA

Chain QY:



- Molecule 55: messenger RNA

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	210.24Å 446.10Å 623.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 3.90 49.68 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.68-3.90) 99.1 (49.68-3.70)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$[1]	1.66 (at 3.67Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.278 0.235 , 0.278	Depositor DCC
R_{free} test set	27641 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å^2)	88.0	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	291950	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 1MG, PAR, ZN, PPU, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	QA	0.43	0/36098	0.95	64/56341 (0.1%)
1	XA	0.48	0/36101	1.01	70/56346 (0.1%)
2	QB	0.35	0/1959	0.65	0/2642
2	XB	0.35	0/1959	0.65	0/2642
3	QC	0.36	0/1629	0.60	0/2195
3	XC	0.37	0/1629	0.60	0/2195
4	QD	0.41	0/1733	0.68	1/2318 (0.0%)
4	XD	0.44	0/1733	0.68	1/2318 (0.0%)
5	QE	0.38	0/1171	0.66	0/1576
5	XE	0.38	0/1171	0.66	0/1576
6	QF	0.43	0/856	0.68	0/1154
6	XF	0.43	0/856	0.68	0/1154
7	QG	0.37	0/1276	0.60	0/1709
7	XG	0.36	0/1276	0.60	0/1709
8	QH	0.40	0/1136	0.69	0/1527
8	XH	0.40	0/1136	0.69	0/1527
9	QI	0.36	0/1029	0.67	0/1379
9	XI	0.36	0/1029	0.67	0/1379
10	QJ	0.35	0/814	0.61	0/1095
10	XJ	0.36	0/814	0.61	0/1095
11	QK	0.40	0/900	0.67	0/1213
11	XK	0.40	0/900	0.67	0/1213
12	QL	0.48	1/991 (0.1%)	0.79	2/1327 (0.2%)
12	XL	0.48	1/991 (0.1%)	0.79	2/1327 (0.2%)
13	QM	0.34	0/974	0.66	0/1303
13	XM	0.34	0/974	0.66	0/1303
14	QN	0.42	0/501	0.68	0/664
14	XN	0.52	0/501	0.67	0/664
15	QO	0.39	0/745	0.67	0/992
15	XO	0.39	0/745	0.66	0/992
16	QP	0.36	0/721	0.67	0/970
16	XP	0.37	0/721	0.67	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	QQ	0.37	0/847	0.68	0/1131
17	XQ	0.38	0/847	0.68	0/1131
18	QR	0.39	0/579	0.72	0/768
18	XR	0.39	0/579	0.72	0/768
19	QS	0.36	0/689	0.84	2/926 (0.2%)
19	XS	0.36	0/689	0.84	2/926 (0.2%)
20	QT	0.33	0/765	0.69	0/1007
20	XT	0.34	0/765	0.69	0/1007
21	QU	0.37	0/221	0.63	0/288
21	XU	0.37	0/221	0.63	0/288
22	RA	0.53	2/69521 (0.0%)	1.06	133/108529 (0.1%)
22	YA	0.59	2/69543 (0.0%)	1.12	219/108563 (0.2%)
23	RB	0.41	0/2878	0.95	4/4490 (0.1%)
23	YB	0.49	0/2878	1.04	4/4490 (0.1%)
24	RD	0.59	2/2165 (0.1%)	0.90	4/2919 (0.1%)
24	YD	0.56	1/2165 (0.0%)	0.90	4/2919 (0.1%)
25	RE	0.52	0/1601	0.91	2/2160 (0.1%)
25	YE	0.52	0/1601	0.91	2/2160 (0.1%)
26	RF	0.50	0/1620	0.76	0/2194
26	YF	0.50	0/1620	0.76	0/2194
27	RG	0.40	0/1499	0.66	0/2016
27	YG	0.40	0/1499	0.66	0/2016
28	RH	0.45	0/1332	0.85	3/1802 (0.2%)
28	YH	0.45	0/1332	0.85	4/1802 (0.2%)
29	RI	0.54	2/1151 (0.2%)	0.68	1/1558 (0.1%)
29	YI	0.34	0/1151	0.61	0/1558
30	RN	0.46	0/1131	0.78	1/1525 (0.1%)
30	YN	0.46	0/1131	0.78	1/1525 (0.1%)
31	RO	0.54	0/943	0.71	0/1269
31	YO	0.53	0/943	0.71	0/1269
32	RP	0.50	0/1162	0.94	3/1544 (0.2%)
32	YP	0.50	0/1162	0.95	3/1544 (0.2%)
33	RQ	0.54	0/1143	0.91	3/1527 (0.2%)
33	YQ	0.54	0/1143	0.89	3/1527 (0.2%)
34	RR	0.45	0/982	0.80	1/1312 (0.1%)
34	YR	0.45	0/982	0.80	1/1312 (0.1%)
35	RS	0.46	0/892	0.82	1/1187 (0.1%)
35	YS	0.45	0/892	0.83	1/1187 (0.1%)
36	RT	0.47	0/1155	0.73	2/1542 (0.1%)
36	YT	0.46	0/1155	0.73	2/1542 (0.1%)
37	RU	0.48	0/982	0.78	0/1306
37	YU	0.48	0/982	0.78	0/1306
38	RV	0.47	0/790	0.82	0/1057

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	YV	0.47	0/790	0.82	0/1057
39	RW	0.45	0/911	0.75	0/1220
39	YW	0.45	0/911	0.75	0/1220
40	RX	0.56	0/739	0.77	0/993
40	YX	0.56	0/739	0.77	0/993
41	RY	0.52	0/798	0.80	0/1064
41	YY	0.52	0/798	0.80	0/1064
42	RZ	0.36	0/1493	0.58	0/2026
42	YZ	0.36	0/1493	0.62	0/2026
43	R0	0.42	0/657	0.63	0/874
43	Y0	0.42	0/657	0.65	0/874
44	R1	0.49	0/770	0.85	1/1022 (0.1%)
44	Y1	0.49	0/770	0.85	1/1022 (0.1%)
45	R2	0.50	0/583	0.84	1/771 (0.1%)
45	Y2	0.51	0/583	0.84	1/771 (0.1%)
46	R3	0.47	0/474	0.72	0/635
46	Y3	0.43	0/474	0.71	0/635
47	R4	0.38	0/594	0.78	1/795 (0.1%)
47	Y4	0.38	0/594	0.78	1/795 (0.1%)
48	R5	0.51	0/473	0.74	0/639
48	Y5	0.50	0/465	0.74	0/629
49	R6	0.42	0/431	0.76	0/575
49	Y6	0.43	0/431	0.76	0/575
50	R7	0.56	0/438	0.76	0/575
50	Y7	0.56	0/438	0.76	0/575
51	R8	0.62	0/525	0.93	1/691 (0.1%)
51	Y8	0.62	0/525	0.93	1/691 (0.1%)
52	R9	0.35	0/310	0.60	0/407
52	Y9	0.37	0/310	0.61	0/407
53	QV	0.51	0/1836	0.99	6/2859 (0.2%)
53	XV	0.51	0/1836	0.99	6/2859 (0.2%)
54	QX	0.74	0/188	0.84	0/290
54	XX	0.48	0/188	0.74	0/290
55	QY	0.78	1/311 (0.3%)	0.88	0/483
55	XY	0.51	0/311	0.88	0/483
56	Z6	0.79	0/40	1.79	1/60 (1.7%)
56	Z8	0.79	0/40	1.83	1/60 (1.7%)
All	All	0.50	12/316321 (0.0%)	0.98	568/472911 (0.1%)

The worst 5 of 12 bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	RD	236	GLY	C-N	8.53	1.53	1.34
29	RI	54	GLN	C-O	-7.01	1.10	1.23
55	QY	36	G	C2-N2	-6.93	1.27	1.34
22	YA	1142(A)	A	N9-C4	-6.45	1.33	1.37
29	RI	55	ALA	C-O	6.04	1.34	1.23

The worst 5 of 568 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	XV	17	C	C2-N1-C1’	11.79	131.77	118.80
53	QV	17	C	C2-N1-C1’	11.74	131.72	118.80
22	YA	761	A	N1-C6-N6	11.29	125.37	118.60
1	XA	328	C	C6-N1-C2	-10.26	116.19	120.30
25	YE	21	VAL	C-N-CD	-10.09	98.39	120.60

There are no chirality outliers.

There are no planarity outliers.

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	16278	672	0
1	XA	32249	0	16278	742	1
2	QB	1924	0	1975	283	0
2	XB	1924	0	1975	290	0
3	QC	1605	0	1668	210	0
3	XC	1605	0	1668	210	0
4	QD	1703	0	1764	247	0
4	XD	1703	0	1765	215	1
5	QE	1155	0	1213	159	0
5	XE	1155	0	1213	133	0
6	QF	843	0	857	92	1
6	XF	843	0	857	96	0
7	QG	1257	0	1296	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	XG	1257	0	1294	147	0
8	QH	1116	0	1175	151	0
8	XH	1116	0	1177	149	0
9	QI	1010	0	1037	140	0
9	XI	1010	0	1037	153	0
10	QJ	801	0	849	149	0
10	XJ	801	0	849	135	0
11	QK	885	0	904	103	0
11	XK	885	0	904	110	0
12	QL	975	0	1062	111	0
12	XL	975	0	1062	116	0
13	QM	964	0	1034	152	0
13	XM	964	0	1034	216	0
14	QN	492	0	529	103	0
14	XN	492	0	529	95	0
15	QO	734	0	771	78	0
15	XO	734	0	771	72	0
16	QP	705	0	725	115	0
16	XP	705	0	725	105	0
17	QQ	834	0	904	77	0
17	XQ	834	0	904	71	0
18	QR	574	0	644	69	0
18	XR	574	0	644	68	0
19	QS	674	0	699	117	0
19	XS	674	0	699	150	0
20	QT	763	0	860	109	0
20	XT	763	0	861	102	0
21	QU	217	0	234	25	0
21	XU	217	0	234	26	0
22	RA	62071	0	31286	1243	0
22	YA	62091	0	31295	1282	0
23	RB	2573	0	1306	68	0
23	YB	2573	0	1306	57	0
24	RD	2115	0	2195	320	0
24	YD	2115	0	2195	323	0
25	RE	1568	0	1634	268	0
25	YE	1568	0	1634	272	0
26	RF	1585	0	1632	178	0
26	YF	1585	0	1632	179	0
27	RG	1474	0	1535	202	0
27	YG	1474	0	1535	204	0
28	RH	1307	0	1382	220	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	YH	1307	0	1382	227	3
29	RI	1136	0	1223	61	1
29	YI	1136	0	1223	57	0
30	RN	1104	0	1180	190	0
30	YN	1104	0	1180	186	0
31	RO	933	0	996	124	0
31	YO	933	0	996	131	0
32	RP	1145	0	1227	247	0
32	YP	1145	0	1228	239	0
33	RQ	1122	0	1179	150	0
33	YQ	1122	0	1178	149	0
34	RR	968	0	1033	110	0
34	YR	968	0	1033	114	0
35	RS	882	0	943	156	0
35	YS	882	0	943	159	0
36	RT	1141	0	1202	156	0
36	YT	1141	0	1202	152	0
37	RU	964	0	1022	128	0
37	YU	964	0	1022	134	0
38	RV	779	0	852	130	0
38	YV	779	0	852	128	0
39	RW	900	0	964	101	0
39	YW	900	0	964	102	0
40	RX	725	0	778	67	0
40	YX	725	0	778	67	0
41	RY	785	0	878	166	0
41	YY	785	0	878	154	3
42	RZ	1461	0	1493	63	0
42	YZ	1461	0	1493	70	0
43	R0	648	0	672	28	0
43	Y0	648	0	672	44	0
44	R1	763	0	848	143	0
44	Y1	763	0	848	140	0
45	R2	581	0	629	80	0
45	Y2	581	0	629	79	0
46	R3	469	0	518	41	0
46	Y3	469	0	518	44	0
47	R4	581	0	574	156	0
47	Y4	581	0	574	225	0
48	R5	459	0	480	74	0
48	Y5	451	0	471	68	0
49	R6	424	0	450	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y6	424	0	450	90	0
50	R7	430	0	480	42	0
50	Y7	430	0	480	44	0
51	R8	517	0	582	102	0
51	Y8	517	0	582	102	0
52	R9	307	0	335	16	0
52	Y9	307	0	336	20	0
53	QV	1644	0	836	63	0
53	XV	1644	0	836	56	0
54	QX	169	0	88	55	0
54	XX	169	0	88	17	0
55	QY	303	0	152	22	0
55	XY	303	0	154	30	0
56	Z6	74	0	51	24	0
56	Z8	74	0	51	14	0
57	QA	65	0	0	0	0
57	QF	1	0	0	0	0
57	QH	1	0	0	0	0
57	QM	1	0	0	0	0
57	QX	1	0	0	0	0
57	R5	1	0	0	0	0
57	R8	1	0	0	0	0
57	RA	244	0	0	0	0
57	RB	2	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RF	1	0	0	0	0
57	RP	2	0	0	0	0
57	RR	1	0	0	0	0
57	RU	1	0	0	0	0
57	XA	72	0	0	0	0
57	XM	1	0	0	0	0
57	XV	2	0	0	0	0
57	XX	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y7	1	0	0	0	0
57	YA	265	0	0	0	0
57	YB	3	0	0	0	0
57	YE	1	0	0	0	0
57	YP	2	0	0	0	0
57	YQ	1	0	0	0	0
57	YX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	QA	42	0	45	4	0
58	XA	42	0	45	2	0
59	QD	1	0	0	0	0
59	QN	1	0	0	0	0
59	R9	1	0	0	0	0
59	XD	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y9	1	0	0	0	0
All	All	291950	0	198321	15633	5

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 32.

The worst 5 of 15633 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1400:C:N4	53:XV:34:C:C6	1.71	1.55
14:XN:32:SER:CB	14:XN:41:ARG:HB3	1.23	1.55
14:XN:32:SER:HB3	14:XN:41:ARG:CB	1.27	1.54
28:RH:127:GLU:CG	28:RH:128:PRO:HD3	1.35	1.53
28:YH:127:GLU:CG	28:YH:128:PRO:HD3	1.35	1.52

All (5) 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)
28:YH:45:VAL:O	41:YY:24:VAL:N[4_445]	1.97	0.23
29:RI:91:SER:OG	1:XA:368:U:OP1[4_555]	2.05	0.15
28:YH:44:VAL:CG2	41:YY:23:ARG:CD[4_445]	2.08	0.12
6:QF:15:ASP:OD2	4:XD:27:TYR:OH[4_555]	2.14	0.06
28:YH:47:GLU:OE2	41:YY:79:CYS:CB[4_445]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	153 (65%)	52 (22%)	30 (13%)	0	5
2	XB	235/256 (92%)	153 (65%)	52 (22%)	30 (13%)	0	5
3	QC	203/239 (85%)	128 (63%)	56 (28%)	19 (9%)	0	12
3	XC	203/239 (85%)	129 (64%)	55 (27%)	19 (9%)	0	12
4	QD	206/209 (99%)	136 (66%)	50 (24%)	20 (10%)	0	11
4	XD	206/209 (99%)	135 (66%)	48 (23%)	23 (11%)	0	7
5	QE	149/162 (92%)	103 (69%)	31 (21%)	15 (10%)	0	10
5	XE	149/162 (92%)	103 (69%)	30 (20%)	16 (11%)	0	8
6	QF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	12
6	XF	99/101 (98%)	66 (67%)	24 (24%)	9 (9%)	1	12
7	QG	153/156 (98%)	101 (66%)	37 (24%)	15 (10%)	0	10
7	XG	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	1	12
8	QH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	8
8	XH	136/138 (99%)	92 (68%)	29 (21%)	15 (11%)	0	8
9	QI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	5
9	XI	125/128 (98%)	77 (62%)	32 (26%)	16 (13%)	0	5
10	QJ	97/105 (92%)	68 (70%)	20 (21%)	9 (9%)	0	12
10	XJ	97/105 (92%)	68 (70%)	19 (20%)	10 (10%)	0	9
11	QK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	18
11	XK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	18
12	QL	123/132 (93%)	84 (68%)	23 (19%)	16 (13%)	0	5
12	XL	123/132 (93%)	84 (68%)	24 (20%)	15 (12%)	0	6
13	QM	119/126 (94%)	71 (60%)	29 (24%)	19 (16%)	0	3
13	XM	119/126 (94%)	71 (60%)	27 (23%)	21 (18%)	0	3
14	QN	58/61 (95%)	31 (53%)	15 (26%)	12 (21%)	0	2
14	XN	58/61 (95%)	33 (57%)	13 (22%)	12 (21%)	0	2
15	QO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	17
15	XO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1	17
16	QP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	4
16	XP	82/88 (93%)	48 (58%)	23 (28%)	11 (13%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	QQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	14
17	XQ	98/105 (93%)	75 (76%)	15 (15%)	8 (8%)	1	14
18	QR	68/88 (77%)	45 (66%)	15 (22%)	8 (12%)	0	6
18	XR	68/88 (77%)	46 (68%)	14 (21%)	8 (12%)	0	6
19	QS	82/93 (88%)	47 (57%)	17 (21%)	18 (22%)	0	1
19	XS	82/93 (88%)	46 (56%)	18 (22%)	18 (22%)	0	1
20	QT	97/106 (92%)	63 (65%)	16 (16%)	18 (19%)	0	2
20	XT	97/106 (92%)	63 (65%)	15 (16%)	19 (20%)	0	2
21	QU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	3
21	XU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	3
24	RD	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	1	17
24	YD	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	1	17
25	RE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
25	YE	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	2
26	RF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	0	10
26	YF	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	0	10
27	RG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	6
27	YG	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	0	6
28	RH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
28	YH	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	1
29	RI	144/148 (97%)	106 (74%)	21 (15%)	17 (12%)	0	6
29	YI	144/148 (97%)	100 (69%)	27 (19%)	17 (12%)	0	6
30	RN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	3
30	YN	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	3
31	RO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	16
31	YO	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	1	16
32	RP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
32	YP	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	1
33	RQ	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	0	10
33	YQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	10
34	RR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	YR	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	0	6
35	RS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	3
35	YS	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	3
36	RT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	4
36	YT	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	4
37	RU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	15
37	YU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	15
38	RV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	10
38	YV	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	0	10
39	RW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	5
39	YW	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	5
40	RX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	21
40	YX	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	2	21
41	RY	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	1
41	YY	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	1
42	RZ	181/206 (88%)	131 (72%)	28 (16%)	22 (12%)	0	6
42	YZ	181/206 (88%)	128 (71%)	35 (19%)	18 (10%)	0	10
43	R0	80/85 (94%)	67 (84%)	12 (15%)	1 (1%)	12	48
43	Y0	80/85 (94%)	67 (84%)	11 (14%)	2 (2%)	5	36
44	R1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	6
44	Y1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	0	6
45	R2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	4
45	Y2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	4
46	R3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	22
46	Y3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	2	22
47	R4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
47	Y4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
48	R5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	1
48	Y5	56/60 (93%)	32 (57%)	9 (16%)	15 (27%)	0	0
49	R6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
49	Y6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	R7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	19
50	Y7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	19
51	R8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	2
51	Y8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	2
52	R9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
52	Y9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	11469/12128 (95%)	7649 (67%)	2333 (20%)	1487 (13%)	0	5

5 of 1487 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	6	THR
2	QB	15	VAL
2	QB	26	PRO
2	QB	84	GLU
2	QB	88	ALA

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%)	181 (88%)	24 (12%)	5	26
2	XB	205/220 (93%)	181 (88%)	24 (12%)	5	26
3	QC	159/188 (85%)	143 (90%)	16 (10%)	7	30
3	XC	159/188 (85%)	143 (90%)	16 (10%)	7	30
4	QD	180/181 (99%)	160 (89%)	20 (11%)	6	27
4	XD	180/181 (99%)	165 (92%)	15 (8%)	11	39
5	QE	116/123 (94%)	107 (92%)	9 (8%)	12	41
5	XE	116/123 (94%)	107 (92%)	9 (8%)	12	41
6	QF	90/90 (100%)	76 (84%)	14 (16%)	2	17
6	XF	90/90 (100%)	76 (84%)	14 (16%)	2	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	QG	126/127 (99%)	114 (90%)	12 (10%)	8	33
7	XG	126/127 (99%)	115 (91%)	11 (9%)	10	37
8	QH	119/119 (100%)	106 (89%)	13 (11%)	6	28
8	XH	119/119 (100%)	106 (89%)	13 (11%)	6	28
9	QI	98/99 (99%)	87 (89%)	11 (11%)	6	27
9	XI	98/99 (99%)	87 (89%)	11 (11%)	6	27
10	QJ	89/92 (97%)	81 (91%)	8 (9%)	9	36
10	XJ	89/92 (97%)	81 (91%)	8 (9%)	9	36
11	QK	90/99 (91%)	81 (90%)	9 (10%)	7	30
11	XK	90/99 (91%)	81 (90%)	9 (10%)	7	30
12	QL	104/109 (95%)	88 (85%)	16 (15%)	2	17
12	XL	104/109 (95%)	89 (86%)	15 (14%)	3	20
13	QM	97/101 (96%)	81 (84%)	16 (16%)	2	15
13	XM	97/101 (96%)	81 (84%)	16 (16%)	2	15
14	QN	49/50 (98%)	40 (82%)	9 (18%)	1	11
14	XN	49/50 (98%)	44 (90%)	5 (10%)	7	30
15	QO	79/80 (99%)	73 (92%)	6 (8%)	13	42
15	XO	79/80 (99%)	73 (92%)	6 (8%)	13	42
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%)	89 (94%)	6 (6%)	18	47
17	XQ	95/97 (98%)	89 (94%)	6 (6%)	18	47
18	QR	61/77 (79%)	54 (88%)	7 (12%)	5	26
18	XR	61/77 (79%)	54 (88%)	7 (12%)	5	26
19	QS	73/80 (91%)	62 (85%)	11 (15%)	3	18
19	XS	73/80 (91%)	62 (85%)	11 (15%)	3	18
20	QT	76/82 (93%)	68 (90%)	8 (10%)	7	29
20	XT	76/82 (93%)	69 (91%)	7 (9%)	9	34
21	QU	20/22 (91%)	19 (95%)	1 (5%)	24	53
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	53
24	RD	214/218 (98%)	177 (83%)	37 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	YD	214/218 (98%)	178 (83%)	36 (17%)	2	15
25	RE	165/166 (99%)	127 (77%)	38 (23%)	1	6
25	YE	165/166 (99%)	127 (77%)	38 (23%)	1	6
26	RF	161/166 (97%)	140 (87%)	21 (13%)	4	23
26	YF	161/166 (97%)	140 (87%)	21 (13%)	4	23
27	RG	155/156 (99%)	130 (84%)	25 (16%)	2	16
27	YG	155/156 (99%)	131 (84%)	24 (16%)	2	17
28	RH	142/148 (96%)	114 (80%)	28 (20%)	1	9
28	YH	142/148 (96%)	114 (80%)	28 (20%)	1	9
29	RI	122/124 (98%)	100 (82%)	22 (18%)	1	12
29	YI	122/124 (98%)	101 (83%)	21 (17%)	2	14
30	RN	117/119 (98%)	98 (84%)	19 (16%)	2	16
30	YN	117/119 (98%)	98 (84%)	19 (16%)	2	16
31	RO	100/100 (100%)	90 (90%)	10 (10%)	7	30
31	YO	100/100 (100%)	90 (90%)	10 (10%)	7	30
32	RP	116/116 (100%)	89 (77%)	27 (23%)	1	5
32	YP	116/116 (100%)	89 (77%)	27 (23%)	1	5
33	RQ	111/111 (100%)	93 (84%)	18 (16%)	2	16
33	YQ	111/111 (100%)	93 (84%)	18 (16%)	2	16
34	RR	101/101 (100%)	84 (83%)	17 (17%)	2	15
34	YR	101/101 (100%)	84 (83%)	17 (17%)	2	15
35	RS	87/88 (99%)	74 (85%)	13 (15%)	3	18
35	YS	87/88 (99%)	74 (85%)	13 (15%)	3	18
36	RT	120/127 (94%)	97 (81%)	23 (19%)	1	10
36	YT	120/127 (94%)	97 (81%)	23 (19%)	1	10
37	RU	93/94 (99%)	80 (86%)	13 (14%)	3	21
37	YU	93/94 (99%)	80 (86%)	13 (14%)	3	21
38	RV	82/82 (100%)	71 (87%)	11 (13%)	4	22
38	YV	82/82 (100%)	71 (87%)	11 (13%)	4	22
39	RW	92/92 (100%)	77 (84%)	15 (16%)	2	16
39	YW	92/92 (100%)	77 (84%)	15 (16%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	RX	74/78 (95%)	63 (85%)	11 (15%)	3	18
40	YX	74/78 (95%)	63 (85%)	11 (15%)	3	18
41	RY	85/91 (93%)	70 (82%)	15 (18%)	2	13
41	YY	85/91 (93%)	70 (82%)	15 (18%)	2	13
42	RZ	162/179 (90%)	141 (87%)	21 (13%)	4	23
42	YZ	162/179 (90%)	139 (86%)	23 (14%)	3	20
43	R0	65/67 (97%)	57 (88%)	8 (12%)	4	24
43	Y0	65/67 (97%)	60 (92%)	5 (8%)	13	42
44	R1	82/83 (99%)	67 (82%)	15 (18%)	1	11
44	Y1	82/83 (99%)	67 (82%)	15 (18%)	1	11
45	R2	64/67 (96%)	57 (89%)	7 (11%)	6	28
45	Y2	64/67 (96%)	57 (89%)	7 (11%)	6	28
46	R3	51/52 (98%)	40 (78%)	11 (22%)	1	7
46	Y3	51/52 (98%)	40 (78%)	11 (22%)	1	7
47	R4	63/63 (100%)	44 (70%)	19 (30%)	0	2
47	Y4	63/63 (100%)	44 (70%)	19 (30%)	0	2
48	R5	51/52 (98%)	39 (76%)	12 (24%)	1	5
48	Y5	50/52 (96%)	38 (76%)	12 (24%)	0	5
49	R6	48/52 (92%)	38 (79%)	10 (21%)	1	7
49	Y6	48/52 (92%)	38 (79%)	10 (21%)	1	7
50	R7	42/42 (100%)	39 (93%)	3 (7%)	14	44
50	Y7	42/42 (100%)	39 (93%)	3 (7%)	14	44
51	R8	54/55 (98%)	39 (72%)	15 (28%)	0	3
51	Y8	54/55 (98%)	39 (72%)	15 (28%)	0	3
52	R9	34/34 (100%)	32 (94%)	2 (6%)	19	49
52	Y9	34/34 (100%)	32 (94%)	2 (6%)	19	49
All	All	9701/10066 (96%)	8295 (86%)	1406 (14%)	3	19

5 of 1406 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	YD	26	LYS
32	YP	144	GLU

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Mol	Chain	Res	Type
24	YD	226	MET
24	YD	17	THR
27	YG	156	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
2	XB	212	GLN
47	Y4	47	GLN
12	XL	9	GLN
46	Y3	32	GLN
39	YW	61	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1499/1522 (98%)	281 (18%)	47 (3%)
1	XA	1498/1522 (98%)	299 (19%)	52 (3%)
22	RA	2879/2916 (98%)	658 (22%)	65 (2%)
22	YA	2880/2916 (98%)	639 (22%)	65 (2%)
23	RB	119/122 (97%)	20 (16%)	2 (1%)
23	YB	119/122 (97%)	25 (21%)	1 (0%)
53	QV	76/77 (98%)	30 (39%)	1 (1%)
53	XV	76/77 (98%)	30 (39%)	1 (1%)
54	QX	7/25 (28%)	5 (71%)	2 (28%)
54	XX	7/25 (28%)	4 (57%)	1 (14%)
55	QY	13/18 (72%)	6 (46%)	2 (15%)
55	XY	13/18 (72%)	5 (38%)	1 (7%)
56	Z6	1/3 (33%)	0	0
56	Z8	1/3 (33%)	0	0
All	All	9188/9366 (98%)	2002 (21%)	240 (2%)

5 of 2002 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	22	G
1	QA	32	A
1	QA	39	G

5 of 240 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	XA	60	A
22	YA	2566	A
1	XA	812	C
22	YA	2481	G
55	QY	39	C

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

4 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	2.56	6 (18%)	33,57,60	2.16	5 (15%)
56	PPU	Z8	76	22,56	32,40,41	2.55	6 (18%)	33,57,60	2.15	5 (15%)
55	1MG	XY	37	55	18,26,27	2.29	2 (11%)	19,39,42	1.55	2 (10%)
55	1MG	QY	37	55	18,26,27	1.05	2 (11%)	19,39,42	1.53	3 (15%)

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	-	2/21/43/44	0/4/4/4
56	PPU	Z8	76	22,56	-	2/21/43/44	0/4/4/4
55	1MG	XY	37	55	-	0/3/25/26	0/3/3/3
55	1MG	QY	37	55	-	0/3/25/26	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z6	76	PPU	O-C	9.30	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z8	76	PPU	O-C	9.27	1.41	1.23
55	XY	37	1MG	C2-N2	7.85	1.48	1.34
56	Z6	76	PPU	C9-N6	-6.00	1.31	1.45
56	Z8	76	PPU	C9-N6	-5.94	1.32	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Z6	76	PPU	C3'-N3'-C	-8.63	110.20	123.21
56	Z8	76	PPU	C3'-N3'-C	-8.59	110.25	123.21
56	Z8	76	PPU	N3-C2-N1	-4.69	121.34	128.68
56	Z6	76	PPU	N3-C2-N1	-4.64	121.42	128.68
55	QY	37	1MG	CM1-N1-C2	4.59	125.48	120.72

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	Z6	76	PPU	O-C-CA-N
56	Z8	76	PPU	O-C-CA-N
56	Z6	76	PPU	N3'-C-CA-N
56	Z8	76	PPU	N3'-C-CA-N

There are no ring outliers.

4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Z6	76	PPU	14	0
56	Z8	76	PPU	11	0
55	XY	37	1MG	7	0
55	QY	37	1MG	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 684 ligands modelled in this entry, 682 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	$\#\|Z\|>2$
58	PAR	QA	1666	-	45,45,45	1.48	7 (15%)	64,67,67	1.39	8 (12%)
58	PAR	XA	1673	-	45,45,45	1.51	7 (15%)	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
58	PAR	QA	1666	-	-	8/18/94/94	0/4/4/4
58	PAR	XA	1673	-	-	6/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	QA	1666	PAR	C64-C54	5.19	1.59	1.52
58	XA	1673	PAR	C64-C54	4.99	1.58	1.52
58	QA	1666	PAR	C52-C42	3.07	1.58	1.52
58	XA	1673	PAR	C52-C42	2.95	1.58	1.52
58	XA	1673	PAR	O54-C14	2.92	1.49	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	XA	1673	PAR	O33-C14-C24	4.73	116.36	108.22
58	XA	1673	PAR	C14-O54-C54	4.31	122.15	113.69
58	QA	1666	PAR	O52-C13-C23	3.86	115.96	107.96
58	QA	1666	PAR	C14-O54-C54	3.83	121.21	113.69
58	QA	1666	PAR	O33-C14-C24	3.75	114.67	108.22

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	QA	1666	PAR	C44-C54-C64-N64
58	QA	1666	PAR	O54-C54-C64-N64
58	QA	1666	PAR	O51-C51-C61-O61
58	XA	1673	PAR	O51-C51-C61-O61
58	QA	1666	PAR	C41-C51-C61-O61

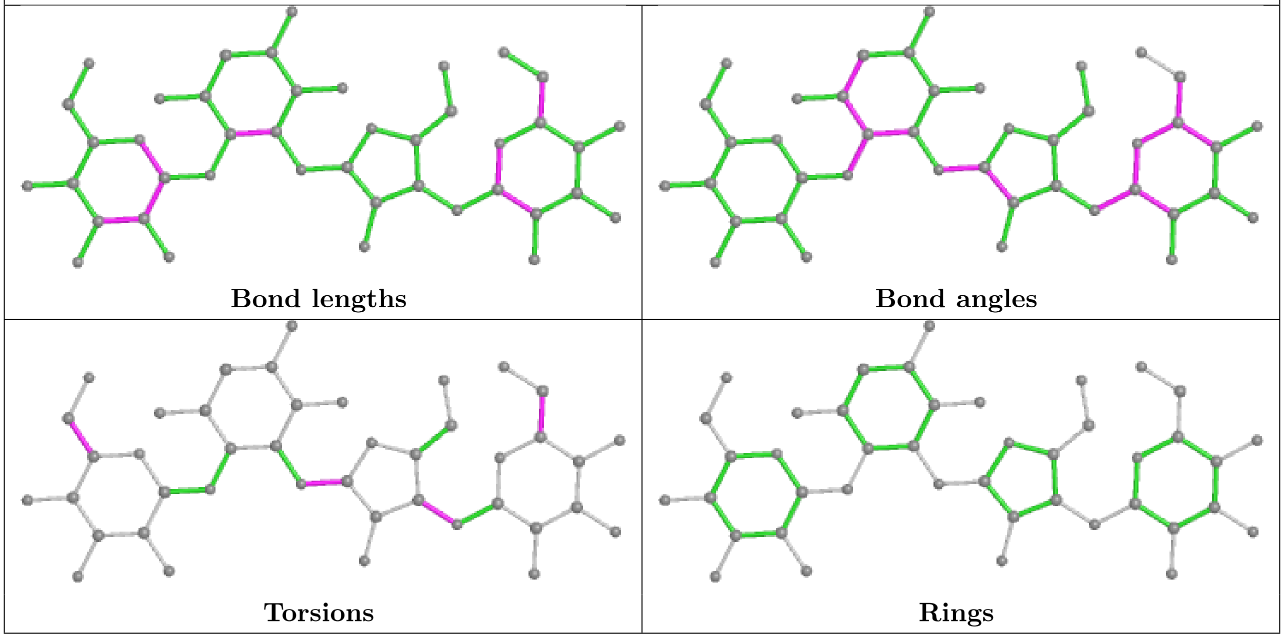
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	QA	1666	PAR	4	0
58	XA	1673	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 1666



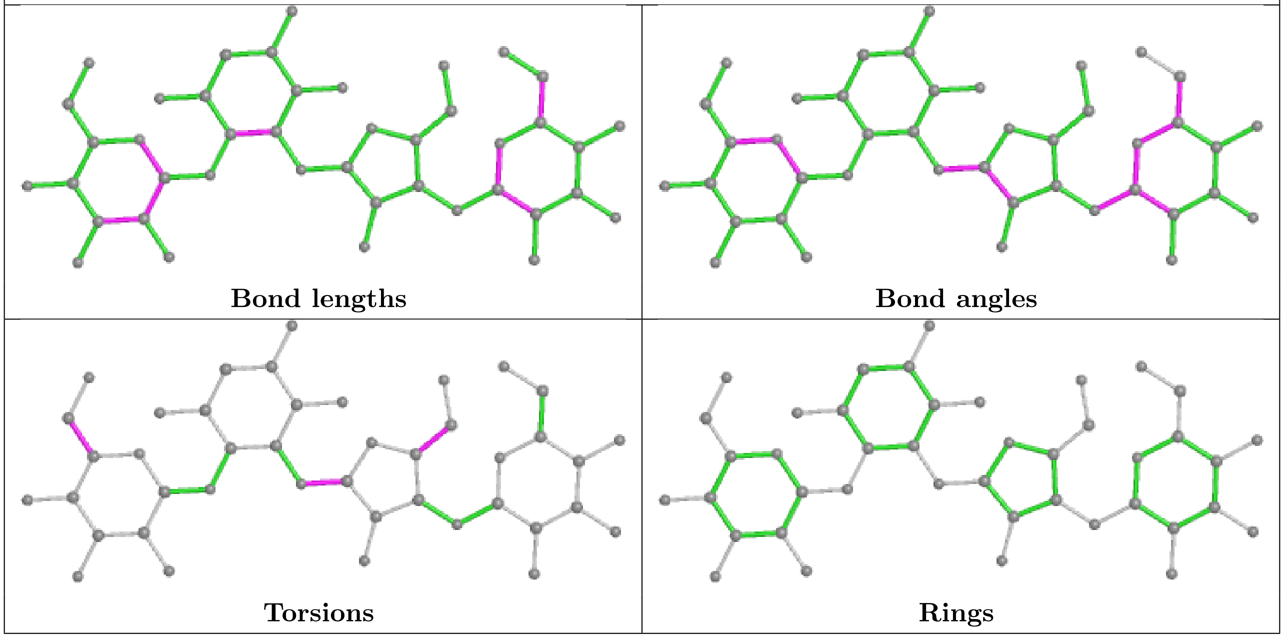
Bond lengths

Bond angles

Torsions

Rings

Ligand PAR XA 1673



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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($\AA^2$)	Q<0.9
1	QA	1500/1522 (98%)	-0.09	27 (1%) 68 59	22, 75, 152, 231	0
1	XA	1500/1522 (98%)	-0.25	9 (0%) 89 84	7, 55, 142, 232	0
2	QB	237/256 (92%)	0.39	16 (6%) 17 12	47, 109, 145, 182	0
2	XB	237/256 (92%)	0.18	9 (3%) 40 31	38, 88, 133, 159	0
3	QC	205/239 (85%)	0.14	4 (1%) 65 55	39, 98, 133, 150	0
3	XC	205/239 (85%)	-0.18	2 (0%) 82 75	20, 67, 110, 138	0
4	QD	208/209 (99%)	0.14	2 (0%) 82 75	29, 79, 128, 167	0
4	XD	208/209 (99%)	0.05	2 (0%) 82 75	10, 72, 110, 139	0
5	QE	151/162 (93%)	0.28	6 (3%) 38 30	25, 85, 122, 159	0
5	XE	151/162 (93%)	-0.03	2 (1%) 77 68	1, 62, 104, 134	0
6	QF	101/101 (100%)	0.15	1 (0%) 82 75	16, 74, 116, 131	0
6	XF	101/101 (100%)	-0.03	1 (0%) 82 75	16, 65, 110, 133	0
7	QG	155/156 (99%)	0.48	17 (10%) 5 5	30, 84, 125, 149	0
7	XG	155/156 (99%)	0.18	6 (3%) 39 30	20, 71, 109, 131	0
8	QH	138/138 (100%)	0.32	3 (2%) 62 51	45, 88, 124, 156	0
8	XH	138/138 (100%)	0.10	1 (0%) 87 82	19, 70, 102, 125	0
9	QI	127/128 (99%)	0.71	13 (10%) 6 6	46, 97, 137, 144	0
9	XI	127/128 (99%)	0.20	3 (2%) 59 48	16, 79, 119, 129	0
10	QJ	99/105 (94%)	1.05	19 (19%) 1 1	44, 108, 142, 161	0
10	XJ	99/105 (94%)	0.56	11 (11%) 5 5	9, 83, 129, 147	0
11	QK	119/129 (92%)	0.40	14 (11%) 4 4	18, 71, 123, 149	0
11	XK	119/129 (92%)	0.26	5 (4%) 36 29	15, 63, 110, 147	0
12	QL	125/132 (94%)	0.45	8 (6%) 19 14	20, 72, 108, 139	0
12	XL	125/132 (94%)	-0.02	2 (1%) 72 62	0, 48, 91, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	QM	121/126 (96%)	0.52	13 (10%) 6 5	39, 96, 131, 170	0
13	XM	121/126 (96%)	-0.00	3 (2%) 57 47	4, 68, 125, 149	0
14	QN	60/61 (98%)	0.64	5 (8%) 11 9	52, 98, 137, 146	0
14	XN	60/61 (98%)	-0.07	0 100 100	4, 60, 100, 120	0
15	QO	88/89 (98%)	0.14	6 (6%) 17 12	30, 79, 120, 136	0
15	XO	88/89 (98%)	0.01	1 (1%) 80 73	10, 64, 93, 107	0
16	QP	84/88 (95%)	0.32	3 (3%) 42 33	12, 68, 103, 138	0
16	XP	84/88 (95%)	0.45	2 (2%) 59 48	30, 70, 106, 135	0
17	QQ	100/105 (95%)	0.56	7 (7%) 16 12	33, 82, 115, 141	0
17	XQ	100/105 (95%)	0.21	0 100 100	14, 64, 102, 124	0
18	QR	70/88 (79%)	0.53	9 (12%) 3 3	18, 78, 119, 147	0
18	XR	70/88 (79%)	0.38	4 (5%) 23 19	22, 67, 109, 135	0
19	QS	84/93 (90%)	0.67	7 (8%) 11 9	60, 102, 132, 147	0
19	XS	84/93 (90%)	0.21	2 (2%) 59 48	15, 73, 112, 164	0
20	QT	99/106 (93%)	0.19	3 (3%) 50 38	3, 77, 111, 131	0
20	XT	99/106 (93%)	0.29	3 (3%) 50 38	19, 77, 117, 126	0
21	QU	25/27 (92%)	1.78	9 (36%) 0 0	37, 85, 131, 145	0
21	XU	25/27 (92%)	0.97	3 (12%) 4 4	30, 75, 103, 134	0
22	RA	2882/2916 (98%)	-0.17	97 (3%) 45 35	2, 45, 174, 236	0
22	YA	2883/2916 (98%)	-0.27	71 (2%) 57 47	1, 35, 165, 227	0
23	RB	120/122 (98%)	-0.17	0 100 100	46, 89, 131, 152	0
23	YB	120/122 (98%)	-0.48	1 (0%) 86 79	18, 58, 93, 139	0
24	RD	272/276 (98%)	-0.11	0 100 100	4, 41, 81, 123	0
24	YD	272/276 (98%)	-0.05	1 (0%) 92 87	1, 33, 74, 140	0
25	RE	205/206 (99%)	0.13	4 (1%) 65 55	7, 62, 112, 141	0
25	YE	205/206 (99%)	0.04	2 (0%) 82 75	6, 56, 103, 125	0
26	RF	202/210 (96%)	-0.04	2 (0%) 82 75	1, 64, 110, 129	0
26	YF	202/210 (96%)	-0.06	2 (0%) 82 75	1, 47, 95, 112	0
27	RG	181/182 (99%)	0.37	9 (4%) 28 24	34, 99, 142, 166	0
27	YG	181/182 (99%)	-0.06	1 (0%) 89 84	9, 66, 115, 163	0
28	RH	170/180 (94%)	1.11	37 (21%) 0 1	32, 108, 152, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	YH	170/180 (94%)	0.20	6 (3%)	44	34	14, 68, 110, 133	0
29	RI	146/148 (98%)	0.36	3 (2%)	63	53	16, 78, 122, 154	0
29	YI	146/148 (98%)	0.17	3 (2%)	63	53	8, 72, 119, 159	0
30	RN	138/140 (98%)	0.31	5 (3%)	42	33	14, 70, 110, 124	0
30	YN	138/140 (98%)	0.03	4 (2%)	51	40	8, 55, 103, 128	0
31	RO	122/122 (100%)	0.15	0	100	100	5, 56, 97, 126	0
31	YO	122/122 (100%)	-0.01	0	100	100	0, 42, 79, 94	0
32	RP	150/150 (100%)	0.49	11 (7%)	15	11	6, 65, 126, 159	0
32	YP	150/150 (100%)	0.04	2 (1%)	77	68	5, 53, 105, 154	0
33	RQ	141/141 (100%)	0.18	3 (2%)	63	53	2, 62, 106, 142	0
33	YQ	141/141 (100%)	-0.12	0	100	100	3, 42, 94, 132	0
34	RR	118/118 (100%)	-0.05	0	100	100	8, 50, 92, 118	0
34	YR	118/118 (100%)	-0.07	0	100	100	6, 43, 89, 109	0
35	RS	111/112 (99%)	0.37	3 (2%)	54	43	35, 78, 114, 141	0
35	YS	111/112 (99%)	0.01	0	100	100	7, 61, 94, 111	0
36	RT	137/146 (93%)	0.11	2 (1%)	73	64	13, 64, 125, 165	0
36	YT	137/146 (93%)	-0.10	1 (0%)	87	82	10, 58, 111, 158	0
37	RU	117/118 (99%)	-0.06	3 (2%)	56	45	10, 61, 104, 147	0
37	YU	117/118 (99%)	-0.16	2 (1%)	70	60	0, 44, 108, 129	0
38	RV	101/101 (100%)	0.07	0	100	100	20, 75, 116, 144	0
38	YV	101/101 (100%)	0.19	2 (1%)	65	55	11, 65, 104, 156	0
39	RW	113/113 (100%)	0.10	0	100	100	3, 43, 93, 149	0
39	YW	113/113 (100%)	-0.09	2 (1%)	68	59	2, 42, 91, 144	0
40	RX	92/96 (95%)	-0.09	1 (1%)	80	73	15, 52, 96, 125	0
40	YX	92/96 (95%)	-0.11	0	100	100	3, 37, 76, 96	0
41	RY	102/110 (92%)	1.27	28 (27%)	0	0	26, 88, 132, 159	0
41	YY	102/110 (92%)	0.34	4 (3%)	39	30	9, 63, 120, 140	0
42	RZ	183/206 (88%)	0.39	10 (5%)	25	20	21, 88, 132, 152	0
42	YZ	183/206 (88%)	0.01	3 (1%)	72	62	20, 70, 123, 155	0
43	R0	82/85 (96%)	0.36	3 (3%)	41	32	14, 48, 79, 112	0
43	Y0	82/85 (96%)	0.18	1 (1%)	79	70	3, 36, 66, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	R1	97/98 (98%)	0.47	4 (4%)	37	29	5, 53, 126, 159	0
44	Y1	97/98 (98%)	0.29	3 (3%)	49	38	5, 43, 104, 139	0
45	R2	69/72 (95%)	0.05	0	100	100	13, 72, 111, 129	0
45	Y2	69/72 (95%)	-0.20	0	100	100	5, 50, 104, 121	0
46	R3	59/60 (98%)	1.17	9 (15%)	2	2	12, 63, 111, 138	0
46	Y3	59/60 (98%)	0.47	5 (8%)	10	8	2, 44, 101, 174	0
47	R4	71/71 (100%)	0.89	12 (16%)	1	1	75, 131, 170, 189	0
47	Y4	71/71 (100%)	0.27	4 (5%)	24	19	46, 102, 154, 161	0
48	R5	59/60 (98%)	0.11	4 (6%)	17	12	6, 55, 133, 141	0
48	Y5	58/60 (96%)	0.14	2 (3%)	45	35	10, 59, 143, 162	0
49	R6	49/54 (90%)	3.21	31 (63%)	0	0	83, 118, 150, 157	0
49	Y6	49/54 (90%)	2.67	31 (63%)	0	0	51, 109, 141, 149	0
50	R7	49/49 (100%)	0.07	2 (4%)	37	29	8, 35, 87, 146	0
50	Y7	49/49 (100%)	0.08	1 (2%)	65	55	1, 29, 71, 121	0
51	R8	64/65 (98%)	0.23	2 (3%)	49	38	1, 52, 96, 158	0
51	Y8	64/65 (98%)	0.01	0	100	100	5, 40, 81, 149	0
52	R9	37/37 (100%)	3.91	32 (86%)	0	0	66, 110, 156, 168	0
52	Y9	37/37 (100%)	4.48	37 (100%)	0	0	78, 107, 132, 166	0
53	QV	77/77 (100%)	0.14	2 (2%)	56	45	46, 99, 145, 169	0
53	XV	77/77 (100%)	0.04	2 (2%)	56	45	28, 72, 119, 180	0
54	QX	8/25 (32%)	3.09	6 (75%)	0	0	103, 130, 144, 183	0
54	XX	8/25 (32%)	1.62	2 (25%)	0	0	56, 75, 115, 190	0
55	QY	13/18 (72%)	1.53	4 (30%)	0	0	112, 161, 199, 206	0
55	XY	13/18 (72%)	1.16	2 (15%)	2	2	72, 116, 180, 193	0
56	Z6	2/3 (66%)	0.35	0	100	100	52, 52, 52, 57	0
56	Z8	2/3 (66%)	0.56	0	100	100	46, 46, 46, 46	0
All	All	20870/21494 (97%)	0.06	789 (3%)	40	31	0, 61, 135, 236	0

The worst 5 of 789 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	R9	11	CYS	11.7
52	Y9	34	GLN	9.8

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Mol	Chain	Res	Type	RSRZ
49	R6	22	ALA	9.7
52	R9	14	CYS	9.5
13	QM	121	LYS	8.4

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, 95th 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
55	1MG	QY	37	24/25	0.84	0.31	125,125,125,125	0
55	1MG	XY	37	24/25	0.89	0.20	64,64,64,64	0
56	PPU	Z6	76	37/38	0.93	0.32	51,51,51,51	0
56	PPU	Z8	76	37/38	0.93	0.33	48,48,48,48	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, 95th 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
59	ZN	R9	101	1/1	0.30	0.76	177,177,177,177	0
57	MG	QH	201	1/1	0.31	0.27	27,27,27,27	0
57	MG	RA	3230	1/1	0.47	0.48	45,45,45,45	0
57	MG	YA	3148	1/1	0.49	0.23	38,38,38,38	0
57	MG	QA	1631	1/1	0.50	0.24	63,63,63,63	0
57	MG	RA	3229	1/1	0.52	0.33	50,50,50,50	0
57	MG	YA	3012	1/1	0.55	1.42	50,50,50,50	0
57	MG	YA	3163	1/1	0.57	0.31	9,9,9,9	0
57	MG	RA	3071	1/1	0.57	0.89	50,50,50,50	0
57	MG	QA	1628	1/1	0.61	0.43	21,21,21,21	0
57	MG	XA	1662	1/1	0.62	0.74	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3235	1/1	0.63	0.47	34,34,34,34	0
57	MG	YA	3156	1/1	0.65	0.24	8,8,8,8	0
57	MG	RA	3217	1/1	0.67	0.91	16,16,16,16	0
57	MG	RA	3186	1/1	0.68	0.72	51,51,51,51	0
57	MG	QF	201	1/1	0.69	0.32	40,40,40,40	0
57	MG	QA	1640	1/1	0.69	0.23	6,6,6,6	0
57	MG	RA	3116	1/1	0.70	0.32	0,0,0,0	0
59	ZN	Y9	101	1/1	0.70	0.53	158,158,158,158	0
57	MG	YA	3150	1/1	0.71	0.59	16,16,16,16	0
57	MG	YA	3117	1/1	0.72	0.80	50,50,50,50	0
57	MG	RA	3004	1/1	0.72	0.44	9,9,9,9	0
57	MG	RA	3065	1/1	0.72	1.22	50,50,50,50	0
57	MG	RA	3127	1/1	0.72	0.52	15,15,15,15	0
57	MG	YA	3151	1/1	0.73	0.55	50,50,50,50	0
57	MG	YA	3153	1/1	0.73	0.28	16,16,16,16	0
57	MG	RA	3181	1/1	0.73	0.33	9,9,9,9	0
57	MG	QA	1638	1/1	0.73	0.20	8,8,8,8	0
57	MG	RA	3205	1/1	0.73	0.46	33,33,33,33	0
57	MG	XA	1635	1/1	0.73	1.57	50,50,50,50	0
57	MG	XA	1650	1/1	0.73	0.31	22,22,22,22	0
57	MG	YA	3247	1/1	0.74	0.59	16,16,16,16	0
57	MG	XA	1601	1/1	0.74	1.10	50,50,50,50	0
57	MG	YA	3070	1/1	0.74	0.30	33,33,33,33	0
57	MG	QA	1665	1/1	0.75	0.48	37,37,37,37	0
57	MG	YA	3126	1/1	0.75	0.33	50,50,50,50	0
57	MG	RA	3223	1/1	0.75	0.33	16,16,16,16	0
57	MG	RA	3064	1/1	0.75	1.71	50,50,50,50	0
57	MG	RA	3140	1/1	0.75	0.24	61,61,61,61	0
57	MG	RA	3212	1/1	0.75	0.26	33,33,33,33	0
57	MG	YA	3250	1/1	0.76	1.15	50,50,50,50	0
57	MG	QA	1643	1/1	0.76	0.14	20,20,20,20	0
57	MG	YA	3223	1/1	0.76	0.93	11,11,11,11	0
57	MG	XA	1649	1/1	0.77	0.39	16,16,16,16	0
57	MG	XA	1605	1/1	0.77	0.61	16,16,16,16	0
57	MG	YA	3043	1/1	0.77	1.09	50,50,50,50	0
57	MG	QA	1602	1/1	0.78	1.00	11,11,11,11	0
57	MG	QA	1664	1/1	0.78	0.35	10,10,10,10	0
57	MG	RA	3034	1/1	0.78	1.60	50,50,50,50	0
57	MG	YA	3259	1/1	0.78	0.67	2,2,2,2	0
57	MG	YA	3261	1/1	0.78	0.96	50,50,50,50	0
57	MG	RA	3164	1/1	0.78	0.55	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3053	1/1	0.78	1.01	50,50,50,50	0
57	MG	QA	1601	1/1	0.79	0.40	21,21,21,21	0
57	MG	RA	3201	1/1	0.79	0.36	41,41,41,41	0
57	MG	RA	3219	1/1	0.79	0.56	40,40,40,40	0
57	MG	YA	3079	1/1	0.79	1.26	50,50,50,50	0
57	MG	RA	3123	1/1	0.79	0.94	50,50,50,50	0
57	MG	XA	1634	1/1	0.79	0.21	11,11,11,11	0
57	MG	YA	3137	1/1	0.79	0.28	22,22,22,22	0
57	MG	XA	1615	1/1	0.80	0.48	50,50,50,50	0
57	MG	RA	3041	1/1	0.80	0.64	50,50,50,50	0
57	MG	QA	1603	1/1	0.80	0.52	10,10,10,10	0
57	MG	QA	1655	1/1	0.80	0.39	66,66,66,66	0
58	PAR	QA	1666	42/42	0.80	0.38	104,104,104,104	0
57	MG	YA	3119	1/1	0.80	0.41	66,66,66,66	0
57	MG	YA	3245	1/1	0.80	0.57	3,3,3,3	0
57	MG	RA	3063	1/1	0.81	0.11	19,19,19,19	0
57	MG	QA	1622	1/1	0.81	0.45	52,52,52,52	0
57	MG	RA	3231	1/1	0.81	0.35	3,3,3,3	0
57	MG	RA	3184	1/1	0.81	0.36	40,40,40,40	0
57	MG	RA	3007	1/1	0.81	1.30	50,50,50,50	0
57	MG	YA	3171	1/1	0.81	0.22	7,7,7,7	0
57	MG	RA	3050	1/1	0.81	0.14	8,8,8,8	0
57	MG	RA	3225	1/1	0.81	0.29	47,47,47,47	0
57	MG	R8	101	1/1	0.82	0.39	6,6,6,6	0
57	MG	YA	3041	1/1	0.82	0.85	50,50,50,50	0
57	MG	YA	3253	1/1	0.82	1.86	50,50,50,50	0
57	MG	YA	3187	1/1	0.82	0.21	47,47,47,47	0
57	MG	YA	3193	1/1	0.82	0.74	7,7,7,7	0
57	MG	RA	3027	1/1	0.82	0.97	50,50,50,50	0
57	MG	RA	3157	1/1	0.82	0.25	39,39,39,39	0
57	MG	XA	1664	1/1	0.82	0.40	27,27,27,27	0
57	MG	YA	3105	1/1	0.83	0.74	8,8,8,8	0
57	MG	QA	1651	1/1	0.83	0.43	16,16,16,16	0
57	MG	YA	3204	1/1	0.83	0.16	11,11,11,11	0
57	MG	XA	1653	1/1	0.83	0.15	29,29,29,29	0
57	MG	RA	3128	1/1	0.83	0.23	10,10,10,10	0
57	MG	RA	3001	1/1	0.83	0.78	1,1,1,1	0
57	MG	XA	1607	1/1	0.83	0.32	17,17,17,17	0
57	MG	YA	3154	1/1	0.84	0.26	5,5,5,5	0
57	MG	YA	3191	1/1	0.84	0.39	14,14,14,14	0
57	MG	XA	1665	1/1	0.84	0.19	18,18,18,18	0
57	MG	YA	3157	1/1	0.84	0.32	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3206	1/1	0.84	0.29	20,20,20,20	0
57	MG	QX	101	1/1	0.84	0.15	6,6,6,6	0
57	MG	YA	3024	1/1	0.84	0.53	50,50,50,50	0
57	MG	YA	3047	1/1	0.84	1.00	50,50,50,50	0
57	MG	YA	3185	1/1	0.84	0.16	74,74,74,74	0
57	MG	RA	3136	1/1	0.85	0.24	14,14,14,14	0
57	MG	QA	1639	1/1	0.85	0.26	27,27,27,27	0
57	MG	YA	3217	1/1	0.85	0.62	52,52,52,52	0
57	MG	RA	3078	1/1	0.85	0.83	50,50,50,50	0
57	MG	RA	3051	1/1	0.85	0.83	50,50,50,50	0
57	MG	XM	201	1/1	0.85	0.17	78,78,78,78	0
57	MG	RA	3119	1/1	0.85	0.25	88,88,88,88	0
57	MG	YA	3168	1/1	0.85	0.16	13,13,13,13	0
57	MG	YA	3125	1/1	0.85	0.45	15,15,15,15	0
57	MG	QA	1637	1/1	0.85	0.26	3,3,3,3	0
57	MG	QA	1610	1/1	0.85	0.57	50,50,50,50	0
57	MG	YB	201	1/1	0.85	0.29	14,14,14,14	0
57	MG	RA	3194	1/1	0.85	0.15	82,82,82,82	0
57	MG	RA	3043	1/1	0.85	0.70	50,50,50,50	0
57	MG	YA	3198	1/1	0.85	0.28	2,2,2,2	0
57	MG	YA	3202	1/1	0.85	0.42	13,13,13,13	0
57	MG	XA	1652	1/1	0.86	0.26	50,50,50,50	0
57	MG	RA	3021	1/1	0.86	1.12	50,50,50,50	0
57	MG	RA	3166	1/1	0.86	0.94	9,9,9,9	0
57	MG	RA	3085	1/1	0.86	0.22	27,27,27,27	0
57	MG	XA	1606	1/1	0.86	0.64	13,13,13,13	0
57	MG	YA	3134	1/1	0.86	0.66	50,50,50,50	0
57	MG	RA	3131	1/1	0.86	0.18	25,25,25,25	0
57	MG	YA	3006	1/1	0.86	0.86	50,50,50,50	0
57	MG	RA	3023	1/1	0.86	0.49	50,50,50,50	0
57	MG	YA	3242	1/1	0.86	0.20	5,5,5,5	0
57	MG	XA	1616	1/1	0.86	0.77	50,50,50,50	0
57	MG	YA	3030	1/1	0.86	0.89	50,50,50,50	0
57	MG	YA	3031	1/1	0.86	1.04	50,50,50,50	0
57	MG	XA	1628	1/1	0.86	0.14	2,2,2,2	0
57	MG	QA	1658	1/1	0.86	0.42	46,46,46,46	0
57	MG	RA	3146	1/1	0.86	0.41	7,7,7,7	0
57	MG	YA	3262	1/1	0.86	0.33	9,9,9,9	0
57	MG	XA	1638	1/1	0.86	0.17	27,27,27,27	0
57	MG	YB	202	1/1	0.86	0.43	5,5,5,5	0
57	MG	QA	1623	1/1	0.86	0.52	13,13,13,13	0
57	MG	YA	3176	1/1	0.86	0.31	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RP	202	1/1	0.86	0.31	75,75,75,75	0
57	MG	YA	3083	1/1	0.86	0.21	16,16,16,16	0
57	MG	XA	1671	1/1	0.87	0.18	28,28,28,28	0
57	MG	RA	3180	1/1	0.87	0.36	1,1,1,1	0
57	MG	XA	1609	1/1	0.87	0.55	8,8,8,8	0
57	MG	RA	3222	1/1	0.87	0.37	4,4,4,4	0
57	MG	RA	3039	1/1	0.87	0.66	50,50,50,50	0
57	MG	RA	3151	1/1	0.87	0.35	37,37,37,37	0
57	MG	YA	3234	1/1	0.87	0.09	2,2,2,2	0
57	MG	RA	3121	1/1	0.87	0.15	0,0,0,0	0
57	MG	RA	3160	1/1	0.87	0.33	2,2,2,2	0
57	MG	RA	3005	1/1	0.87	0.80	50,50,50,50	0
57	MG	XA	1641	1/1	0.87	0.33	14,14,14,14	0
57	MG	YA	3249	1/1	0.87	0.70	5,5,5,5	0
57	MG	RA	3237	1/1	0.87	0.23	4,4,4,4	0
57	MG	YA	3162	1/1	0.87	0.29	30,30,30,30	0
57	MG	RA	3241	1/1	0.87	0.38	0,0,0,0	0
57	MG	YA	3074	1/1	0.87	0.61	4,4,4,4	0
57	MG	YA	3169	1/1	0.87	0.86	7,7,7,7	0
57	MG	YA	3264	1/1	0.87	0.53	14,14,14,14	0
57	MG	RA	3003	1/1	0.87	1.15	50,50,50,50	0
57	MG	RA	3206	1/1	0.87	0.25	11,11,11,11	0
57	MG	RA	3211	1/1	0.87	0.25	11,11,11,11	0
57	MG	YA	3115	1/1	0.87	0.29	15,15,15,15	0
58	PAR	XA	1673	42/42	0.87	0.32	132,132,132,132	0
57	MG	RA	3174	1/1	0.87	0.15	40,40,40,40	0
57	MG	RA	3175	1/1	0.87	0.28	12,12,12,12	0
57	MG	YA	3236	1/1	0.88	0.20	12,12,12,12	0
57	MG	RA	3196	1/1	0.88	0.33	22,22,22,22	0
57	MG	YA	3138	1/1	0.88	0.49	4,4,4,4	0
57	MG	YA	3183	1/1	0.88	0.19	17,17,17,17	0
57	MG	RA	3228	1/1	0.88	0.15	7,7,7,7	0
57	MG	RA	3020	1/1	0.88	0.71	50,50,50,50	0
57	MG	YA	3113	1/1	0.88	0.48	50,50,50,50	0
57	MG	YA	3254	1/1	0.88	0.37	0,0,0,0	0
57	MG	RA	3139	1/1	0.88	0.54	18,18,18,18	0
57	MG	YA	3197	1/1	0.88	1.38	50,50,50,50	0
57	MG	YA	3045	1/1	0.88	0.55	0,0,0,0	0
57	MG	XA	1625	1/1	0.88	0.48	50,50,50,50	0
57	MG	RA	3069	1/1	0.88	0.26	9,9,9,9	0
57	MG	QA	1618	1/1	0.88	0.42	8,8,8,8	0
57	MG	Y7	101	1/1	0.88	0.27	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	YA	3128	1/1	0.88	0.23	0,0,0,0	0
57	MG	YA	3220	1/1	0.88	0.15	26,26,26,26	0
57	MG	YA	3131	1/1	0.88	0.50	17,17,17,17	0
57	MG	XA	1656	1/1	0.88	0.89	12,12,12,12	0
57	MG	YA	3170	1/1	0.88	0.28	8,8,8,8	0
57	MG	YA	3207	1/1	0.89	0.25	0,0,0,0	0
57	MG	YA	3215	1/1	0.89	0.25	2,2,2,2	0
57	MG	RA	3202	1/1	0.89	0.31	2,2,2,2	0
57	MG	YA	3062	1/1	0.89	0.23	0,0,0,0	0
57	MG	QA	1612	1/1	0.89	0.38	4,4,4,4	0
57	MG	YA	3232	1/1	0.89	0.22	15,15,15,15	0
57	MG	RA	3178	1/1	0.89	0.37	5,5,5,5	0
57	MG	RA	3207	1/1	0.89	0.25	5,5,5,5	0
57	MG	RA	3091	1/1	0.89	0.49	2,2,2,2	0
57	MG	YA	3085	1/1	0.89	0.81	50,50,50,50	0
57	MG	YA	3103	1/1	0.89	0.15	31,31,31,31	0
57	MG	YA	3246	1/1	0.89	0.51	2,2,2,2	0
57	MG	YA	3001	1/1	0.89	1.16	50,50,50,50	0
57	MG	YA	3005	1/1	0.89	0.21	2,2,2,2	0
57	MG	RA	3240	1/1	0.89	0.67	12,12,12,12	0
57	MG	YA	3116	1/1	0.89	0.40	11,11,11,11	0
57	MG	RA	3156	1/1	0.89	0.16	7,7,7,7	0
57	MG	YA	3178	1/1	0.89	0.52	32,32,32,32	0
57	MG	YA	3180	1/1	0.89	0.71	5,5,5,5	0
57	MG	RD	301	1/1	0.89	0.28	15,15,15,15	0
57	MG	YA	3027	1/1	0.89	0.17	1,1,1,1	0
57	MG	RA	3114	1/1	0.89	0.18	3,3,3,3	0
57	MG	RA	3054	1/1	0.89	0.31	4,4,4,4	0
57	MG	YA	3130	1/1	0.89	0.10	3,3,3,3	0
57	MG	YA	3040	1/1	0.89	0.69	50,50,50,50	0
57	MG	XX	101	1/1	0.89	0.17	88,88,88,88	0
57	MG	RA	3221	1/1	0.89	0.69	79,79,79,79	0
57	MG	QA	1657	1/1	0.89	0.10	19,19,19,19	0
57	MG	QA	1608	1/1	0.89	0.23	63,63,63,63	0
57	MG	RA	3122	1/1	0.89	0.30	19,19,19,19	0
57	MG	RA	3149	1/1	0.90	0.62	17,17,17,17	0
57	MG	YA	3226	1/1	0.90	0.23	10,10,10,10	0
57	MG	YA	3112	1/1	0.90	0.21	19,19,19,19	0
57	MG	QA	1633	1/1	0.90	0.43	1,1,1,1	0
57	MG	RA	3153	1/1	0.90	0.41	36,36,36,36	0
57	MG	RA	3216	1/1	0.90	0.29	1,1,1,1	0
57	MG	RA	3092	1/1	0.90	0.23	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3173	1/1	0.90	0.20	14,14,14,14	0
57	MG	RA	3093	1/1	0.90	0.71	50,50,50,50	0
57	MG	RA	3220	1/1	0.90	0.15	25,25,25,25	0
57	MG	XA	1603	1/1	0.90	0.95	50,50,50,50	0
57	MG	RA	3038	1/1	0.90	0.73	50,50,50,50	0
57	MG	XA	1659	1/1	0.90	0.16	15,15,15,15	0
57	MG	RA	3010	1/1	0.90	0.31	56,56,56,56	0
57	MG	YA	3190	1/1	0.90	0.51	17,17,17,17	0
57	MG	YA	3055	1/1	0.90	0.19	24,24,24,24	0
57	MG	RA	3197	1/1	0.90	0.16	9,9,9,9	0
57	MG	RA	3072	1/1	0.90	0.35	0,0,0,0	0
57	MG	YA	3145	1/1	0.90	0.22	25,25,25,25	0
57	MG	YA	3073	1/1	0.90	0.29	4,4,4,4	0
57	MG	RA	3167	1/1	0.90	0.09	26,26,26,26	0
57	MG	YA	3075	1/1	0.90	1.18	50,50,50,50	0
57	MG	RA	3203	1/1	0.90	0.20	34,34,34,34	0
57	MG	YA	3213	1/1	0.90	0.31	15,15,15,15	0
57	MG	RA	3006	1/1	0.90	1.06	50,50,50,50	0
57	MG	RA	3030	1/1	0.90	0.73	50,50,50,50	0
57	MG	XA	1629	1/1	0.90	0.14	32,32,32,32	0
57	MG	YA	3205	1/1	0.91	0.24	40,40,40,40	0
57	MG	RA	3182	1/1	0.91	0.50	10,10,10,10	0
57	MG	YA	3143	1/1	0.91	0.23	11,11,11,11	0
57	MG	RA	3014	1/1	0.91	0.90	50,50,50,50	0
57	MG	YA	3214	1/1	0.91	0.24	23,23,23,23	0
57	MG	RA	3218	1/1	0.91	0.35	10,10,10,10	0
57	MG	XA	1660	1/1	0.91	0.10	19,19,19,19	0
57	MG	QA	1627	1/1	0.91	0.15	1,1,1,1	0
57	MG	YA	3221	1/1	0.91	0.24	7,7,7,7	0
57	MG	RA	3188	1/1	0.91	0.13	16,16,16,16	0
57	MG	RA	3190	1/1	0.91	0.14	4,4,4,4	0
57	MG	XA	1667	1/1	0.91	0.14	4,4,4,4	0
57	MG	RA	3087	1/1	0.91	0.43	0,0,0,0	0
57	MG	YA	3080	1/1	0.91	0.83	50,50,50,50	0
57	MG	YA	3081	1/1	0.91	0.28	7,7,7,7	0
57	MG	RA	3090	1/1	0.91	0.45	4,4,4,4	0
57	MG	YA	3244	1/1	0.91	0.48	6,6,6,6	0
57	MG	RA	3035	1/1	0.91	0.81	50,50,50,50	0
57	MG	YA	3098	1/1	0.91	0.84	50,50,50,50	0
57	MG	QA	1617	1/1	0.91	0.44	2,2,2,2	0
57	MG	YA	3248	1/1	0.91	0.87	15,15,15,15	0
57	MG	YA	3172	1/1	0.91	0.14	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	RA	3134	1/1	0.91	0.09	23,23,23,23	0
57	MG	QA	1611	1/1	0.91	0.27	4,4,4,4	0
57	MG	YA	3016	1/1	0.91	0.20	8,8,8,8	0
57	MG	YA	3179	1/1	0.91	0.27	20,20,20,20	0
57	MG	YA	3019	1/1	0.91	0.80	50,50,50,50	0
57	MG	YA	3020	1/1	0.91	0.58	6,6,6,6	0
57	MG	RA	3026	1/1	0.91	0.17	13,13,13,13	0
57	MG	RA	3011	1/1	0.91	0.38	7,7,7,7	0
57	MG	YA	3189	1/1	0.91	0.42	7,7,7,7	0
57	MG	RA	3239	1/1	0.91	0.79	10,10,10,10	0
57	MG	RA	3118	1/1	0.91	0.20	1,1,1,1	0
57	MG	YA	3035	1/1	0.91	0.80	50,50,50,50	0
57	MG	XA	1648	1/1	0.91	0.19	10,10,10,10	0
57	MG	RA	3210	1/1	0.91	0.15	11,11,11,11	0
57	MG	RA	3148	1/1	0.91	0.13	0,0,0,0	0
57	MG	RA	3028	1/1	0.91	0.23	23,23,23,23	0
57	MG	RA	3195	1/1	0.92	0.14	23,23,23,23	0
57	MG	XA	1621	1/1	0.92	0.57	6,6,6,6	0
57	MG	YA	3149	1/1	0.92	0.76	7,7,7,7	0
57	MG	YA	3071	1/1	0.92	0.32	6,6,6,6	0
57	MG	XA	1666	1/1	0.92	0.21	34,34,34,34	0
57	MG	RA	3238	1/1	0.92	0.71	3,3,3,3	0
57	MG	XA	1669	1/1	0.92	0.08	15,15,15,15	0
57	MG	QA	1646	1/1	0.92	0.58	11,11,11,11	0
57	MG	QA	1626	1/1	0.92	0.17	17,17,17,17	0
57	MG	YA	3160	1/1	0.92	0.38	4,4,4,4	0
57	MG	YA	3227	1/1	0.92	0.17	15,15,15,15	0
57	MG	XA	1630	1/1	0.92	0.31	1,1,1,1	0
57	MG	XA	1631	1/1	0.92	0.18	10,10,10,10	0
57	MG	RA	3045	1/1	0.92	0.28	0,0,0,0	0
57	MG	YA	3086	1/1	0.92	0.42	19,19,19,19	0
57	MG	RA	3244	1/1	0.92	0.20	9,9,9,9	0
57	MG	YA	3099	1/1	0.92	0.79	50,50,50,50	0
57	MG	RA	3013	1/1	0.92	0.35	0,0,0,0	0
57	MG	QA	1614	1/1	0.92	0.24	21,21,21,21	0
57	MG	XA	1643	1/1	0.92	0.75	50,50,50,50	0
57	MG	XA	1646	1/1	0.92	0.17	8,8,8,8	0
57	MG	RA	3162	1/1	0.92	0.21	18,18,18,18	0
57	MG	RA	3185	1/1	0.92	0.19	3,3,3,3	0
57	MG	YA	3182	1/1	0.92	0.63	14,14,14,14	0
57	MG	XA	1602	1/1	0.92	0.92	50,50,50,50	0
57	MG	YA	3258	1/1	0.92	0.52	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3032	1/1	0.92	0.52	50,50,50,50	0
57	MG	XA	1651	1/1	0.92	0.17	84,84,84,84	0
57	MG	YA	3188	1/1	0.92	0.12	36,36,36,36	0
57	MG	RA	3224	1/1	0.92	0.17	16,16,16,16	0
57	MG	RA	3142	1/1	0.92	0.43	8,8,8,8	0
57	MG	QA	1656	1/1	0.92	0.09	63,63,63,63	0
57	MG	XA	1657	1/1	0.92	0.26	4,4,4,4	0
57	MG	YA	3194	1/1	0.92	0.19	15,15,15,15	0
57	MG	XV	101	1/1	0.92	0.39	1,1,1,1	0
57	MG	RA	3101	1/1	0.92	0.27	9,9,9,9	0
57	MG	RA	3056	1/1	0.92	0.20	0,0,0,0	0
57	MG	YA	3054	1/1	0.92	0.59	50,50,50,50	0
57	MG	YA	3140	1/1	0.92	0.22	19,19,19,19	0
57	MG	RA	3214	1/1	0.92	0.21	43,43,43,43	0
57	MG	YA	3090	1/1	0.93	0.22	17,17,17,17	0
57	MG	YA	3158	1/1	0.93	0.24	6,6,6,6	0
57	MG	YA	3219	1/1	0.93	0.10	22,22,22,22	0
57	MG	RA	3008	1/1	0.93	0.28	0,0,0,0	0
57	MG	XA	1654	1/1	0.93	0.43	17,17,17,17	0
57	MG	YA	3100	1/1	0.93	0.71	0,0,0,0	0
57	MG	YA	3102	1/1	0.93	0.84	6,6,6,6	0
57	MG	XA	1614	1/1	0.93	0.31	25,25,25,25	0
57	MG	RA	3187	1/1	0.93	0.16	10,10,10,10	0
57	MG	YA	3036	1/1	0.93	0.19	3,3,3,3	0
57	MG	RA	3233	1/1	0.93	1.47	50,50,50,50	0
57	MG	RA	3234	1/1	0.93	0.85	50,50,50,50	0
57	MG	RA	3031	1/1	0.93	0.77	50,50,50,50	0
57	MG	YA	3243	1/1	0.93	0.77	50,50,50,50	0
57	MG	RA	3215	1/1	0.93	0.28	14,14,14,14	0
57	MG	RA	3046	1/1	0.93	0.45	0,0,0,0	0
57	MG	YA	3048	1/1	0.93	0.46	50,50,50,50	0
57	MG	RA	3147	1/1	0.93	0.24	6,6,6,6	0
57	MG	RA	3171	1/1	0.93	0.44	15,15,15,15	0
57	MG	XA	1633	1/1	0.93	0.18	13,13,13,13	0
57	MG	YA	3056	1/1	0.93	0.88	50,50,50,50	0
57	MG	YA	3132	1/1	0.93	0.37	26,26,26,26	0
57	MG	XA	1670	1/1	0.93	0.19	44,44,44,44	0
57	MG	YA	3255	1/1	0.93	1.37	50,50,50,50	0
57	MG	RA	3172	1/1	0.93	0.27	17,17,17,17	0
57	MG	QA	1642	1/1	0.93	0.16	9,9,9,9	0
57	MG	YA	3072	1/1	0.93	0.49	50,50,50,50	0
57	MG	YA	3142	1/1	0.93	0.27	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	QA	1659	1/1	0.93	0.19	4,4,4,4	0
57	MG	YA	3265	1/1	0.93	0.65	11,11,11,11	0
57	MG	RA	3104	1/1	0.93	0.13	5,5,5,5	0
57	MG	YA	3199	1/1	0.93	0.18	11,11,11,11	0
57	MG	RA	3108	1/1	0.93	0.24	5,5,5,5	0
57	MG	RA	3154	1/1	0.93	0.45	6,6,6,6	0
57	MG	QA	1650	1/1	0.93	0.23	8,8,8,8	0
57	MG	RA	3226	1/1	0.93	0.32	29,29,29,29	0
57	MG	QA	1605	1/1	0.93	0.52	4,4,4,4	0
57	MG	YA	3211	1/1	0.93	0.13	3,3,3,3	0
57	MG	RA	3016	1/1	0.93	0.65	50,50,50,50	0
57	MG	XA	1608	1/1	0.93	0.18	50,50,50,50	0
57	MG	RA	3200	1/1	0.94	0.20	31,31,31,31	0
57	MG	RA	3173	1/1	0.94	0.35	3,3,3,3	0
57	MG	RA	3120	1/1	0.94	0.20	31,31,31,31	0
57	MG	RA	3037	1/1	0.94	0.43	0,0,0,0	0
57	MG	YA	3141	1/1	0.94	0.10	18,18,18,18	0
57	MG	RA	3176	1/1	0.94	0.28	30,30,30,30	0
57	MG	YA	3065	1/1	0.94	0.75	8,8,8,8	0
57	MG	RA	3048	1/1	0.94	1.15	50,50,50,50	0
57	MG	YA	3147	1/1	0.94	0.17	0,0,0,0	0
57	MG	XA	1619	1/1	0.94	0.41	8,8,8,8	0
57	MG	RA	3232	1/1	0.94	0.30	5,5,5,5	0
57	MG	RA	3002	1/1	0.94	0.19	8,8,8,8	0
57	MG	QA	1661	1/1	0.94	0.10	44,44,44,44	0
57	MG	YA	3222	1/1	0.94	0.11	2,2,2,2	0
57	MG	RA	3103	1/1	0.94	0.22	8,8,8,8	0
57	MG	RA	3130	1/1	0.94	0.17	19,19,19,19	0
57	MG	YA	3003	1/1	0.94	0.46	50,50,50,50	0
57	MG	RA	3213	1/1	0.94	0.31	10,10,10,10	0
57	MG	RA	3052	1/1	0.94	0.48	50,50,50,50	0
57	MG	YA	3084	1/1	0.94	0.28	2,2,2,2	0
57	MG	YA	3007	1/1	0.94	0.22	1,1,1,1	0
57	MG	YA	3241	1/1	0.94	0.27	13,13,13,13	0
57	MG	RA	3075	1/1	0.94	0.36	37,37,37,37	0
57	MG	YA	3166	1/1	0.94	0.13	14,14,14,14	0
57	MG	RA	3242	1/1	0.94	0.61	8,8,8,8	0
57	MG	YA	3093	1/1	0.94	0.48	4,4,4,4	0
57	MG	YA	3018	1/1	0.94	0.82	50,50,50,50	0
57	MG	RA	3243	1/1	0.94	0.38	18,18,18,18	0
57	MG	XA	1640	1/1	0.94	0.14	119,119,119,119	0
57	MG	RA	3113	1/1	0.94	0.30	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	YA	3026	1/1	0.94	1.28	50,50,50,50	0
57	MG	YA	3251	1/1	0.94	1.32	50,50,50,50	0
57	MG	QA	1621	1/1	0.94	0.19	35,35,35,35	0
57	MG	YA	3109	1/1	0.94	0.20	9,9,9,9	0
57	MG	YA	3111	1/1	0.94	0.24	7,7,7,7	0
57	MG	YA	3181	1/1	0.94	0.57	5,5,5,5	0
57	MG	RE	302	1/1	0.94	0.20	15,15,15,15	0
57	MG	YA	3260	1/1	0.94	0.57	50,50,50,50	0
57	MG	RF	301	1/1	0.94	0.27	10,10,10,10	0
57	MG	RA	3189	1/1	0.94	0.17	16,16,16,16	0
57	MG	YA	3186	1/1	0.94	0.18	10,10,10,10	0
57	MG	RU	201	1/1	0.94	0.16	86,86,86,86	0
57	MG	QA	1630	1/1	0.94	0.13	14,14,14,14	0
57	MG	RA	3193	1/1	0.94	0.15	17,17,17,17	0
57	MG	YE	301	1/1	0.94	0.24	1,1,1,1	0
57	MG	RA	3061	1/1	0.94	0.77	50,50,50,50	0
57	MG	RA	3168	1/1	0.94	0.23	10,10,10,10	0
57	MG	RA	3144	1/1	0.94	0.18	29,29,29,29	0
57	MG	XV	102	1/1	0.94	0.16	16,16,16,16	0
57	MG	RA	3019	1/1	0.94	1.19	50,50,50,50	0
57	MG	YA	3195	1/1	0.94	0.19	21,21,21,21	0
57	MG	XA	1658	1/1	0.94	0.28	17,17,17,17	0
57	MG	YA	3049	1/1	0.94	1.10	50,50,50,50	0
59	ZN	XD	301	1/1	0.94	0.39	50,50,50,50	0
57	MG	YA	3133	1/1	0.94	0.08	12,12,12,12	0
57	MG	RA	3102	1/1	0.95	0.13	10,10,10,10	0
57	MG	RA	3208	1/1	0.95	0.14	50,50,50,50	0
57	MG	XA	1642	1/1	0.95	0.23	11,11,11,11	0
57	MG	RA	3135	1/1	0.95	0.13	28,28,28,28	0
57	MG	XA	1645	1/1	0.95	0.45	8,8,8,8	0
57	MG	QA	1624	1/1	0.95	0.29	16,16,16,16	0
57	MG	YA	3203	1/1	0.95	0.40	29,29,29,29	0
57	MG	YA	3033	1/1	0.95	0.73	50,50,50,50	0
57	MG	YA	3124	1/1	0.95	0.27	13,13,13,13	0
57	MG	YA	3034	1/1	0.95	0.34	7,7,7,7	0
57	MG	XA	1647	1/1	0.95	0.34	11,11,11,11	0
57	MG	YA	3209	1/1	0.95	0.20	9,9,9,9	0
57	MG	QA	1625	1/1	0.95	0.08	74,74,74,74	0
57	MG	YA	3037	1/1	0.95	0.34	3,3,3,3	0
57	MG	YA	3039	1/1	0.95	0.23	0,0,0,0	0
57	MG	RA	3107	1/1	0.95	0.27	9,9,9,9	0
57	MG	RP	201	1/1	0.95	0.43	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3076	1/1	0.95	0.17	3,3,3,3	0
57	MG	YA	3135	1/1	0.95	0.39	9,9,9,9	0
57	MG	YA	3044	1/1	0.95	0.53	16,16,16,16	0
57	MG	RA	3177	1/1	0.95	0.27	30,30,30,30	0
57	MG	R5	101	1/1	0.95	0.15	14,14,14,14	0
57	MG	RA	3143	1/1	0.95	0.08	12,12,12,12	0
57	MG	RA	3179	1/1	0.95	0.24	10,10,10,10	0
57	MG	YA	3229	1/1	0.95	0.13	5,5,5,5	0
57	MG	RA	3077	1/1	0.95	0.39	50,50,50,50	0
57	MG	YA	3233	1/1	0.95	0.10	3,3,3,3	0
57	MG	YA	3144	1/1	0.95	0.54	6,6,6,6	0
57	MG	QA	1652	1/1	0.95	0.21	24,24,24,24	0
57	MG	RA	3080	1/1	0.95	0.16	5,5,5,5	0
57	MG	RA	3057	1/1	0.95	0.77	50,50,50,50	0
57	MG	YA	3057	1/1	0.95	0.50	8,8,8,8	0
57	MG	YA	3059	1/1	0.95	0.30	3,3,3,3	0
57	MG	QA	1653	1/1	0.95	0.11	6,6,6,6	0
57	MG	YA	3064	1/1	0.95	0.17	4,4,4,4	0
57	MG	RA	3089	1/1	0.95	0.38	0,0,0,0	0
57	MG	QA	1613	1/1	0.95	0.42	1,1,1,1	0
57	MG	RA	3047	1/1	0.95	0.16	2,2,2,2	0
57	MG	RA	3155	1/1	0.95	0.19	9,9,9,9	0
57	MG	XA	1668	1/1	0.95	0.27	6,6,6,6	0
57	MG	QA	1604	1/1	0.95	0.37	7,7,7,7	0
57	MG	RA	3126	1/1	0.95	0.22	14,14,14,14	0
57	MG	RA	3158	1/1	0.95	0.26	15,15,15,15	0
57	MG	XA	1672	1/1	0.95	0.26	5,5,5,5	0
57	MG	XA	1624	1/1	0.95	0.60	8,8,8,8	0
57	MG	YA	3082	1/1	0.95	0.58	50,50,50,50	0
57	MG	QA	1619	1/1	0.95	0.25	29,29,29,29	0
57	MG	YA	3002	1/1	0.95	0.73	50,50,50,50	0
57	MG	RA	3161	1/1	0.95	0.14	8,8,8,8	0
57	MG	RA	3098	1/1	0.95	0.40	4,4,4,4	0
57	MG	YA	3089	1/1	0.95	0.24	13,13,13,13	0
57	MG	RA	3100	1/1	0.95	1.01	50,50,50,50	0
57	MG	YA	3091	1/1	0.95	0.58	12,12,12,12	0
57	MG	YA	3092	1/1	0.95	0.40	2,2,2,2	0
57	MG	YX	101	1/1	0.95	0.41	50,50,50,50	0
57	MG	Y5	101	1/1	0.95	0.14	2,2,2,2	0
57	MG	RA	3165	1/1	0.95	0.25	3,3,3,3	0
57	MG	YA	3097	1/1	0.95	0.70	50,50,50,50	0
57	MG	YA	3008	1/1	0.95	0.21	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	XA	1632	1/1	0.95	0.41	2,2,2,2	0
57	MG	QA	1649	1/1	0.95	0.10	19,19,19,19	0
57	MG	RA	3132	1/1	0.95	0.38	7,7,7,7	0
57	MG	RA	3133	1/1	0.95	0.14	4,4,4,4	0
57	MG	RA	3169	1/1	0.95	0.12	19,19,19,19	0
57	MG	YA	3106	1/1	0.95	0.49	50,50,50,50	0
59	ZN	XN	101	1/1	0.95	0.18	59,59,59,59	0
57	MG	YA	3021	1/1	0.95	0.56	50,50,50,50	0
57	MG	RA	3138	1/1	0.96	0.37	8,8,8,8	0
57	MG	RA	3009	1/1	0.96	0.57	7,7,7,7	0
57	MG	RA	3235	1/1	0.96	0.14	2,2,2,2	0
57	MG	RA	3170	1/1	0.96	0.41	2,2,2,2	0
57	MG	YA	3061	1/1	0.96	0.49	9,9,9,9	0
57	MG	RA	3111	1/1	0.96	0.44	4,4,4,4	0
57	MG	RA	3141	1/1	0.96	0.45	5,5,5,5	0
57	MG	YA	3210	1/1	0.96	0.30	30,30,30,30	0
57	MG	RA	3112	1/1	0.96	0.38	2,2,2,2	0
57	MG	YA	3212	1/1	0.96	0.24	8,8,8,8	0
57	MG	YA	3139	1/1	0.96	0.27	13,13,13,13	0
57	MG	YA	3069	1/1	0.96	0.10	8,8,8,8	0
57	MG	RA	3081	1/1	0.96	0.34	10,10,10,10	0
57	MG	RA	3083	1/1	0.96	0.39	3,3,3,3	0
57	MG	RA	3022	1/1	0.96	0.25	5,5,5,5	0
57	MG	RA	3086	1/1	0.96	0.30	50,50,50,50	0
57	MG	RA	3060	1/1	0.96	0.70	13,13,13,13	0
57	MG	YA	3146	1/1	0.96	0.21	6,6,6,6	0
57	MG	YA	3009	1/1	0.96	0.74	50,50,50,50	0
57	MG	YA	3225	1/1	0.96	0.36	23,23,23,23	0
57	MG	YA	3076	1/1	0.96	0.39	1,1,1,1	0
57	MG	RE	301	1/1	0.96	0.13	2,2,2,2	0
57	MG	YA	3013	1/1	0.96	0.37	1,1,1,1	0
57	MG	YA	3014	1/1	0.96	0.39	1,1,1,1	0
57	MG	YA	3152	1/1	0.96	0.39	7,7,7,7	0
57	MG	YA	3015	1/1	0.96	0.77	50,50,50,50	0
57	MG	QA	1647	1/1	0.96	0.15	55,55,55,55	0
57	MG	YA	3155	1/1	0.96	0.18	8,8,8,8	0
57	MG	YA	3237	1/1	0.96	0.20	38,38,38,38	0
57	MG	YA	3017	1/1	0.96	0.28	7,7,7,7	0
57	MG	RA	3042	1/1	0.96	0.58	50,50,50,50	0
57	MG	RA	3152	1/1	0.96	0.16	26,26,26,26	0
57	MG	XA	1644	1/1	0.96	0.30	11,11,11,11	0
57	MG	QA	1662	1/1	0.96	0.08	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3012	1/1	0.96	0.27	1,1,1,1	0
57	MG	RA	3124	1/1	0.96	0.29	19,19,19,19	0
57	MG	QA	1648	1/1	0.96	0.19	16,16,16,16	0
57	MG	YA	3094	1/1	0.96	0.38	8,8,8,8	0
57	MG	RA	3097	1/1	0.96	0.60	11,11,11,11	0
57	MG	QA	1620	1/1	0.96	0.12	21,21,21,21	0
57	MG	QA	1615	1/1	0.96	0.18	54,54,54,54	0
57	MG	XA	1604	1/1	0.96	1.07	50,50,50,50	0
57	MG	YA	3175	1/1	0.96	0.12	2,2,2,2	0
57	MG	YA	3256	1/1	0.96	0.14	9,9,9,9	0
57	MG	RA	3073	1/1	0.96	0.28	36,36,36,36	0
57	MG	RA	3192	1/1	0.96	0.16	27,27,27,27	0
57	MG	XA	1655	1/1	0.96	0.22	7,7,7,7	0
57	MG	RA	3033	1/1	0.96	0.60	16,16,16,16	0
57	MG	RA	3227	1/1	0.96	0.14	39,39,39,39	0
57	MG	RA	3163	1/1	0.96	0.18	38,38,38,38	0
57	MG	XA	1610	1/1	0.96	0.26	1,1,1,1	0
57	MG	XA	1611	1/1	0.96	0.33	1,1,1,1	0
57	MG	YA	3114	1/1	0.96	0.29	16,16,16,16	0
57	MG	YB	203	1/1	0.96	0.18	17,17,17,17	0
57	MG	RA	3018	1/1	0.96	0.28	3,3,3,3	0
57	MG	YQ	201	1/1	0.96	0.20	79,79,79,79	0
57	MG	XA	1663	1/1	0.96	0.17	3,3,3,3	0
57	MG	QA	1644	1/1	0.96	0.29	24,24,24,24	0
57	MG	RA	3105	1/1	0.96	0.21	1,1,1,1	0
57	MG	YA	3120	1/1	0.96	0.16	16,16,16,16	0
57	MG	YA	3192	1/1	0.96	0.15	15,15,15,15	0
57	MG	YA	3121	1/1	0.96	0.15	8,8,8,8	0
57	MG	YA	3123	1/1	0.96	0.18	0,0,0,0	0
57	MG	XA	1617	1/1	0.96	0.26	2,2,2,2	0
57	MG	YA	3050	1/1	0.96	0.50	50,50,50,50	0
59	ZN	QN	101	1/1	0.96	0.13	56,56,56,56	0
57	MG	QA	1641	1/1	0.96	0.08	3,3,3,3	0
57	MG	XA	1620	1/1	0.96	0.15	0,0,0,0	0
57	MG	YA	3200	1/1	0.96	0.15	35,35,35,35	0
57	MG	YA	3201	1/1	0.96	0.16	10,10,10,10	0
57	MG	RA	3062	1/1	0.97	0.49	2,2,2,2	0
57	MG	RA	3145	1/1	0.97	0.42	3,3,3,3	0
57	MG	YA	3077	1/1	0.97	0.22	0,0,0,0	0
57	MG	YA	3078	1/1	0.97	0.26	10,10,10,10	0
57	MG	YA	3231	1/1	0.97	0.35	11,11,11,11	0
57	MG	YA	3177	1/1	0.97	0.07	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3040	1/1	0.97	0.23	11,11,11,11	0
57	MG	YA	3129	1/1	0.97	0.11	1,1,1,1	0
57	MG	XA	1612	1/1	0.97	0.22	23,23,23,23	0
57	MG	XA	1613	1/1	0.97	0.08	16,16,16,16	0
57	MG	RA	3183	1/1	0.97	0.49	11,11,11,11	0
57	MG	RA	3032	1/1	0.97	0.68	50,50,50,50	0
57	MG	YA	3184	1/1	0.97	0.32	50,50,50,50	0
57	MG	RA	3095	1/1	0.97	0.42	24,24,24,24	0
57	MG	YA	3004	1/1	0.97	0.43	5,5,5,5	0
57	MG	RA	3025	1/1	0.97	0.25	7,7,7,7	0
57	MG	YA	3088	1/1	0.97	0.26	3,3,3,3	0
57	MG	XA	1618	1/1	0.97	0.31	4,4,4,4	0
57	MG	RA	3115	1/1	0.97	0.16	8,8,8,8	0
57	MG	YA	3046	1/1	0.97	0.27	12,12,12,12	0
57	MG	QA	1632	1/1	0.97	0.11	71,71,71,71	0
57	MG	RR	201	1/1	0.97	0.27	9,9,9,9	0
57	MG	YA	3252	1/1	0.97	0.15	4,4,4,4	0
57	MG	YA	3010	1/1	0.97	0.60	50,50,50,50	0
57	MG	YA	3095	1/1	0.97	0.32	8,8,8,8	0
57	MG	YA	3196	1/1	0.97	0.27	76,76,76,76	0
57	MG	RA	3117	1/1	0.97	0.35	4,4,4,4	0
57	MG	YA	3257	1/1	0.97	0.78	50,50,50,50	0
57	MG	YA	3052	1/1	0.97	0.33	5,5,5,5	0
57	MG	RA	3084	1/1	0.97	0.31	6,6,6,6	0
57	MG	XA	1627	1/1	0.97	0.35	9,9,9,9	0
57	MG	RA	3015	1/1	0.97	0.29	15,15,15,15	0
57	MG	QM	201	1/1	0.97	0.10	34,34,34,34	0
57	MG	YA	3263	1/1	0.97	0.29	2,2,2,2	0
57	MG	RA	3059	1/1	0.97	0.50	50,50,50,50	0
57	MG	RA	3236	1/1	0.97	0.49	2,2,2,2	0
57	MG	RA	3088	1/1	0.97	0.25	10,10,10,10	0
57	MG	YA	3110	1/1	0.97	0.16	5,5,5,5	0
57	MG	RA	3017	1/1	0.97	0.30	0,0,0,0	0
57	MG	YA	3208	1/1	0.97	0.16	0,0,0,0	0
57	MG	YP	202	1/1	0.97	0.33	5,5,5,5	0
57	MG	QA	1616	1/1	0.97	0.28	10,10,10,10	0
57	MG	YA	3022	1/1	0.97	0.75	50,50,50,50	0
57	MG	YA	3159	1/1	0.97	0.19	22,22,22,22	0
57	MG	YA	3068	1/1	0.97	0.27	1,1,1,1	0
57	MG	RA	3198	1/1	0.97	0.06	35,35,35,35	0
57	MG	XA	1636	1/1	0.97	0.23	9,9,9,9	0
57	MG	YA	3164	1/1	0.97	0.76	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	YA	3216	1/1	0.97	0.25	30,30,30,30	0
57	MG	YA	3165	1/1	0.97	0.20	42,42,42,42	0
57	MG	XA	1637	1/1	0.97	0.27	13,13,13,13	0
57	MG	YA	3029	1/1	0.97	0.32	6,6,6,6	0
57	MG	RA	3125	1/1	0.97	0.08	14,14,14,14	0
57	MG	XA	1639	1/1	0.97	0.06	11,11,11,11	0
57	MG	YA	3122	1/1	0.97	0.58	50,50,50,50	0
57	MG	YA	3224	1/1	0.97	0.80	50,50,50,50	0
57	MG	RA	3044	1/1	0.98	0.23	8,8,8,8	0
57	MG	YA	3239	1/1	0.98	0.12	13,13,13,13	0
57	MG	YA	3101	1/1	0.98	0.12	11,11,11,11	0
57	MG	YA	3060	1/1	0.98	0.09	9,9,9,9	0
57	MG	QA	1645	1/1	0.98	0.27	37,37,37,37	0
57	MG	YA	3104	1/1	0.98	0.14	11,11,11,11	0
57	MG	YA	3023	1/1	0.98	0.46	5,5,5,5	0
57	MG	RA	3099	1/1	0.98	0.33	20,20,20,20	0
57	MG	YA	3107	1/1	0.98	0.45	2,2,2,2	0
57	MG	YA	3108	1/1	0.98	0.12	10,10,10,10	0
57	MG	YA	3025	1/1	0.98	0.27	3,3,3,3	0
57	MG	QA	1609	1/1	0.98	0.12	10,10,10,10	0
57	MG	RA	3036	1/1	0.98	0.40	0,0,0,0	0
57	MG	YA	3028	1/1	0.98	0.22	8,8,8,8	0
57	MG	QA	1606	1/1	0.98	0.06	23,23,23,23	0
57	MG	RA	3204	1/1	0.98	0.53	15,15,15,15	0
57	MG	RA	3082	1/1	0.98	0.14	5,5,5,5	0
57	MG	QA	1635	1/1	0.98	0.14	11,11,11,11	0
57	MG	RA	3129	1/1	0.98	0.10	19,19,19,19	0
57	MG	YA	3161	1/1	0.98	0.35	14,14,14,14	0
57	MG	YA	3118	1/1	0.98	0.46	12,12,12,12	0
57	MG	RA	3029	1/1	0.98	0.24	5,5,5,5	0
57	MG	RA	3209	1/1	0.98	0.12	44,44,44,44	0
57	MG	RA	3066	1/1	0.98	0.24	23,23,23,23	0
57	MG	RA	3067	1/1	0.98	0.17	6,6,6,6	0
57	MG	YA	3167	1/1	0.98	0.18	39,39,39,39	0
57	MG	RA	3109	1/1	0.98	0.25	11,11,11,11	0
57	MG	RA	3110	1/1	0.98	0.10	15,15,15,15	0
57	MG	RA	3068	1/1	0.98	0.48	4,4,4,4	0
57	MG	YA	3042	1/1	0.98	0.46	50,50,50,50	0
57	MG	YA	3218	1/1	0.98	0.27	5,5,5,5	0
57	MG	YP	201	1/1	0.98	0.05	83,83,83,83	0
57	MG	YA	3127	1/1	0.98	0.10	12,12,12,12	0
57	MG	QA	1654	1/1	0.98	0.12	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	RA	3070	1/1	0.98	0.15	21,21,21,21	0
57	MG	RA	3053	1/1	0.98	0.63	50,50,50,50	0
57	MG	RB	201	1/1	0.98	0.08	38,38,38,38	0
57	MG	RB	202	1/1	0.98	0.20	15,15,15,15	0
57	MG	QA	1636	1/1	0.98	0.18	11,11,11,11	0
57	MG	RA	3191	1/1	0.98	0.26	38,38,38,38	0
57	MG	XA	1622	1/1	0.98	0.11	6,6,6,6	0
57	MG	YA	3136	1/1	0.98	0.12	1,1,1,1	0
57	MG	QA	1663	1/1	0.98	0.09	19,19,19,19	0
59	ZN	QD	301	1/1	0.98	0.19	12,12,12,12	0
57	MG	RA	3074	1/1	0.98	0.19	20,20,20,20	0
57	MG	XA	1626	1/1	0.98	0.21	1,1,1,1	0
57	MG	RA	3094	1/1	0.98	0.36	3,3,3,3	0
57	MG	RA	3024	1/1	0.98	0.36	15,15,15,15	0
57	MG	RA	3096	1/1	0.98	0.48	11,11,11,11	0
57	MG	YA	3230	1/1	0.99	0.20	19,19,19,19	0
57	MG	XA	1623	1/1	0.99	0.22	23,23,23,23	0
57	MG	RA	3058	1/1	0.99	0.29	0,0,0,0	0
57	MG	QA	1607	1/1	0.99	0.06	30,30,30,30	0
57	MG	YA	3063	1/1	0.99	0.29	15,15,15,15	0
57	MG	YA	3011	1/1	0.99	0.41	3,3,3,3	0
57	MG	YA	3087	1/1	0.99	0.37	6,6,6,6	0
57	MG	RA	3106	1/1	0.99	0.26	3,3,3,3	0
57	MG	YA	3238	1/1	0.99	0.10	33,33,33,33	0
57	MG	YA	3066	1/1	0.99	0.19	9,9,9,9	0
57	MG	YA	3240	1/1	0.99	0.14	15,15,15,15	0
57	MG	YA	3067	1/1	0.99	0.45	7,7,7,7	0
57	MG	QA	1660	1/1	0.99	0.33	16,16,16,16	0
57	MG	RA	3049	1/1	0.99	0.34	1,1,1,1	0
57	MG	RA	3055	1/1	0.99	0.28	12,12,12,12	0
57	MG	RA	3137	1/1	0.99	0.10	3,3,3,3	0
57	MG	RA	3159	1/1	0.99	0.14	18,18,18,18	0
57	MG	YA	3096	1/1	0.99	0.24	17,17,17,17	0
57	MG	YA	3051	1/1	0.99	0.21	5,5,5,5	0
57	MG	QA	1629	1/1	0.99	0.08	38,38,38,38	0
57	MG	XA	1661	1/1	0.99	0.07	14,14,14,14	0
57	MG	QA	1634	1/1	0.99	0.12	44,44,44,44	0
57	MG	RA	3150	1/1	0.99	0.26	4,4,4,4	0
57	MG	YA	3174	1/1	0.99	0.37	3,3,3,3	0
57	MG	YA	3038	1/1	0.99	0.25	5,5,5,5	0
57	MG	RA	3199	1/1	0.99	0.16	1,1,1,1	0
57	MG	YA	3058	1/1	0.99	0.20	13,13,13,13	0

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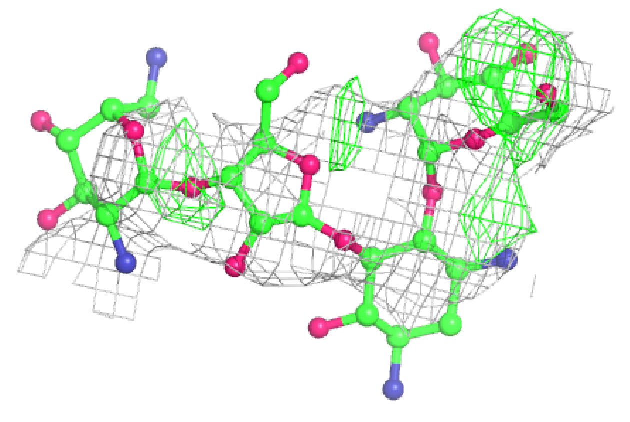
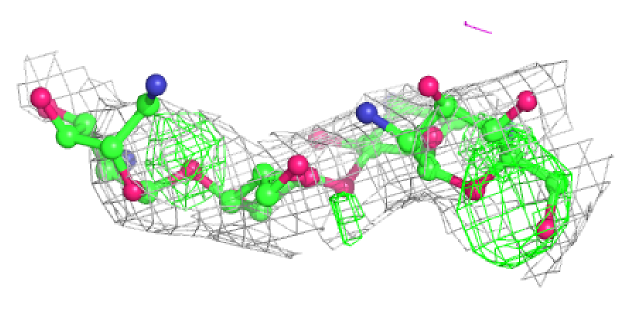
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	YA	3228	1/1	0.99	0.17	67,67,67,67	0
57	MG	RA	3079	1/1	0.99	0.40	0,0,0,0	0

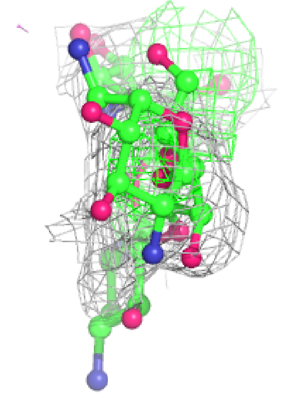
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAR QA 1666:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

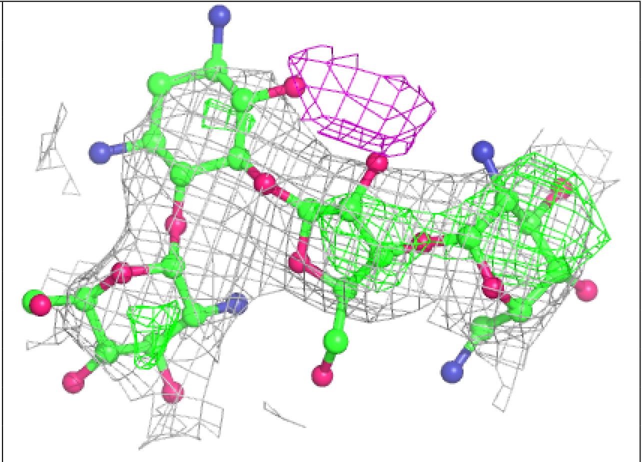


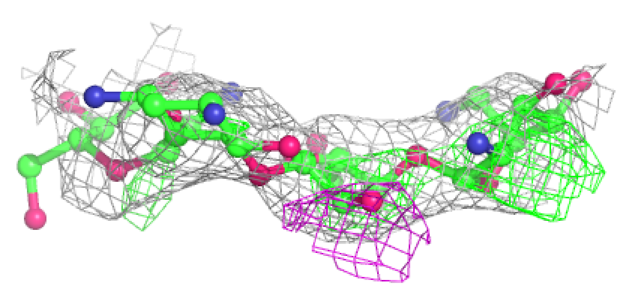


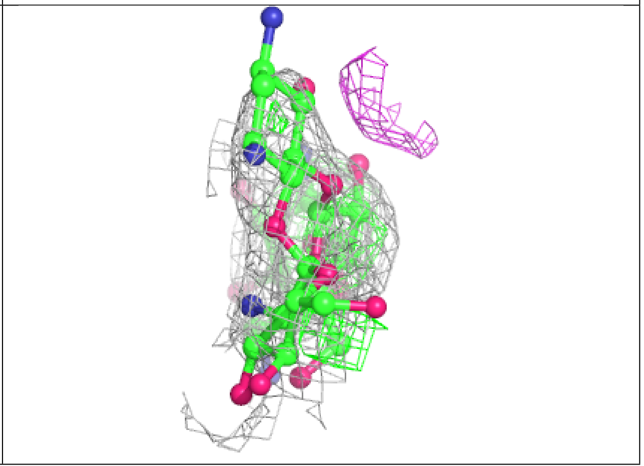


Electron density around PAR XA 1673:

$2mF_o$-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.