wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 17, 2023 – 09:32 AM EDT

PDB ID : 4WWW
Title : Crystal structure of the E. coli ribosome bound to CEM-101
Authors : Dunkle, J.A.; Zhang, W.; Cate, J.H.D.; Mankin, A.S.
Deposited on : 2014-11-12
Resolution : 3.10 Å(reported)

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

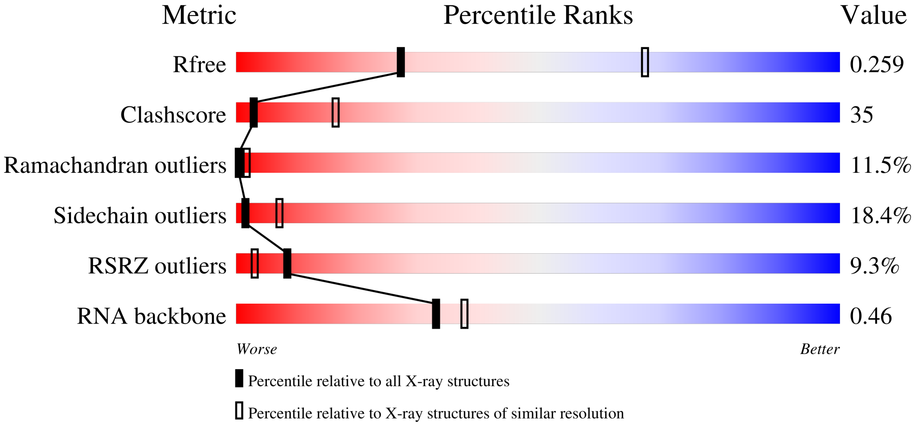
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance ⓘ

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

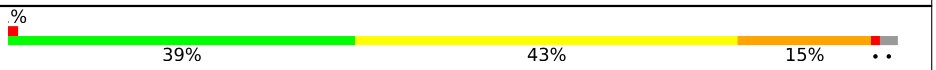
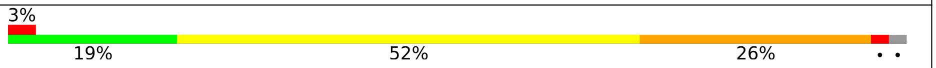
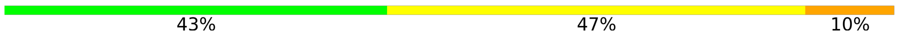
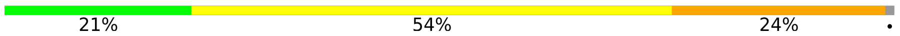
The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	RA	2904	
1	YA	2904	
2	RB	118	
2	YB	118	

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Mol	Chain	Length	Quality of chain
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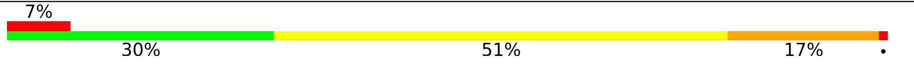
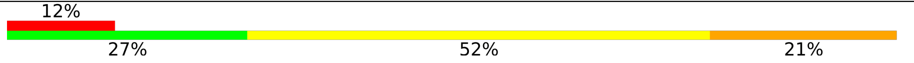
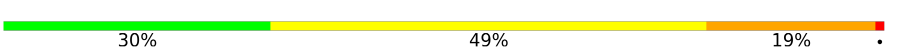
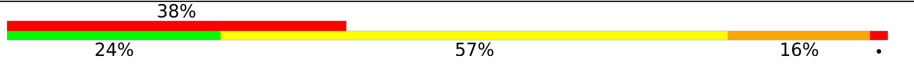
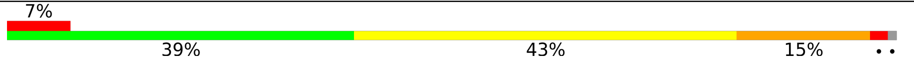
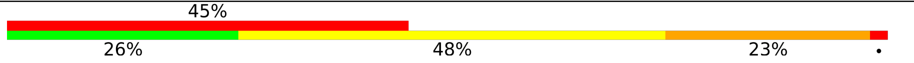
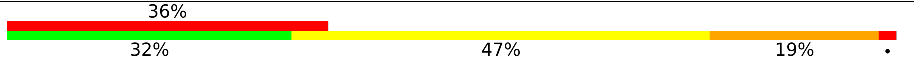
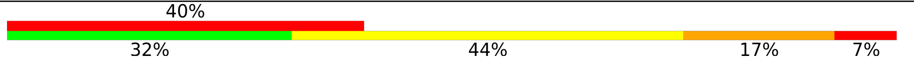
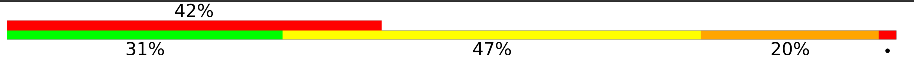
3	YC	271	
4	RD	209	
4	YD	209	
5	RE	201	
5	YE	201	
6	RF	178	
6	YF	178	
7	RG	176	
7	YG	176	
8	RH	149	
8	YH	149	
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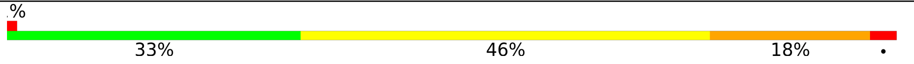
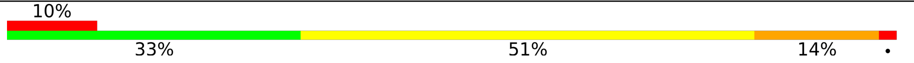
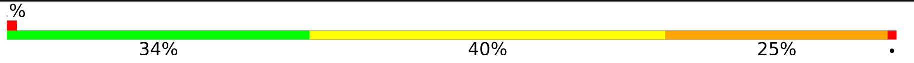
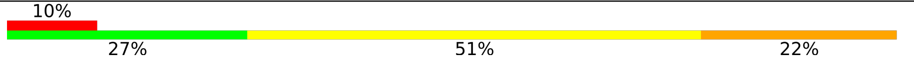
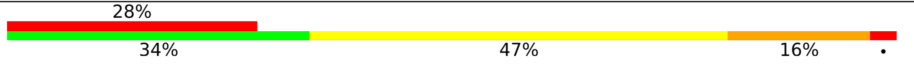
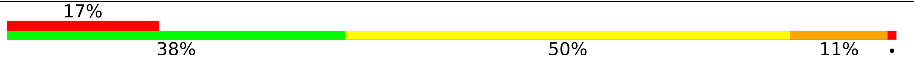
9	YI	141	
10	RJ	142	
10	YJ	142	
11	RK	122	
11	YK	122	
12	RL	143	
12	YL	143	
13	RM	136	
13	YM	136	
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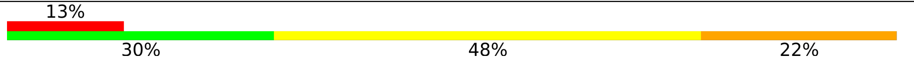
14	YN	120	
15	RO	116	

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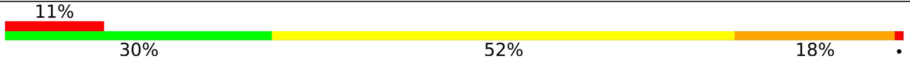
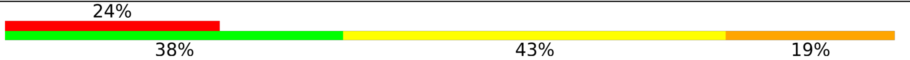
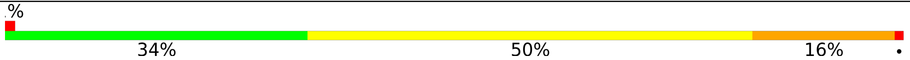
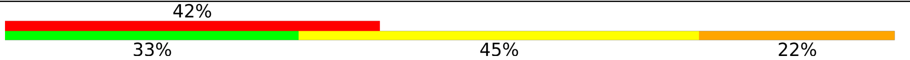
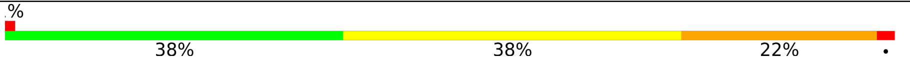
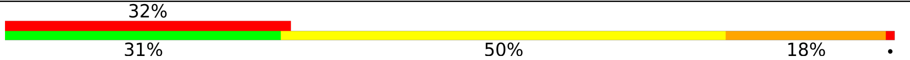
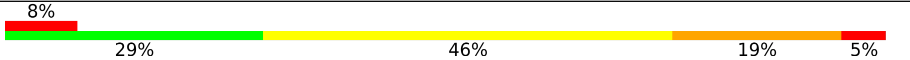
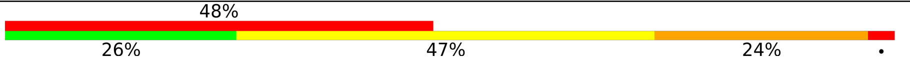
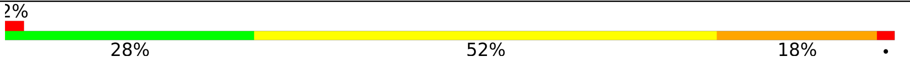
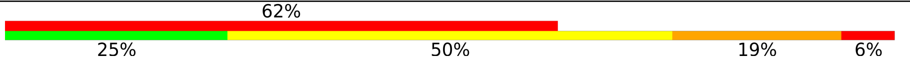
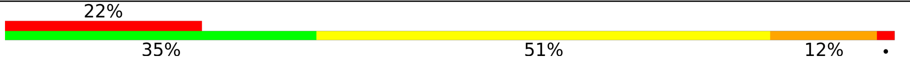
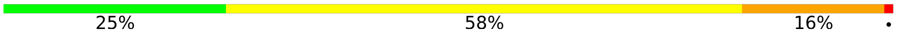
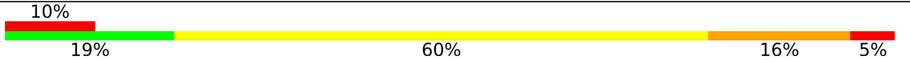
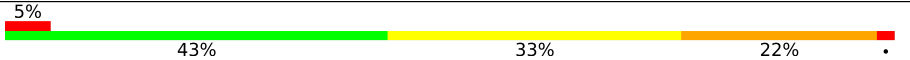
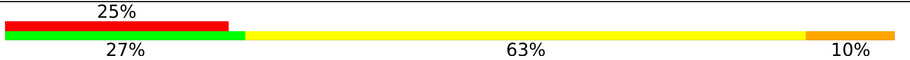
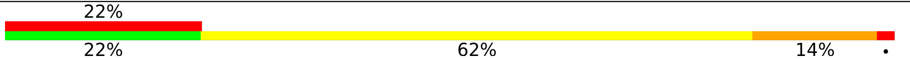
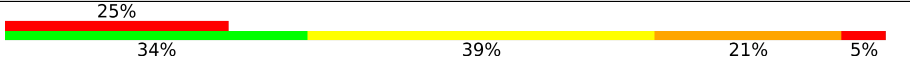
Mol	Chain	Length	Quality of chain
15	YO	116	
16	RP	114	
16	YP	114	
17	RQ	117	
17	YQ	117	
18	RR	103	
18	YR	103	
19	RS	110	
19	YS	110	
20	RT	93	
20	YT	93	
21	RU	102	
21	YU	102	
22	RV	94	
22	YV	94	
23	RW	79	
23	YW	79	
24	RX	77	
24	YX	77	
25	RY	63	
25	YY	63	
26	RZ	58	
26	YZ	58	
27	R0	56	
27	Y0	56	

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Mol	Chain	Length	Quality of chain
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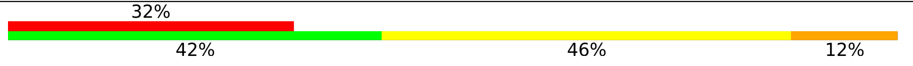
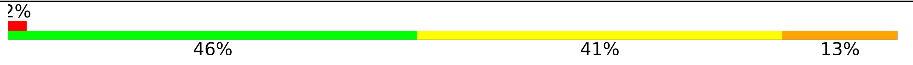
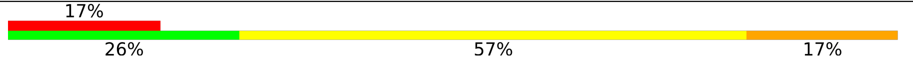
28	Y1	50	
29	R2	46	
29	Y2	46	
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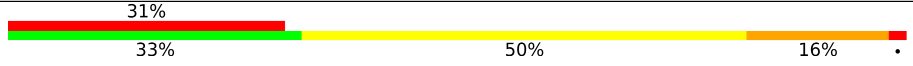
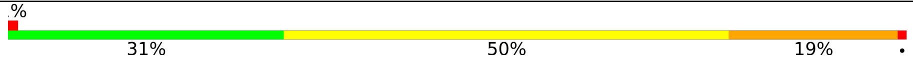
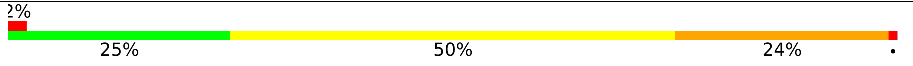
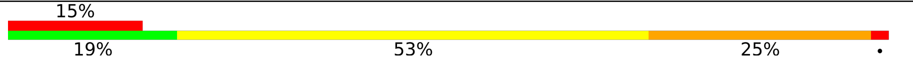
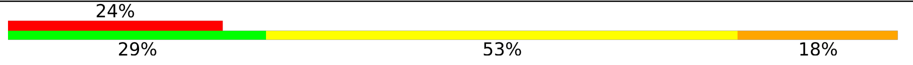
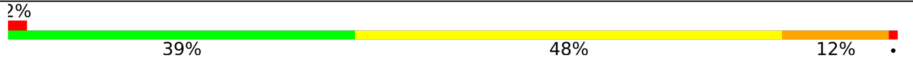
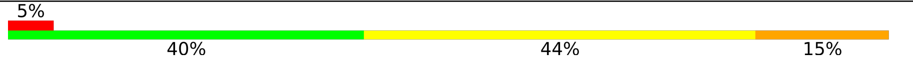
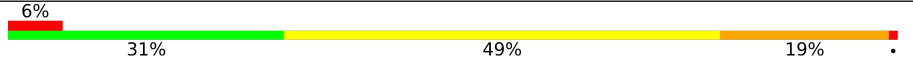
30	Y3	64	
31	R4	38	
31	Y4	38	
32	QA	1533	
32	XA	1533	
33	QB	218	
33	XB	218	
34	QC	206	
34	XC	206	
35	QD	205	
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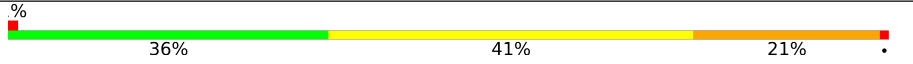
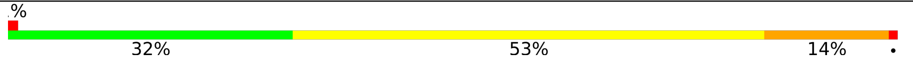
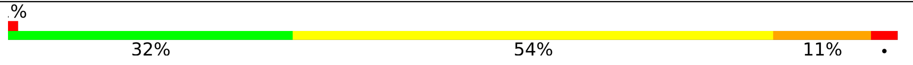
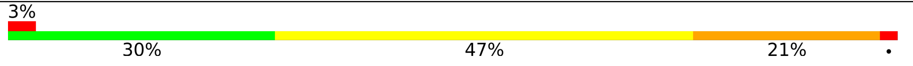
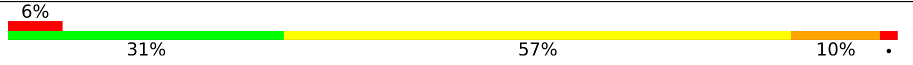
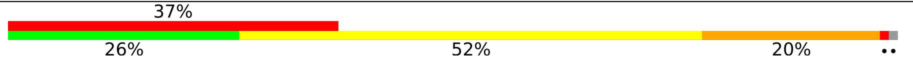
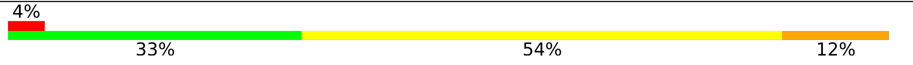
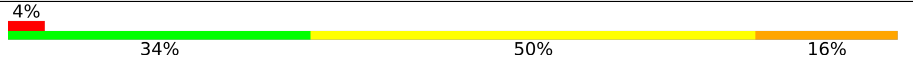
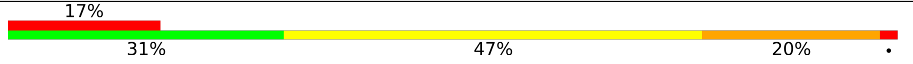
36	QE	150	
36	XE	150	
37	QF	100	
37	XF	100	
38	QG	151	
38	XG	151	
39	QH	129	
39	XH	129	
40	QI	127	

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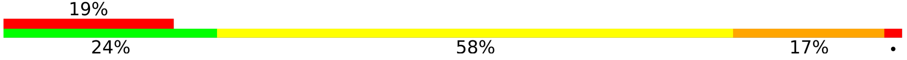
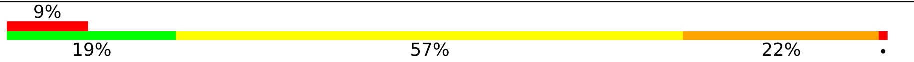
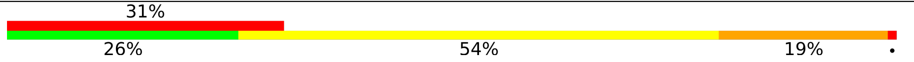
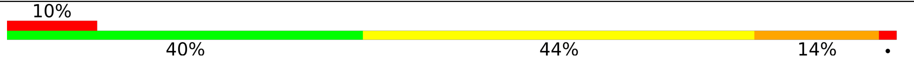
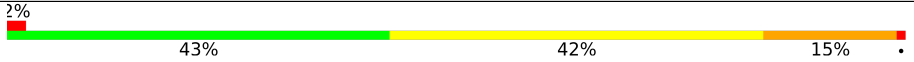
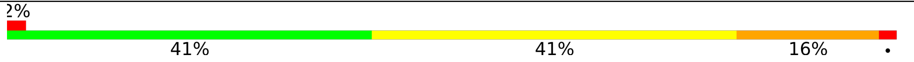
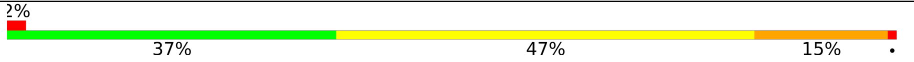
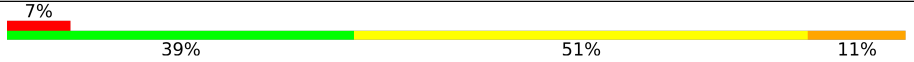
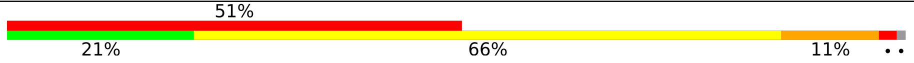
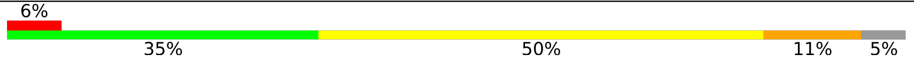
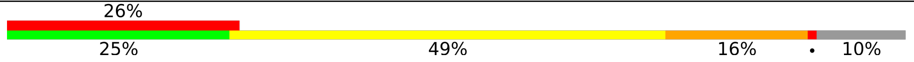
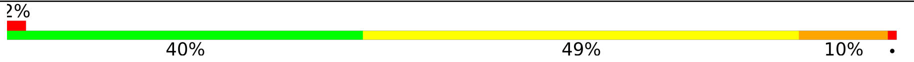
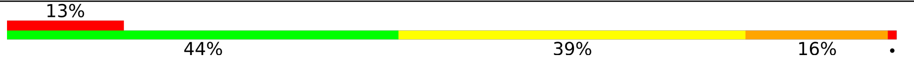
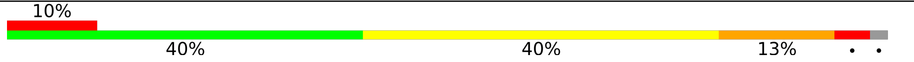
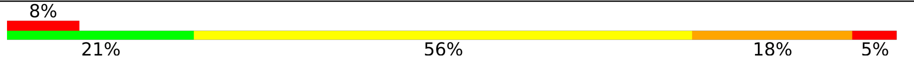
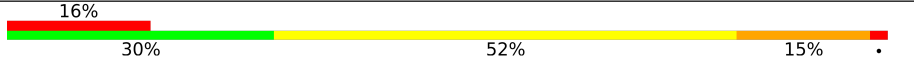
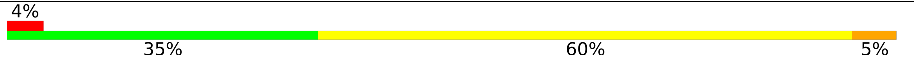
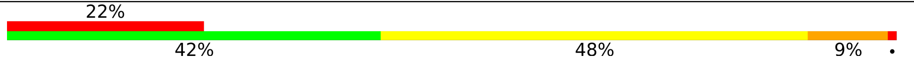
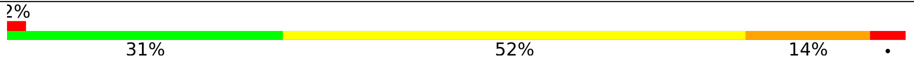
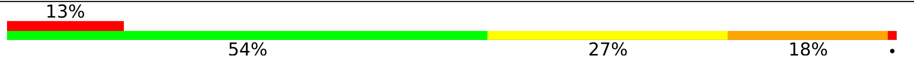
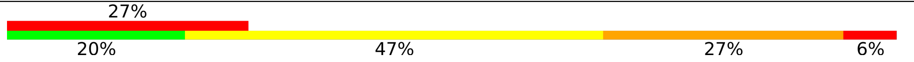
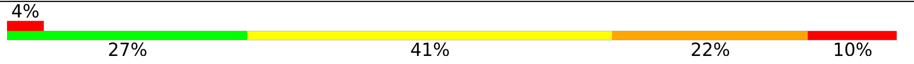
Mol	Chain	Length	Quality of chain
40	XI	127	
41	QJ	98	
41	XJ	98	
42	QK	117	
42	XK	117	
43	QL	123	
43	XL	123	
44	QM	114	
44	XM	114	
45	QN	101	
45	XN	101	
46	QO	88	
46	XO	88	
47	QP	82	
47	XP	82	
48	QQ	80	
48	XQ	80	
49	QR	55	
49	XR	55	
50	QS	79	
50	XS	79	
51	QT	85	
51	XT	85	
52	QU	51	
52	XU	51	

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
53	MG	QA	1619	-	-	-	X
53	MG	RA	3129	-	-	-	X
53	MG	XA	1614	-	-	-	X
53	MG	XA	1616	-	-	-	X
53	MG	YA	3002	-	-	-	X
53	MG	YA	3003	-	-	-	X
53	MG	YA	3005	-	-	-	X
53	MG	YA	3019	-	-	-	X
53	MG	YA	3049	-	-	-	X
53	MG	YA	3062	-	-	-	X
53	MG	YA	3063	-	-	-	X
53	MG	YA	3064	-	-	-	X
53	MG	YA	3074	-	-	-	X
53	MG	YA	3108	-	-	-	X
53	MG	YA	3109	-	-	-	X
53	MG	YA	3127	-	-	-	X
53	MG	YA	3129	-	-	-	X
53	MG	YA	3130	-	-	-	X
53	MG	YJ	201	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284464 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 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	RA	2854	61274	27334	11279	19807	2854	0	0	0
1	YA	2841	60995	27210	11229	19715	2841	0	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	RB	118	2529	1126	464	821	118	0	0	0
2	YB	117	2507	1116	459	815	117	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	RC	271	2082	1288	423	364	7	0	0	0
3	YC	271	2082	1288	423	364	7	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	RD	209	1565	979	288	294	4	0	0	0
4	YD	209	1565	979	288	294	4	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	RE	201	1552	974	283	290	5	0	0	0
5	YE	201	1552	974	283	290	5	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	RF	177	1410	899	249	256	6	0	0	0
6	YF	178	1420	905	251	258	6	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	RG	176	1323	832	243	246	2	0	0	0
7	YG	176	1323	832	243	246	2	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	RH	149	1111	699	197	214	1	0	0	0
8	YH	149	1111	699	197	214	1	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	RI	141	1032	651	179	196	6	0	0	0
9	YI	141	1032	651	179	196	6	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	RJ	142	1129	714	212	199	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	YJ	142	Total 1129	C 714	N 212	O 199	S 4	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	RK	122	Total 938	C 587	N 180	O 165	S 6	0	0	0
11	YK	122	Total 938	C 587	N 180	O 165	S 6	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	RL	143	Total 1045	C 649	N 206	O 189	S 1	0	0	0
12	YL	143	Total 1045	C 649	N 206	O 189	S 1	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	RM	136	Total 1074	C 686	N 205	O 177	S 6	0	0	0
13	YM	136	Total 1074	C 686	N 205	O 177	S 6	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	RN	120	Total 960	C 593	N 196	O 166	S 5	0	0	0
14	YN	120	Total 960	C 593	N 196	O 166	S 5	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	RO	116	Total 892	C 552	N 178	O 162	0	0	0
15	YO	116	Total 892	C 552	N 178	O 162	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	RP	114	917	574	179	163	1	0	0	0
			Total	C	N	O	S			
16	YP	114	917	574	179	163	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	RQ	117	947	604	192	151	0	0	0
			Total	C	N	O			
17	YQ	117	947	604	192	151	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	RR	103	816	516	153	145	2	0	0	0
			Total	C	N	O	S			
18	YR	103	816	516	153	145	2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	RS	110	857	532	166	156	3	0	0	0
			Total	C	N	O	S			
19	YS	110	857	532	166	156	3	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	RT	93	738	466	139	131	2	0	0	0
			Total	C	N	O	S			
20	YT	93	738	466	139	131	2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	RU	102	Total C N O 779 492 146 141	0	0	0
21	YU	102	Total C N O 779 492 146 141	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	RV	94	Total C N O S 753 479 137 134 3	0	0	0
22	YV	94	Total C N O S 753 479 137 134 3	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	RW	79	Total C N O S 596 367 120 108 1	0	0	0
23	YW	79	Total C N O S 596 367 120 108 1	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	RX	77	Total C N O S 625 388 129 106 2	0	0	0
24	YX	77	Total C N O S 625 388 129 106 2	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	RY	63	Total C N O S 509 313 99 95 2	0	0	0
25	YY	63	Total C N O S 509 313 99 95 2	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	RZ	58	Total C N O S 449 281 87 79 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	YZ	58	449	281	87	79	2	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	R0	56	444	269	94	80	1	0	0	0
27	Y0	56	444	269	94	80	1	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
28	R1	50	409	263	75	71	0	0	0
28	Y1	50	409	263	75	71	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	R2	46	377	228	90	57	2	0	0	0
29	Y2	46	377	228	90	57	2	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	R3	64	504	323	105	74	2	0	0	0
30	Y3	64	504	323	105	74	2	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	R4	38	302	185	65	48	4	0	0	0
31	Y4	38	302	185	65	48	4	0	0	0

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	QA	1533	Total 32895	C 14671	N 6036	O 10655	P 1533	0	0	0
32	XA	1530	Total 32831	C 14642	N 6024	O 10635	P 1530	0	0	0

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	QB	218	Total 1704	C 1081	N 305	O 311	S 7	0	0	0
33	XB	218	Total 1704	C 1081	N 305	O 311	S 7	0	0	0

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	QC	206	Total 1624	C 1028	N 305	O 288	S 3	0	0	0
34	XC	206	Total 1624	C 1028	N 305	O 288	S 3	0	0	0

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	QD	205	Total 1643	C 1026	N 315	O 298	S 4	0	0	0
35	XD	205	Total 1643	C 1026	N 315	O 298	S 4	0	0	0

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	QE	150	Total 1105	C 687	N 211	O 201	S 6	0	0	0
36	XE	150	Total 1105	C 687	N 211	O 201	S 6	0	0	0

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	QF	100	817	515	148	148	6	0	0	0
37	XF	100	817	515	148	148	6	0	0	0

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	QG	151	1181	735	227	215	4	0	0	0
38	XG	150	1174	730	226	214	4	0	0	0

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	QH	129	979	616	173	184	6	0	0	0
39	XH	129	979	616	173	184	6	0	0	0

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	QI	127	1022	634	206	179	3	0	0	0
40	XI	127	1022	634	206	179	3	0	0	0

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	QJ	98	786	493	150	142	1	0	0	0
41	XJ	98	786	493	150	142	1	0	0	0

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	QK	117	877	540	174	160	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	XK	117	Total 877	C 540	N 174	O 160	S 3	0	0	0

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	QL	123	Total 955	C 590	N 196	O 165	S 4	0	0	0
43	XL	123	Total 955	C 590	N 196	O 165	S 4	0	0	0

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	QM	114	Total 883	C 546	N 178	O 156	S 3	0	0	0
44	XM	113	Total 876	C 541	N 177	O 155	S 3	0	0	0

- Molecule 45 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	QN	96	Total 774	C 483	N 160	O 128	S 3	0	0	0
45	XN	91	Total 735	C 461	N 151	O 120	S 3	0	0	0

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	QO	88	Total 714	C 439	N 144	O 130	S 1	0	0	0
46	XO	88	Total 714	C 439	N 144	O 130	S 1	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	QP	82	Total 649	C 406	N 128	O 114	S 1	0	0	0
47	XP	80	Total 638	C 400	N 126	O 111	S 1	0	0	0

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
48	QQ	80	Total C N O S 648 411 121 113 3	0	0	0
48	XQ	80	Total C N O S 648 411 121 113 3	0	0	0

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
49	QR	55	Total C N O 455 288 86 81	0	0	0
49	XR	55	Total C N O 455 288 86 81	0	0	0

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
50	QS	79	Total C N O S 637 408 120 107 2	0	0	0
50	XS	79	Total C N O S 637 408 120 107 2	0	0	0

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
51	QT	85	Total C N O S 665 411 137 114 3	0	0	0
51	XT	85	Total C N O S 665 411 137 114 3	0	0	0

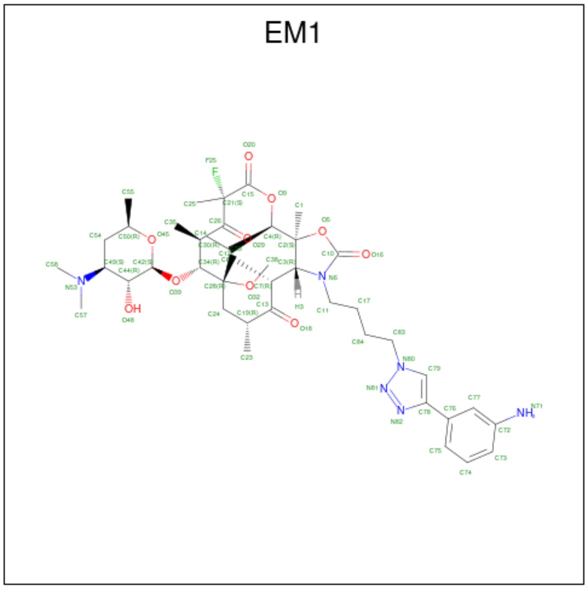
- Molecule 52 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
52	QU	51	Total C N O S 425 265 86 73 1	0	0	0
52	XU	51	Total C N O S 425 265 86 73 1	0	0	0

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	RA	135	Total 135	Mg 135	0	0
53	RB	4	Total 4	Mg 4	0	0
53	QA	43	Total 43	Mg 43	0	0
53	XA	42	Total 42	Mg 42	0	0
53	YA	134	Total 134	Mg 134	0	0
53	YB	1	Total 1	Mg 1	0	0
53	YE	1	Total 1	Mg 1	0	0
53	YJ	1	Total 1	Mg 1	0	0

- Molecule 54 is (3aS,4R,7S,9R,10R,11R,13R,15R,15aR)-1-{4-[4-(3-aminophenyl)-1H-1,2,3-triazol-1-yl]butyl}-4-ethyl-7-fluoro-11-methoxy-3a ,7,9,11,13,15-hexamethyl-2,6,8,14-tetraoxotetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-10-yl 3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranoside (three-letter code: EM1) (formula: $C_{43}H_{65}FN_6O_{10}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
54	RA	1	Total 60	C 43	F 1	N 6	O 10	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	R4	1	Total Zn 1 1	0	0
55	Y4	1	Total Zn 1 1	0	0

- Molecule 56 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	RA	606	Total O 606 606	0	0
56	RB	20	Total O 20 20	0	0
56	RC	9	Total O 9 9	0	0
56	RD	1	Total O 1 1	0	0
56	RL	4	Total O 4 4	0	0
56	RN	3	Total O 3 3	0	0
56	RT	2	Total O 2 2	0	0
56	R2	1	Total O 1 1	0	0
56	R3	2	Total O 2 2	0	0
56	R4	2	Total O 2 2	0	0
56	QA	200	Total O 200 200	0	0
56	QL	1	Total O 1 1	0	0
56	QN	5	Total O 5 5	0	0
56	QT	1	Total O 1 1	0	0
56	QU	1	Total O 1 1	0	0
56	XA	194	Total O 194 194	0	0
56	XE	5	Total O 5 5	0	0
56	XI	1	Total O 1 1	0	0

Continued on next page...

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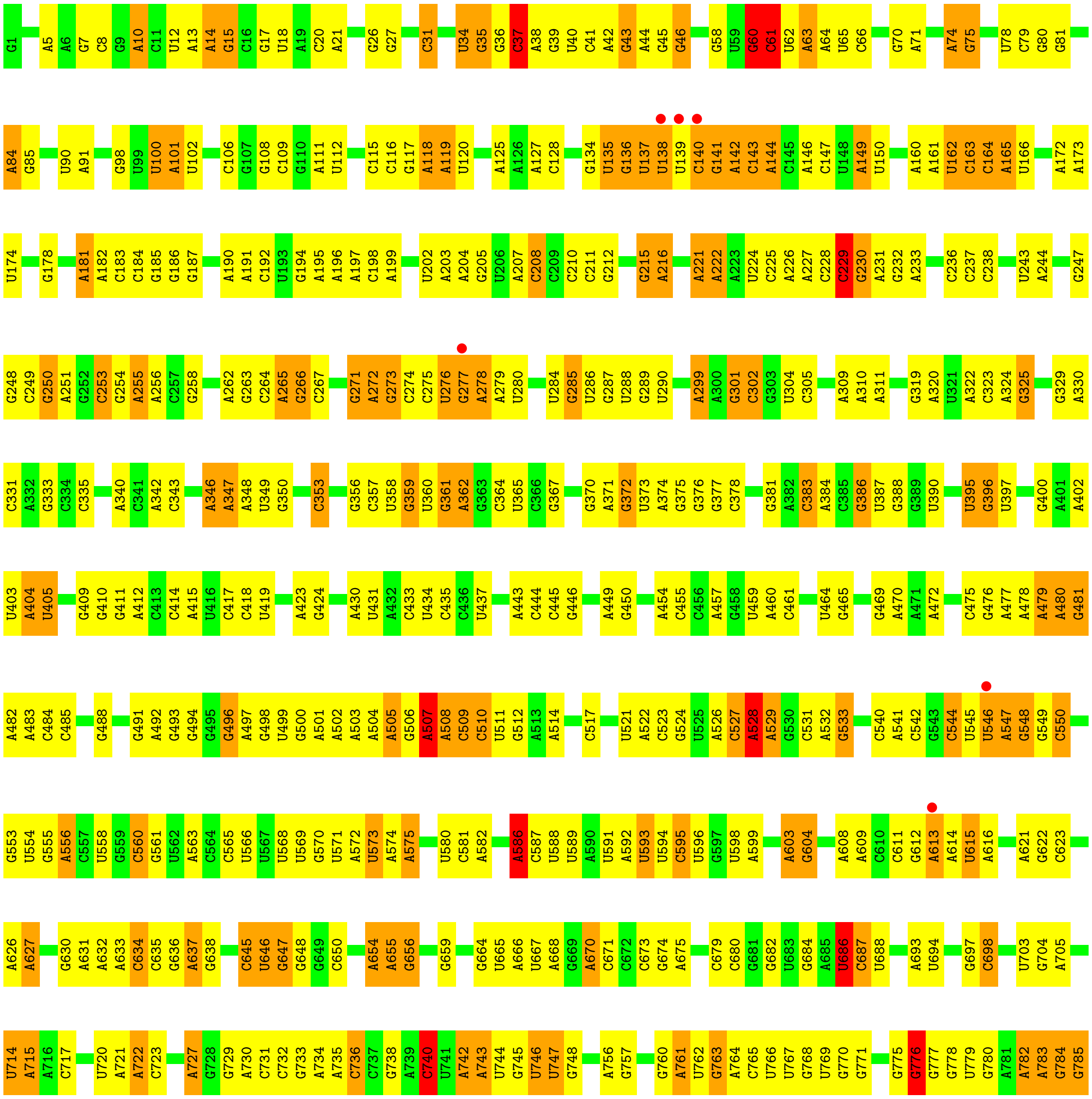
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	XL	1	Total O 1 1	0	0
56	XN	3	Total O 3 3	0	0
56	XT	2	Total O 2 2	0	0
56	XU	1	Total O 1 1	0	0
56	YA	605	Total O 605 605	0	0
56	YB	4	Total O 4 4	0	0
56	YC	8	Total O 8 8	0	0
56	YD	3	Total O 3 3	0	0
56	YE	3	Total O 3 3	0	0
56	YJ	3	Total O 3 3	0	0
56	YL	4	Total O 4 4	0	0
56	YN	1	Total O 1 1	0	0
56	YT	2	Total O 2 2	0	0
56	YU	2	Total O 2 2	0	0
56	YV	1	Total O 1 1	0	0
56	Y2	1	Total O 1 1	0	0
56	Y3	1	Total O 1 1	0	0
56	Y4	5	Total O 5 5	0	0

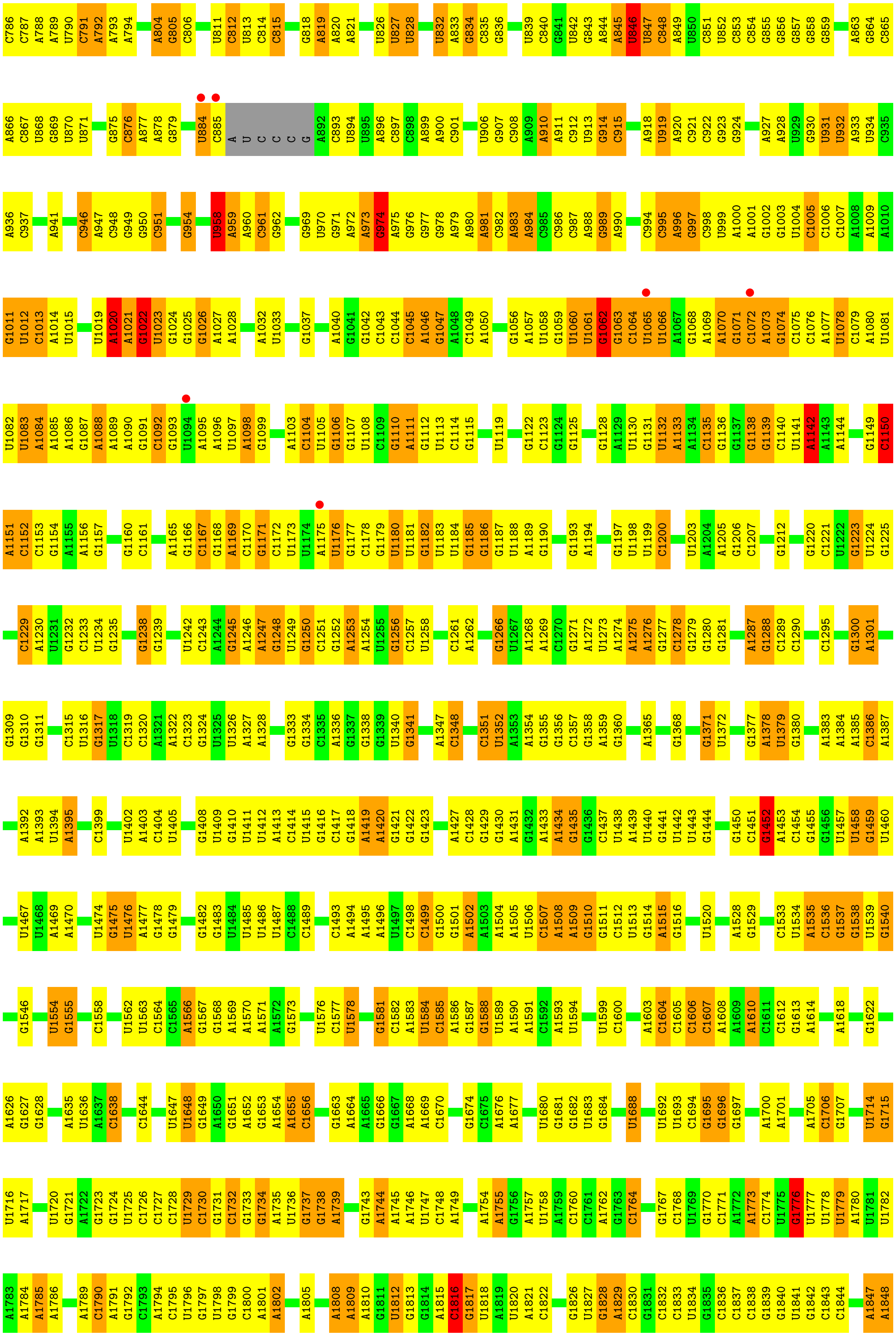
3 Residue-property plots

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: 23S rRNA

Chain RA:

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A866 C867 U868 G869 U870 U871 G875 C876 A877 A878 G879 U884 C885 A U C C C G A892 C893 U894 U895 A896 C897 C898 A899 A900 C901 U906 G907 C908 A909 A910 A911 G912 U913 G914 C915 A918 U919 A920 C921 G922 G923 G924 A927 A928 U929 G930 U931 U932 A933 U934 C935
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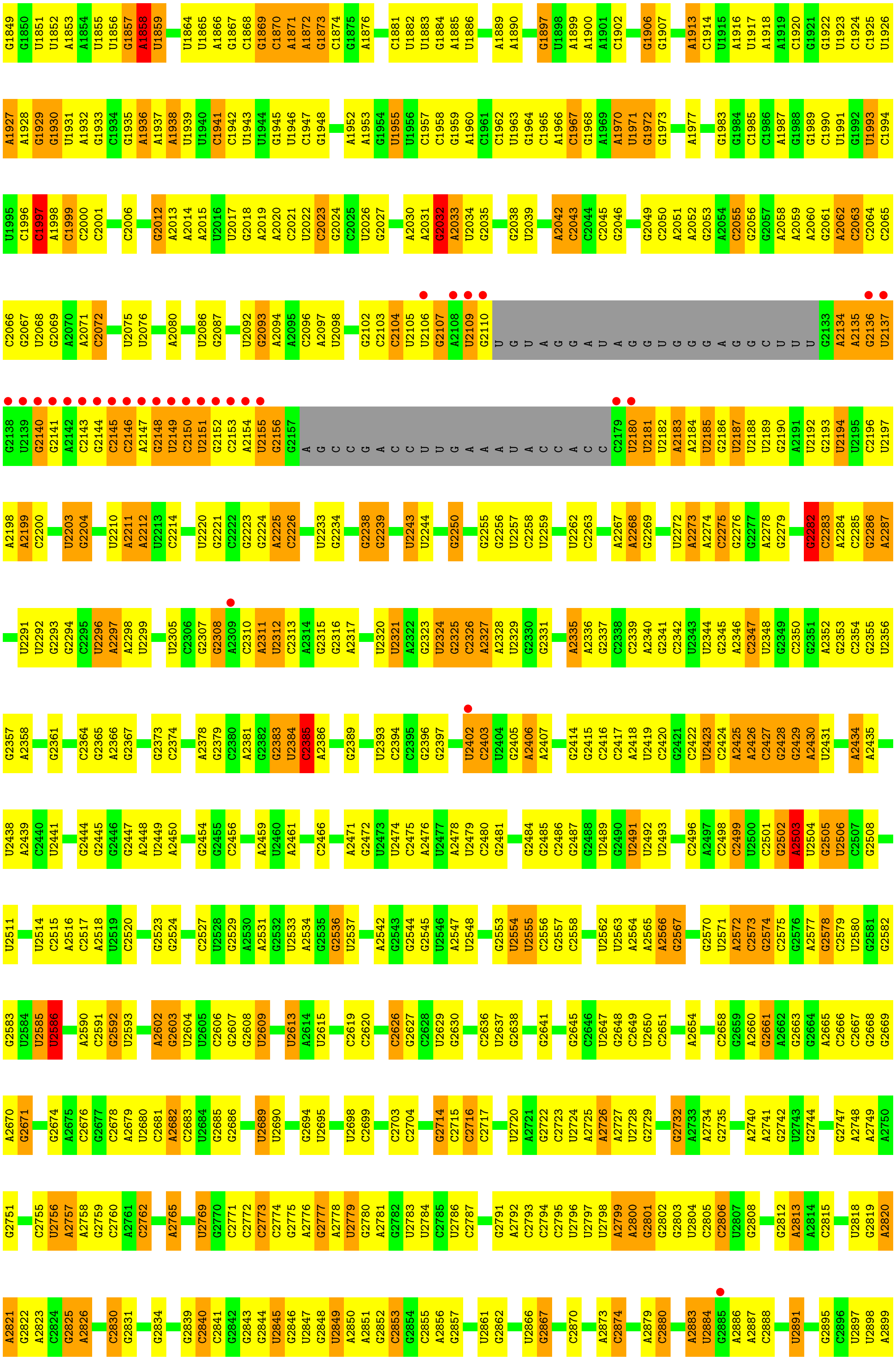
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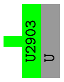
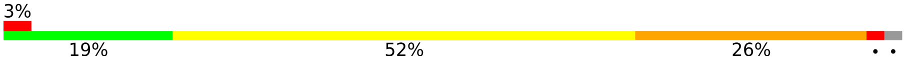
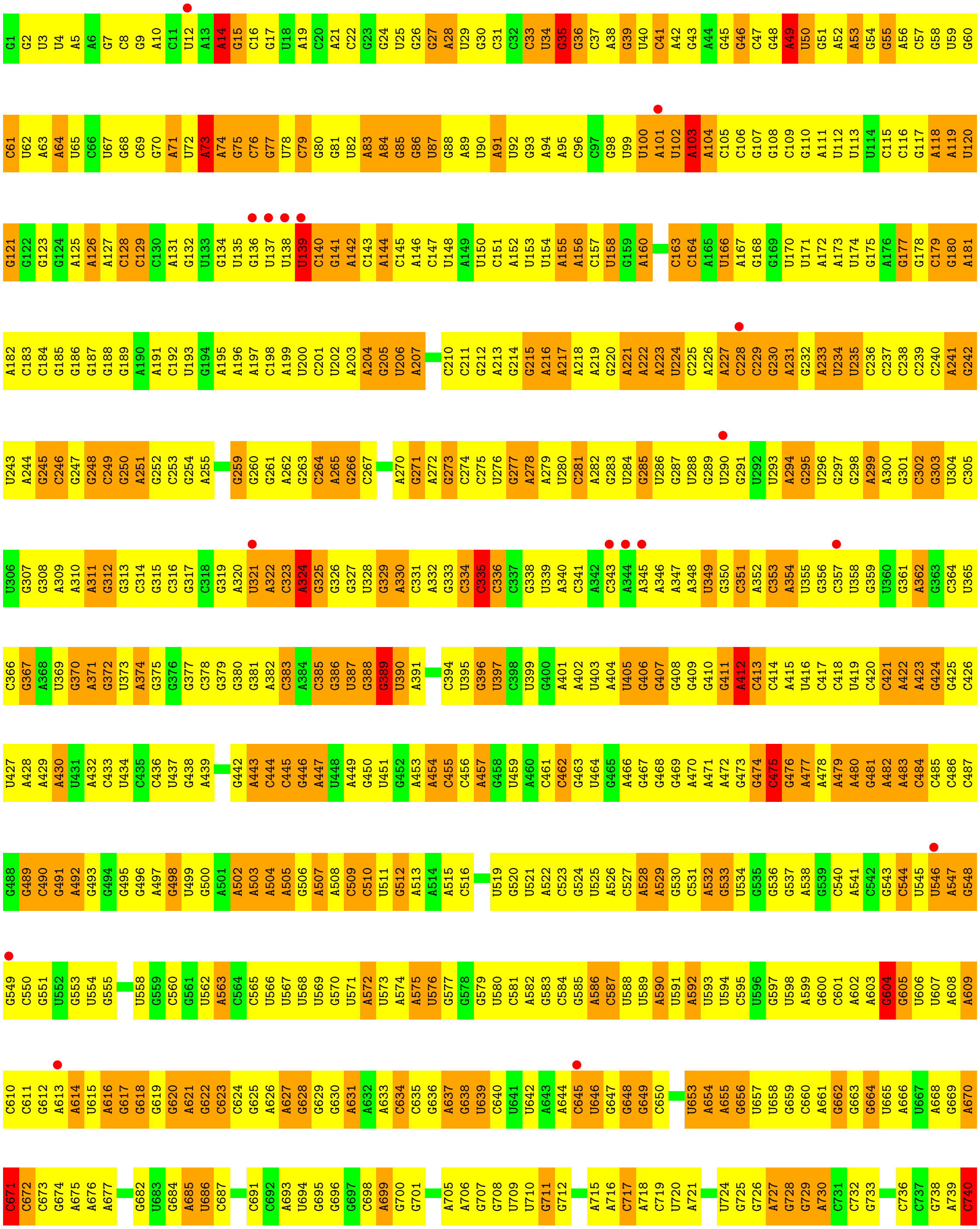
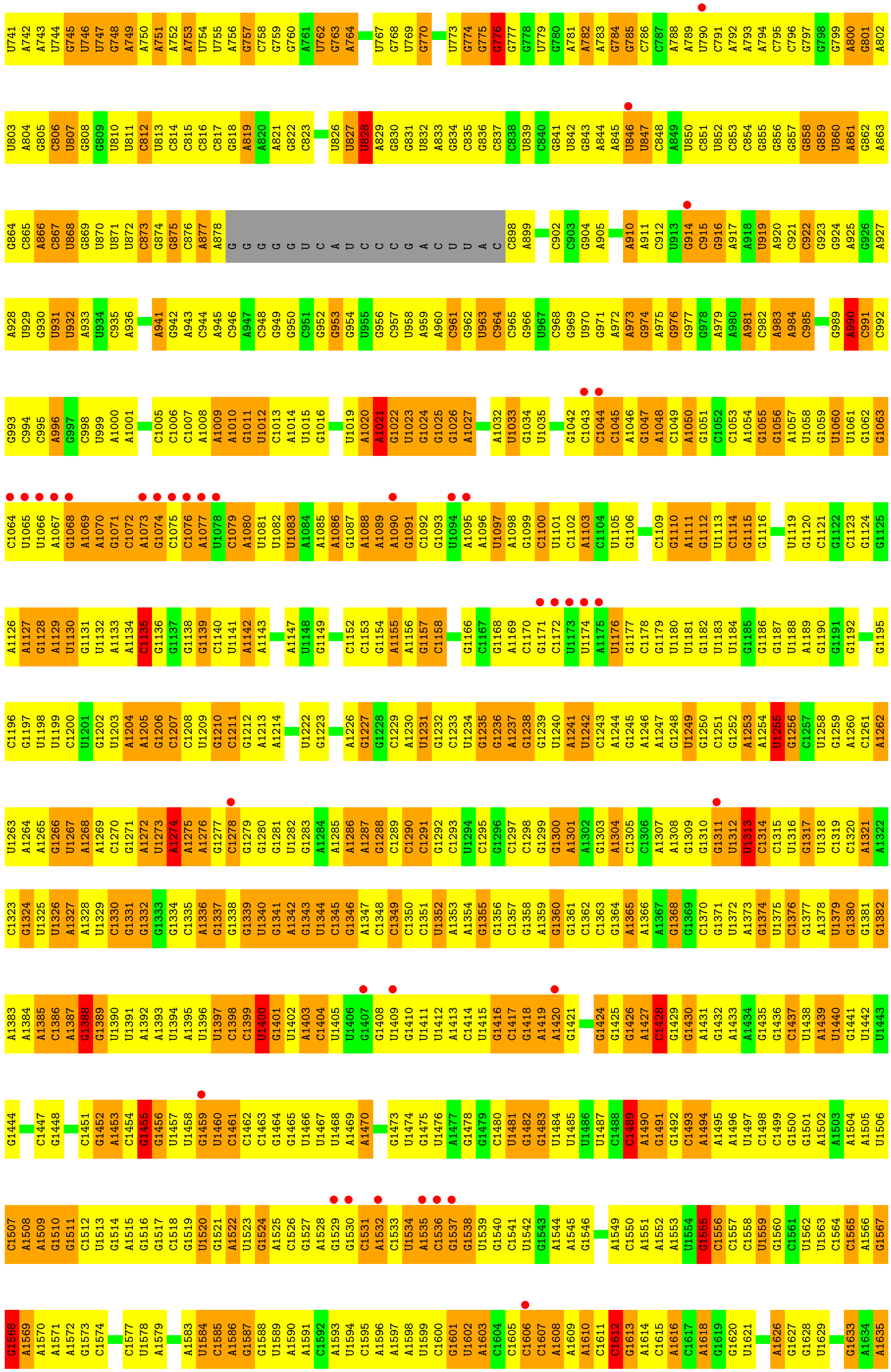


- Molecule 1: 23S rRNA

Chain YA:



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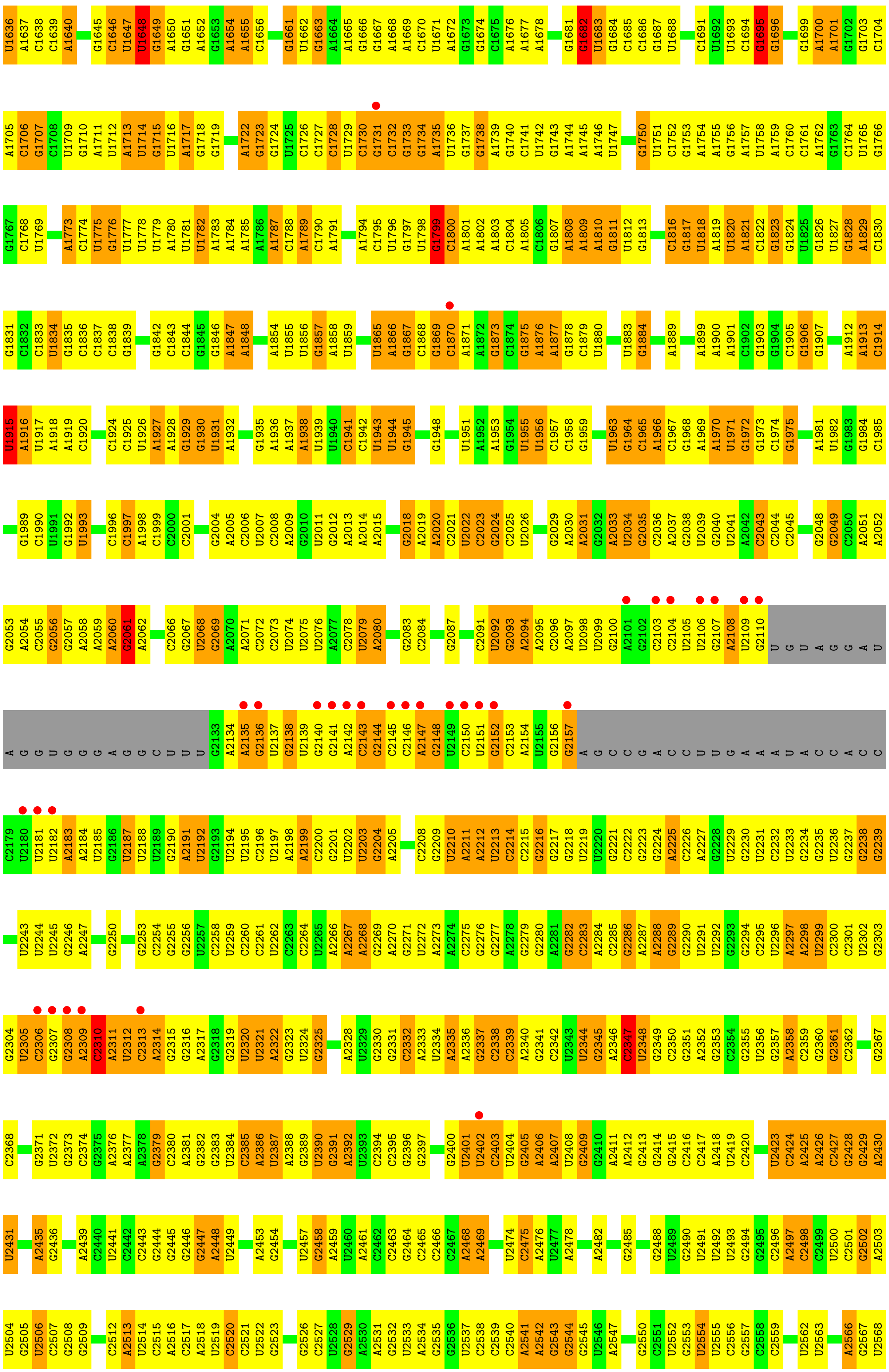
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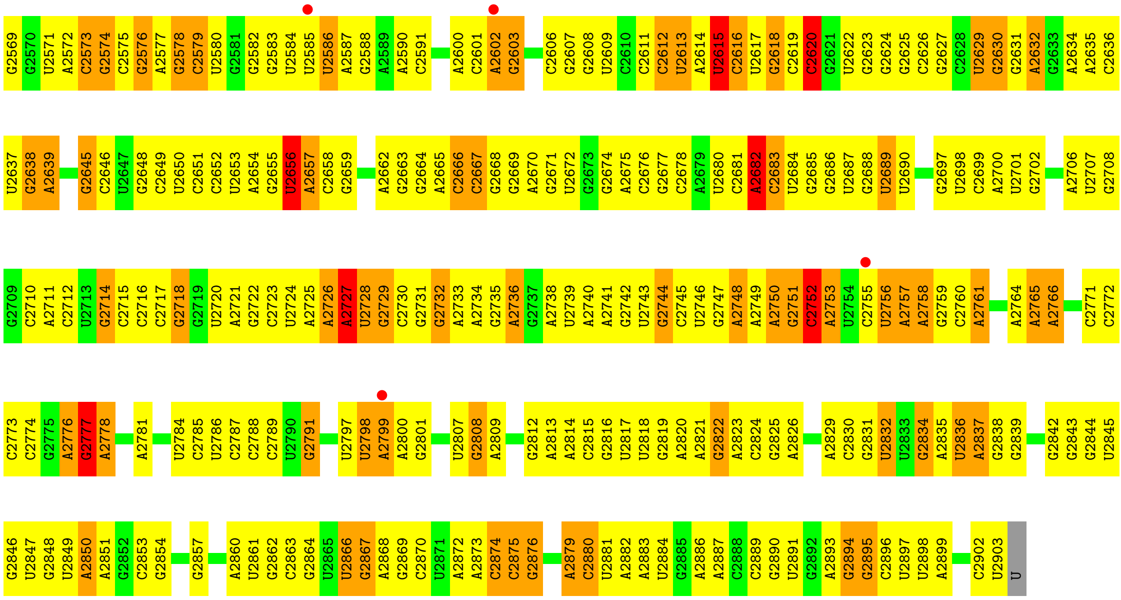

- Molecule 2: 5S rRNA

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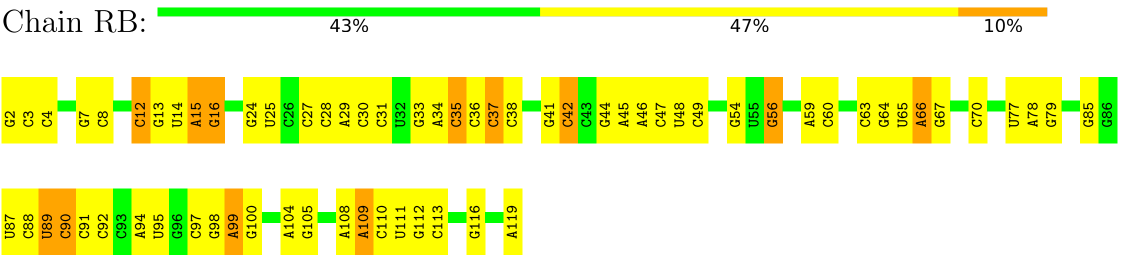

- Molecule 2: 5S rRNA

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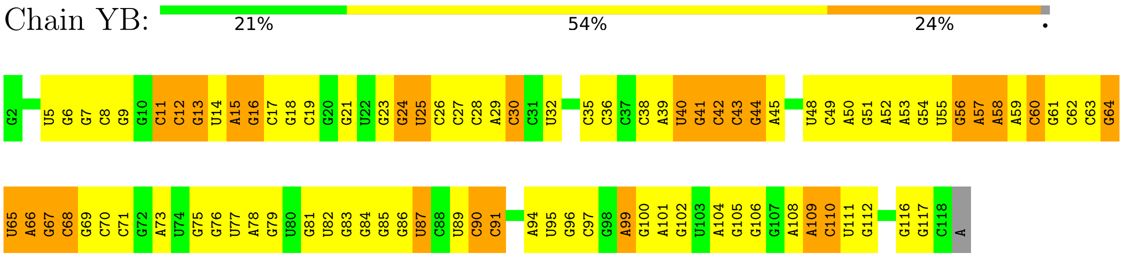
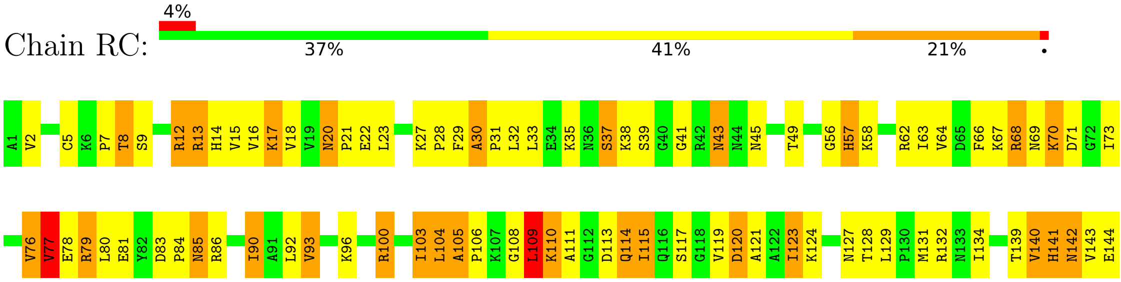
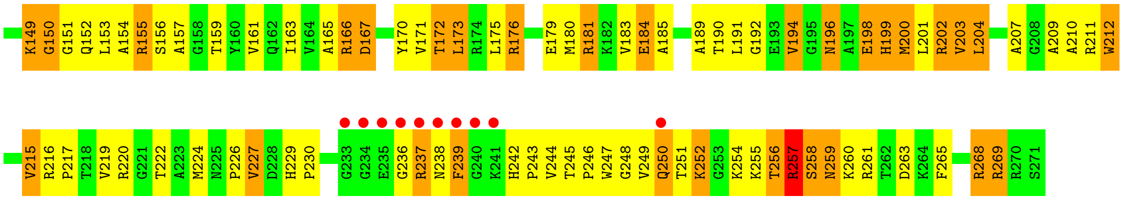


- Molecule 3: 50S ribosomal protein L2

Chain RC:





- Molecule 3: 50S ribosomal protein L2

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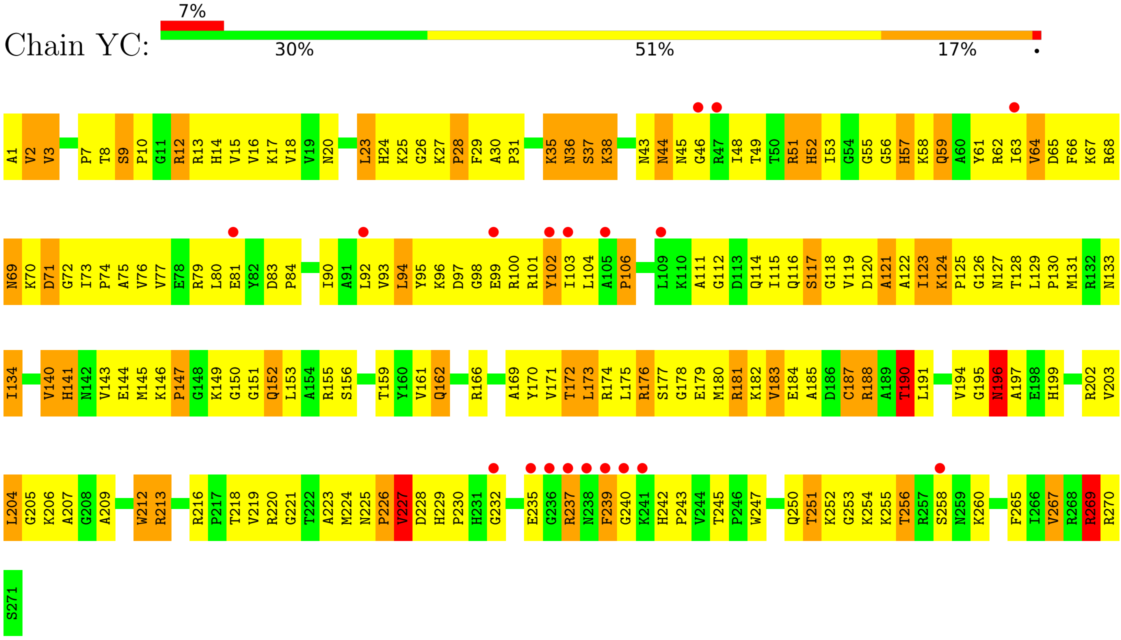
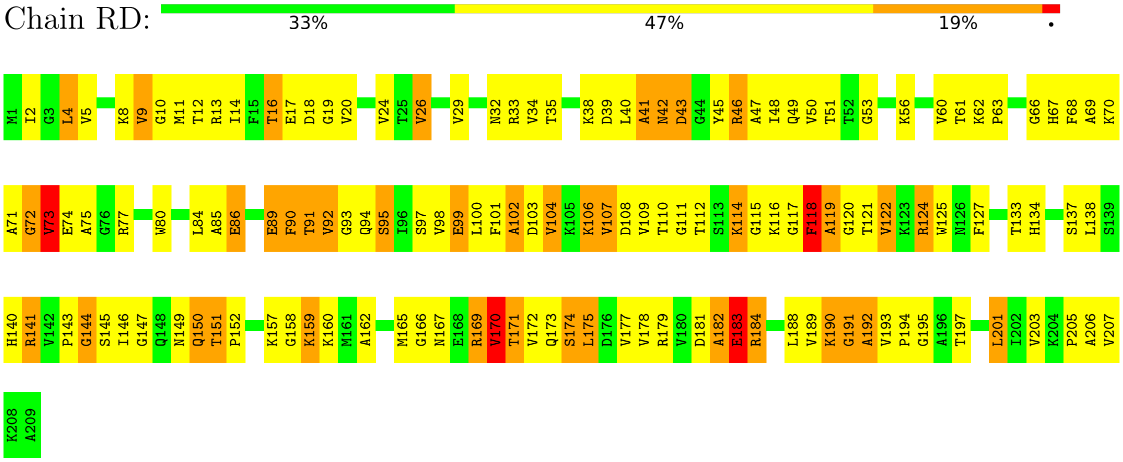


- Molecule 4: 50S ribosomal protein L3

Chain RD:



- Molecule 4: 50S ribosomal protein L3

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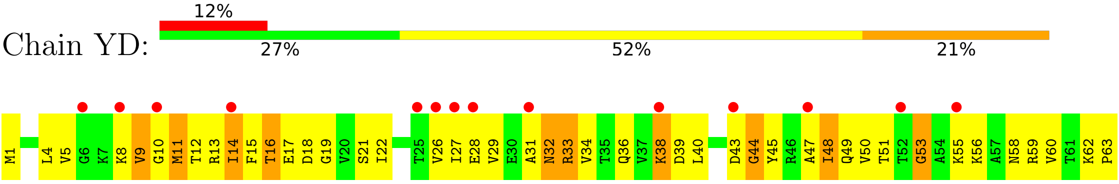
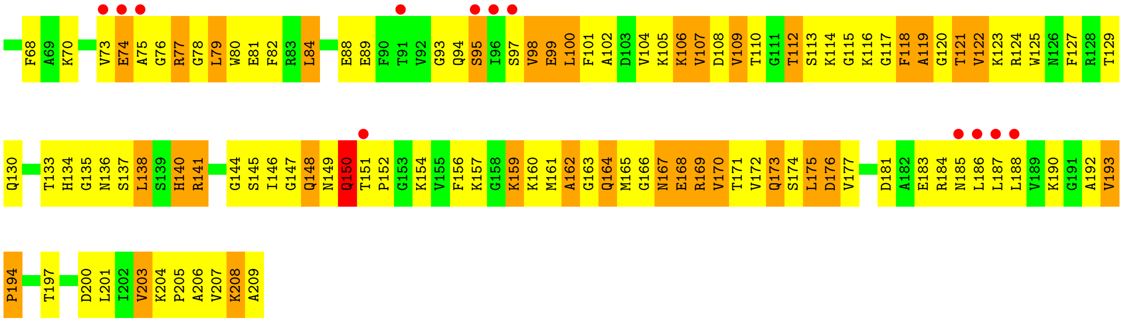
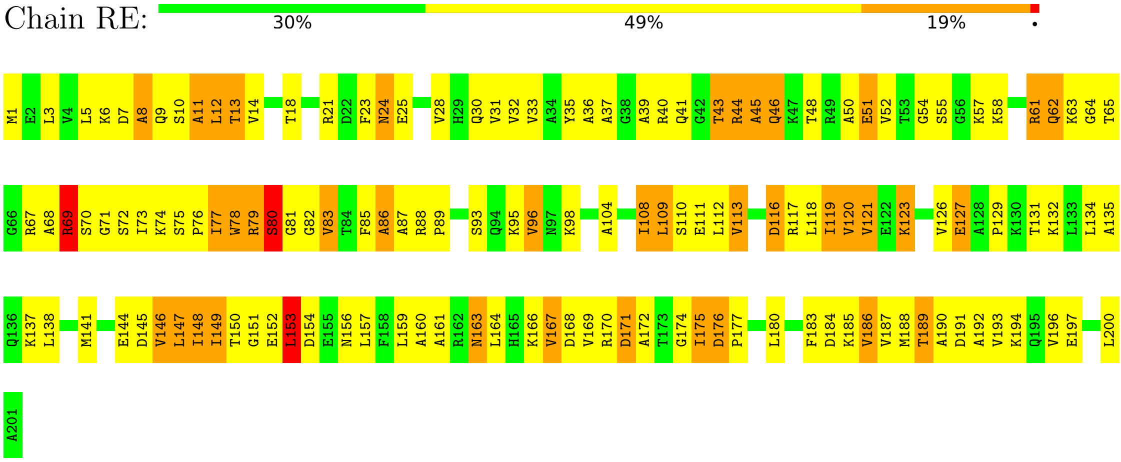




- Molecule 5: 50S ribosomal protein L4

Chain RE:



- Molecule 5: 50S ribosomal protein L4

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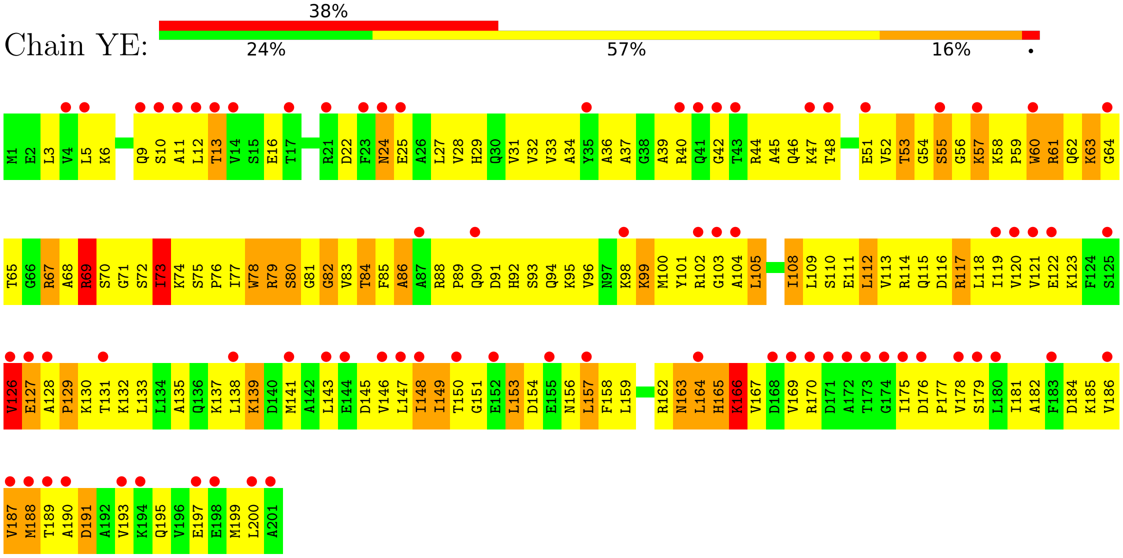
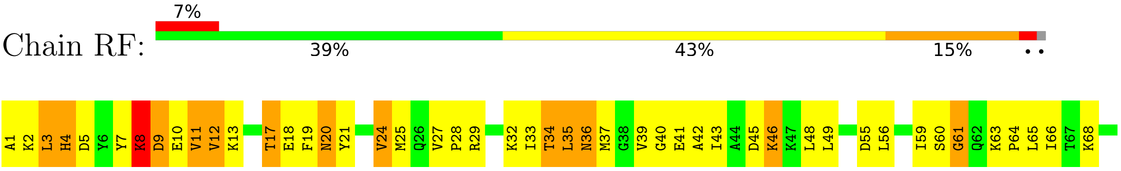
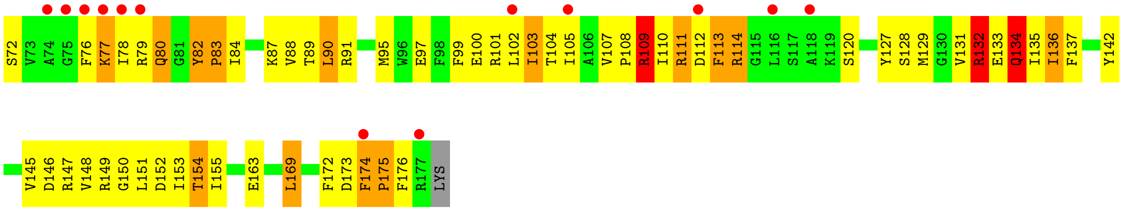


- Molecule 6: 50S ribosomal protein L5

Chain RF:





- Molecule 6: 50S ribosomal protein L5

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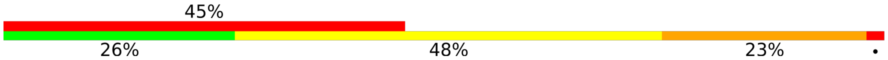

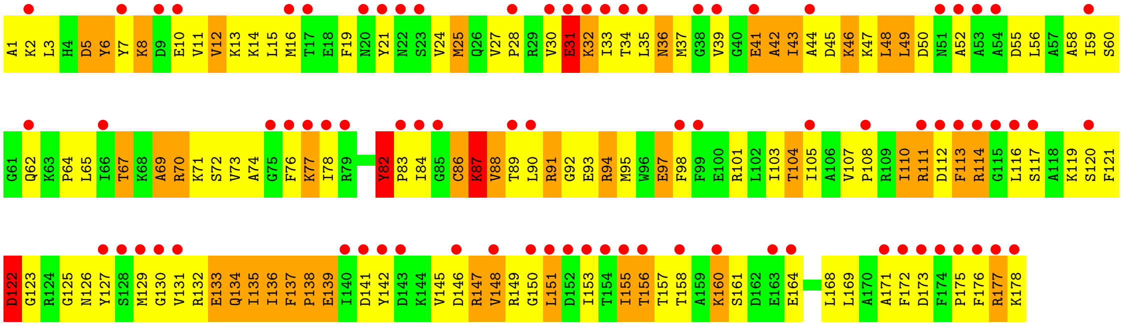

- Molecule 7: 50S ribosomal protein L6

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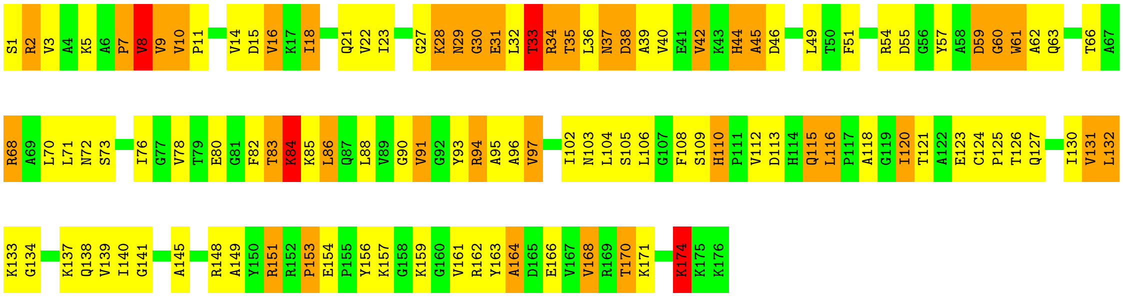

- Molecule 7: 50S ribosomal protein L6

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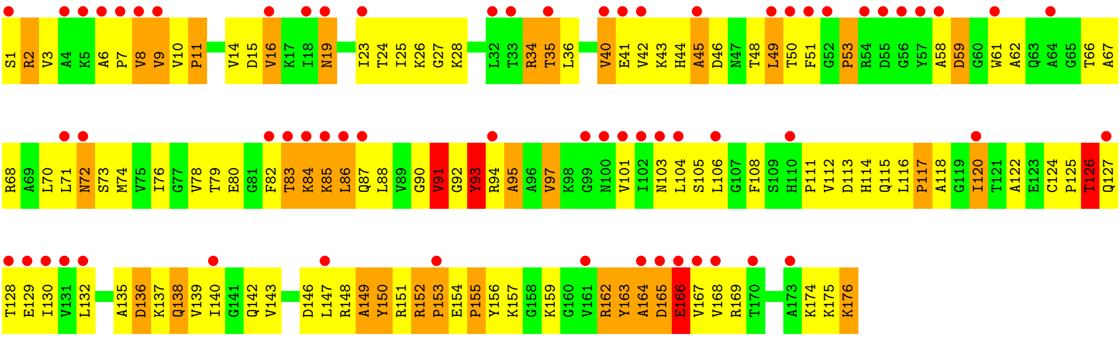
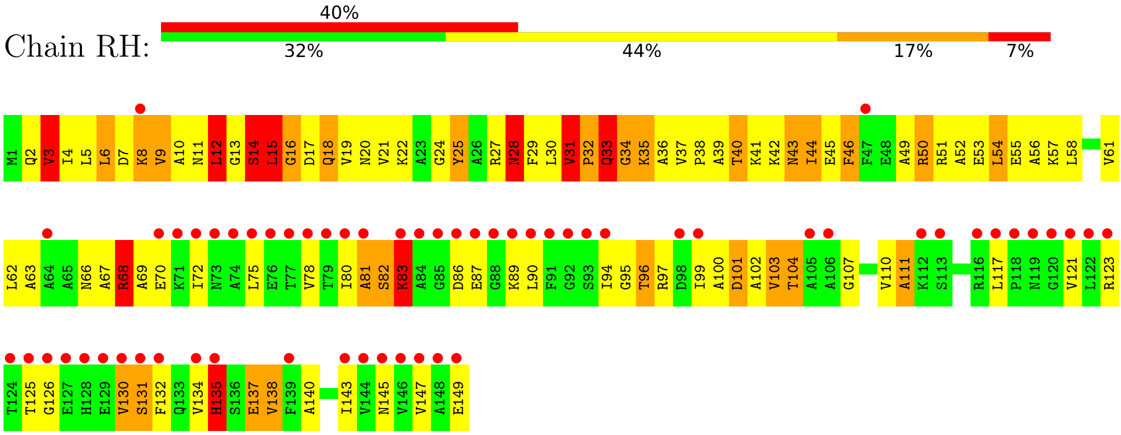
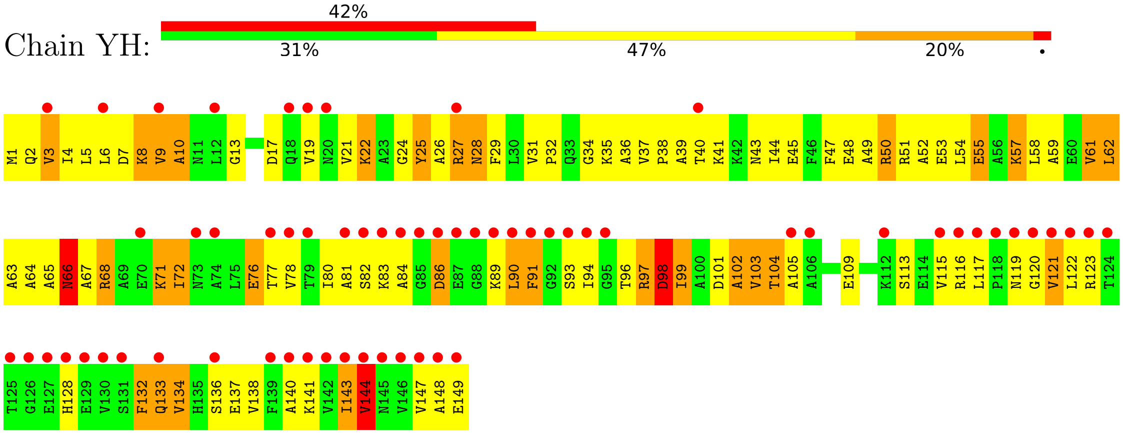


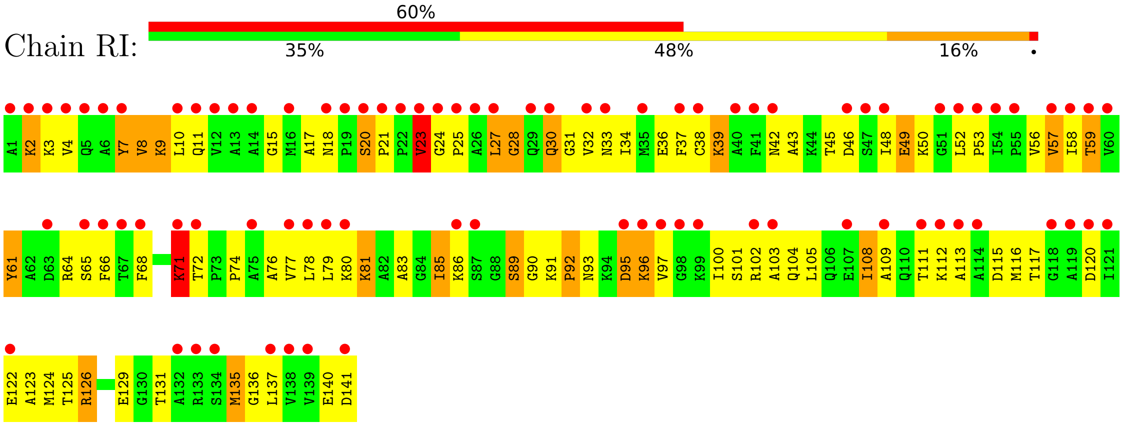
- Molecule 8: 50S ribosomal protein L9



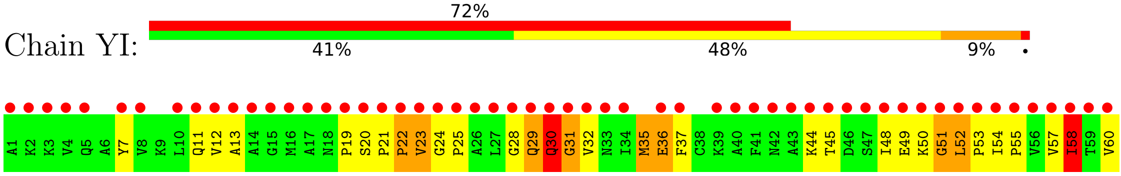
- Molecule 8: 50S ribosomal protein L9

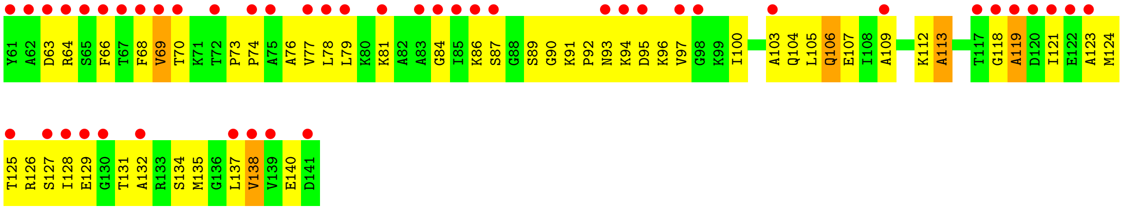


- Molecule 9: 50S ribosomal protein L11



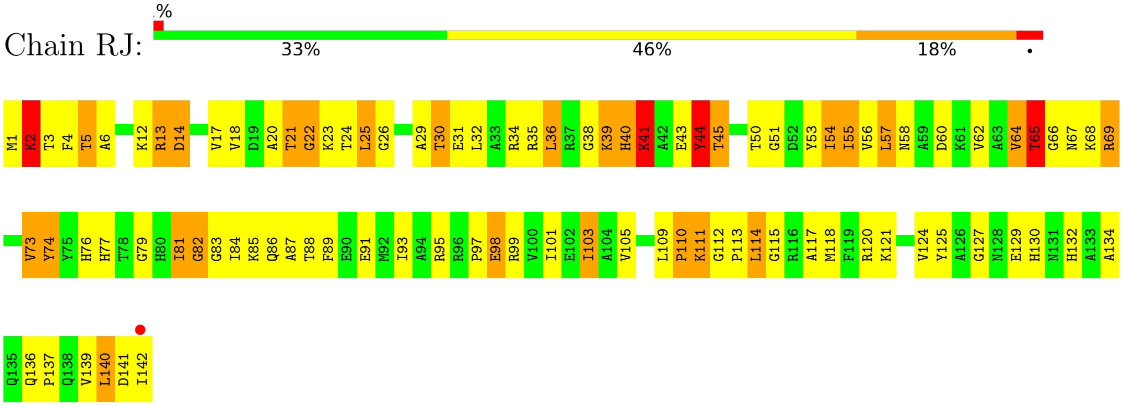
- Molecule 9: 50S ribosomal protein L11





- Molecule 10: 50S ribosomal protein L13

Chain RJ:



- Molecule 10: 50S ribosomal protein L13

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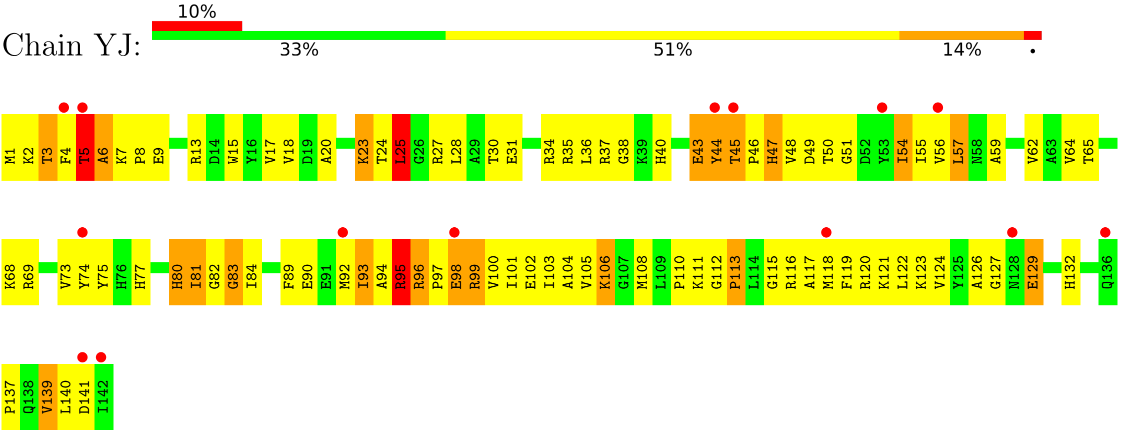

- Molecule 11: 50S ribosomal protein L14

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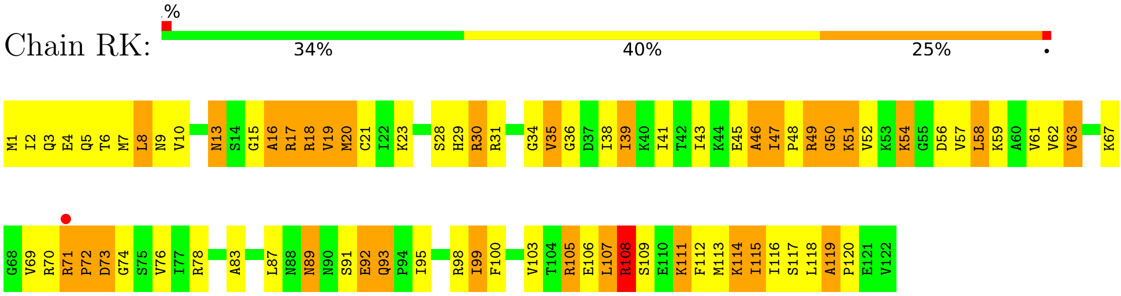

- Molecule 11: 50S ribosomal protein L14

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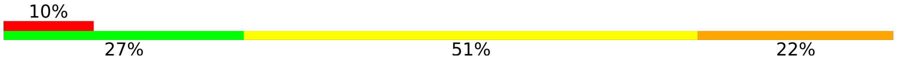
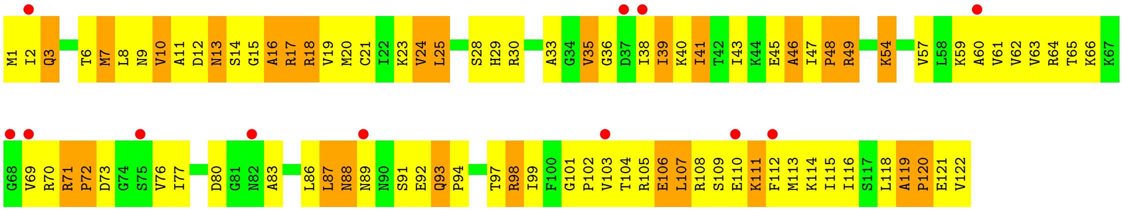
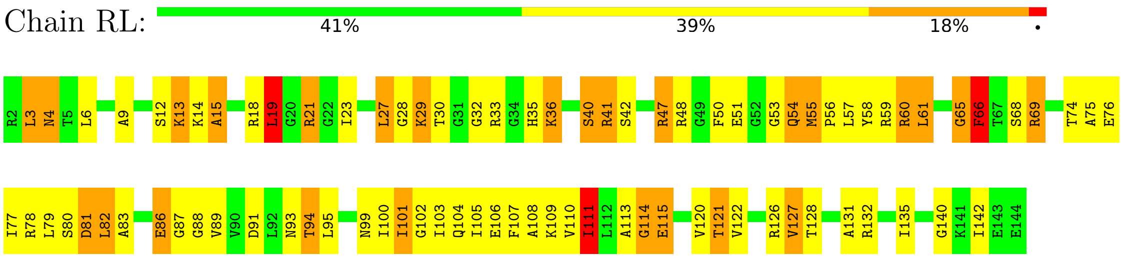
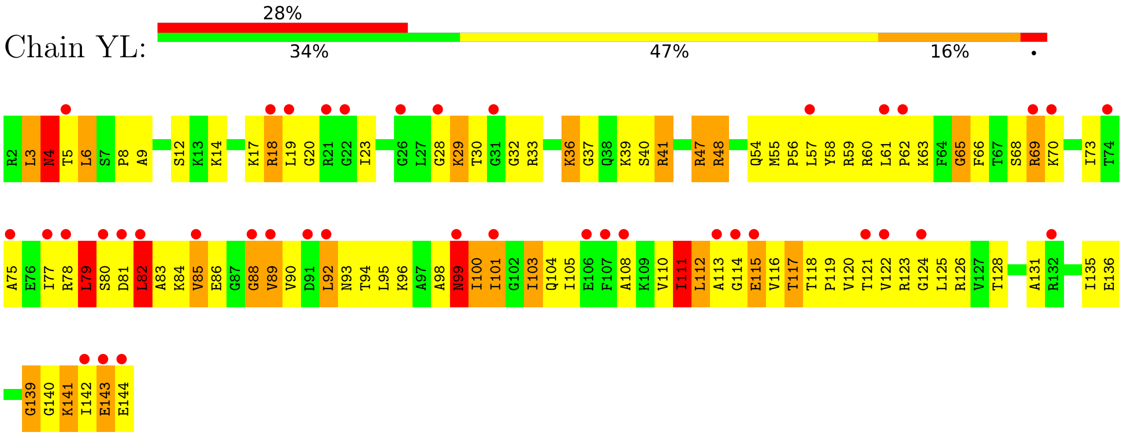




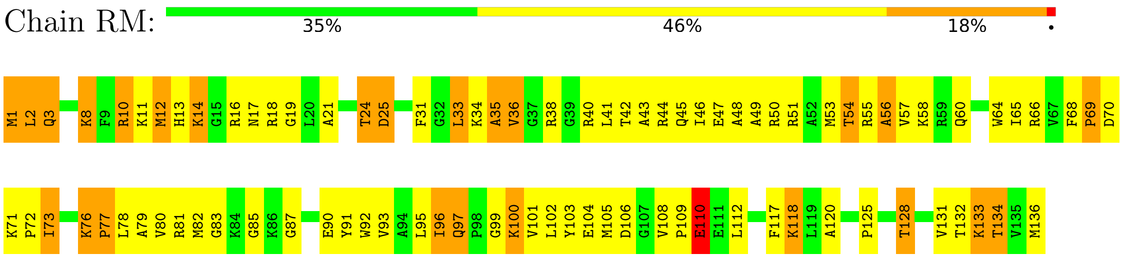
- Molecule 12: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16



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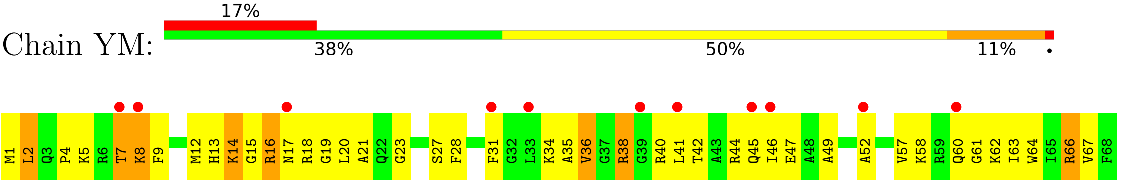
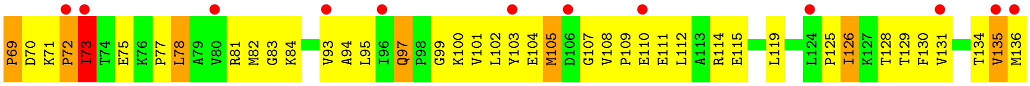
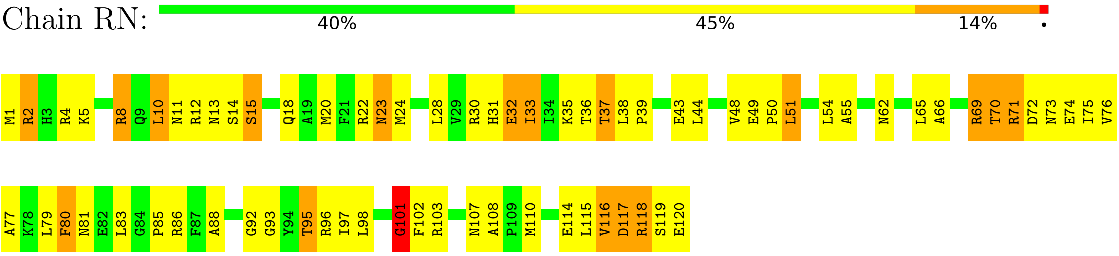
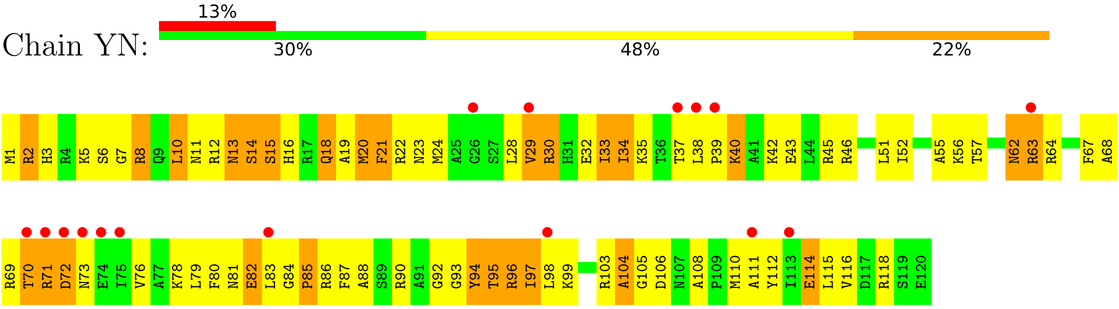




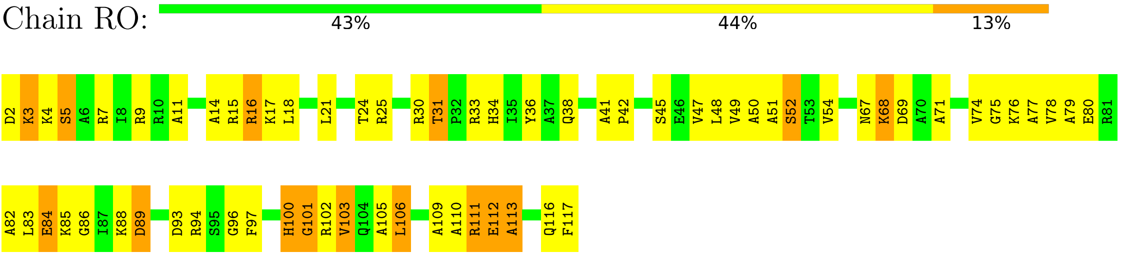
- Molecule 14: 50S ribosomal protein L17



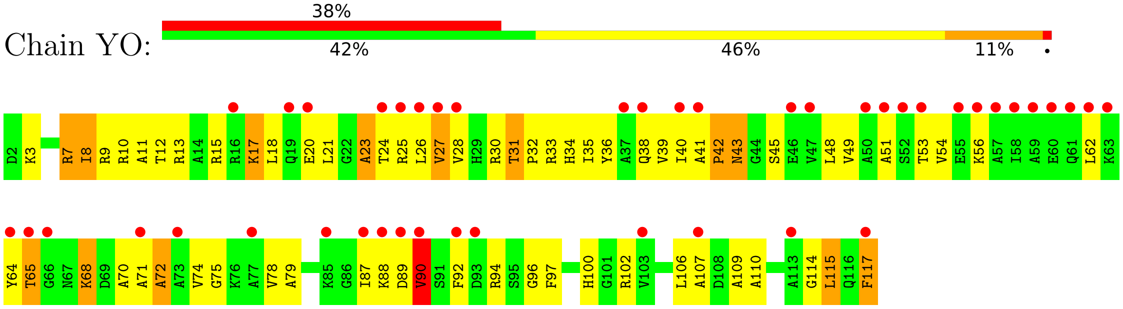
- Molecule 14: 50S ribosomal protein L17



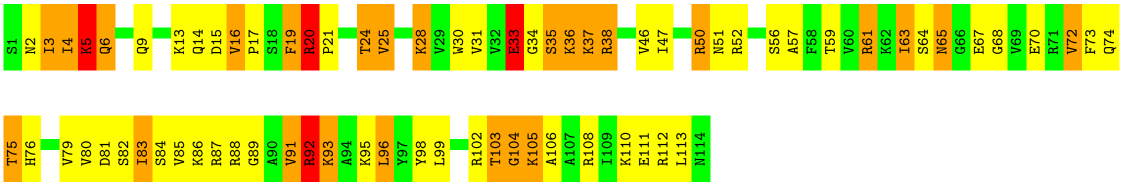
- Molecule 15: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L18



- Molecule 16: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L19

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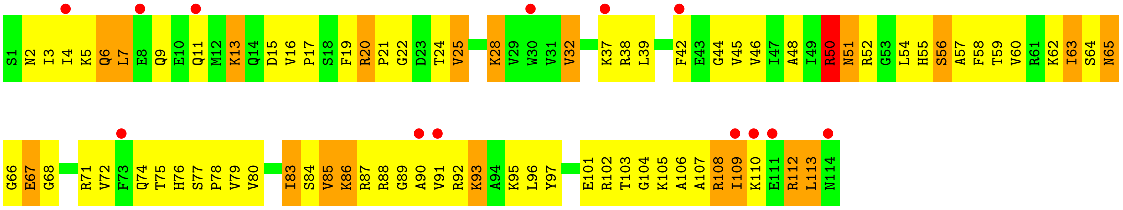
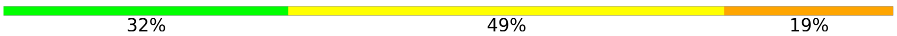
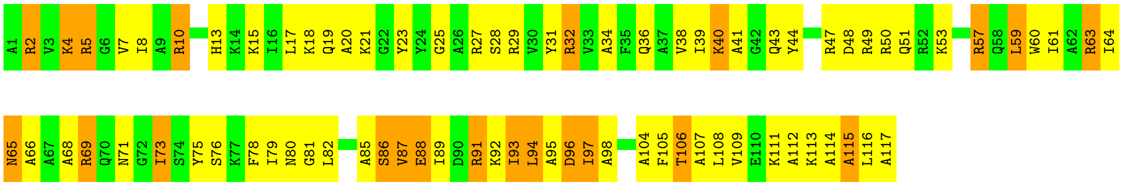


- Molecule 17: 50S ribosomal protein L20

Chain RQ:





- Molecule 17: 50S ribosomal protein L20

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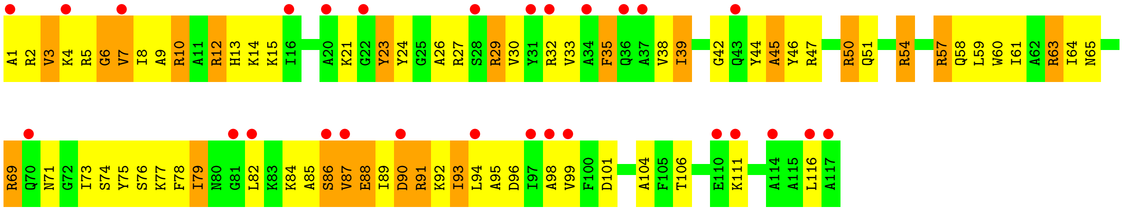

- Molecule 18: 50S ribosomal protein L21

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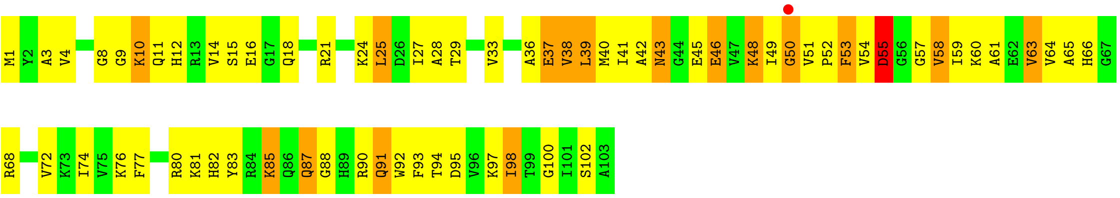
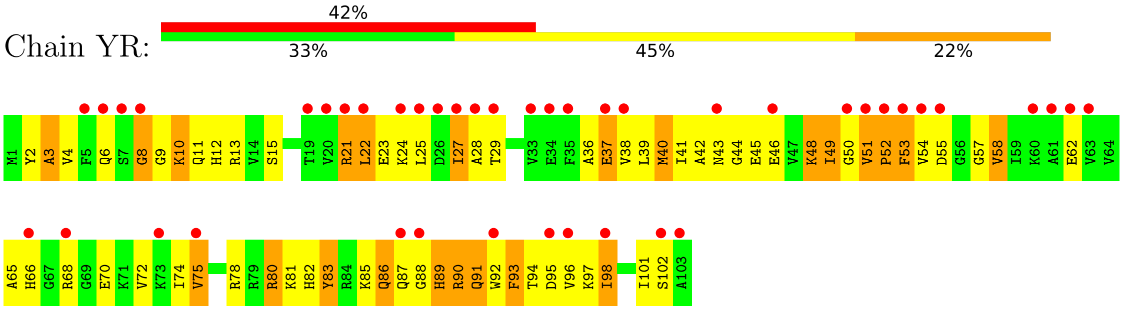
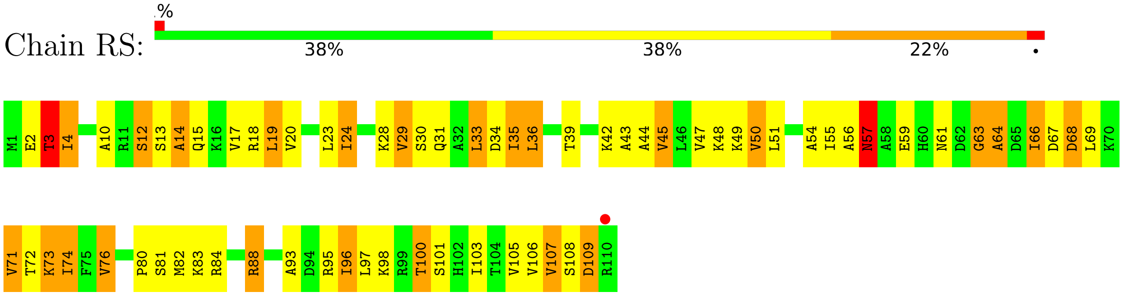


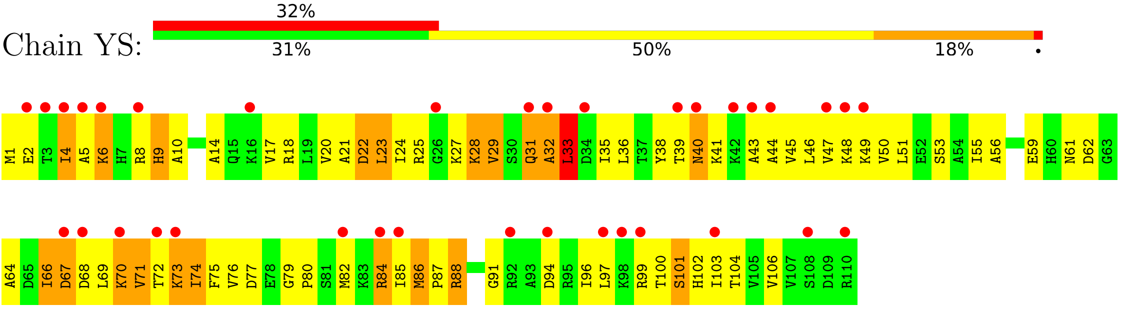
- Molecule 18: 50S ribosomal protein L21



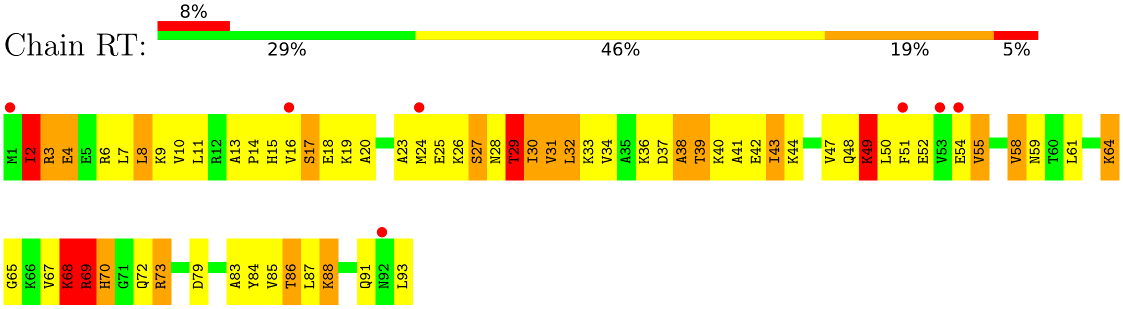
- Molecule 19: 50S ribosomal protein L22



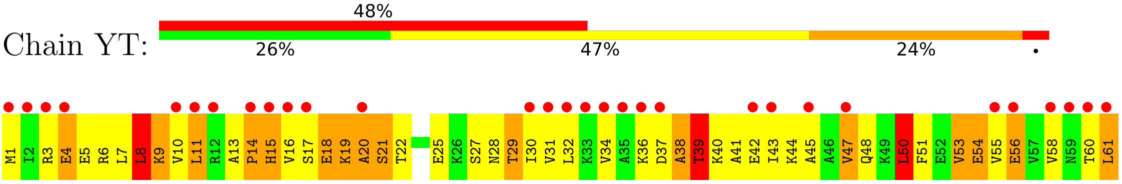
- Molecule 19: 50S ribosomal protein L22

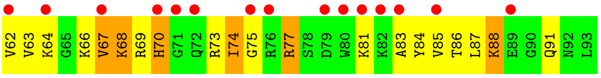


- Molecule 20: 50S ribosomal protein L23

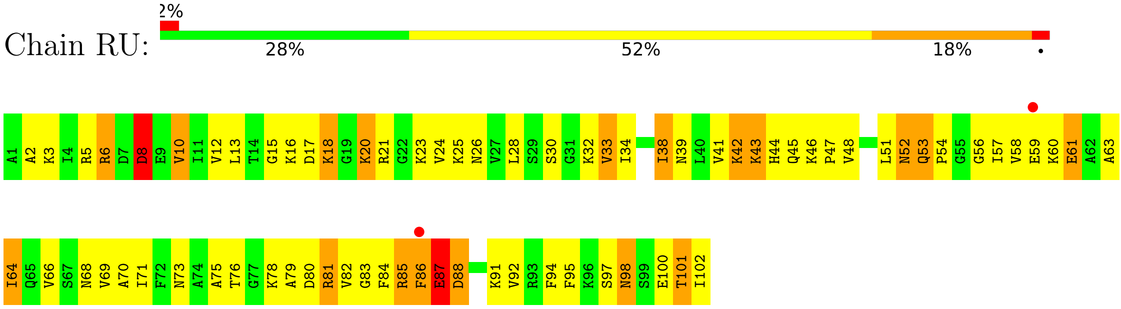


- Molecule 20: 50S ribosomal protein L23

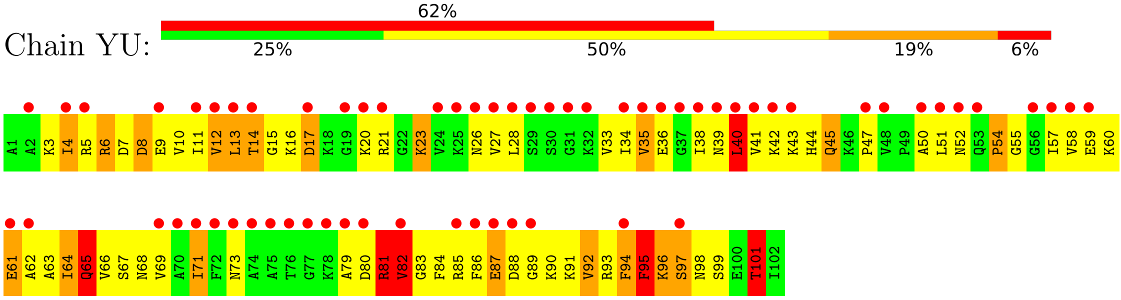




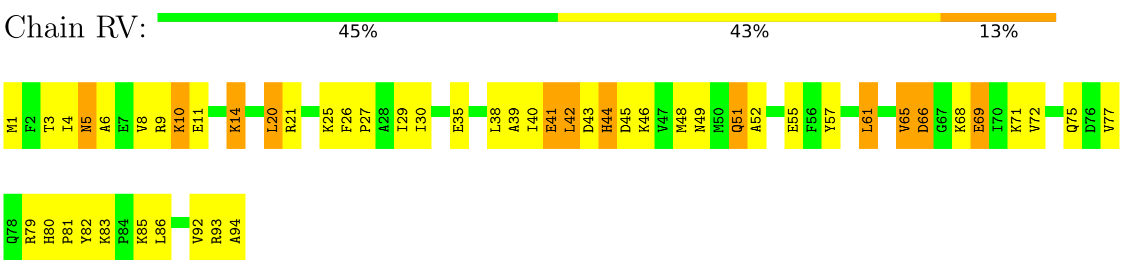
- Molecule 21: 50S ribosomal protein L24



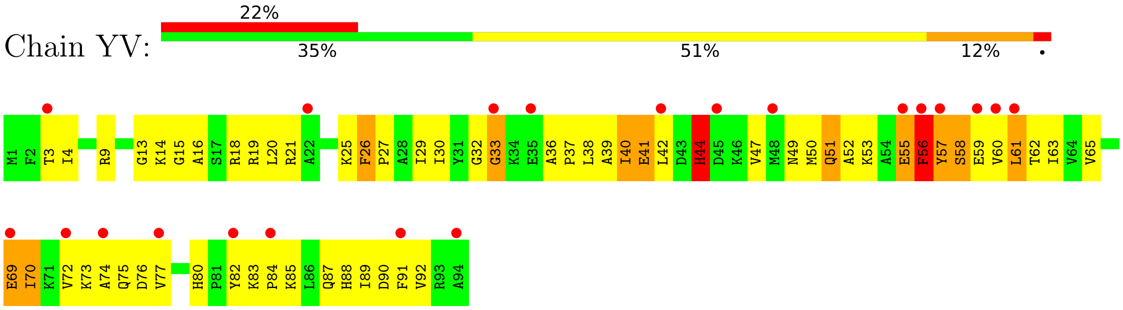
- Molecule 21: 50S ribosomal protein L24



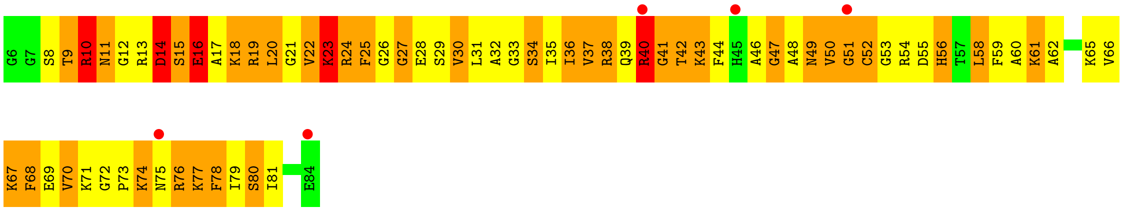
- Molecule 22: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L25

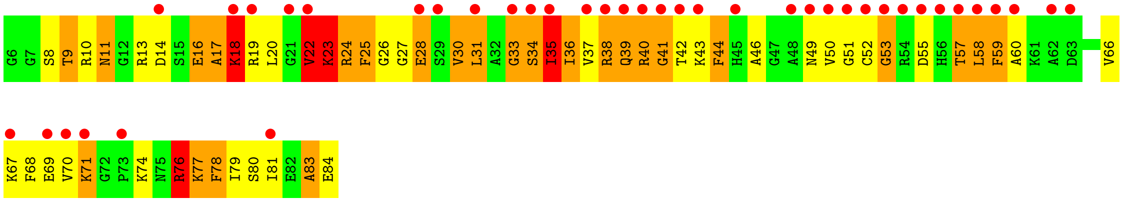


- Molecule 23: 50S ribosomal protein L27



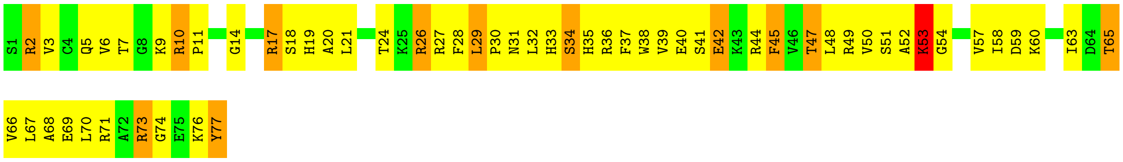
- Molecule 23: 50S ribosomal protein L27

Chain YW:



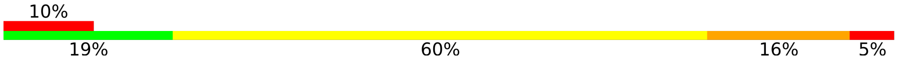
- Molecule 24: 50S ribosomal protein L28

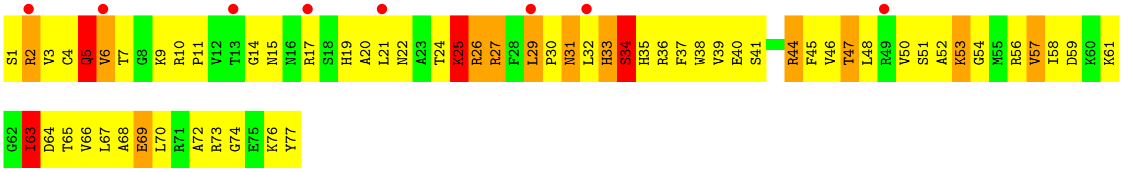
Chain RX:



- Molecule 24: 50S ribosomal protein L28

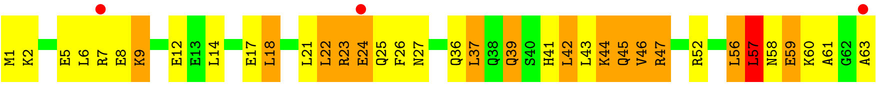
Chain YX:





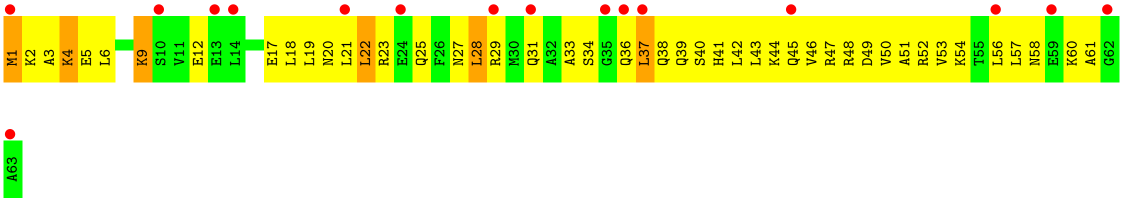
- Molecule 25: 50S ribosomal protein L29

Chain RY:

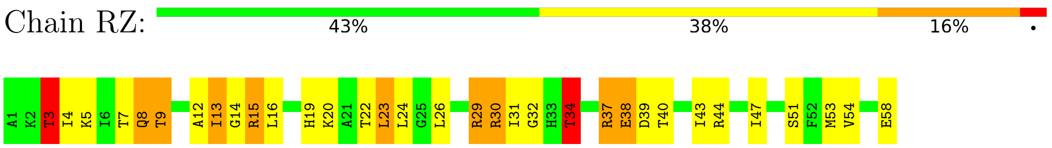


- Molecule 25: 50S ribosomal protein L29

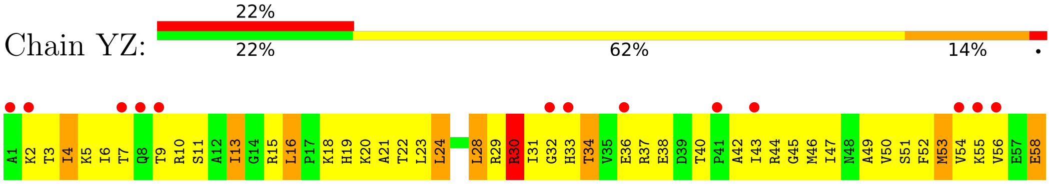
Chain YY:



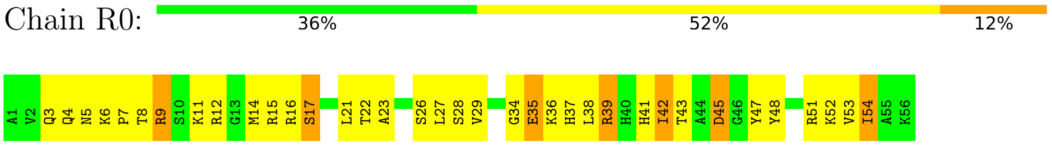
- Molecule 26: 50S ribosomal protein L30



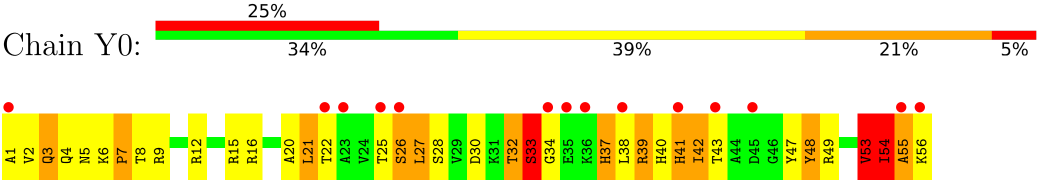
- Molecule 26: 50S ribosomal protein L30



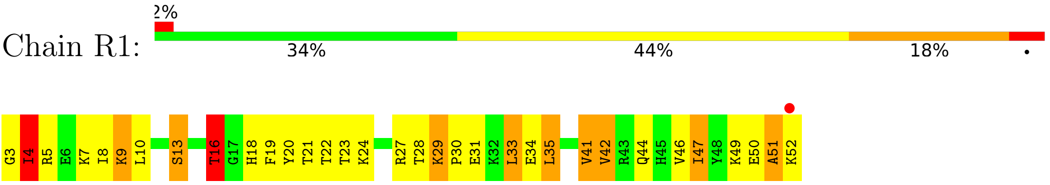
- Molecule 27: 50S ribosomal protein L32



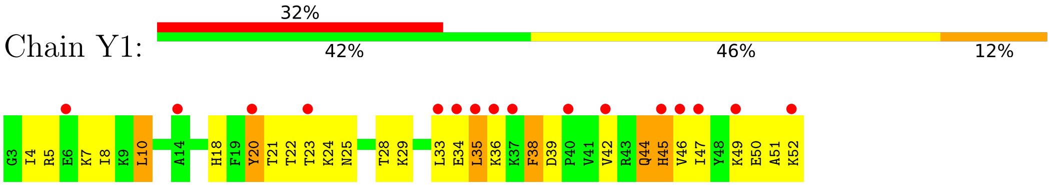
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

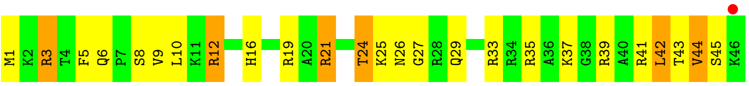


- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

Chain R2:



- Molecule 29: 50S ribosomal protein L34

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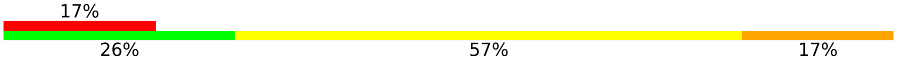
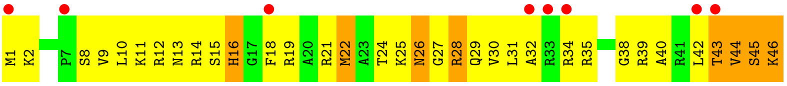
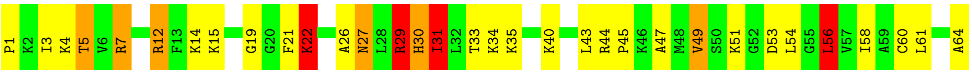




- Molecule 30: 50S ribosomal protein L35

Chain R3:

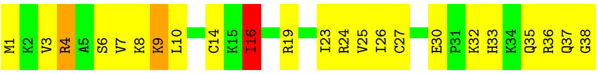


- Molecule 30: 50S ribosomal protein L35

Chain Y3:

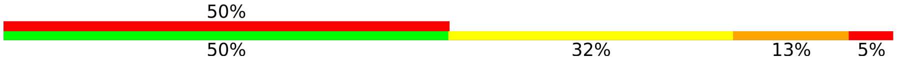
- Molecule 31: 50S ribosomal protein L36

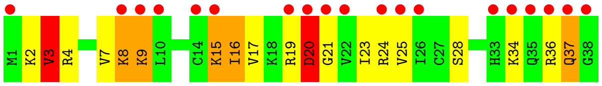
Chain R4:



- Molecule 31: 50S ribosomal protein L36

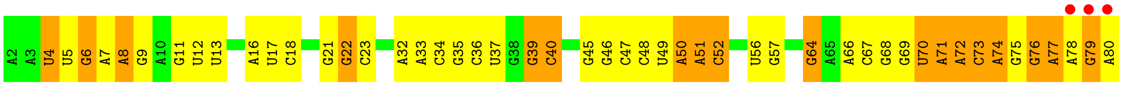
Chain Y4:

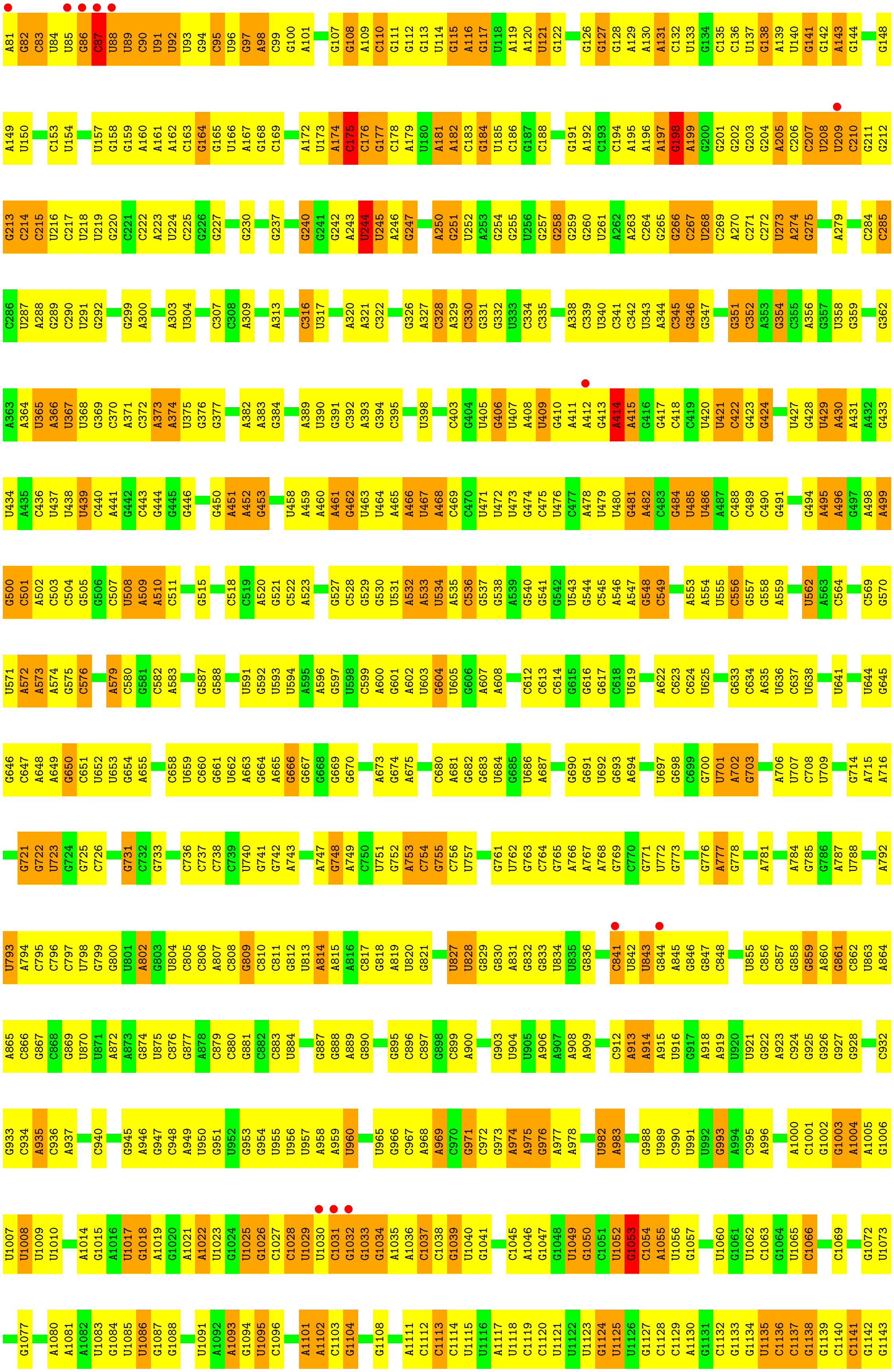




- Molecule 32: 16S rRNA

Chain QA:

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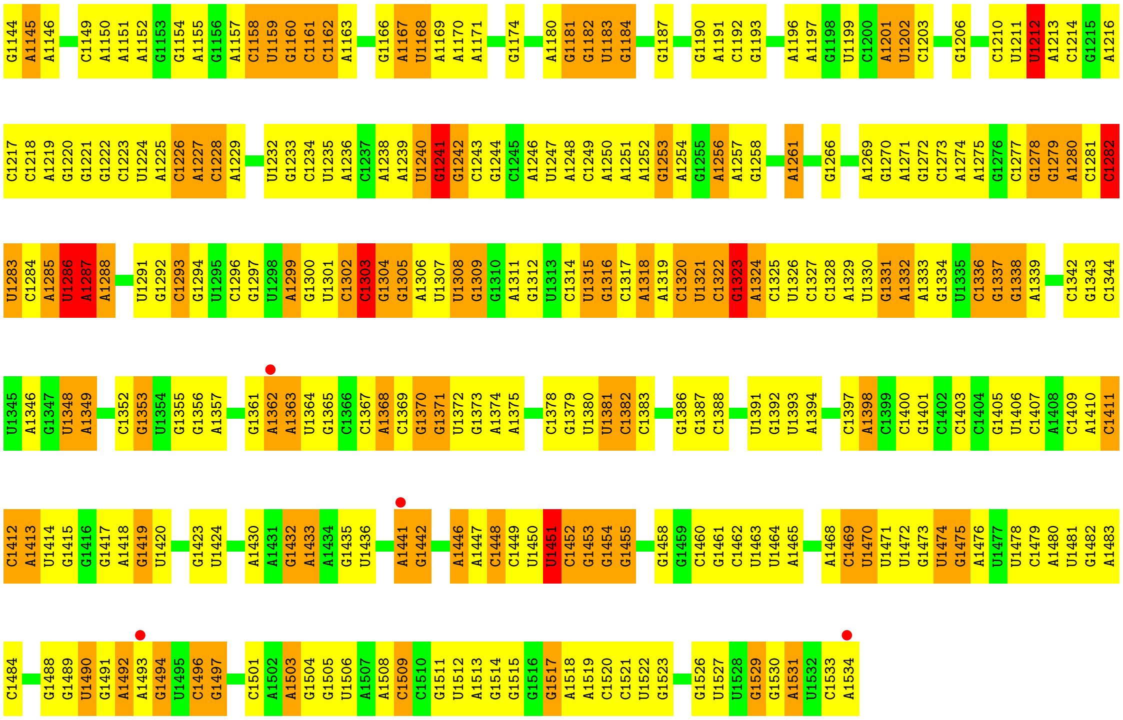
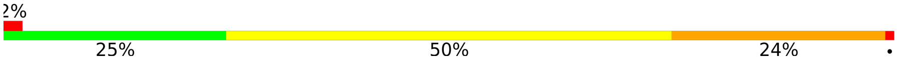
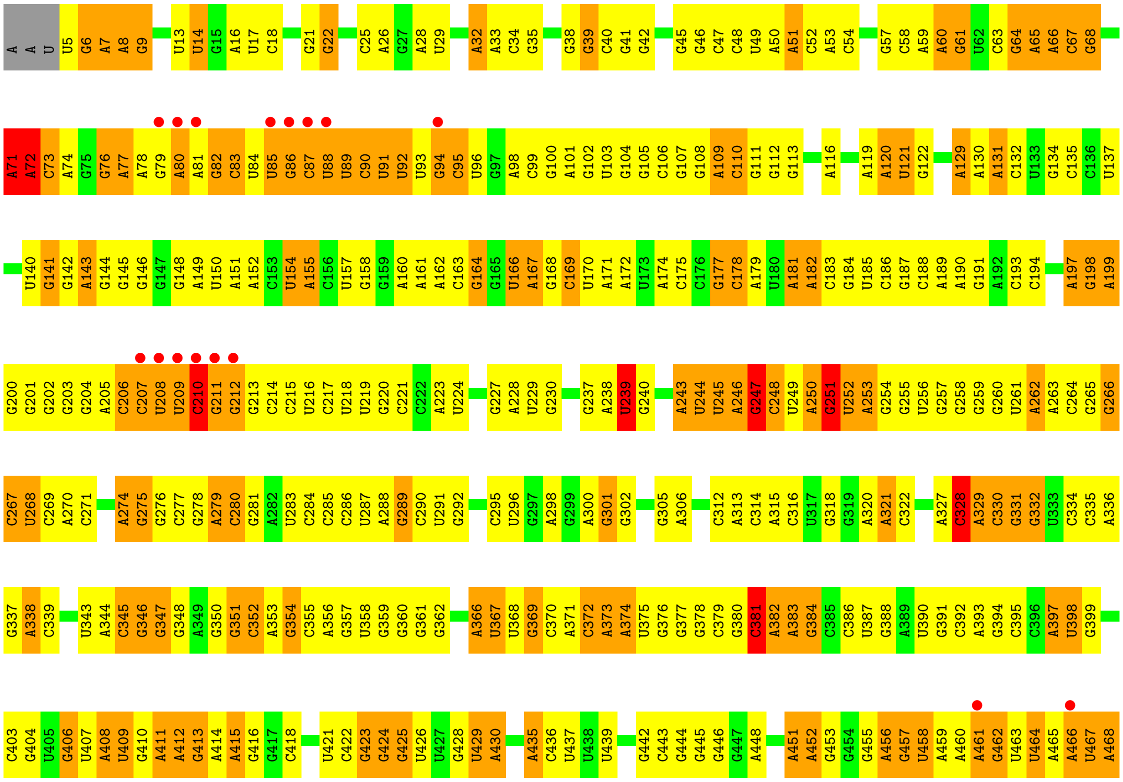
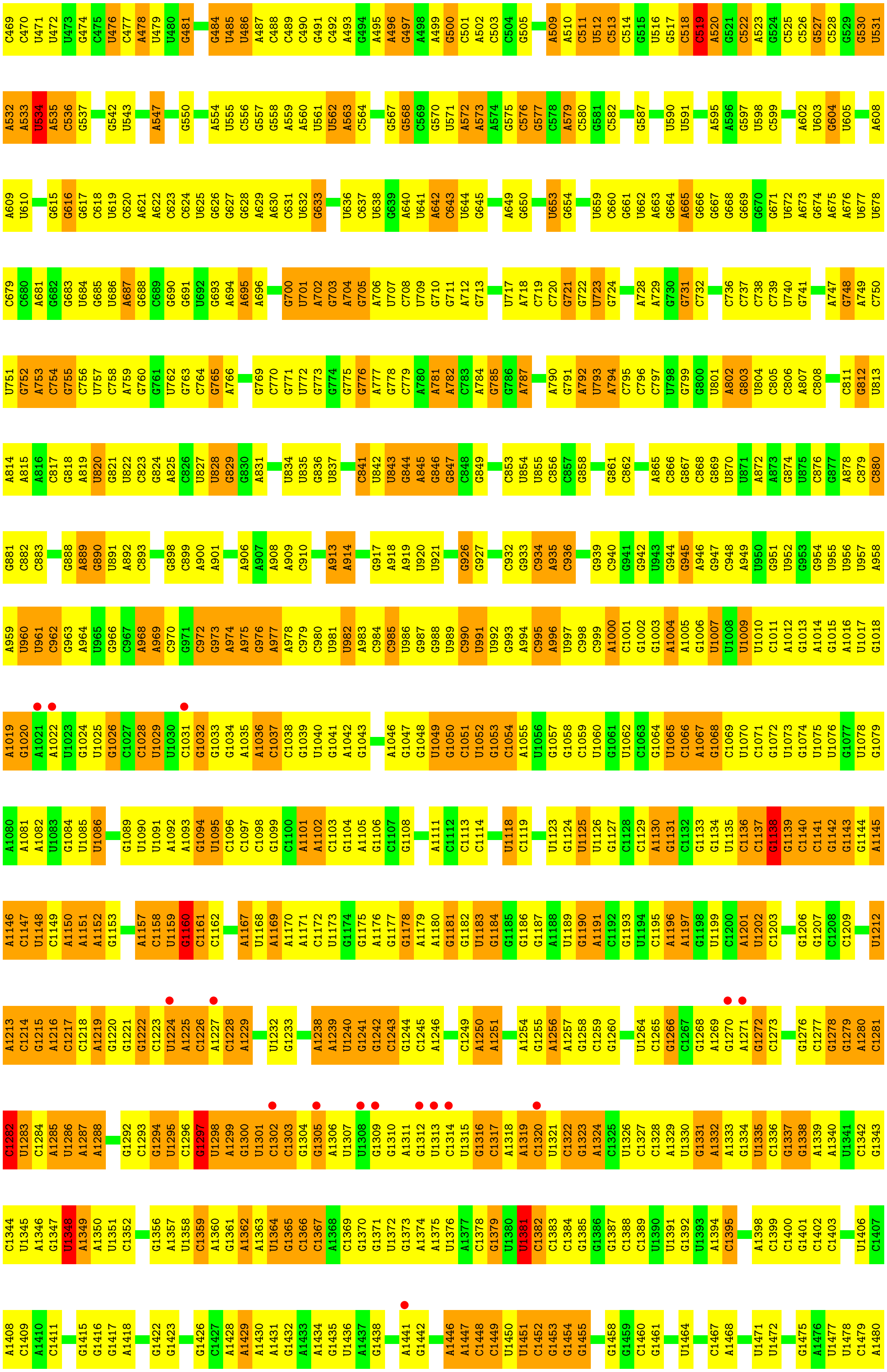


- Molecule 32: 16S rRNA

Chain XA:



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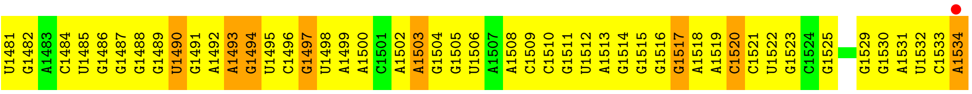
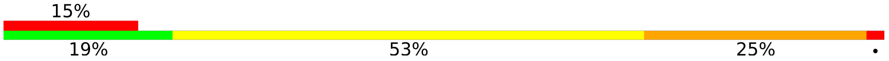
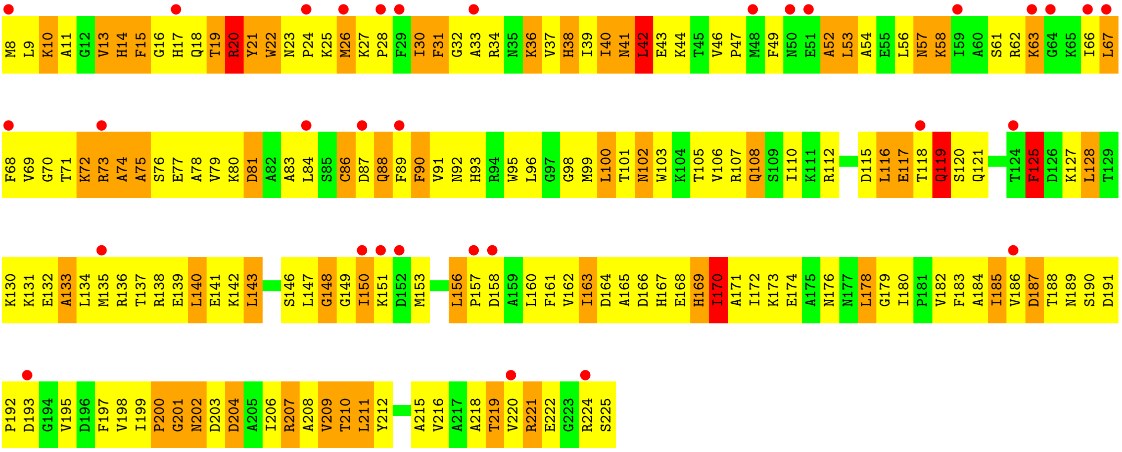
A1213 C1214 G1215 A1216 C1217 C1218 A1219 G1220 G1221 G1222 C1223 U1224 A1225 C1226 A1227 C1228 A1229 U1232 G1233 A1238 U1239 U1240 G1241 G1242 C1243 G1244 C1245 A1246 C1249 U1250 A1251 A1254 G1255 A1256 A1257 G1258 C1259 G1260 U1264 C1265 G1266 C1267 G1268 A1269 G1270 A1271 G1272 C1273 G1276 C1277 G1278 G1279 A1280 C1281
C1282 U1283 C1284 A1285 U1286 A1287 A1288 G1292 C1293 G1294 U1295 C1296 G1297 U1298 A1299 G1300 U1301 C1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309 G1310 A1311 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 U1321 C1322 G1323 G1324 C1325 U1326 C1327 C1328 A1329 U1330 G1331 A1332 A1333 G1334 U1335 C1336 G1337 G1338 A1339 A1340 U1341 C1342 G1343
C1344 U1345 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1356 A1357 U1358 C1359 A1360 G1361 A1362 A1363 U1364 G1365 C1366 C1367 A1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377 C1378 G1379 U1380 U1381 C1382 C1383 C1384 G1385 G1386 G1387 C1388 C1389 U1390 U1391 G1392 U1393 A1394 C1395 A1398 C1399 C1400 G1401 C1402 C1403 U1406 C1407
A1408 C1409 A1410 C1411 G1415 G1416 G1417 A1418 G1422 G1423 G1426 C1427 A1428 A1429 A1430 A1431 G1432 A1433 A1434 G1435 U1436 A1437 G1438 A1441 G1442 A1446 A1447 C1448 C1449 U1450 U1451 C1452 G1453 G1454 G1455 G1458 G1459 C1460 G1461 U1464 C1467 A1468 U1471 U1472 G1475 A1476 U1477 U1478 C1479 A1480



- Molecule 33: 30S ribosomal protein S2

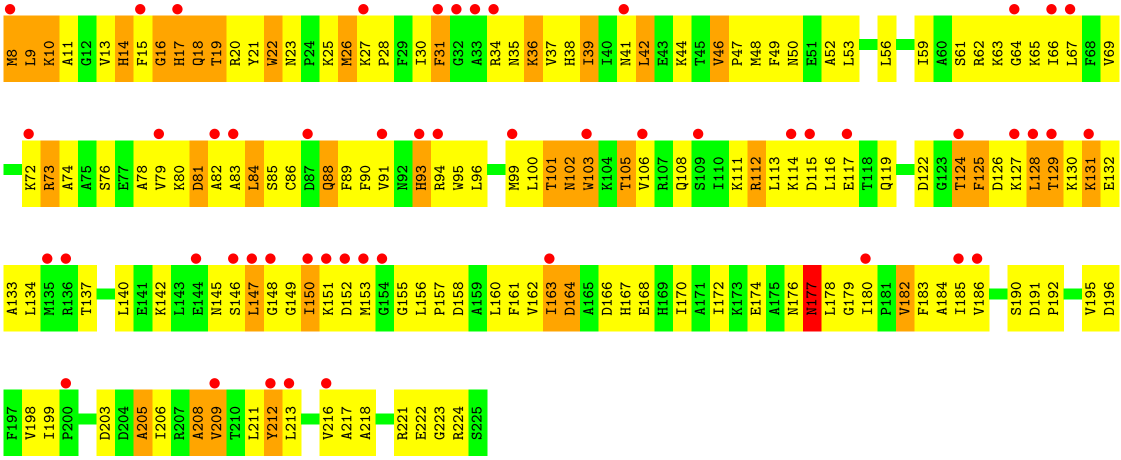
Chain QB:





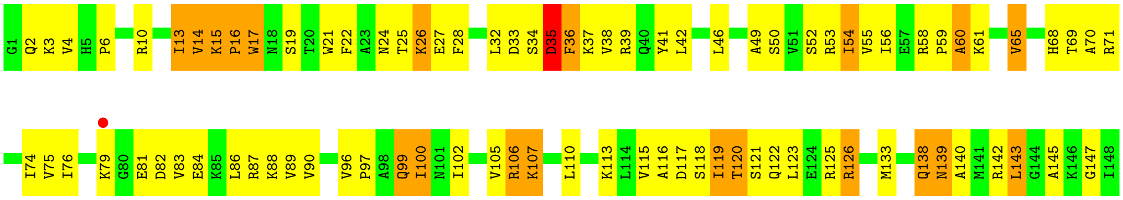
- Molecule 33: 30S ribosomal protein S2

Chain XB:



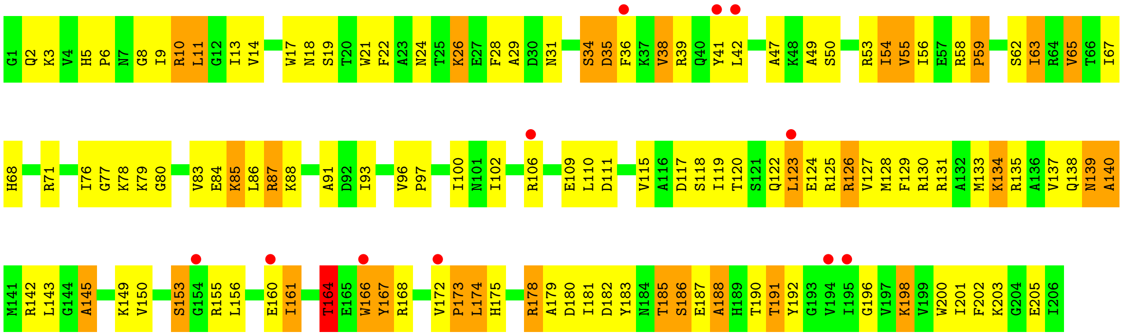
- Molecule 34: 30S ribosomal protein S3

Chain QC:



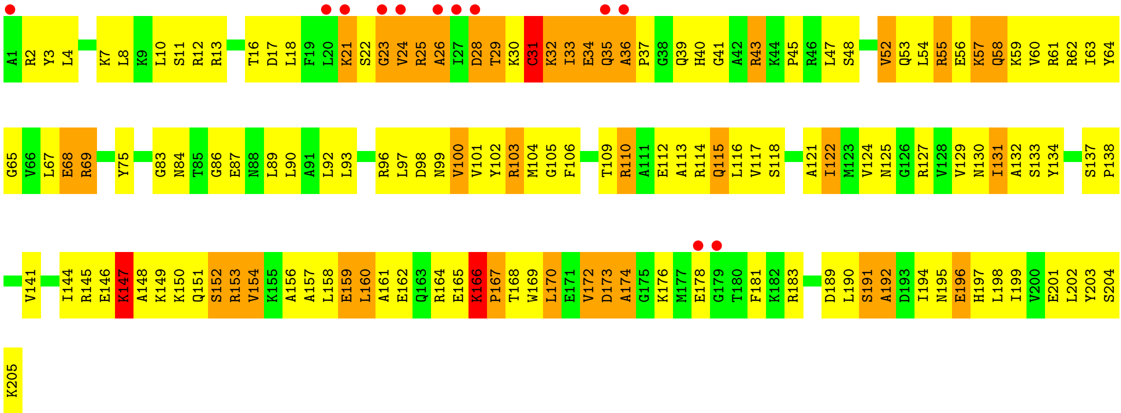
- Molecule 34: 30S ribosomal protein S3

Chain XC:



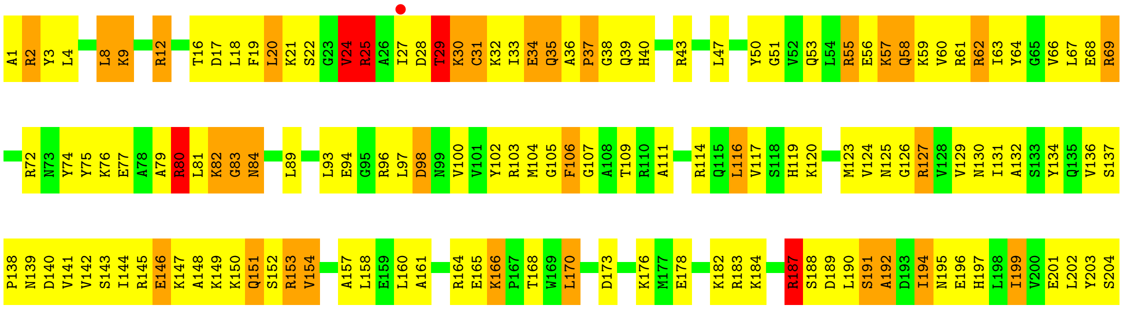
- Molecule 35: 30S ribosomal protein S4

Chain QD:

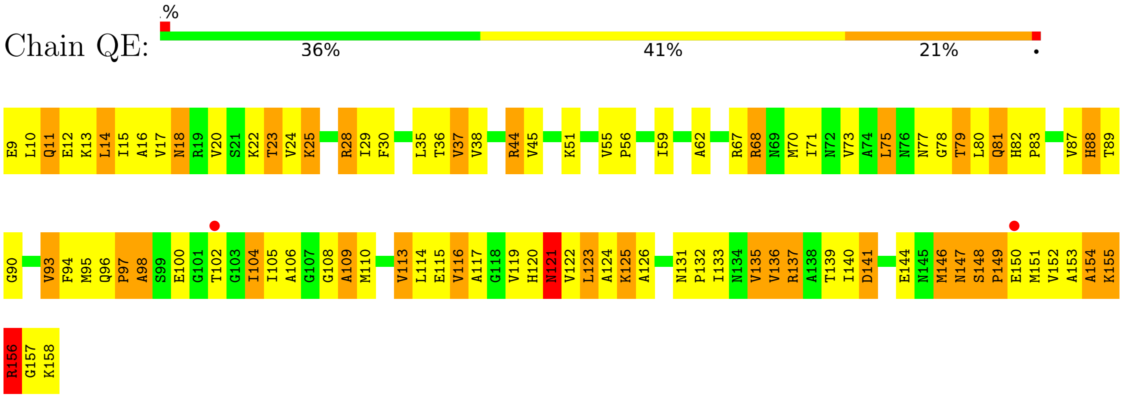


- Molecule 35: 30S ribosomal protein S4

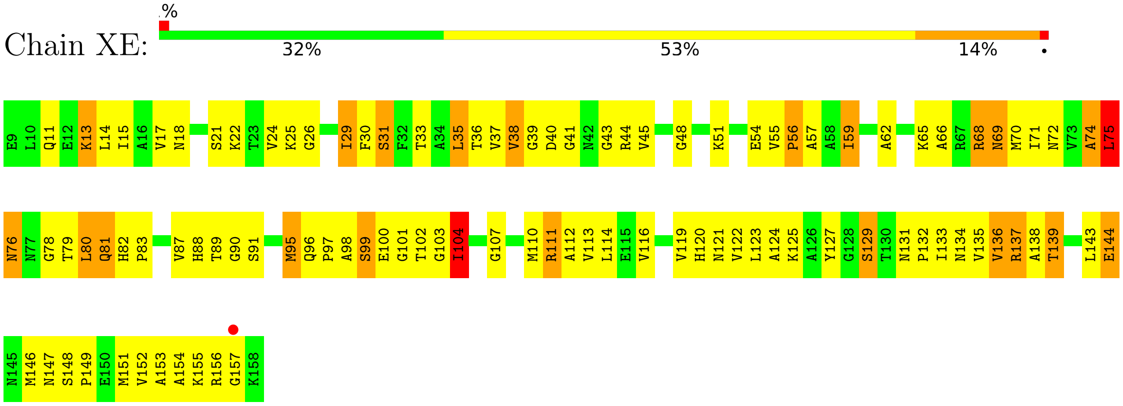
Chain XD:



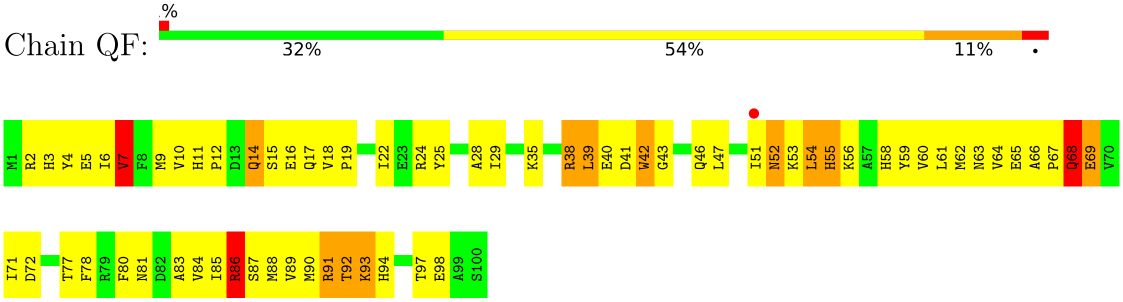
- Molecule 36: 30S ribosomal protein S5



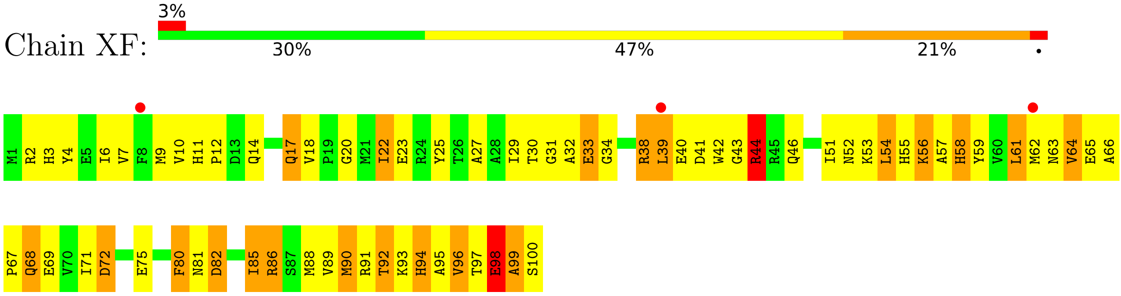
- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6

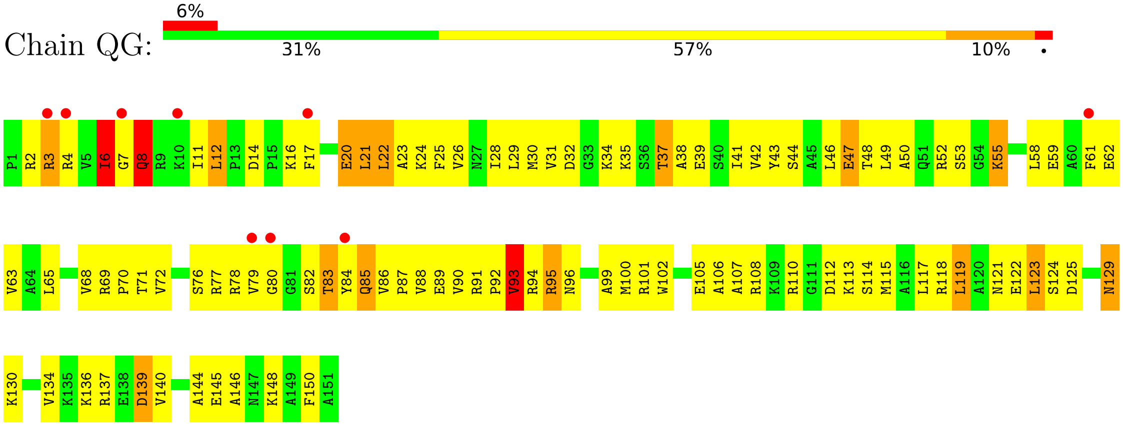


- Molecule 37: 30S ribosomal protein S6



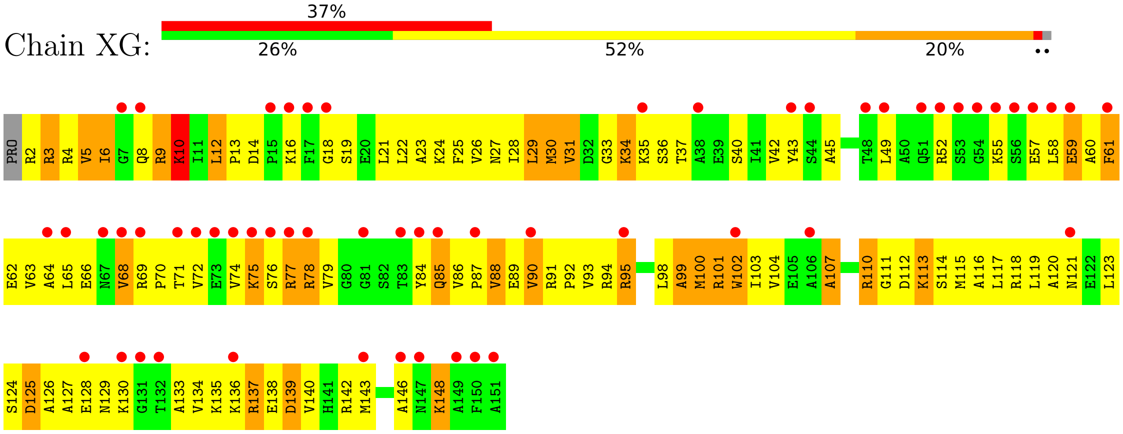
- Molecule 38: 30S ribosomal protein S7

Chain QG:



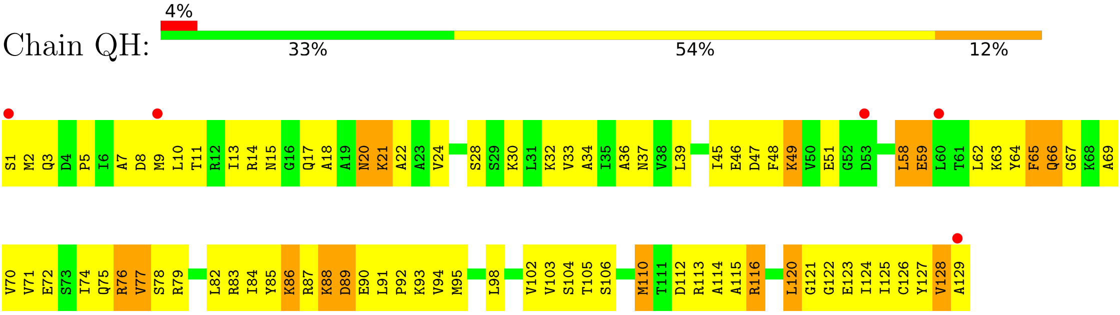
- Molecule 38: 30S ribosomal protein S7

Chain XG:



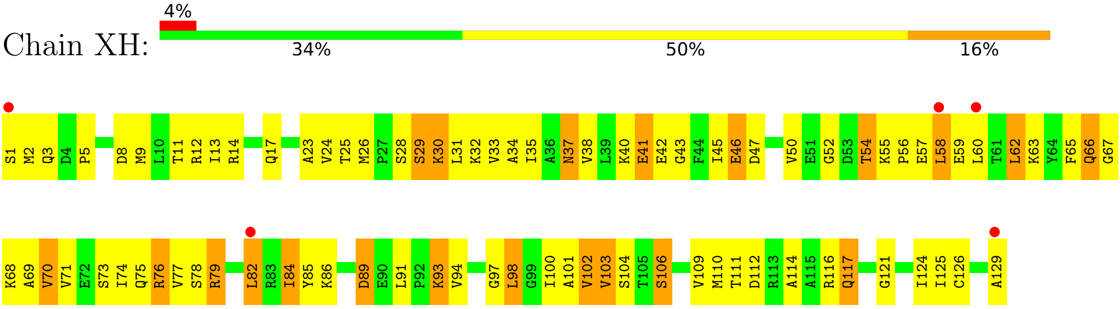
- Molecule 39: 30S ribosomal protein S8

Chain QH:



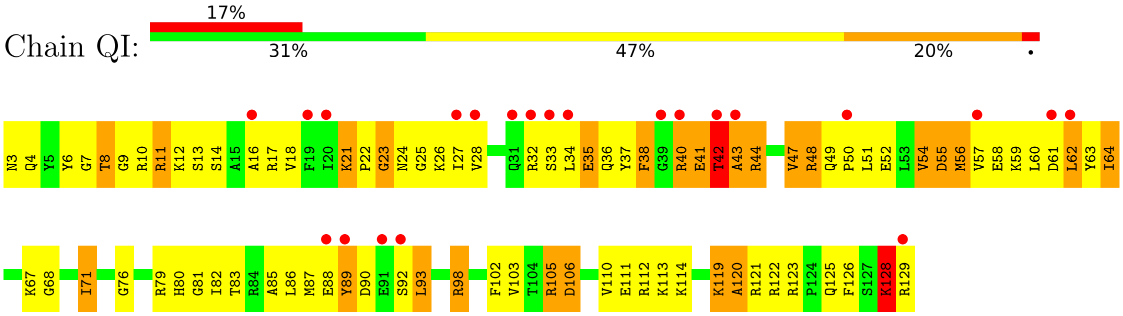
- Molecule 39: 30S ribosomal protein S8

Chain XH:



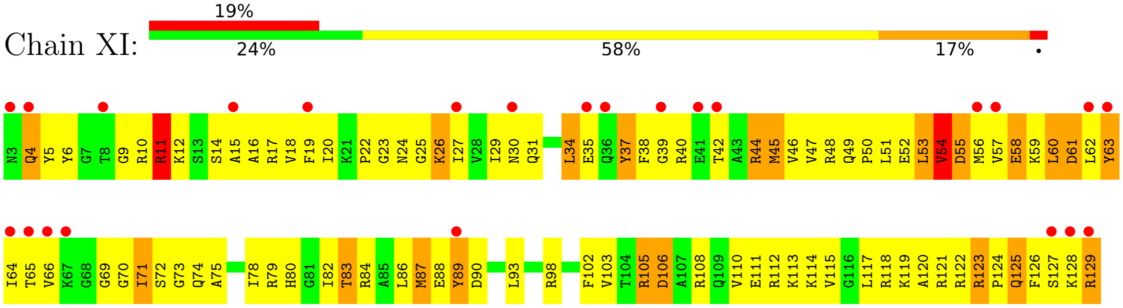
- Molecule 40: 30S ribosomal protein S9

Chain QI:



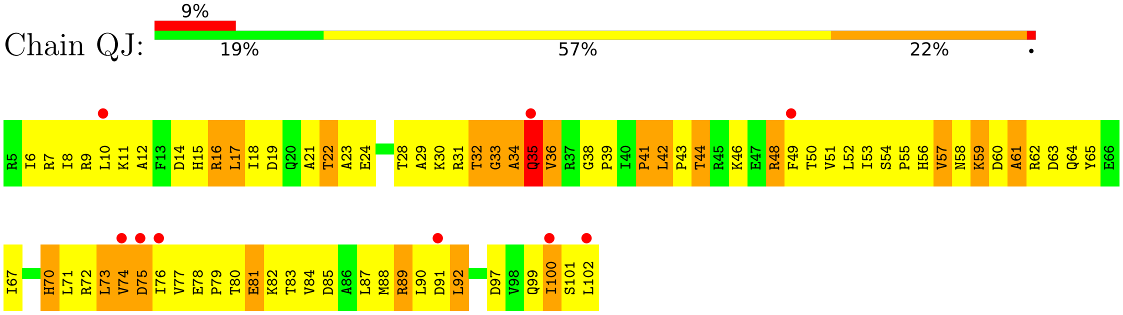
- Molecule 40: 30S ribosomal protein S9

Chain XI:



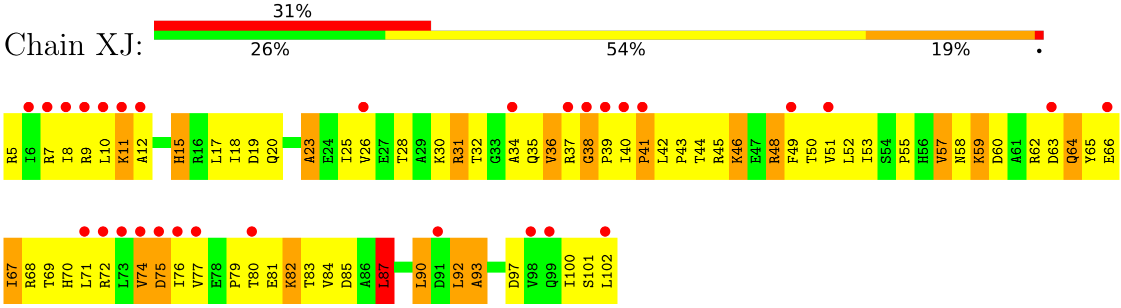
- Molecule 41: 30S ribosomal protein S10

Chain QJ:



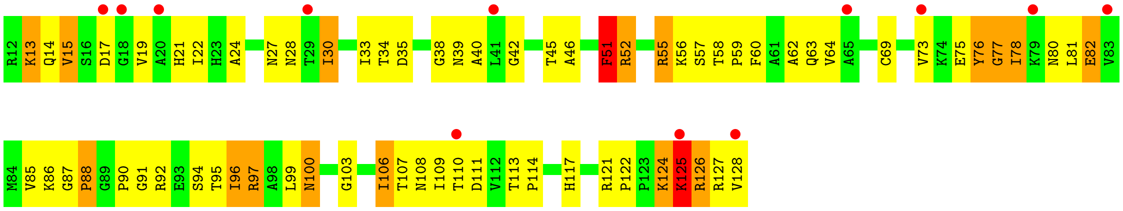
- Molecule 41: 30S ribosomal protein S10

Chain XJ:

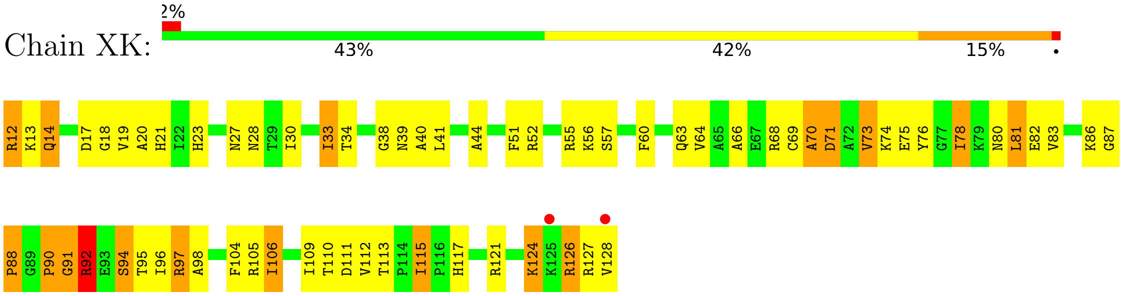


- Molecule 42: 30S ribosomal protein S11

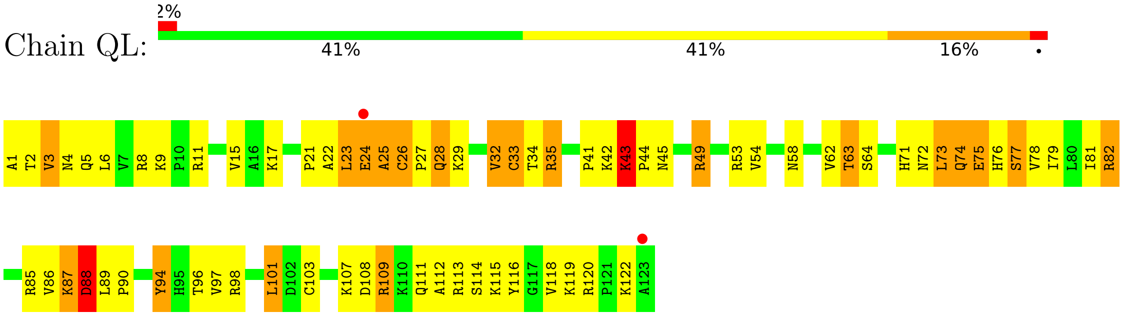
Chain QK:



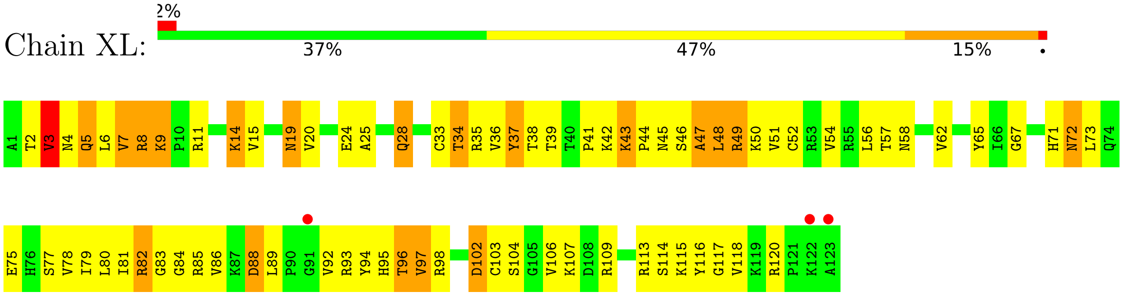
- Molecule 42: 30S ribosomal protein S11



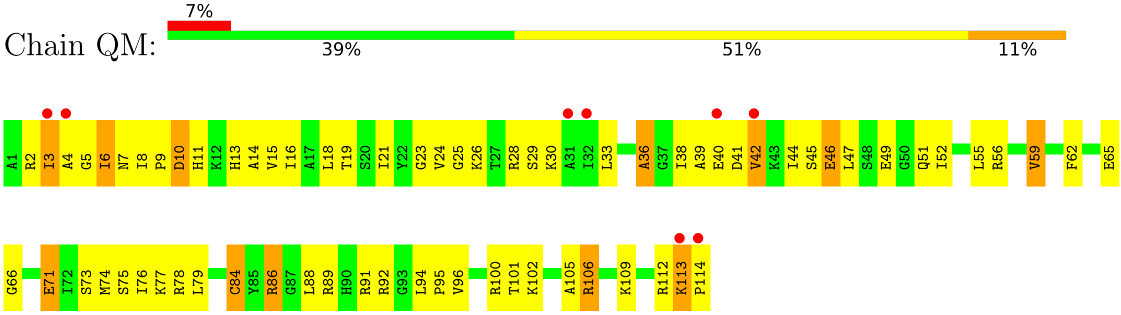
- Molecule 43: 30S ribosomal protein S12



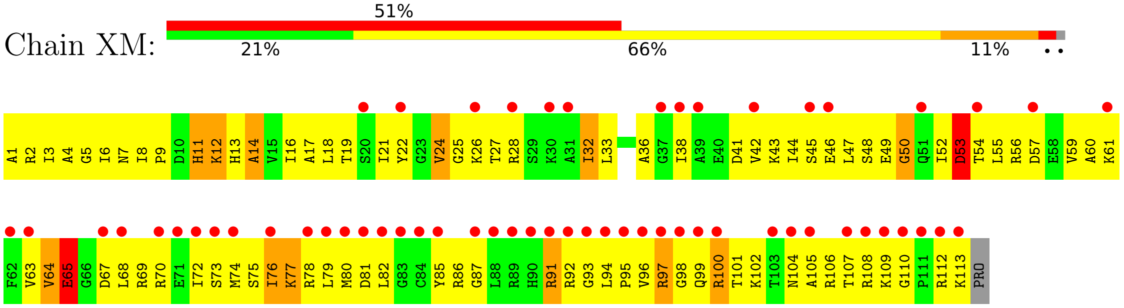
- Molecule 43: 30S ribosomal protein S12



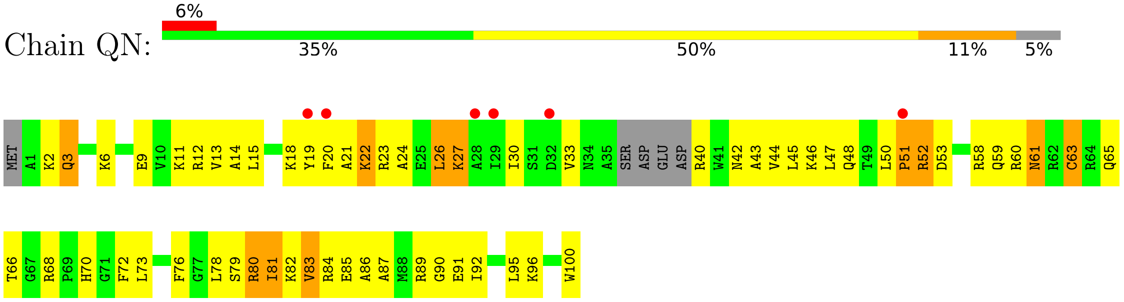
- Molecule 44: 30S ribosomal protein S13



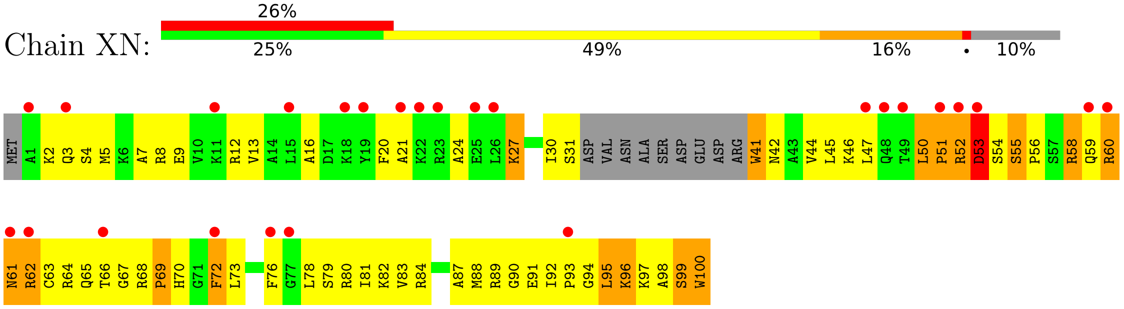
- Molecule 44: 30S ribosomal protein S13



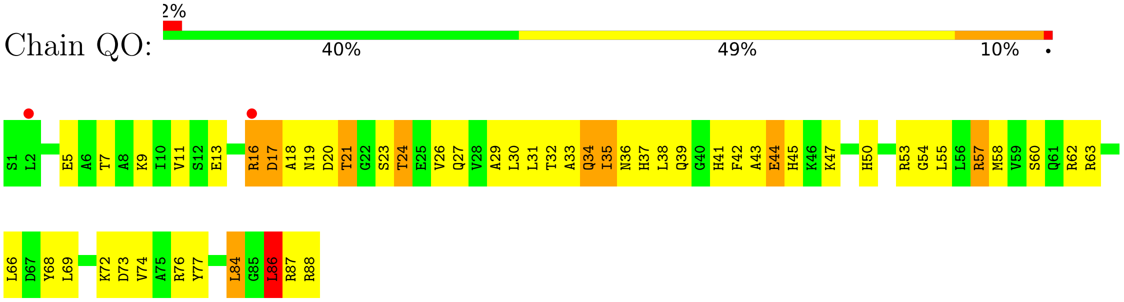
- Molecule 45: 30S ribosomal protein S14



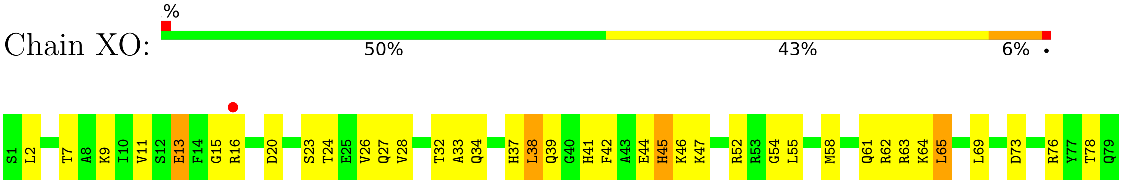
- Molecule 45: 30S ribosomal protein S14

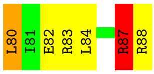


- Molecule 46: 30S ribosomal protein S15



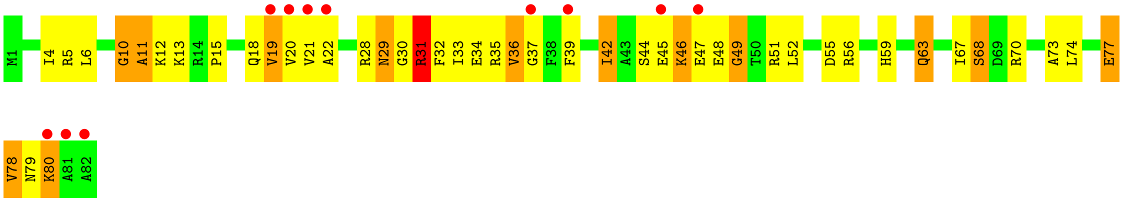
- Molecule 46: 30S ribosomal protein S15





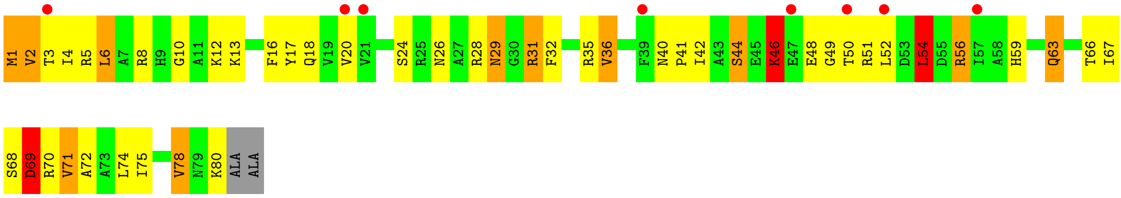
- Molecule 47: 30S ribosomal protein S16

Chain QP:



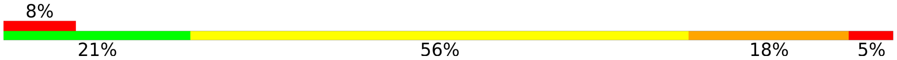
- Molecule 47: 30S ribosomal protein S16

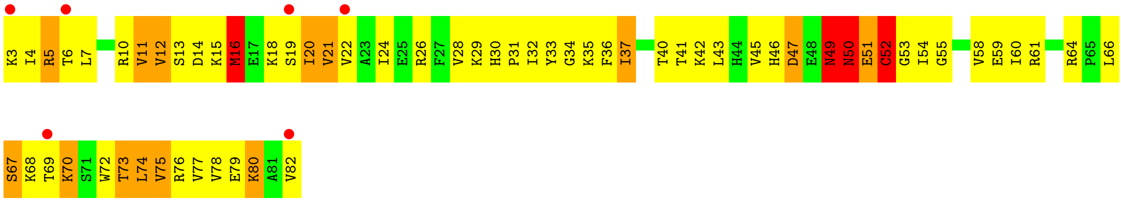
Chain XP:



- Molecule 48: 30S ribosomal protein S17

Chain QQ:



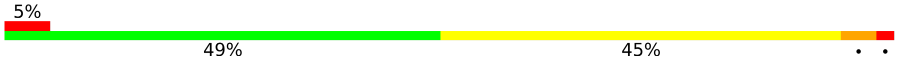


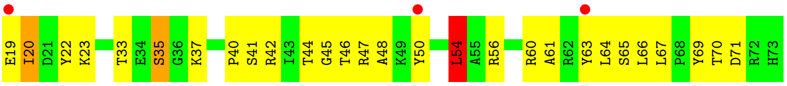
- Molecule 48: 30S ribosomal protein S17

Chain XQ:

- Molecule 49: 30S ribosomal protein S18

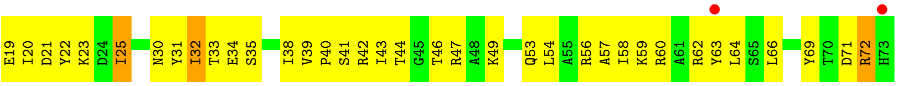
Chain QR:





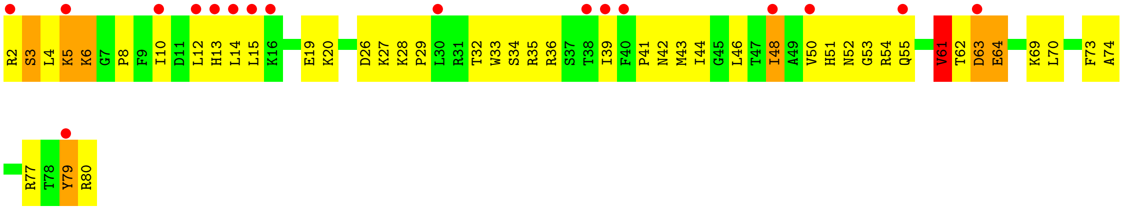
- Molecule 49: 30S ribosomal protein S18

Chain XR:



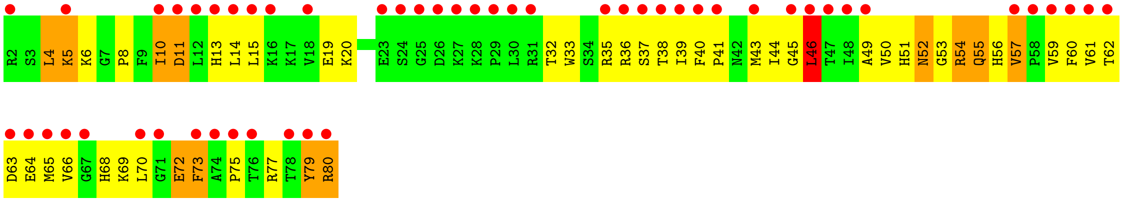
- Molecule 50: 30S ribosomal protein S19

Chain QS:



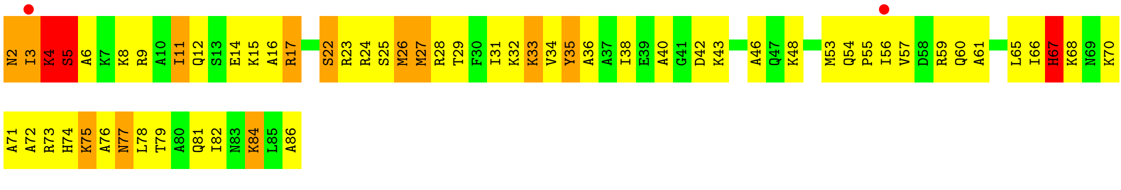
- Molecule 50: 30S ribosomal protein S19

Chain XS:



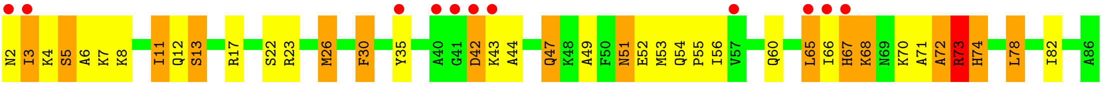
- Molecule 51: 30S ribosomal protein S20

Chain QT:



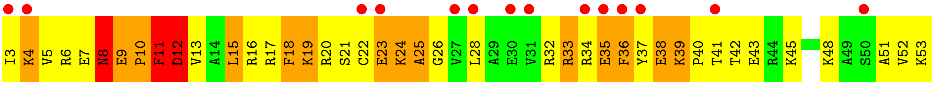
- Molecule 51: 30S ribosomal protein S20

Chain XT:



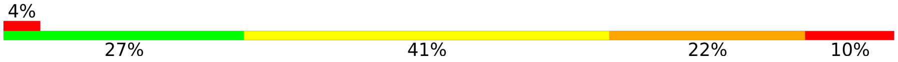
- Molecule 52: 30S ribosomal protein S21

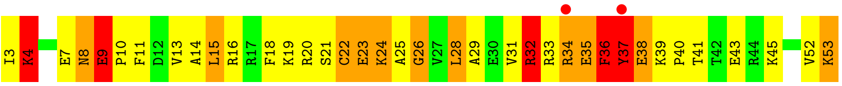
Chain QU:



- Molecule 52: 30S ribosomal protein S21

Chain XU:





4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.76Å 433.27Å 618.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.78 – 3.10 69.78 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.8 (69.78-3.10) 95.9 (69.78-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 3.13Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.200 , 0.252 0.210 , 0.259	Depositor DCC
R_{free} test set	19579 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	68.1	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 91.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	284464	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EM1, ZN, 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	RA	0.73	7/68626 (0.0%)	1.08	288/107056 (0.3%)
1	YA	0.38	0/68314	0.83	60/106569 (0.1%)
2	RB	0.64	0/2828	0.94	1/4410 (0.0%)
2	YB	0.30	0/2803	0.76	1/4371 (0.0%)
3	RC	0.47	0/2121	0.72	1/2852 (0.0%)
3	YC	0.32	0/2121	0.55	0/2852
4	RD	0.56	0/1586	0.80	1/2134 (0.0%)
4	YD	0.31	0/1586	0.57	0/2134
5	RE	0.43	0/1571	0.66	0/2113
5	YE	0.27	0/1571	0.51	0/2113
6	RF	0.32	0/1434	0.53	0/1926
6	YF	0.24	0/1444	0.50	0/1937
7	RG	0.40	0/1343	0.65	0/1816
7	YG	0.24	0/1343	0.50	0/1816
8	RH	0.32	0/1122	0.56	0/1515
8	YH	0.29	0/1122	0.52	0/1515
9	RI	0.23	0/1046	0.48	0/1410
9	YI	0.22	0/1046	0.47	0/1410
10	RJ	0.57	0/1152	0.82	1/1551 (0.1%)
10	YJ	0.29	0/1152	0.60	1/1551 (0.1%)
11	RK	0.54	0/947	0.80	0/1268
11	YK	0.34	0/947	0.58	0/1268
12	RL	0.44	0/1054	0.75	1/1403 (0.1%)
12	YL	0.28	0/1054	0.56	0/1403
13	RM	0.50	0/1093	0.71	0/1460
13	YM	0.29	0/1093	0.50	0/1460
14	RN	0.49	0/973	0.72	0/1301
14	YN	0.30	0/973	0.53	0/1301
15	RO	0.41	0/902	0.63	0/1209
15	YO	0.24	0/902	0.45	0/1209
16	RP	0.48	0/929	0.73	0/1242
16	YP	0.32	0/929	0.52	0/1242

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	RQ	0.58	0/960	0.75	0/1278
17	YQ	0.30	0/960	0.47	0/1278
18	RR	0.59	0/829	0.80	0/1107
18	YR	0.30	0/829	0.52	0/1107
19	RS	0.54	0/864	0.76	0/1156
19	YS	0.29	0/864	0.54	1/1156 (0.1%)
20	RT	0.47	0/744	0.72	0/994
20	YT	0.26	0/744	0.54	0/994
21	RU	0.43	0/787	0.68	0/1051
21	YU	0.26	0/787	0.51	0/1051
22	RV	0.42	0/766	0.61	0/1025
22	YV	0.24	0/766	0.44	0/1025
23	RW	0.67	1/603 (0.2%)	0.96	2/797 (0.3%)
23	YW	0.29	0/603	0.54	0/797
24	RX	0.44	0/635	0.69	0/848
24	YX	0.28	0/635	0.58	0/848
25	RY	0.35	0/510	0.61	0/677
25	YY	0.23	0/510	0.50	0/677
26	RZ	0.56	0/453	0.77	0/605
26	YZ	0.28	0/453	0.53	0/605
27	R0	0.45	0/450	0.74	0/599
27	Y0	0.30	0/450	0.52	0/599
28	R1	0.39	0/416	0.63	0/554
28	Y1	0.27	0/416	0.49	0/554
29	R2	0.52	0/380	0.76	0/498
29	Y2	0.30	0/380	0.54	0/498
30	R3	0.46	0/513	0.73	1/676 (0.1%)
30	Y3	0.29	0/513	0.56	0/676
31	R4	0.52	0/303	0.73	0/397
31	Y4	0.33	0/303	0.53	0/397
32	QA	0.43	0/36834	0.82	31/57462 (0.1%)
32	XA	0.39	0/36762	0.80	29/57350 (0.1%)
33	QB	0.30	0/1735	0.55	0/2338
33	XB	0.26	0/1735	0.49	0/2338
34	QC	0.30	0/1651	0.53	1/2225 (0.0%)
34	XC	0.26	0/1651	0.48	0/2225
35	QD	0.32	0/1665	0.54	0/2227
35	XD	0.40	0/1665	0.63	0/2227
36	QE	0.38	0/1118	0.63	0/1504
36	XE	0.35	0/1118	0.60	0/1504
37	QF	0.31	0/835	0.51	0/1128
37	XF	0.30	0/835	0.54	0/1128
38	QG	0.27	0/1195	0.47	0/1602

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\lvert Z\rvert >5$	RMSZ	$\#\lvert Z\rvert >5$
38	XG	0.25	0/1187	0.48	0/1591
39	QH	0.35	0/989	0.56	0/1326
39	XH	0.30	0/989	0.51	0/1326
40	QI	0.27	0/1034	0.51	0/1375
40	XI	0.26	0/1034	0.48	0/1375
41	QJ	0.30	0/796	0.52	0/1077
41	XJ	0.26	0/796	0.50	0/1077
42	QK	0.29	0/893	0.54	0/1205
42	XK	0.29	0/893	0.55	0/1205
43	QL	0.35	0/969	0.67	0/1300
43	XL	0.34	0/969	0.58	0/1300
44	QM	0.26	0/892	0.50	0/1193
44	XM	0.22	0/884	0.44	0/1181
45	QN	0.29	0/785	0.51	0/1043
45	XN	0.23	0/746	0.42	0/990
46	QO	0.31	0/722	0.49	0/964
46	XO	0.27	0/722	0.46	0/964
47	QP	0.29	0/659	0.51	0/884
47	XP	0.31	0/648	0.53	0/870
48	QQ	0.39	0/657	0.63	0/881
48	XQ	0.32	0/657	0.53	0/881
49	QR	0.30	0/462	0.52	0/621
49	XR	0.35	0/462	0.50	0/621
50	QS	0.26	0/652	0.48	0/877
50	XS	0.22	0/652	0.45	0/877
51	QT	0.38	0/671	0.58	0/888
51	XT	0.27	0/671	0.52	0/888
52	QU	0.33	0/430	0.50	0/570
52	XU	0.38	0/430	0.64	0/570
All	All	0.48	8/306703 (0.0%)	0.84	420/458519 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	RD	0	1
10	RJ	0	1
14	RN	0	1
30	R3	0	1
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	RA	984	A	N9-C4	-8.71	1.32	1.37
1	RA	1142	A	N9-C4	-8.61	1.32	1.37
1	RA	1936	A	N9-C4	-6.89	1.33	1.37
23	RW	32	ALA	CA-CB	5.66	1.64	1.52
1	RA	984	A	C5-C6	-5.54	1.36	1.41

The worst 5 of 420 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	RA	974	G	C5-N7-C8	-11.14	98.73	104.30
1	RA	1142	A	C2-N3-C4	-10.75	105.23	110.60
1	RA	974	G	N7-C8-N9	10.43	118.31	113.10
1	RA	1990	C	C6-N1-C2	10.42	124.47	120.30
1	RA	560	C	N3-C4-C5	10.30	126.02	121.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	R3	29	ARG	Peptide
4	RD	9	VAL	Peptide
10	RJ	110	PRO	Peptide
14	RN	101	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	61274	0	30819	1808	0
1	YA	60995	0	30679	3669	0
2	RB	2529	0	1281	57	0
2	YB	2507	0	1270	166	0
3	RC	2082	0	2157	207	0
3	YC	2082	0	2157	227	0
4	RD	1565	0	1616	201	0
4	YD	1565	0	1616	202	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	RE	1552	0	1619	151	0
5	YE	1552	0	1619	188	0
6	RF	1410	0	1447	128	0
6	YF	1420	0	1460	158	0
7	RG	1323	0	1374	138	0
7	YG	1323	0	1374	144	0
8	RH	1111	0	1148	97	0
8	YH	1111	0	1148	119	0
9	RI	1032	0	1088	108	0
9	YI	1032	0	1088	83	0
10	RJ	1129	0	1162	151	0
10	YJ	1129	0	1162	132	0
11	RK	938	0	1012	91	0
11	YK	938	0	1012	107	0
12	RL	1045	0	1117	110	0
12	YL	1045	0	1117	136	0
13	RM	1074	0	1157	94	0
13	YM	1074	0	1157	91	0
14	RN	960	0	1000	77	0
14	YN	960	0	1000	141	0
15	RO	892	0	923	50	0
15	YO	892	0	923	76	0
16	RP	917	0	965	122	0
16	YP	917	0	965	123	0
17	RQ	947	0	1022	139	0
17	YQ	947	0	1022	124	0
18	RR	816	0	839	102	0
18	YR	816	0	839	94	0
19	RS	857	0	922	83	0
19	YS	857	0	922	69	0
20	RT	738	0	807	107	0
20	YT	738	0	807	104	0
21	RU	779	0	834	61	0
21	YU	779	0	834	98	0
22	RV	753	0	780	47	0
22	YV	753	0	780	62	0
23	RW	596	0	610	191	0
23	YW	596	0	610	127	0
24	RX	625	0	655	53	0
24	YX	625	0	655	77	0
25	RY	509	0	543	40	0
25	YY	509	0	543	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	RZ	449	0	491	33	0
26	YZ	449	0	491	42	0
27	R0	444	0	461	29	0
27	Y0	444	0	461	54	0
28	R1	409	0	440	42	0
28	Y1	409	0	440	39	0
29	R2	377	0	418	25	0
29	Y2	377	0	418	52	0
30	R3	504	0	574	42	0
30	Y3	504	0	574	52	0
31	R4	302	0	340	29	0
31	Y4	302	0	342	22	0
32	QA	32895	0	16553	1244	0
32	XA	32831	0	16521	1591	0
33	QB	1704	0	1732	225	0
33	XB	1704	0	1732	160	0
34	QC	1624	0	1699	109	0
34	XC	1624	0	1699	125	0
35	QD	1643	0	1710	153	0
35	XD	1643	0	1710	156	0
36	QE	1105	0	1148	135	0
36	XE	1105	0	1148	106	0
37	QF	817	0	808	83	0
37	XF	817	0	808	85	0
38	QG	1181	0	1240	93	0
38	XG	1174	0	1230	130	0
39	QH	979	0	1034	86	0
39	XH	979	0	1034	97	0
40	QI	1022	0	1070	99	0
40	XI	1022	0	1070	127	0
41	QJ	786	0	828	93	0
41	XJ	786	0	828	96	0
42	QK	877	0	887	83	0
42	XK	877	0	887	74	0
43	QL	955	0	1019	88	0
43	XL	955	0	1019	86	0
44	QM	883	0	944	67	0
44	XM	876	0	937	106	0
45	QN	774	0	827	78	0
45	XN	735	0	790	97	0
46	QO	714	0	737	54	0
46	XO	714	0	737	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	QP	649	0	666	48	0
47	XP	638	0	656	51	0
48	QQ	648	0	691	89	0
48	XQ	648	0	691	56	0
49	QR	455	0	478	21	0
49	XR	455	0	478	39	0
50	QS	637	0	665	54	0
50	XS	637	0	665	87	0
51	QT	665	0	714	85	0
51	XT	665	0	714	40	0
52	QU	425	0	449	79	0
52	XU	425	0	449	76	0
53	QA	43	0	0	0	0
53	RA	135	0	0	0	0
53	RB	4	0	0	0	0
53	XA	42	0	0	0	0
53	YA	134	0	0	0	0
53	YB	1	0	0	0	0
53	YE	1	0	0	0	0
53	YJ	1	0	0	0	0
54	RA	60	0	65	4	0
55	R4	1	0	0	0	0
55	Y4	1	0	0	0	0
56	QA	200	0	0	4	0
56	QL	1	0	0	0	0
56	QN	5	0	0	1	0
56	QT	1	0	0	0	0
56	QU	1	0	0	0	0
56	R2	1	0	0	0	0
56	R3	2	0	0	0	0
56	R4	2	0	0	0	0
56	RA	606	0	0	39	0
56	RB	20	0	0	0	0
56	RC	9	0	0	0	0
56	RD	1	0	0	0	0
56	RL	4	0	0	0	0
56	RN	3	0	0	0	0
56	RT	2	0	0	0	0
56	XA	194	0	0	7	0
56	XE	5	0	0	1	0
56	XI	1	0	0	0	0
56	XL	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	XN	3	0	0	0	0
56	XT	2	0	0	0	0
56	XU	1	0	0	0	0
56	Y2	1	0	0	1	0
56	Y3	1	0	0	0	0
56	Y4	5	0	0	0	0
56	YA	605	0	0	35	0
56	YB	4	0	0	1	0
56	YC	8	0	0	0	0
56	YD	3	0	0	0	0
56	YE	3	0	0	0	0
56	YJ	3	0	0	0	0
56	YL	4	0	0	0	0
56	YN	1	0	0	0	0
56	YT	2	0	0	0	0
56	YU	2	0	0	0	0
56	YV	1	0	0	0	0
All	All	284464	0	190873	16435	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

The worst 5 of 16435 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)
17:RQ:63:ARG:NH1	17:RQ:96:ASP:HA	1.42	1.33
43:XL:43:LYS:HB3	43:XL:44:PRO:HD2	1.18	1.17
1:RA:1073:A:H3’	1:RA:1074:G:H5”	1.20	1.17
32:XA:120:A:C3’	32:XA:121:U:H5”	1.75	1.17
37:QF:16:GLU:HG2	35:XD:191:SER:HB2	1.20	1.17

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	RC	269/271 (99%)	198 (74%)	43 (16%)	28 (10%)	0	3
3	YC	269/271 (99%)	180 (67%)	60 (22%)	29 (11%)	0	2
4	RD	207/209 (99%)	147 (71%)	31 (15%)	29 (14%)	0	1
4	YD	207/209 (99%)	128 (62%)	45 (22%)	34 (16%)	0	0
5	RE	199/201 (99%)	146 (73%)	32 (16%)	21 (11%)	0	3
5	YE	199/201 (99%)	117 (59%)	55 (28%)	27 (14%)	0	1
6	RF	175/178 (98%)	138 (79%)	22 (13%)	15 (9%)	1	4
6	YF	176/178 (99%)	102 (58%)	42 (24%)	32 (18%)	0	0
7	RG	174/176 (99%)	121 (70%)	26 (15%)	27 (16%)	0	0
7	YG	174/176 (99%)	104 (60%)	36 (21%)	34 (20%)	0	0
8	RH	147/149 (99%)	64 (44%)	49 (33%)	34 (23%)	0	0
8	YH	147/149 (99%)	73 (50%)	59 (40%)	15 (10%)	0	3
9	RI	139/141 (99%)	84 (60%)	42 (30%)	13 (9%)	0	3
9	YI	139/141 (99%)	85 (61%)	37 (27%)	17 (12%)	0	1
10	RJ	140/142 (99%)	107 (76%)	19 (14%)	14 (10%)	0	3
10	YJ	140/142 (99%)	98 (70%)	28 (20%)	14 (10%)	0	3
11	RK	120/122 (98%)	87 (72%)	16 (13%)	17 (14%)	0	1
11	YK	120/122 (98%)	83 (69%)	20 (17%)	17 (14%)	0	1
12	RL	141/143 (99%)	98 (70%)	27 (19%)	16 (11%)	0	2
12	YL	141/143 (99%)	77 (55%)	45 (32%)	19 (14%)	0	1
13	RM	134/136 (98%)	97 (72%)	22 (16%)	15 (11%)	0	2
13	YM	134/136 (98%)	92 (69%)	28 (21%)	14 (10%)	0	3
14	RN	118/120 (98%)	96 (81%)	14 (12%)	8 (7%)	1	7
14	YN	118/120 (98%)	72 (61%)	30 (25%)	16 (14%)	0	1
15	RO	114/116 (98%)	89 (78%)	17 (15%)	8 (7%)	1	7
15	YO	114/116 (98%)	74 (65%)	29 (25%)	11 (10%)	0	3
16	RP	112/114 (98%)	78 (70%)	18 (16%)	16 (14%)	0	1
16	YP	112/114 (98%)	70 (62%)	25 (22%)	17 (15%)	0	0
17	RQ	115/117 (98%)	93 (81%)	17 (15%)	5 (4%)	2	16
17	YQ	115/117 (98%)	77 (67%)	27 (24%)	11 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	RR	101/103 (98%)	82 (81%)	11 (11%)	8 (8%)	1	5
18	YR	101/103 (98%)	66 (65%)	22 (22%)	13 (13%)	0	1
19	RS	108/110 (98%)	88 (82%)	10 (9%)	10 (9%)	0	3
19	YS	108/110 (98%)	75 (69%)	22 (20%)	11 (10%)	0	3
20	RT	91/93 (98%)	51 (56%)	25 (28%)	15 (16%)	0	0
20	YT	91/93 (98%)	42 (46%)	27 (30%)	22 (24%)	0	0
21	RU	100/102 (98%)	69 (69%)	16 (16%)	15 (15%)	0	0
21	YU	100/102 (98%)	53 (53%)	23 (23%)	24 (24%)	0	0
22	RV	92/94 (98%)	81 (88%)	9 (10%)	2 (2%)	6	29
22	YV	92/94 (98%)	61 (66%)	23 (25%)	8 (9%)	1	4
23	RW	77/79 (98%)	34 (44%)	16 (21%)	27 (35%)	0	0
23	YW	77/79 (98%)	30 (39%)	27 (35%)	20 (26%)	0	0
24	RX	75/77 (97%)	58 (77%)	14 (19%)	3 (4%)	3	17
24	YX	75/77 (97%)	45 (60%)	22 (29%)	8 (11%)	0	2
25	RY	61/63 (97%)	38 (62%)	15 (25%)	8 (13%)	0	1
25	YY	61/63 (97%)	37 (61%)	20 (33%)	4 (7%)	1	7
26	RZ	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	3	20
26	YZ	56/58 (97%)	34 (61%)	16 (29%)	6 (11%)	0	2
27	R0	54/56 (96%)	42 (78%)	9 (17%)	3 (6%)	2	11
27	Y0	54/56 (96%)	38 (70%)	7 (13%)	9 (17%)	0	0
28	R1	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	1	5
28	Y1	48/50 (96%)	33 (69%)	10 (21%)	5 (10%)	0	3
29	R2	44/46 (96%)	37 (84%)	5 (11%)	2 (4%)	2	15
29	Y2	44/46 (96%)	29 (66%)	9 (20%)	6 (14%)	0	1
30	R3	62/64 (97%)	50 (81%)	8 (13%)	4 (6%)	1	8
30	Y3	62/64 (97%)	43 (69%)	13 (21%)	6 (10%)	0	3
31	R4	36/38 (95%)	29 (81%)	5 (14%)	2 (6%)	2	11
31	Y4	36/38 (95%)	22 (61%)	8 (22%)	6 (17%)	0	0
33	QB	216/218 (99%)	129 (60%)	51 (24%)	36 (17%)	0	0
33	XB	216/218 (99%)	146 (68%)	49 (23%)	21 (10%)	0	3
34	QC	204/206 (99%)	159 (78%)	26 (13%)	19 (9%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	XC	204/206 (99%)	137 (67%)	44 (22%)	23 (11%)	0	2
35	QD	203/205 (99%)	135 (66%)	39 (19%)	29 (14%)	0	1
35	XD	203/205 (99%)	141 (70%)	44 (22%)	18 (9%)	1	4
36	QE	148/150 (99%)	108 (73%)	25 (17%)	15 (10%)	0	3
36	XE	148/150 (99%)	110 (74%)	24 (16%)	14 (10%)	0	3
37	QF	98/100 (98%)	62 (63%)	28 (29%)	8 (8%)	1	5
37	XF	98/100 (98%)	59 (60%)	28 (29%)	11 (11%)	0	2
38	QG	149/151 (99%)	108 (72%)	33 (22%)	8 (5%)	2	12
38	XG	148/151 (98%)	86 (58%)	46 (31%)	16 (11%)	0	2
39	QH	127/129 (98%)	95 (75%)	25 (20%)	7 (6%)	2	11
39	XH	127/129 (98%)	92 (72%)	25 (20%)	10 (8%)	1	5
40	QI	125/127 (98%)	88 (70%)	25 (20%)	12 (10%)	0	3
40	XI	125/127 (98%)	91 (73%)	25 (20%)	9 (7%)	1	6
41	QJ	96/98 (98%)	64 (67%)	17 (18%)	15 (16%)	0	0
41	XJ	96/98 (98%)	61 (64%)	22 (23%)	13 (14%)	0	1
42	QK	115/117 (98%)	83 (72%)	22 (19%)	10 (9%)	1	4
42	XK	115/117 (98%)	87 (76%)	18 (16%)	10 (9%)	1	4
43	QL	121/123 (98%)	87 (72%)	23 (19%)	11 (9%)	1	4
43	XL	121/123 (98%)	90 (74%)	22 (18%)	9 (7%)	1	6
44	QM	112/114 (98%)	83 (74%)	20 (18%)	9 (8%)	1	5
44	XM	111/114 (97%)	64 (58%)	33 (30%)	14 (13%)	0	1
45	QN	92/101 (91%)	57 (62%)	25 (27%)	10 (11%)	0	2
45	XN	87/101 (86%)	58 (67%)	18 (21%)	11 (13%)	0	1
46	QO	86/88 (98%)	55 (64%)	26 (30%)	5 (6%)	1	10
46	XO	86/88 (98%)	64 (74%)	18 (21%)	4 (5%)	2	14
47	QP	80/82 (98%)	55 (69%)	17 (21%)	8 (10%)	0	3
47	XP	78/82 (95%)	52 (67%)	18 (23%)	8 (10%)	0	3
48	QQ	78/80 (98%)	55 (70%)	11 (14%)	12 (15%)	0	0
48	XQ	78/80 (98%)	63 (81%)	6 (8%)	9 (12%)	0	2
49	QR	53/55 (96%)	41 (77%)	10 (19%)	2 (4%)	3	19
49	XR	53/55 (96%)	37 (70%)	15 (28%)	1 (2%)	8	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	QS	77/79 (98%)	57 (74%)	14 (18%)	6 (8%)	1	5
50	XS	77/79 (98%)	47 (61%)	25 (32%)	5 (6%)	1	8
51	QT	83/85 (98%)	61 (74%)	16 (19%)	6 (7%)	1	6
51	XT	83/85 (98%)	59 (71%)	18 (22%)	6 (7%)	1	6
52	QU	49/51 (96%)	25 (51%)	14 (29%)	10 (20%)	0	0
52	XU	49/51 (96%)	21 (43%)	12 (24%)	16 (33%)	0	0
All	All	11234/11454 (98%)	7596 (68%)	2346 (21%)	1292 (12%)	0	2

5 of 1292 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	RC	104	LEU
3	RC	121	ALA
3	RC	200	MET
3	RC	239	PHE
3	RC	243	PRO

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	
3	RC	216/216 (100%)	164 (76%)	52 (24%)	0	2
3	YC	216/216 (100%)	181 (84%)	35 (16%)	2	10
4	RD	164/164 (100%)	138 (84%)	26 (16%)	2	11
4	YD	164/164 (100%)	142 (87%)	22 (13%)	4	16
5	RE	165/165 (100%)	126 (76%)	39 (24%)	1	2
5	YE	165/165 (100%)	140 (85%)	25 (15%)	3	12
6	RF	148/149 (99%)	121 (82%)	27 (18%)	1	7
6	YF	149/149 (100%)	120 (80%)	29 (20%)	1	6
7	RG	137/137 (100%)	108 (79%)	29 (21%)	1	5
7	YG	137/137 (100%)	119 (87%)	18 (13%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	RH	114/114 (100%)	93 (82%)	21 (18%)	1	7
8	YH	114/114 (100%)	91 (80%)	23 (20%)	1	5
9	RI	109/109 (100%)	89 (82%)	20 (18%)	1	7
9	YI	109/109 (100%)	102 (94%)	7 (6%)	17	48
10	RJ	116/116 (100%)	86 (74%)	30 (26%)	0	1
10	YJ	116/116 (100%)	99 (85%)	17 (15%)	3	13
11	RK	103/103 (100%)	81 (79%)	22 (21%)	1	4
11	YK	103/103 (100%)	84 (82%)	19 (18%)	1	7
12	RL	102/102 (100%)	80 (78%)	22 (22%)	1	4
12	YL	102/102 (100%)	85 (83%)	17 (17%)	2	9
13	RM	109/109 (100%)	89 (82%)	20 (18%)	1	7
13	YM	109/109 (100%)	98 (90%)	11 (10%)	7	28
14	RN	100/100 (100%)	82 (82%)	18 (18%)	1	7
14	YN	100/100 (100%)	85 (85%)	15 (15%)	3	12
15	RO	86/86 (100%)	67 (78%)	19 (22%)	1	4
15	YO	86/86 (100%)	79 (92%)	7 (8%)	11	39
16	RP	99/99 (100%)	76 (77%)	23 (23%)	1	3
16	YP	99/99 (100%)	89 (90%)	10 (10%)	7	28
17	RQ	89/89 (100%)	69 (78%)	20 (22%)	1	3
17	YQ	89/89 (100%)	75 (84%)	14 (16%)	2	11
18	RR	84/84 (100%)	70 (83%)	14 (17%)	2	9
18	YR	84/84 (100%)	67 (80%)	17 (20%)	1	5
19	RS	93/93 (100%)	70 (75%)	23 (25%)	0	2
19	YS	93/93 (100%)	73 (78%)	20 (22%)	1	4
20	RT	80/80 (100%)	62 (78%)	18 (22%)	1	3
20	YT	80/80 (100%)	71 (89%)	9 (11%)	6	23
21	RU	83/83 (100%)	63 (76%)	20 (24%)	0	2
21	YU	83/83 (100%)	68 (82%)	15 (18%)	1	7
22	RV	78/78 (100%)	62 (80%)	16 (20%)	1	5
22	YV	78/78 (100%)	67 (86%)	11 (14%)	3	15
23	RW	59/59 (100%)	37 (63%)	22 (37%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	YW	59/59 (100%)	41 (70%)	18 (30%)	0	0
24	RX	67/67 (100%)	50 (75%)	17 (25%)	0	1
24	YX	67/67 (100%)	52 (78%)	15 (22%)	1	3
25	RY	55/55 (100%)	44 (80%)	11 (20%)	1	5
25	YY	55/55 (100%)	51 (93%)	4 (7%)	14	43
26	RZ	48/48 (100%)	33 (69%)	15 (31%)	0	0
26	YZ	48/48 (100%)	37 (77%)	11 (23%)	1	3
27	R0	47/47 (100%)	38 (81%)	9 (19%)	1	6
27	Y0	47/47 (100%)	34 (72%)	13 (28%)	0	1
28	R1	45/45 (100%)	34 (76%)	11 (24%)	0	2
28	Y1	45/45 (100%)	41 (91%)	4 (9%)	9	34
29	R2	38/38 (100%)	30 (79%)	8 (21%)	1	5
29	Y2	38/38 (100%)	32 (84%)	6 (16%)	2	11
30	R3	51/51 (100%)	42 (82%)	9 (18%)	2	8
30	Y3	51/51 (100%)	38 (74%)	13 (26%)	0	1
31	R4	34/34 (100%)	30 (88%)	4 (12%)	5	21
31	Y4	34/34 (100%)	27 (79%)	7 (21%)	1	5
33	QB	180/180 (100%)	138 (77%)	42 (23%)	1	3
33	XB	180/180 (100%)	148 (82%)	32 (18%)	2	8
34	QC	170/170 (100%)	142 (84%)	28 (16%)	2	10
34	XC	170/170 (100%)	148 (87%)	22 (13%)	4	18
35	QD	172/172 (100%)	142 (83%)	30 (17%)	2	9
35	XD	172/172 (100%)	133 (77%)	39 (23%)	1	3
36	QE	113/113 (100%)	86 (76%)	27 (24%)	0	2
36	XE	113/113 (100%)	89 (79%)	24 (21%)	1	5
37	QF	87/87 (100%)	71 (82%)	16 (18%)	1	7
37	XF	87/87 (100%)	69 (79%)	18 (21%)	1	5
38	QG	124/124 (100%)	105 (85%)	19 (15%)	2	12
38	XG	123/124 (99%)	94 (76%)	29 (24%)	1	2
39	QH	104/104 (100%)	85 (82%)	19 (18%)	1	7
39	XH	104/104 (100%)	84 (81%)	20 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	QI	105/105 (100%)	82 (78%)	23 (22%)	1	4
40	XI	105/105 (100%)	82 (78%)	23 (22%)	1	4
41	QJ	86/86 (100%)	69 (80%)	17 (20%)	1	5
41	XJ	86/86 (100%)	70 (81%)	16 (19%)	1	7
42	QK	90/90 (100%)	73 (81%)	17 (19%)	1	6
42	XK	90/90 (100%)	76 (84%)	14 (16%)	2	11
43	QL	103/103 (100%)	85 (82%)	18 (18%)	2	8
43	XL	103/103 (100%)	84 (82%)	19 (18%)	1	7
44	QM	92/92 (100%)	85 (92%)	7 (8%)	13	41
44	XM	91/92 (99%)	81 (89%)	10 (11%)	6	25
45	QN	79/84 (94%)	74 (94%)	5 (6%)	18	48
45	XN	75/84 (89%)	64 (85%)	11 (15%)	3	13
46	QO	76/76 (100%)	66 (87%)	10 (13%)	4	17
46	XO	76/76 (100%)	69 (91%)	7 (9%)	9	33
47	QP	65/65 (100%)	55 (85%)	10 (15%)	2	11
47	XP	65/65 (100%)	51 (78%)	14 (22%)	1	4
48	QQ	74/74 (100%)	57 (77%)	17 (23%)	1	3
48	XQ	74/74 (100%)	57 (77%)	17 (23%)	1	3
49	QR	48/48 (100%)	44 (92%)	4 (8%)	11	38
49	XR	48/48 (100%)	42 (88%)	6 (12%)	4	18
50	QS	70/70 (100%)	61 (87%)	9 (13%)	4	18
50	XS	70/70 (100%)	60 (86%)	10 (14%)	3	14
51	QT	65/65 (100%)	48 (74%)	17 (26%)	0	1
51	XT	65/65 (100%)	48 (74%)	17 (26%)	0	1
52	QU	44/44 (100%)	32 (73%)	12 (27%)	0	1
52	XU	44/44 (100%)	36 (82%)	8 (18%)	1	7
All	All	9327/9344 (100%)	7607 (82%)	1720 (18%)	1	7

5 of 1720 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	QU	18	PHE
41	XJ	64	GLN

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Mol	Chain	Res	Type
20	YT	50	LEU
33	XB	124	THR
52	QU	15	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 309 such sidechains are listed below:

Mol	Chain	Res	Type
3	YC	59	GLN
19	YS	31	GLN
4	YD	36	GLN
11	YK	89	ASN
25	YY	15	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2850/2904 (98%)	547 (19%)	74 (2%)
1	YA	2837/2904 (97%)	870 (30%)	153 (5%)
2	RB	117/118 (99%)	22 (18%)	0
2	YB	116/118 (98%)	31 (26%)	6 (5%)
32	QA	1532/1533 (99%)	372 (24%)	56 (3%)
32	XA	1529/1533 (99%)	442 (28%)	70 (4%)
All	All	8981/9110 (98%)	2284 (25%)	359 (3%)

5 of 2284 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	RA	10	A
1	RA	12	U
1	RA	13	A
1	RA	14	A
1	RA	15	G

5 of 359 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	YA	454	A
1	YA	1537	G
1	YA	575	A
1	YA	1023	U

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Mol	Chain	Res	Type
1	YA	1775	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 364 ligands modelled in this entry, 363 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
54	EM1	RA	3135	-	58,64,64	1.85	13 (22%)	71,97,97	2.91	23 (32%)

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
54	EM1	RA	3135	-	-	10/71/112/112	0/4/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	RA	3135	EM1	C21-C15	-5.52	1.49	1.53
54	RA	3135	EM1	N81-N80	-4.50	1.25	1.34
54	RA	3135	EM1	N82-N81	-4.46	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	RA	3135	EM1	O5-C2	-4.02	1.41	1.47
54	RA	3135	EM1	C77-C72	-3.77	1.32	1.39

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	RA	3135	EM1	C8-C4-C2	-11.37	99.56	115.23
54	RA	3135	EM1	N82-N81-N80	9.48	114.46	107.31
54	RA	3135	EM1	C72-C77-C76	-8.31	115.50	121.11
54	RA	3135	EM1	O20-C15-C21	-5.88	117.22	123.51
54	RA	3135	EM1	C2-O5-C10	-4.91	105.41	109.29

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	RA	3135	EM1	O9-C4-C8-C14
54	RA	3135	EM1	C21-C15-O9-C4
54	RA	3135	EM1	O9-C15-C21-C26
54	RA	3135	EM1	O20-C15-C21-C26
54	RA	3135	EM1	O20-C15-O9-C4

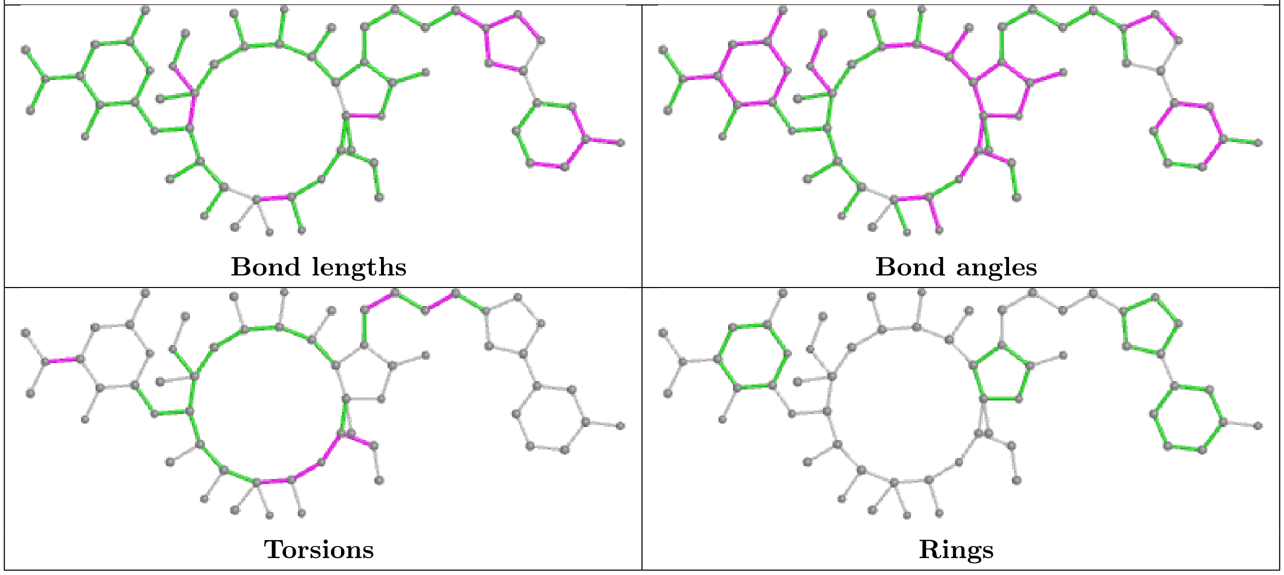
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	RA	3135	EM1	4	0

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

Ligand EM1 RA 3135



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	RA	2854/2904 (98%)	-0.43	41 (1%)	75	56	19, 47, 175, 400	0
1	YA	2841/2904 (97%)	0.15	90 (3%)	47	25	64, 140, 260, 408	0
2	RB	118/118 (100%)	-0.63	0	100	100	32, 61, 95, 115	0
2	YB	117/118 (99%)	-0.18	0	100	100	111, 185, 242, 277	0
3	RC	271/271 (100%)	-0.25	10 (3%)	41	21	25, 57, 97, 202	0
3	YC	271/271 (100%)	0.43	19 (7%)	16	7	64, 107, 154, 181	0
4	RD	209/209 (100%)	-0.36	0	100	100	19, 41, 90, 149	0
4	YD	209/209 (100%)	0.83	26 (12%)	4	1	71, 122, 174, 236	0
5	RE	201/201 (100%)	-0.24	0	100	100	23, 58, 116, 177	0
5	YE	201/201 (100%)	1.85	76 (37%)	0	0	91, 214, 335, 378	0
6	RF	177/178 (99%)	0.22	13 (7%)	15	6	52, 93, 166, 225	0
6	YF	178/178 (100%)	2.02	80 (44%)	0	0	154, 229, 270, 299	0
7	RG	176/176 (100%)	-0.05	0	100	100	41, 75, 129, 161	0
7	YG	176/176 (100%)	1.88	64 (36%)	0	0	129, 198, 270, 312	0
8	RH	149/149 (100%)	2.56	60 (40%)	0	0	59, 178, 260, 278	0
8	YH	149/149 (100%)	2.43	63 (42%)	0	0	100, 197, 252, 272	0
9	RI	141/141 (100%)	3.30	84 (59%)	0	0	149, 241, 292, 339	0
9	YI	141/141 (100%)	4.31	102 (72%)	0	0	231, 317, 353, 360	0
10	RJ	142/142 (100%)	-0.48	1 (0%)	87	75	21, 40, 76, 139	0
10	YJ	142/142 (100%)	0.47	14 (9%)	7	2	75, 126, 168, 193	0
11	RK	122/122 (100%)	-0.36	1 (0%)	86	72	23, 45, 94, 191	0
11	YK	122/122 (100%)	0.55	12 (9%)	7	2	66, 107, 155, 228	0
12	RL	143/143 (100%)	-0.42	0	100	100	18, 55, 93, 123	0
12	YL	143/143 (100%)	1.37	40 (27%)	0	0	86, 169, 242, 284	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	RM	136/136 (100%)	-0.43	0	100	100	17, 45, 85, 146	0
13	YM	136/136 (100%)	1.04	23 (16%)	1	0	78, 131, 175, 208	0
14	RN	120/120 (100%)	-0.46	0	100	100	18, 41, 63, 132	0
14	YN	120/120 (100%)	0.89	16 (13%)	3	1	88, 136, 190, 237	0
15	RO	116/116 (100%)	-0.23	0	100	100	40, 64, 97, 124	0
15	YO	116/116 (100%)	1.88	44 (37%)	0	0	134, 182, 227, 252	0
16	RP	114/114 (100%)	-0.33	0	100	100	29, 53, 104, 149	0
16	YP	114/114 (100%)	0.65	13 (11%)	5	2	82, 121, 160, 197	0
17	RQ	117/117 (100%)	-0.54	0	100	100	19, 34, 63, 108	0
17	YQ	117/117 (100%)	1.17	28 (23%)	0	0	88, 126, 203, 287	0
18	RR	103/103 (100%)	-0.42	1 (0%)	82	67	20, 48, 92, 115	0
18	YR	103/103 (100%)	2.09	43 (41%)	0	0	98, 154, 219, 274	0
19	RS	110/110 (100%)	-0.42	1 (0%)	84	69	20, 38, 83, 143	0
19	YS	110/110 (100%)	1.55	35 (31%)	0	0	86, 141, 208, 266	0
20	RT	93/93 (100%)	0.34	7 (7%)	14	5	35, 69, 134, 207	0
20	YT	93/93 (100%)	2.30	45 (48%)	0	0	133, 215, 282, 315	0
21	RU	102/102 (100%)	0.02	2 (1%)	65	44	38, 72, 160, 192	0
21	YU	102/102 (100%)	3.27	63 (61%)	0	0	151, 251, 347, 416	0
22	RV	94/94 (100%)	-0.21	0	100	100	31, 61, 102, 114	0
22	YV	94/94 (100%)	1.08	21 (22%)	0	0	107, 157, 199, 222	0
23	RW	79/79 (100%)	0.10	5 (6%)	20	8	22, 53, 114, 195	0
23	YW	79/79 (100%)	2.25	40 (50%)	0	0	108, 163, 232, 250	0
24	RX	77/77 (100%)	-0.16	0	100	100	32, 58, 110, 124	0
24	YX	77/77 (100%)	0.84	8 (10%)	6	2	88, 134, 182, 237	0
25	RY	63/63 (100%)	0.23	3 (4%)	30	14	53, 90, 153, 175	0
25	YY	63/63 (100%)	1.45	16 (25%)	0	0	167, 286, 366, 383	0
26	RZ	58/58 (100%)	-0.36	0	100	100	19, 40, 87, 117	0
26	YZ	58/58 (100%)	1.02	13 (22%)	0	0	104, 143, 200, 247	0
27	R0	56/56 (100%)	-0.51	0	100	100	17, 42, 85, 150	0
27	Y0	56/56 (100%)	1.20	14 (25%)	0	0	87, 161, 210, 255	0
28	R1	50/50 (100%)	0.23	1 (2%)	65	44	45, 65, 111, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	Y1	50/50 (100%)	1.57	16 (32%) 0 0	106, 161, 203, 255	0
29	R2	46/46 (100%)	-0.38	1 (2%) 62 41	30, 42, 69, 166	0
29	Y2	46/46 (100%)	1.09	8 (17%) 1 0	95, 128, 162, 176	0
30	R3	64/64 (100%)	-0.45	0 100 100	25, 44, 64, 91	0
30	Y3	64/64 (100%)	1.76	20 (31%) 0 0	96, 140, 173, 212	0
31	R4	38/38 (100%)	0.06	0 100 100	40, 58, 98, 108	0
31	Y4	38/38 (100%)	2.50	19 (50%) 0 0	94, 155, 195, 203	0
32	QA	1533/1533 (100%)	-0.46	19 (1%) 79 61	46, 97, 198, 345	0
32	XA	1530/1533 (99%)	-0.17	33 (2%) 62 41	55, 113, 259, 356	0
33	QB	218/218 (100%)	0.84	32 (14%) 2 1	82, 141, 198, 243	0
33	XB	218/218 (100%)	1.19	52 (23%) 0 0	93, 145, 201, 251	0
34	QC	206/206 (100%)	0.11	4 (1%) 66 46	71, 107, 156, 198	0
34	XC	206/206 (100%)	0.47	11 (5%) 26 12	86, 136, 185, 215	0
35	QD	205/205 (100%)	0.33	12 (5%) 22 10	57, 114, 174, 236	0
35	XD	205/205 (100%)	-0.20	1 (0%) 91 81	41, 78, 132, 212	0
36	QE	150/150 (100%)	-0.13	2 (1%) 77 59	59, 90, 147, 217	0
36	XE	150/150 (100%)	-0.19	1 (0%) 87 75	55, 92, 141, 191	0
37	QF	100/100 (100%)	0.03	1 (1%) 82 67	80, 126, 168, 190	0
37	XF	100/100 (100%)	0.14	3 (3%) 50 27	82, 119, 176, 211	0
38	QG	151/151 (100%)	0.33	9 (5%) 21 10	98, 138, 186, 203	0
38	XG	150/151 (99%)	1.68	56 (37%) 0 0	121, 195, 245, 277	0
39	QH	129/129 (100%)	0.22	5 (3%) 39 20	62, 101, 142, 189	0
39	XH	129/129 (100%)	0.10	5 (3%) 39 20	77, 115, 152, 209	0
40	QI	127/127 (100%)	0.93	22 (17%) 1 0	82, 137, 209, 250	0
40	XI	127/127 (100%)	1.19	24 (18%) 1 0	114, 158, 225, 259	0
41	QJ	98/98 (100%)	0.40	9 (9%) 9 3	71, 121, 175, 200	0
41	XJ	98/98 (100%)	1.57	30 (30%) 0 0	117, 166, 211, 238	0
42	QK	117/117 (100%)	0.85	12 (10%) 6 2	54, 123, 177, 206	0
42	XK	117/117 (100%)	0.02	2 (1%) 70 49	67, 115, 162, 186	0
43	QL	123/123 (100%)	0.05	2 (1%) 72 51	50, 79, 123, 189	0
43	XL	123/123 (100%)	0.26	3 (2%) 59 37	61, 89, 142, 202	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	QM	114/114 (100%)	0.34	8 (7%)	16	7	94, 142, 198, 217	0
44	XM	113/114 (99%)	2.49	58 (51%)	0	0	218, 370, 442, 470	0
45	QN	96/101 (95%)	0.45	6 (6%)	20	8	80, 116, 187, 224	0
45	XN	91/101 (90%)	1.46	26 (28%)	0	0	107, 180, 260, 287	0
46	QO	88/88 (100%)	0.05	2 (2%)	60	39	64, 102, 139, 188	0
46	XO	88/88 (100%)	-0.12	1 (1%)	80	64	76, 116, 160, 209	0
47	QP	82/82 (100%)	0.84	11 (13%)	3	1	78, 99, 166, 223	0
47	XP	80/82 (97%)	0.78	8 (10%)	7	2	72, 107, 158, 222	0
48	QQ	80/80 (100%)	0.65	6 (7%)	14	5	62, 96, 136, 164	0
48	XQ	80/80 (100%)	1.17	13 (16%)	1	1	78, 115, 144, 155	0
49	QR	55/55 (100%)	0.50	3 (5%)	25	11	90, 110, 168, 218	0
49	XR	55/55 (100%)	0.07	2 (3%)	42	22	74, 103, 171, 243	0
50	QS	79/79 (100%)	1.06	17 (21%)	0	0	110, 143, 197, 208	0
50	XS	79/79 (100%)	3.78	52 (65%)	0	0	205, 346, 411, 424	0
51	QT	85/85 (100%)	0.35	2 (2%)	59	37	74, 103, 147, 179	0
51	XT	85/85 (100%)	1.04	11 (12%)	3	1	91, 134, 190, 216	0
52	QU	51/51 (100%)	1.11	14 (27%)	0	0	96, 139, 187, 225	0
52	XU	51/51 (100%)	0.21	2 (3%)	39	20	83, 120, 184, 224	0
All	All	20427/20564 (99%)	0.31	1894 (9%)	8	3	17, 111, 252, 470	0

The worst 5 of 1894 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	YH	91	PHE	19.3
9	RI	52	LEU	17.1
8	RH	92	GLY	16.3
9	YI	57	VAL	16.2
6	YF	129	MET	16.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
53	MG	YA	3108	1/1	-0.03	0.81	217,217,217,217	0
53	MG	YA	3049	1/1	-0.02	0.45	243,243,243,243	0
53	MG	YJ	201	1/1	0.21	2.54	319,319,319,319	0
53	MG	XA	1636	1/1	0.27	0.37	224,224,224,224	0
53	MG	YA	3120	1/1	0.33	0.21	124,124,124,124	0
53	MG	YA	3109	1/1	0.37	1.54	227,227,227,227	0
53	MG	YA	3003	1/1	0.40	1.59	238,238,238,238	0
53	MG	YA	3002	1/1	0.43	0.53	231,231,231,231	0
53	MG	YA	3019	1/1	0.48	0.66	278,278,278,278	0
53	MG	XA	1617	1/1	0.49	0.12	202,202,202,202	0
53	MG	YA	3091	1/1	0.51	0.21	184,184,184,184	0
53	MG	YA	3125	1/1	0.52	0.36	200,200,200,200	0
53	MG	YA	3129	1/1	0.53	0.74	261,261,261,261	0
53	MG	QA	1627	1/1	0.54	0.16	132,132,132,132	0
53	MG	YA	3006	1/1	0.55	0.10	237,237,237,237	0
53	MG	YA	3087	1/1	0.57	0.10	199,199,199,199	0
53	MG	XA	1622	1/1	0.58	0.09	187,187,187,187	0
53	MG	YA	3063	1/1	0.58	1.61	273,273,273,273	0
53	MG	YA	3076	1/1	0.60	0.19	195,195,195,195	0
53	MG	YA	3023	1/1	0.62	0.09	130,130,130,130	0
53	MG	YA	3133	1/1	0.63	0.30	220,220,220,220	0
53	MG	YA	3078	1/1	0.65	0.26	214,214,214,214	0
53	MG	QA	1619	1/1	0.66	0.54	230,230,230,230	0
53	MG	YA	3005	1/1	0.66	0.86	282,282,282,282	0
53	MG	YA	3057	1/1	0.67	0.30	205,205,205,205	0
53	MG	YA	3028	1/1	0.67	0.33	222,222,222,222	0
53	MG	YA	3127	1/1	0.67	1.29	248,248,248,248	0
53	MG	RA	3058	1/1	0.68	0.22	100,100,100,100	0
53	MG	YA	3073	1/1	0.68	0.18	193,193,193,193	0
53	MG	YA	3130	1/1	0.69	1.80	271,271,271,271	0
53	MG	QA	1637	1/1	0.69	0.15	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
53	MG	YA	3062	1/1	0.69	0.55	190,190,190,190	0
53	MG	RA	3047	1/1	0.70	0.13	122,122,122,122	0
53	MG	YA	3085	1/1	0.71	0.23	158,158,158,158	0
53	MG	YA	3074	1/1	0.71	0.56	260,260,260,260	0
53	MG	YA	3033	1/1	0.71	0.30	151,151,151,151	0
53	MG	RA	3129	1/1	0.71	1.07	285,285,285,285	0
53	MG	YA	3064	1/1	0.72	0.88	256,256,256,256	0
53	MG	YA	3045	1/1	0.72	0.22	206,206,206,206	0
53	MG	YA	3097	1/1	0.72	0.21	159,159,159,159	0
53	MG	YA	3122	1/1	0.73	0.15	104,104,104,104	0
53	MG	QA	1602	1/1	0.74	0.12	177,177,177,177	0
53	MG	XA	1619	1/1	0.74	0.12	212,212,212,212	0
53	MG	RA	3134	1/1	0.74	0.27	210,210,210,210	0
53	MG	YA	3059	1/1	0.74	0.18	232,232,232,232	0
53	MG	XA	1614	1/1	0.74	0.64	236,236,236,236	0
53	MG	RA	3054	1/1	0.76	0.36	198,198,198,198	0
53	MG	YA	3008	1/1	0.77	0.24	147,147,147,147	0
53	MG	XA	1602	1/1	0.77	0.13	139,139,139,139	0
53	MG	YA	3031	1/1	0.77	0.21	80,80,80,80	0
53	MG	YA	3110	1/1	0.77	0.07	120,120,120,120	0
53	MG	XA	1634	1/1	0.78	0.13	165,165,165,165	0
53	MG	RA	3068	1/1	0.78	0.12	175,175,175,175	0
53	MG	YA	3017	1/1	0.79	0.13	185,185,185,185	0
53	MG	YA	3088	1/1	0.79	0.35	222,222,222,222	0
53	MG	YA	3036	1/1	0.79	0.16	205,205,205,205	0
53	MG	YA	3083	1/1	0.79	0.10	214,214,214,214	0
53	MG	YA	3039	1/1	0.79	0.19	105,105,105,105	0
53	MG	XA	1629	1/1	0.80	0.15	190,190,190,190	0
53	MG	XA	1616	1/1	0.80	0.62	195,195,195,195	0
53	MG	YA	3123	1/1	0.80	0.36	217,217,217,217	0
53	MG	YA	3050	1/1	0.80	0.16	154,154,154,154	0
53	MG	RA	3089	1/1	0.80	0.16	127,127,127,127	0
53	MG	YA	3101	1/1	0.80	0.20	96,96,96,96	0
53	MG	YA	3010	1/1	0.80	1.07	272,272,272,272	0
53	MG	XA	1610	1/1	0.80	0.13	168,168,168,168	0
53	MG	RB	202	1/1	0.80	0.11	82,82,82,82	0
53	MG	RA	3096	1/1	0.81	0.18	169,169,169,169	0
53	MG	RA	3069	1/1	0.81	0.24	197,197,197,197	0
53	MG	RA	3024	1/1	0.81	0.47	210,210,210,210	0
53	MG	XA	1620	1/1	0.82	0.19	182,182,182,182	0
53	MG	RA	3011	1/1	0.82	0.18	129,129,129,129	0
53	MG	RA	3060	1/1	0.82	0.47	236,236,236,236	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
53	MG	YA	3082	1/1	0.82	0.19	164,164,164,164	0
53	MG	RA	3086	1/1	0.82	0.09	151,151,151,151	0
53	MG	YA	3084	1/1	0.82	0.16	168,168,168,168	0
53	MG	XA	1624	1/1	0.83	0.37	146,146,146,146	0
53	MG	YA	3038	1/1	0.83	0.07	234,234,234,234	0
53	MG	YA	3079	1/1	0.83	0.79	225,225,225,225	0
53	MG	YA	3007	1/1	0.83	0.45	232,232,232,232	0
53	MG	RA	3082	1/1	0.83	0.14	86,86,86,86	0
53	MG	YA	3047	1/1	0.83	0.18	174,174,174,174	0
53	MG	RA	3085	1/1	0.83	0.17	133,133,133,133	0
53	MG	XA	1635	1/1	0.83	0.11	76,76,76,76	0
53	MG	RA	3090	1/1	0.84	0.17	135,135,135,135	0
53	MG	YA	3128	1/1	0.84	0.81	163,163,163,163	0
53	MG	XA	1632	1/1	0.84	0.10	122,122,122,122	0
53	MG	YA	3106	1/1	0.84	0.17	218,218,218,218	0
53	MG	QA	1610	1/1	0.84	0.11	197,197,197,197	0
53	MG	YE	301	1/1	0.84	0.29	199,199,199,199	0
53	MG	YA	3071	1/1	0.84	0.20	102,102,102,102	0
53	MG	YA	3043	1/1	0.85	0.23	155,155,155,155	0
53	MG	YA	3098	1/1	0.85	0.21	183,183,183,183	0
53	MG	QA	1632	1/1	0.85	0.15	85,85,85,85	0
53	MG	YA	3020	1/1	0.85	0.21	53,53,53,53	0
53	MG	YA	3060	1/1	0.85	0.76	235,235,235,235	0
53	MG	RA	3020	1/1	0.85	0.37	200,200,200,200	0
53	MG	RA	3056	1/1	0.86	0.12	148,148,148,148	0
53	MG	RA	3004	1/1	0.86	0.19	184,184,184,184	0
53	MG	XA	1601	1/1	0.86	0.08	106,106,106,106	0
53	MG	YA	3026	1/1	0.86	0.77	242,242,242,242	0
53	MG	YA	3072	1/1	0.86	0.12	183,183,183,183	0
53	MG	YA	3004	1/1	0.86	0.17	134,134,134,134	0
53	MG	QA	1630	1/1	0.86	0.14	196,196,196,196	0
53	MG	QA	1641	1/1	0.87	0.16	171,171,171,171	0
53	MG	YA	3093	1/1	0.87	0.36	188,188,188,188	0
53	MG	YA	3025	1/1	0.87	0.15	162,162,162,162	0
53	MG	YA	3022	1/1	0.87	0.23	149,149,149,149	0
53	MG	YA	3100	1/1	0.88	0.13	124,124,124,124	0
53	MG	QA	1638	1/1	0.88	0.13	67,67,67,67	0
53	MG	YA	3132	1/1	0.88	0.49	240,240,240,240	0
53	MG	YA	3027	1/1	0.89	0.23	194,194,194,194	0
53	MG	RA	3131	1/1	0.89	0.60	187,187,187,187	0
53	MG	QA	1624	1/1	0.89	0.14	143,143,143,143	0
53	MG	RA	3091	1/1	0.89	0.10	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
53	MG	YA	3015	1/1	0.89	0.19	219,219,219,219	0
53	MG	XA	1638	1/1	0.89	0.15	204,204,204,204	0
53	MG	YA	3070	1/1	0.89	0.13	91,91,91,91	0
53	MG	YA	3001	1/1	0.89	0.15	141,141,141,141	0
53	MG	YA	3092	1/1	0.89	0.16	169,169,169,169	0
53	MG	RA	3070	1/1	0.89	0.34	137,137,137,137	0
53	MG	XA	1606	1/1	0.89	0.13	93,93,93,93	0
53	MG	RA	3103	1/1	0.89	0.15	30,30,30,30	0
53	MG	XA	1611	1/1	0.89	0.11	110,110,110,110	0
53	MG	YA	3077	1/1	0.89	0.07	109,109,109,109	0
53	MG	RA	3035	1/1	0.89	0.33	189,189,189,189	0
53	MG	XA	1618	1/1	0.90	0.11	136,136,136,136	0
53	MG	YA	3042	1/1	0.90	0.17	81,81,81,81	0
53	MG	QA	1625	1/1	0.90	0.14	101,101,101,101	0
53	MG	QA	1605	1/1	0.90	0.18	72,72,72,72	0
53	MG	YA	3080	1/1	0.90	0.18	154,154,154,154	0
53	MG	RA	3003	1/1	0.90	0.14	77,77,77,77	0
53	MG	XA	1623	1/1	0.90	0.11	108,108,108,108	0
53	MG	RA	3130	1/1	0.90	0.24	118,118,118,118	0
53	MG	YA	3054	1/1	0.90	0.12	86,86,86,86	0
53	MG	RA	3055	1/1	0.90	0.33	252,252,252,252	0
53	MG	YA	3058	1/1	0.90	0.39	249,249,249,249	0
53	MG	YA	3114	1/1	0.90	0.12	182,182,182,182	0
53	MG	RA	3014	1/1	0.91	0.18	38,38,38,38	0
53	MG	YA	3011	1/1	0.91	0.21	150,150,150,150	0
53	MG	YA	3111	1/1	0.91	0.14	202,202,202,202	0
53	MG	YA	3089	1/1	0.91	0.21	101,101,101,101	0
53	MG	QA	1643	1/1	0.91	0.11	67,67,67,67	0
53	MG	RA	3051	1/1	0.91	0.16	70,70,70,70	0
53	MG	XA	1628	1/1	0.91	0.44	224,224,224,224	0
53	MG	YA	3094	1/1	0.91	0.14	145,145,145,145	0
53	MG	YA	3126	1/1	0.91	0.19	120,120,120,120	0
53	MG	YA	3096	1/1	0.91	0.14	127,127,127,127	0
53	MG	YA	3029	1/1	0.91	0.21	178,178,178,178	0
53	MG	YA	3030	1/1	0.91	0.13	130,130,130,130	0
53	MG	YA	3069	1/1	0.91	0.23	267,267,267,267	0
53	MG	RB	201	1/1	0.91	0.33	255,255,255,255	0
53	MG	YA	3104	1/1	0.91	0.22	52,52,52,52	0
53	MG	XA	1615	1/1	0.91	0.20	187,187,187,187	0
53	MG	YA	3034	1/1	0.91	0.09	88,88,88,88	0
53	MG	QA	1640	1/1	0.92	0.05	79,79,79,79	0
53	MG	QA	1606	1/1	0.92	0.13	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
53	MG	YA	3044	1/1	0.92	0.15	87,87,87,87	0
53	MG	QA	1609	1/1	0.92	0.08	77,77,77,77	0
53	MG	YA	3115	1/1	0.92	0.26	176,176,176,176	0
53	MG	YA	3116	1/1	0.92	0.12	84,84,84,84	0
53	MG	RA	3119	1/1	0.92	0.08	56,56,56,56	0
53	MG	XA	1640	1/1	0.92	0.17	137,137,137,137	0
53	MG	YA	3013	1/1	0.92	0.39	241,241,241,241	0
53	MG	YA	3124	1/1	0.92	0.16	82,82,82,82	0
53	MG	YA	3051	1/1	0.92	0.14	88,88,88,88	0
53	MG	XA	1625	1/1	0.92	0.23	111,111,111,111	0
53	MG	YA	3016	1/1	0.92	0.10	60,60,60,60	0
53	MG	XA	1627	1/1	0.92	0.23	197,197,197,197	0
53	MG	QA	1616	1/1	0.92	0.18	98,98,98,98	0
53	MG	YA	3081	1/1	0.92	0.10	83,83,83,83	0
53	MG	YA	3103	1/1	0.92	0.13	86,86,86,86	0
53	MG	RA	3100	1/1	0.92	0.27	119,119,119,119	0
53	MG	YA	3021	1/1	0.92	0.28	183,183,183,183	0
53	MG	RA	3110	1/1	0.92	0.15	84,84,84,84	0
53	MG	QA	1636	1/1	0.93	0.37	218,218,218,218	0
53	MG	XA	1642	1/1	0.93	0.10	139,139,139,139	0
53	MG	RA	3050	1/1	0.93	0.18	39,39,39,39	0
53	MG	XA	1612	1/1	0.93	0.19	125,125,125,125	0
53	MG	RB	203	1/1	0.93	0.12	58,58,58,58	0
53	MG	YA	3035	1/1	0.93	0.09	90,90,90,90	0
53	MG	QA	1621	1/1	0.93	0.13	131,131,131,131	0
53	MG	RA	3046	1/1	0.93	0.08	176,176,176,176	0
53	MG	RA	3083	1/1	0.93	0.16	53,53,53,53	0
53	MG	YA	3041	1/1	0.93	0.15	119,119,119,119	0
53	MG	RA	3031	1/1	0.93	0.14	37,37,37,37	0
53	MG	YA	3067	1/1	0.93	0.11	72,72,72,72	0
53	MG	RA	3113	1/1	0.93	0.14	190,190,190,190	0
53	MG	YA	3009	1/1	0.93	0.28	157,157,157,157	0
53	MG	XA	1604	1/1	0.93	0.10	96,96,96,96	0
53	MG	RA	3117	1/1	0.93	0.16	162,162,162,162	0
54	EM1	RA	3135	60/60	0.93	0.26	0,23,85,88	0
53	MG	RA	3122	1/1	0.94	0.70	164,164,164,164	0
53	MG	RA	3045	1/1	0.94	0.14	25,25,25,25	0
53	MG	QA	1634	1/1	0.94	0.15	94,94,94,94	0
53	MG	YA	3118	1/1	0.94	0.17	100,100,100,100	0
53	MG	YA	3119	1/1	0.94	0.12	60,60,60,60	0
53	MG	XA	1613	1/1	0.94	0.17	147,147,147,147	0
53	MG	QA	1607	1/1	0.94	0.13	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
53	MG	RA	3017	1/1	0.94	0.09	57,57,57,57	0
53	MG	RA	3061	1/1	0.94	0.12	18,18,18,18	0
53	MG	RA	3133	1/1	0.94	0.28	116,116,116,116	0
53	MG	XA	1637	1/1	0.94	0.13	94,94,94,94	0
53	MG	QA	1618	1/1	0.94	0.12	78,78,78,78	0
53	MG	XA	1639	1/1	0.94	0.05	159,159,159,159	0
53	MG	RA	3018	1/1	0.94	0.34	32,32,32,32	0
53	MG	RA	3001	1/1	0.94	0.09	98,98,98,98	0
53	MG	RA	3057	1/1	0.94	0.08	71,71,71,71	0
53	MG	YA	3040	1/1	0.94	0.17	72,72,72,72	0
53	MG	RA	3118	1/1	0.94	0.15	48,48,48,48	0
53	MG	RA	3072	1/1	0.94	0.05	61,61,61,61	0
53	MG	YA	3113	1/1	0.94	0.07	128,128,128,128	0
53	MG	RA	3088	1/1	0.95	0.08	59,59,59,59	0
53	MG	YA	3037	1/1	0.95	0.13	81,81,81,81	0
53	MG	YA	3112	1/1	0.95	0.09	79,79,79,79	0
53	MG	RA	3030	1/1	0.95	0.11	56,56,56,56	0
53	MG	RA	3052	1/1	0.95	0.14	34,34,34,34	0
53	MG	YA	3086	1/1	0.95	0.13	109,109,109,109	0
53	MG	XA	1631	1/1	0.95	0.23	82,82,82,82	0
53	MG	YA	3065	1/1	0.95	0.13	88,88,88,88	0
53	MG	YA	3066	1/1	0.95	0.17	105,105,105,105	0
53	MG	RA	3041	1/1	0.95	0.14	38,38,38,38	0
53	MG	QA	1629	1/1	0.95	0.06	97,97,97,97	0
53	MG	RA	3084	1/1	0.95	0.15	26,26,26,26	0
53	MG	QA	1613	1/1	0.95	0.07	76,76,76,76	0
53	MG	RA	3121	1/1	0.95	0.17	45,45,45,45	0
53	MG	XA	1621	1/1	0.95	0.13	57,57,57,57	0
53	MG	YA	3048	1/1	0.95	0.10	103,103,103,103	0
53	MG	YA	3075	1/1	0.95	0.54	209,209,209,209	0
53	MG	XA	1607	1/1	0.95	0.13	167,167,167,167	0
53	MG	QA	1635	1/1	0.95	0.10	87,87,87,87	0
53	MG	YA	3131	1/1	0.95	0.14	94,94,94,94	0
53	MG	YA	3032	1/1	0.95	0.13	162,162,162,162	0
53	MG	RA	3002	1/1	0.95	0.10	75,75,75,75	0
53	MG	YA	3134	1/1	0.95	0.33	201,201,201,201	0
53	MG	YA	3107	1/1	0.95	0.20	91,91,91,91	0
53	MG	RA	3071	1/1	0.95	0.11	16,16,16,16	0
53	MG	YA	3018	1/1	0.95	0.10	185,185,185,185	0
53	MG	RA	3005	1/1	0.96	0.12	74,74,74,74	0
53	MG	YA	3012	1/1	0.96	0.09	72,72,72,72	0
53	MG	RA	3120	1/1	0.96	0.31	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
53	MG	RA	3059	1/1	0.96	0.43	207,207,207,207	0
53	MG	XA	1630	1/1	0.96	0.16	160,160,160,160	0
53	MG	RA	3074	1/1	0.96	0.10	93,93,93,93	0
53	MG	RA	3095	1/1	0.96	0.16	139,139,139,139	0
53	MG	XA	1633	1/1	0.96	0.10	79,79,79,79	0
53	MG	RA	3075	1/1	0.96	0.05	43,43,43,43	0
53	MG	RA	3099	1/1	0.96	0.19	34,34,34,34	0
53	MG	QA	1622	1/1	0.96	0.17	54,54,54,54	0
53	MG	QA	1623	1/1	0.96	0.11	77,77,77,77	0
53	MG	YA	3053	1/1	0.96	0.18	127,127,127,127	0
53	MG	RA	3008	1/1	0.96	0.14	45,45,45,45	0
53	MG	YA	3056	1/1	0.96	0.07	85,85,85,85	0
53	MG	RA	3028	1/1	0.96	0.14	92,92,92,92	0
53	MG	RA	3105	1/1	0.96	0.21	66,66,66,66	0
53	MG	QA	1628	1/1	0.96	0.24	142,142,142,142	0
53	MG	RA	3065	1/1	0.96	0.15	35,35,35,35	0
53	MG	RA	3112	1/1	0.96	0.10	49,49,49,49	0
53	MG	QA	1631	1/1	0.96	0.19	228,228,228,228	0
53	MG	RB	204	1/1	0.96	0.14	45,45,45,45	0
53	MG	YA	3095	1/1	0.96	0.15	138,138,138,138	0
53	MG	RA	3048	1/1	0.96	0.17	25,25,25,25	0
53	MG	QA	1604	1/1	0.96	0.04	139,139,139,139	0
53	MG	RA	3116	1/1	0.96	0.10	72,72,72,72	0
53	MG	YA	3099	1/1	0.96	0.17	188,188,188,188	0
53	MG	RA	3049	1/1	0.96	0.14	76,76,76,76	0
53	MG	RA	3029	1/1	0.96	0.19	14,14,14,14	0
53	MG	YA	3102	1/1	0.96	0.10	118,118,118,118	0
53	MG	QA	1608	1/1	0.96	0.26	61,61,61,61	0
55	ZN	Y4	101	1/1	0.96	0.07	169,169,169,169	0
53	MG	RA	3063	1/1	0.97	0.13	26,26,26,26	0
53	MG	RA	3064	1/1	0.97	0.14	28,28,28,28	0
53	MG	QA	1620	1/1	0.97	0.08	116,116,116,116	0
53	MG	RA	3037	1/1	0.97	0.14	30,30,30,30	0
53	MG	RA	3067	1/1	0.97	0.14	28,28,28,28	0
53	MG	RA	3053	1/1	0.97	0.17	55,55,55,55	0
53	MG	RA	3124	1/1	0.97	0.20	63,63,63,63	0
53	MG	YA	3061	1/1	0.97	0.14	110,110,110,110	0
53	MG	RA	3126	1/1	0.97	0.14	40,40,40,40	0
53	MG	YA	3105	1/1	0.97	0.19	97,97,97,97	0
53	MG	RA	3127	1/1	0.97	0.09	8,8,8,8	0
53	MG	RA	3006	1/1	0.97	0.13	54,54,54,54	0
53	MG	RA	3025	1/1	0.97	0.06	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
53	MG	YA	3024	1/1	0.97	0.15	102,102,102,102	0
53	MG	RA	3016	1/1	0.97	0.11	22,22,22,22	0
53	MG	RA	3132	1/1	0.97	0.12	20,20,20,20	0
53	MG	RA	3010	1/1	0.97	0.12	31,31,31,31	0
53	MG	RA	3097	1/1	0.97	0.13	54,54,54,54	0
53	MG	RA	3098	1/1	0.97	0.07	49,49,49,49	0
53	MG	RA	3073	1/1	0.97	0.24	43,43,43,43	0
53	MG	RA	3007	1/1	0.97	0.13	112,112,112,112	0
53	MG	YA	3117	1/1	0.97	0.17	73,73,73,73	0
53	MG	RA	3101	1/1	0.97	0.11	48,48,48,48	0
53	MG	QA	1639	1/1	0.97	0.18	118,118,118,118	0
53	MG	RA	3019	1/1	0.97	0.06	34,34,34,34	0
53	MG	YA	3121	1/1	0.97	0.17	168,168,168,168	0
53	MG	RA	3077	1/1	0.97	0.10	63,63,63,63	0
53	MG	QA	1642	1/1	0.97	0.13	79,79,79,79	0
53	MG	RA	3108	1/1	0.97	0.13	95,95,95,95	0
53	MG	RA	3109	1/1	0.97	0.16	46,46,46,46	0
53	MG	RA	3079	1/1	0.97	0.15	32,32,32,32	0
53	MG	XA	1603	1/1	0.97	0.09	136,136,136,136	0
53	MG	RA	3080	1/1	0.97	0.07	60,60,60,60	0
53	MG	XA	1605	1/1	0.97	0.19	54,54,54,54	0
53	MG	RA	3081	1/1	0.97	0.17	99,99,99,99	0
53	MG	RA	3114	1/1	0.97	0.19	28,28,28,28	0
53	MG	XA	1609	1/1	0.97	0.15	98,98,98,98	0
53	MG	YA	3046	1/1	0.97	0.22	73,73,73,73	0
53	MG	QA	1611	1/1	0.97	0.14	57,57,57,57	0
53	MG	YB	201	1/1	0.97	0.09	111,111,111,111	0
53	MG	QA	1612	1/1	0.97	0.18	113,113,113,113	0
53	MG	RA	3012	1/1	0.97	0.12	20,20,20,20	0
53	MG	QA	1614	1/1	0.97	0.15	159,159,159,159	0
53	MG	RA	3036	1/1	0.97	0.18	23,23,23,23	0
53	MG	RA	3038	1/1	0.98	0.17	19,19,19,19	0
53	MG	RA	3039	1/1	0.98	0.24	7,7,7,7	0
53	MG	RA	3066	1/1	0.98	0.16	32,32,32,32	0
53	MG	RA	3123	1/1	0.98	0.11	24,24,24,24	0
53	MG	RA	3040	1/1	0.98	0.13	47,47,47,47	0
53	MG	QA	1615	1/1	0.98	0.11	152,152,152,152	0
53	MG	YA	3068	1/1	0.98	0.07	98,98,98,98	0
53	MG	RA	3125	1/1	0.98	0.14	40,40,40,40	0
53	MG	QA	1617	1/1	0.98	0.17	129,129,129,129	0
53	MG	RA	3009	1/1	0.98	0.14	38,38,38,38	0
53	MG	XA	1641	1/1	0.98	0.15	116,116,116,116	0

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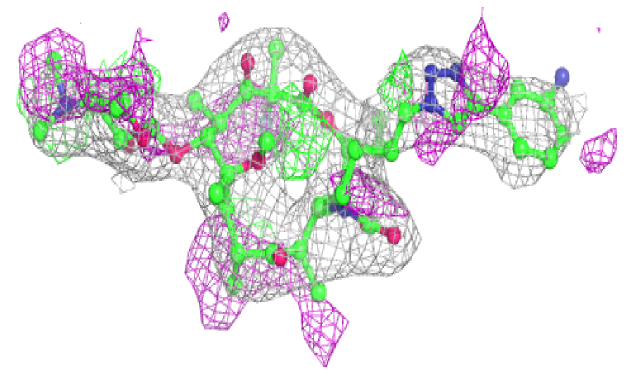
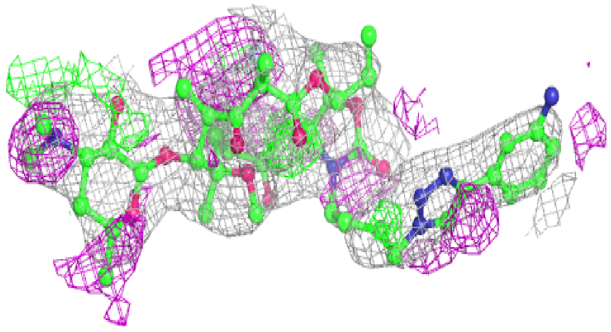
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
53	MG	XA	1608	1/1	0.98	0.27	46,46,46,46	0
53	MG	RA	3102	1/1	0.98	0.17	24,24,24,24	0
53	MG	RA	3042	1/1	0.98	0.07	60,60,60,60	0
53	MG	RA	3104	1/1	0.98	0.17	23,23,23,23	0
53	MG	RA	3044	1/1	0.98	0.14	34,34,34,34	0
53	MG	RA	3106	1/1	0.98	0.19	13,13,13,13	0
53	MG	RA	3107	1/1	0.98	0.22	17,17,17,17	0
53	MG	RA	3026	1/1	0.98	0.17	143,143,143,143	0
53	MG	RA	3136	1/1	0.98	0.07	61,61,61,61	0
53	MG	RA	3087	1/1	0.98	0.08	47,47,47,47	0
53	MG	RA	3032	1/1	0.98	0.14	23,23,23,23	0
53	MG	RA	3111	1/1	0.98	0.15	31,31,31,31	0
53	MG	RA	3033	1/1	0.98	0.15	159,159,159,159	0
53	MG	QA	1601	1/1	0.98	0.07	94,94,94,94	0
53	MG	YA	3014	1/1	0.98	0.20	113,113,113,113	0
53	MG	QA	1633	1/1	0.98	0.12	70,70,70,70	0
53	MG	RA	3027	1/1	0.98	0.12	33,33,33,33	0
53	MG	YA	3090	1/1	0.98	0.10	112,112,112,112	0
53	MG	YA	3052	1/1	0.98	0.07	72,72,72,72	0
53	MG	QA	1603	1/1	0.98	0.09	65,65,65,65	0
53	MG	RA	3022	1/1	0.98	0.12	27,27,27,27	0
53	MG	YA	3055	1/1	0.98	0.16	103,103,103,103	0
53	MG	XA	1626	1/1	0.98	0.24	20,20,20,20	0
53	MG	RA	3115	1/1	0.98	0.07	22,22,22,22	0
53	MG	RA	3093	1/1	0.98	0.08	45,45,45,45	0
53	MG	RA	3094	1/1	0.98	0.10	32,32,32,32	0
53	MG	RA	3015	1/1	0.98	0.06	65,65,65,65	0
53	MG	RA	3078	1/1	0.98	0.13	58,58,58,58	0
53	MG	RA	3021	1/1	0.99	0.12	24,24,24,24	0
53	MG	RA	3034	1/1	0.99	0.10	11,11,11,11	0
53	MG	RA	3092	1/1	0.99	0.09	68,68,68,68	0
53	MG	RA	3128	1/1	0.99	0.16	33,33,33,33	0
53	MG	RA	3043	1/1	0.99	0.26	11,11,11,11	0
53	MG	RA	3013	1/1	0.99	0.16	18,18,18,18	0
53	MG	RA	3076	1/1	0.99	0.07	107,107,107,107	0
53	MG	RA	3023	1/1	0.99	0.12	22,22,22,22	0
55	ZN	R4	101	1/1	0.99	0.10	108,108,108,108	0
53	MG	QA	1626	1/1	0.99	0.20	29,29,29,29	0
53	MG	RA	3062	1/1	1.00	0.15	19,19,19,19	0

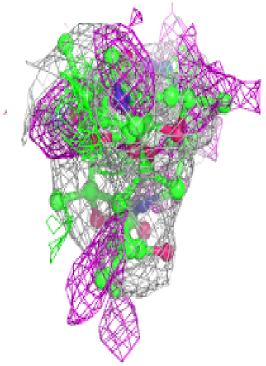
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EM1 RA 3135:

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.