



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 12:40 AM UTC

PDB ID : 4WWW / pdb_00004www
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)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

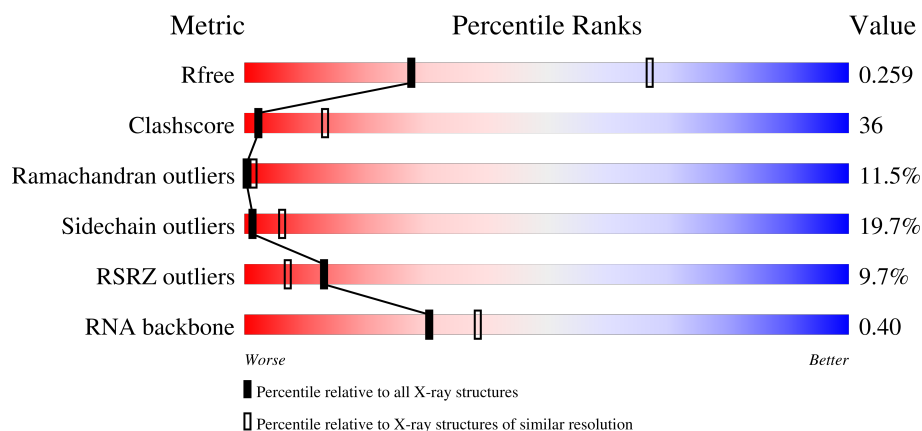
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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 $\leq 5\%$. 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	41% 43% 14% •
1	YA	2904	11% 19% 52% 27% •
2	RB	118	44% 46% 10%
2	YB	118	21% 53% 25% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	RC	271	
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	
9	RI	141	
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	
14	RN	120	
14	YN	120	
15	RO	116	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	R1	50	
28	Y1	50	
29	R2	46	
29	Y2	46	
30	R3	64	
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	
35	XD	205	
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	

Continued on next page...

Continued from previous page...

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	YA	3026	-	-	-	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
1	RA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
1	YA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	0	0	0
			753	479	137	134	3			
22	YV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- 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	0	0	0
			596	367	120	108	1			
23	YW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- 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	0	0	0
			625	388	129	106	2			
24	YX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- 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	0	0	0
			509	313	99	95	2			
25	YY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- 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	0	0	0
			449	281	87	79	2			

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

- 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	0	0	0
			648	411	121	113	3			
48	XQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

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

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

- 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	0	0	0
			637	408	120	107	2			
50	XS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- 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	0	0	0
			665	411	137	114	3			
51	XT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

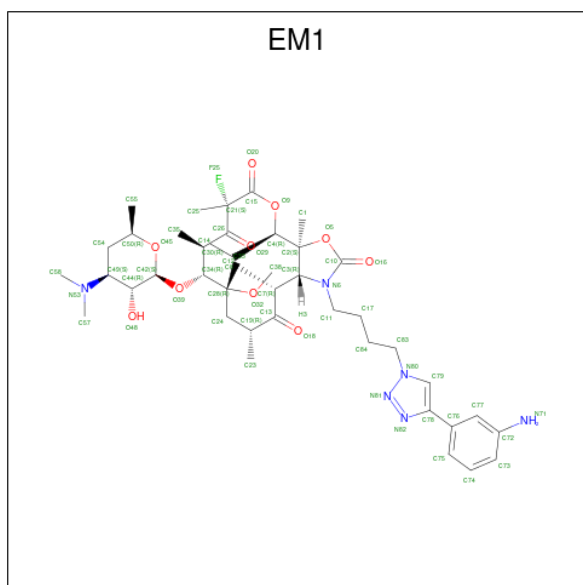
- Molecule 52 is a protein called 30S ribosomal protein S21.

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

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 54 is (3a*S*,4*R*,7*S*,9*R*,10*R*,11*R*,13*R*,15*R*,15a*R*)-1-{4-[4-(3-aminophenyl)-1*H*-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-2*H*-oxacyclotetradecino[4,3-*d*][1,3]oxazol-10-yl 3,4,6-trideoxy-3-(dimethylamino)-β-D-xylo-hexopyranoside (CCD ID: EM1) (formula: C₄₃H₆₅FN₆O₁₀).



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...

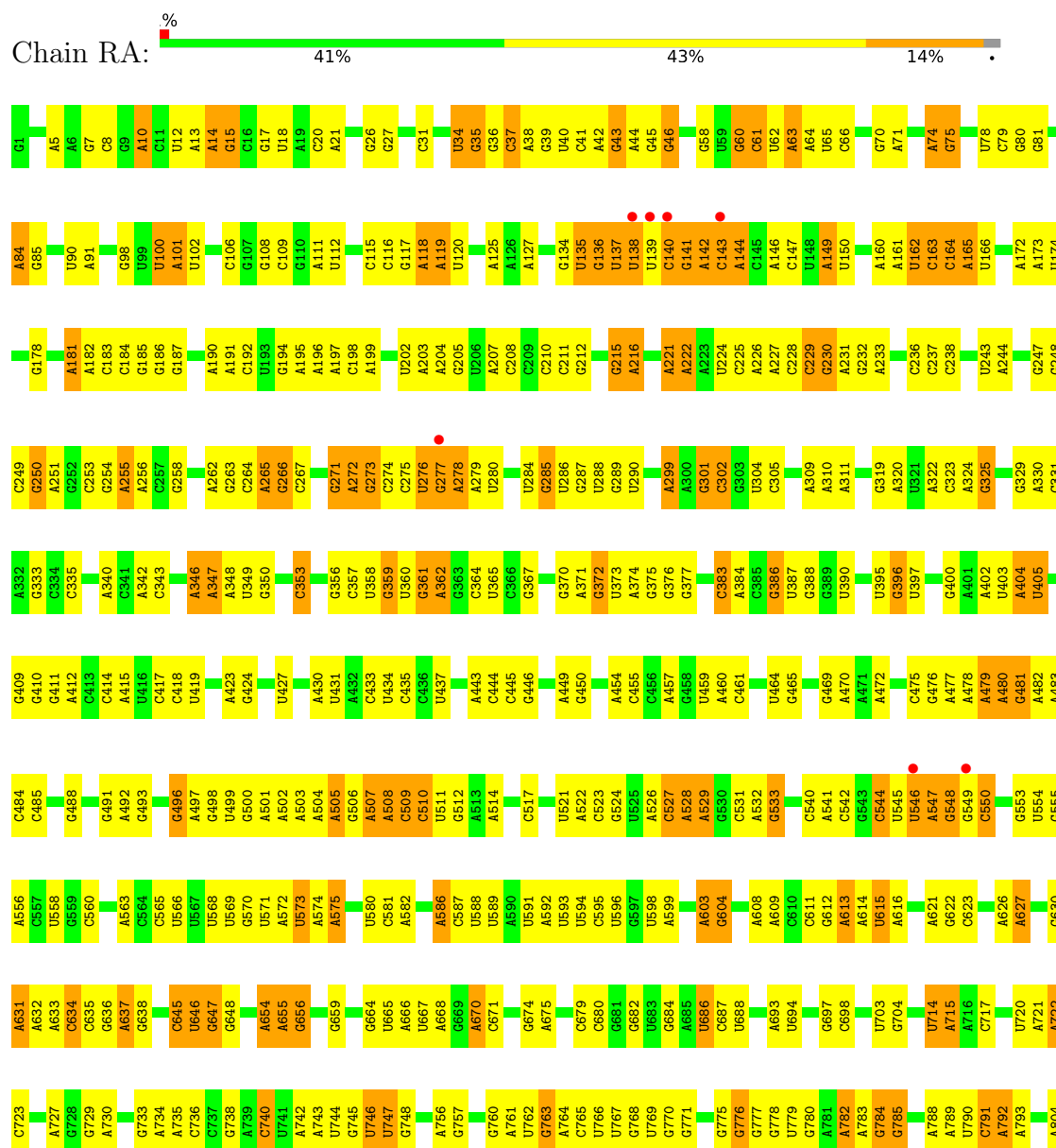
Continued from previous page...

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

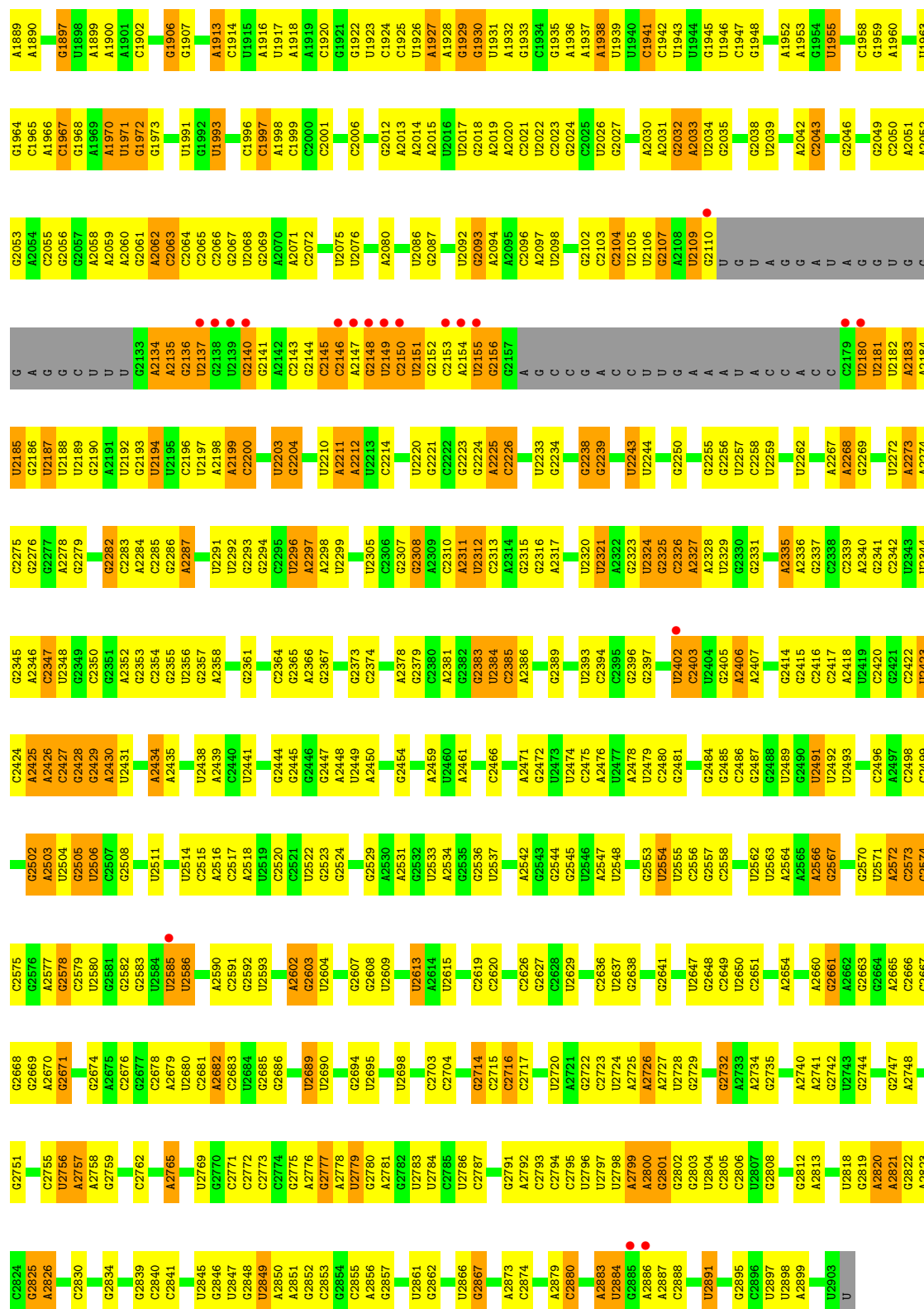
3 Residue-property plots

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.

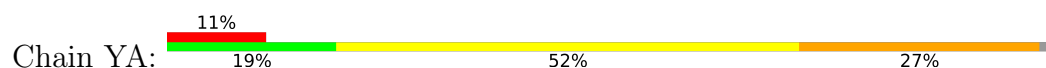
• Molecule 1: 23S rRNA

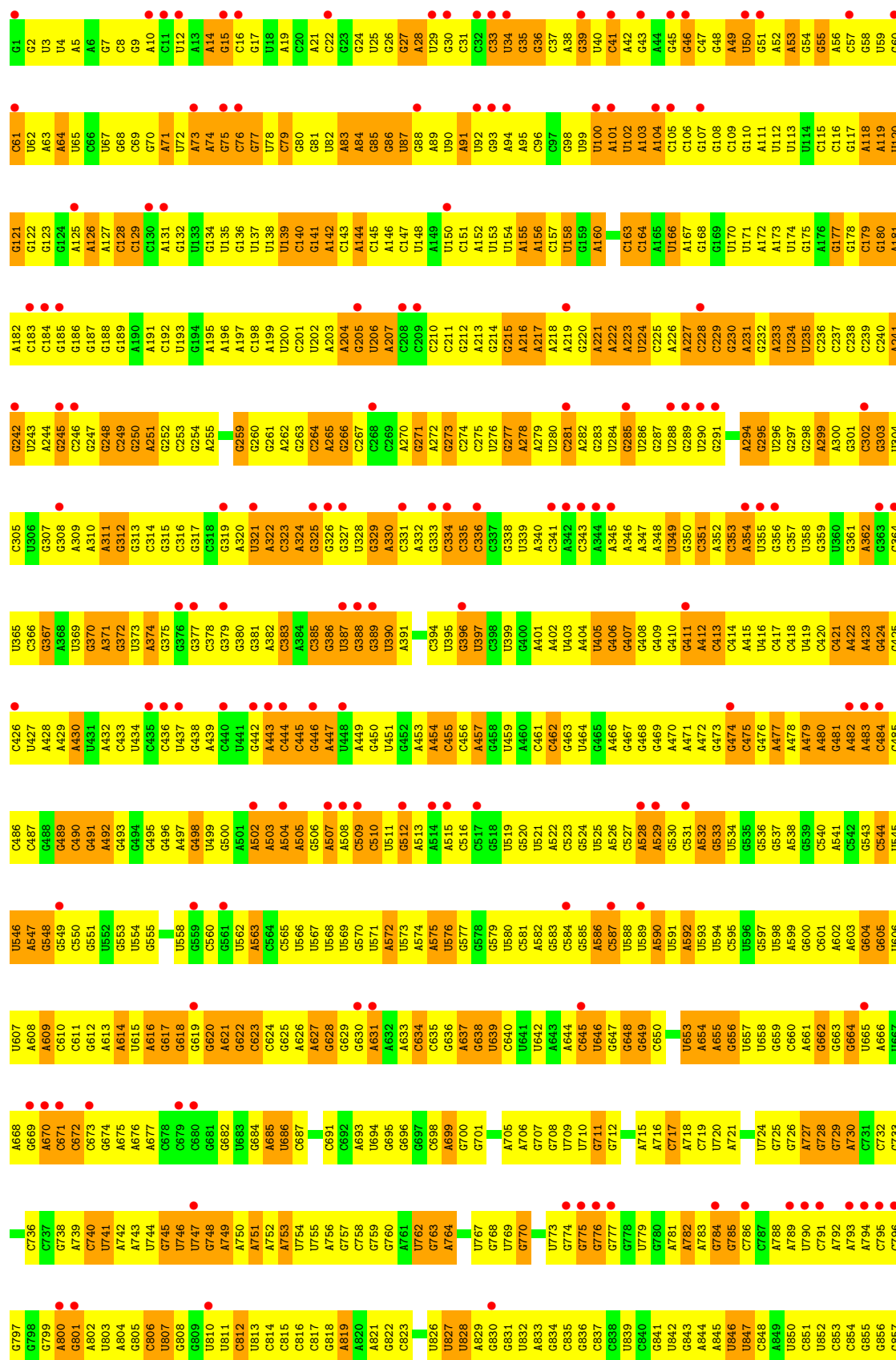


G1817	A1746	C1670	U1578	C1488	G1414	A1328	A1247	G1171	U1097	A1028	A959	C885	G805
U1818	U1747	C1674	G1581	C1489	U1415	G1333	G1248	C1172	A1098	A1028	A960	A	C806
A1819	C1748	G1675	G1582	C1493	G1416	G1334	U1249	U1173	G1099	U1033	G961	U	U811
U1820	A1749	A1676	A1583	C1494	C1417	C1335	G1250	U1174	A1103	C	G962	C	C812
A1821	A1754	A1677	A1584	A1495	G1418	C1336	C1251	A1175	C1104	G1037	G969	C	U813
C1822	A1755	A1677	C1585	A1496	A1419	G1337	G1252	U1176	U1105	A1040	U970	G	C814
G1826	U1756	U1680	A1586	U1497	A1420	G1338	A1253	G1177	G1106	A1040	G971	A892	C815
U1827	G1756	G1681	G1587	C1498	G1421	G1339	U1255	C1178	G1107	G1041	A972	C893	G818
G1828	A1757	G1682	G1588	C1499	G1422	G1340	U1256	U1179	U1108	G1042	A973	U894	C819
A1829	A1762	U1683	U1589	G1500	G1423	G1341	C1257	U1181	C1109	C1043	A974	U895	A819
G1832	G1763	G1684	A1590	A1501	U1427	G1342	U1258	G1182	G1110	C1044	A975	C896	A820
C1833	C1764	U1688	A1591	G1502	A1428	A1347	C1261	U1183	A1111	C1045	G976	C897	A821
U1834	G1767	U1688	C1592	A1503	G1429	C1348	A1262	U1184	G1112	A1046	G977	C898	U826
C1837	C1768	U1692	A1593	A1504	G1430	C1351	U1266	G1185	U1113	G1047	A978	A899	U827
G1838	U1769	U1693	U1594	A1505	A1431	G1352	A1267	G1186	C1114	A1048	A979	A900	U828
G1839	G1770	C1694	G1597	C1506	G1432	A1353	U1267	U1187	G1115	C1049	A981	C901	
C1840	A1773	G1695	A1598	U1507	A1434	A1354	A1268	A1188	U1119	A1050	A982	C902	U832
U1841	C1774	G1696	C1600	A1509	G1435	G1355	A1269	G1190	G1122	G1056	A983	C908	U833
C1842	U1775	A1700	A1603	G1511	U1437	C1357	G1271	G1193	G1125	U1057	A984	A910	G834
C1843	G1776	A1701	C1604	C1512	U1438	G1358	A1272	A1194	U1128	U1058	C985	A911	U839
C1844	U1777	G1706	C1605	U1513	A1439	A1359	U1273	G1199	G1130	G1063	C986	C912	C840
A1847	U1778	A1707	C1606	G1514	U1440	G1360	A1274	U1198	U1131	U1065	C987	C913	G841
A1848	U1779	A1708	A1608	A1515	G1441	G1365	A1275	U1199	G1132	U1066	A988	G914	U842
U1849	U1780	C1706	A1609	G1516	U1442	A1365	A1276	C1200	U1133	G1067	C994	C915	G843
G1850	U1781	A1610	A1610	U1528	U1443	G1368	G1277	G1201	U1134	U1068	C995	A918	A845
U1851	A1782	C1611	C1612	G1529	G1444	G1371	G1280	U1203	U1135	A1067	A996	A920	U846
A1852	U1783	G1613	G1613	C1533	G1450	U1372	G1281	A1205	G1136	G1068	C997	C921	U847
A1853	A1784	A1614	G1622	U1534	C1451	G1377	A1287	G1206	G1137	A1070	C998	C922	C848
A1854	A1785	G1715	G1626	C1535	G1452	A1378	G1288	C1207	U1138	G1071	U999	G924	A849
U1855	A1786	U1716	G1627	G1537	C1453	U1379	C1289	G1212	G1139	C1072	A1000	A1001	U850
U1856	U1789	C1790	U1628	G1538	G1454	G1380	G1290	U1141	C1140	A1073	A1002	A927	G855
G1857	A1791	G1720	G1628	U1539	U1457	A1383	C1295	G1220	U1141	G1074	G1003	A928	G856
U1858	G1792	G1721	G1628	G1540	U1458	A1384	U1221	C1221	A1142	C1075	U1004	U929	G857
U1859	C1793	A1722	A1635	G1546	G1459	A1385	G1300	G1222	A1143	C1076	C1005	U930	G858
U1864	U1794	G1723	U1636	U1554	U1460	C1386	U1224	U1224	G1144	A1077	C1006	U931	G859
U1865	C1795	G1724	A1637	G1554	U1467	A1387	A1301	G1225	G1149	U1078	A1008	U932	
A1866	U1796	U1725	C1638	G1555	U1468	A1392	G1309	G1229	C1150	A1080	A1009	U934	A863
G1867	G1797	C1726	G1638	C1558	A1469	A1393	G1310	C1238	A1151	U1081	A1010	C935	G864
C1868	U1798	C1727	C1644	C1564	A1470	U1394	G1311	U1230	C1152	U1082	G1011	A936	C865
G1869	G1799	U1728	U1647	U1562	U1471	A1395	C1315	U1231	C1153	U1083	U1012	C937	A866
C1870	A1800	G1730	U1648	C1565	U1474	A1403	U1316	G1232	G1154	A1084	C1013	A941	C867
A1871	G1731	G1732	G1649	C1566	U1475	U1402	G1317	U1234	G1157	A1085	A1014	U1015	U868
G1872	A1802	G1733	A1652	C1568	U1476	A1403	U1318	G1235	G1160	A1086	U1016	C946	G869
C1873	U1805	G1734	G1653	C1569	U1477	U1405	C1319	U1239	C1161	U1088	U1019	A947	U870
C1874	A1808	A1735	A1654	G1567	G1478	U1406	A1321	G1238	U1165	A1089	A1020	C948	U871
G1875	U1809	U1736	A1654	U1568	G1479	U1407	G1320	U1239	A1166	A1090	A1021	C949	G875
A1876	A1810	G1737	C1656	A1569	G1482	G1408	A1322	U1242	C1167	G1091	G1022	C950	C876
C1881	U1882	G1738	A1664	A1571	U1483	G1410	C1323	C1243	A1165	C1092	U1023	C951	A877
U1883	U1882	A1739	U1485	A1571	U1484	G1411	U1325	A1244	G1168	G1093	G1024	G1025	A878
G1884	G1813	G1743	U1486	U1576	U1486	U1412	U1326	A1245	U1169	U1094	G1026	G1095	G879
U1885	G1814	A1668	A1669	C1577	U1487	A1413	A1327	A1246	C1170	A1096	A1027	U958	U884
U1886	C1816	A1745											



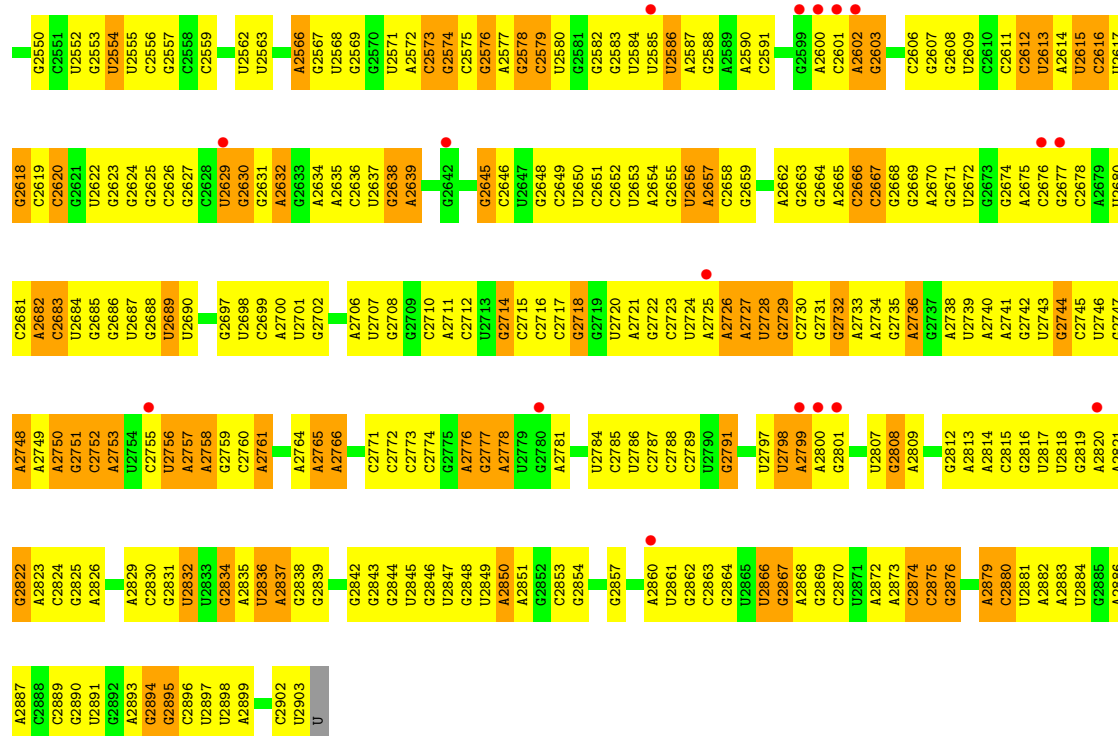
- Molecule 1: 23S rRNA





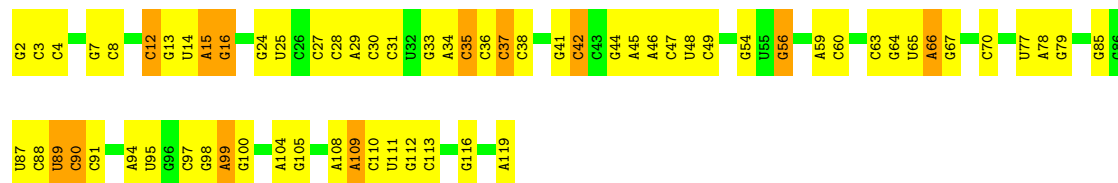
G1619	G1620	G1621	G1622	G1623	G1624	G1625	G1626	G1627	G1628	G1629	G1633	G1634	G1635	G1636	G1637	G1638	G1639	G1640	G1644	G1645	G1646	G1647	G1648	G1649	G1650	G1651	G1652	G1653	G1654	G1655	G1656	G1660	G1661	G1662	G1663	G1664	G1665	G1666	G1667	G1668	G1669	G1670	G1671	G1672	G1673	G1674	G1675	G1676	G1677	G1678	G1681	G1682	G1683	G1684	G1685						
C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1577	C1578	C1579	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618				
A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542	A1543	A1544	A1545	A1546	A1549	C1550	A1551	A1552	A1553	A1554	A1555			
G1432	A1433	A1434	G1435	G1436	G1437	G1438	A1439	G1440	G1441	G1442	G1443	G1444	C1447	G1448	C1451	G1452	A1453	A1454	G1455	G1456	G1457	G1458	G1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	G1473	G1474	G1475	G1476	G1477	G1478	G1479	C1480	G1481	G1482	G1483	G1484	A1485	A1486	G1487	G1488	G1489	A1490	A1491	A1492	A1493	A1494					
G1371	G1372	A1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	A1383	A1384	C1385	G1386	A1387	G1388	G1389	G1390	G1391	A1392	A1393	G1394	A1395	G1396	G1397	G1398	G1399	G1400	G1401	A1402	A1403	A1404	A1405	G1406	G1407	G1408	G1409	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	A1419	A1420	G1421	G1424	G1425	G1426	A1427	G1428	G1429	G1430	A1431			
G1311	G1312	G1313	C1314	C1315	G1316	G1317	G1318	G1319	C1320	A1321	A1322	C1323	G1324	G1325	G1326	A1327	A1328	G1329	C1330	G1331	G1332	G1333	G1334	G1335	A1336	G1337	G1338	G1339	G1340	G1341	A1342	G1343	G1344	C1345	G1346	A1347	C1348	G1349	C1350	C1351	G1352	A1353	A1354	G1355	G1356	C1357	G1358	A1359	G1360	G1361	G1362	C1363	G1364	A1365	A1366	A1367	G1368	G1369	C1370		
C1251	G1252	A1253	A1254	G1255	G1256	C1257	G1258	G1259	A1260	C1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	G1270	G1271	A1272	A1273	A1274	A1275	A1276	G1277	A1278	G1279	G1280	G1281	G1282	G1283	A1284	A1285	A1286	A1287	G1288	C1289	C1290	C1291	G1292	G1293	C1294	G1295	G1296	G1297	G1298	G1299	G1300	A1301	A1302	A1303	A1304	C1305	C1306	A1307	A1308	G1309	G1310		
U1188	A1189	G1190	G1191	G1192	G1193	A1194	G1195	G1196	G1197	U1198	U1199	G1200	U1201	G1202	U1203	A1204	A1205	G1206	C1207	C1208	U1209	G1210	A1211	G1212	A1213	A1214	G1215	G1216	U1217	U1222	G1223	U1224	G1225	A1226	G1227	G1228	C1229	A1230	U1231	G1232	G1233	U1234	G1235	U1236	A1237	U1238	G1239	U1240	A1241	U1242	C1243	A1244	G1245	A1246	A1247	G1248	U1249	G1250			
U1058	G1059	U1061	G1062	G1063	G1064	C1065	U1066	U1067	G1068	A1069	A1070	G1071	C1072	A1073	G1074	G1075	G1076	A1077	U1078	G1079	A1080	U1081	G1082	U1083	A1084	A1085	A1086	G1087	U1088	A1089	A1090	G1091	C1092	G1093	U1094	A1095	U1096	A1097	C1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	A1106	C1107	G1108	G1109	G1110	A1111	G1112	U1113	U1114	G1115	G1116	C1117	C1118		
C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	A1000	A1001	C1005	C1006	C1007	A1008	A1009	A1010	G1011	U1012	C1013	A1014	U1015	G1016	C995	U1019	A1020	A1021	C997	U1022	U1023	G1024	G1025	A1026	C991	C992	U1027	A1032	U1033	G1034	U1035	G1042	C1043	C1044	C1045	A1046	G1047	A1048	A1049	A1050	G1051	C1052	A1053	A1054	G1055	A1056	A1057
C922	G923	G924	A925	G926	G927	A928	U929	U930	U931	U932	A933	U934	C935	A936	A941	A942	A943	A944	A945	A946	A947	A948	G949	G950	C951	G952	C953	C954	U955	G956	C957	U958	A959	A960	C961	C962	U963	C964	C965	C966	U967	C968	C969	U970	G971	A972	A973	G974	A975	A976	A977	C978	C979	A980	A981	C982	A983	A984			
G858	G859	U860	A861	G862	A863	G864	G865	G866	C867	U868	G869	U870	U871	U872	C873	G874	G875	C876	A877	A878	G	G	G	G	G	U	C	A	U	C	C	C	U	U	C	A	C	C898	A899	C902	C903	G904	A905	A910	A911	C912	C913	C914	C915	G916	A917	A918	U919	A920	C921						





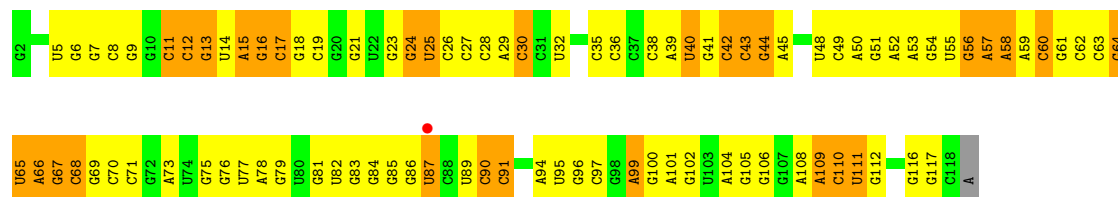
• Molecule 2: 5S rRNA

Chain RB: 44% 46% 10%



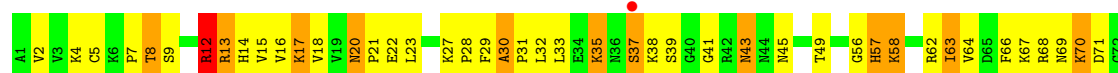
• Molecule 2: 5S rRNA

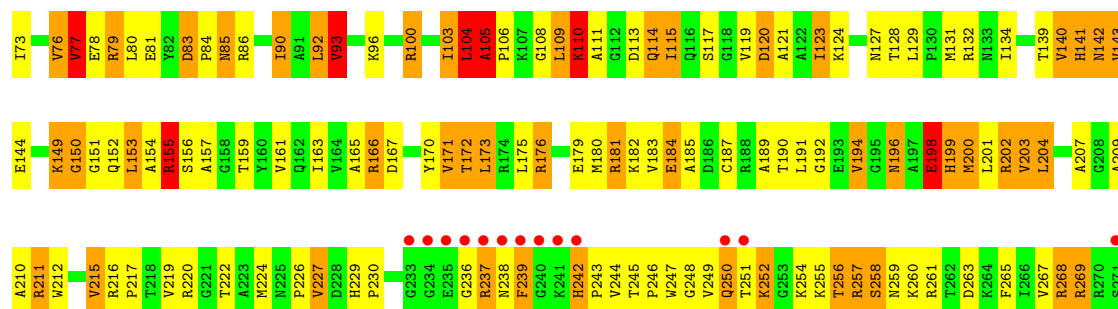
Chain YB: 21% 53% 25%



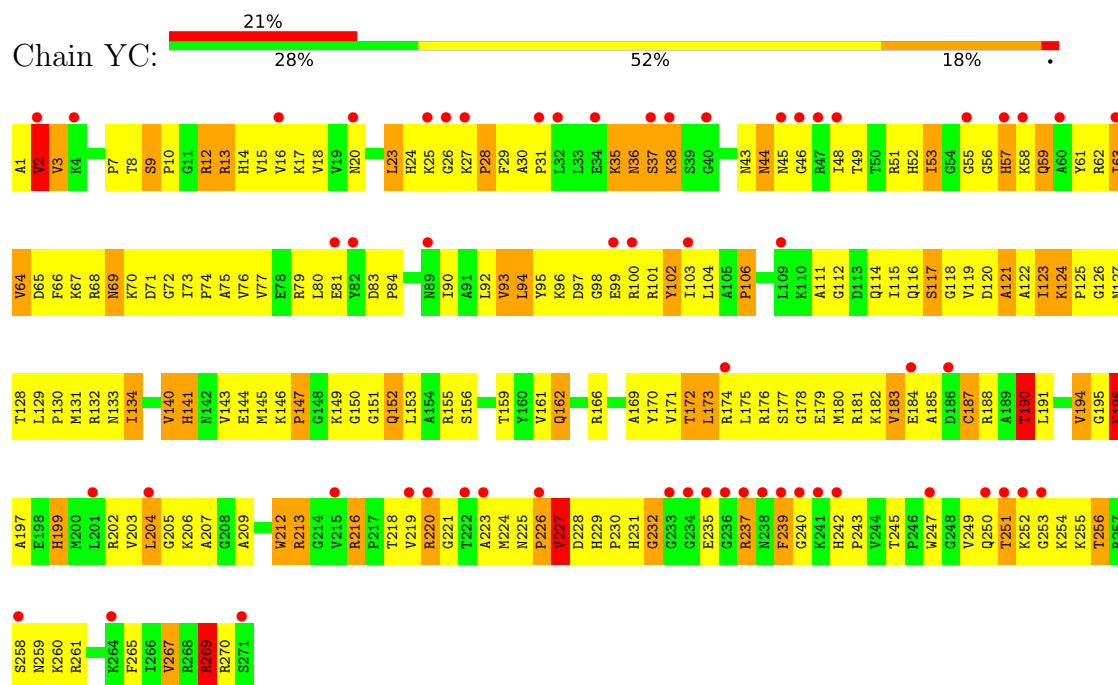
• Molecule 3: 50S ribosomal protein L2

Chain RC: 5% 35% 40% 22%

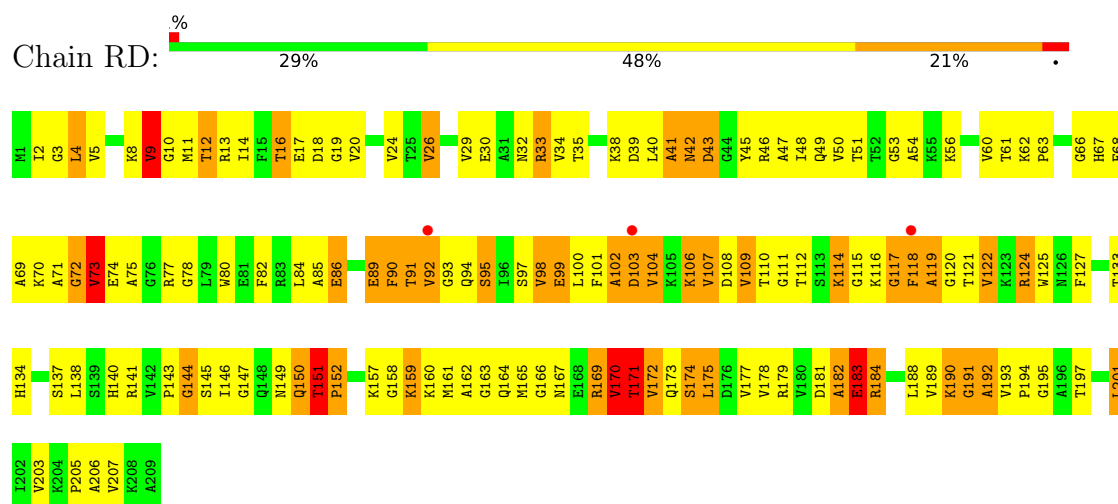




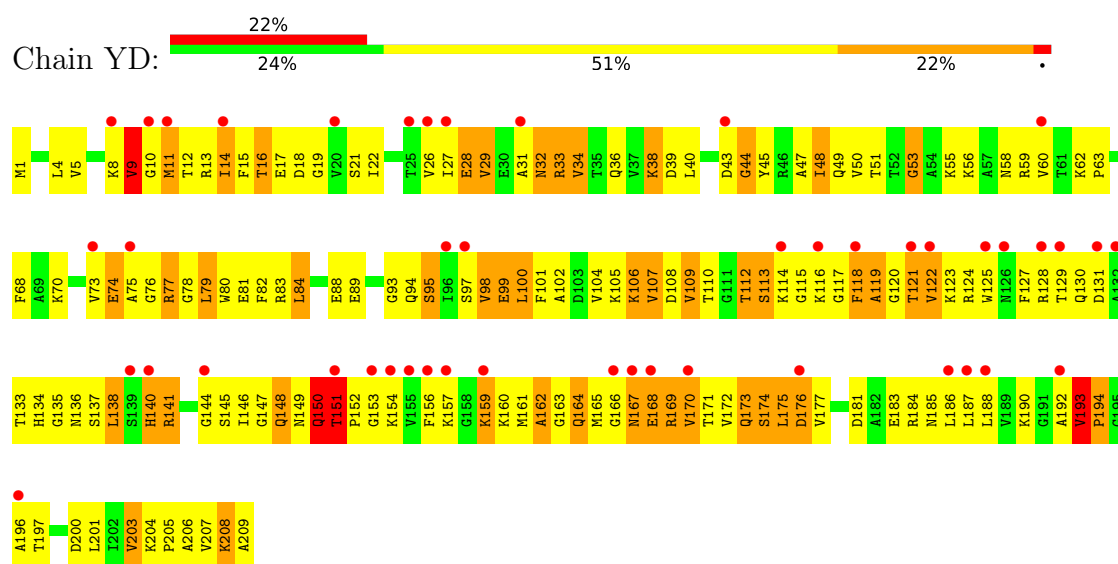
• Molecule 3: 50S ribosomal protein L2



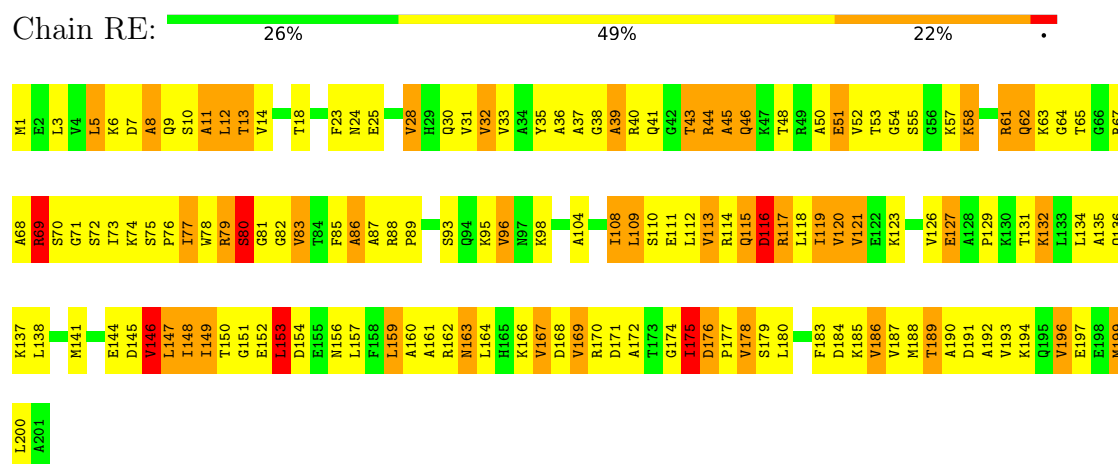
• Molecule 4: 50S ribosomal protein L3



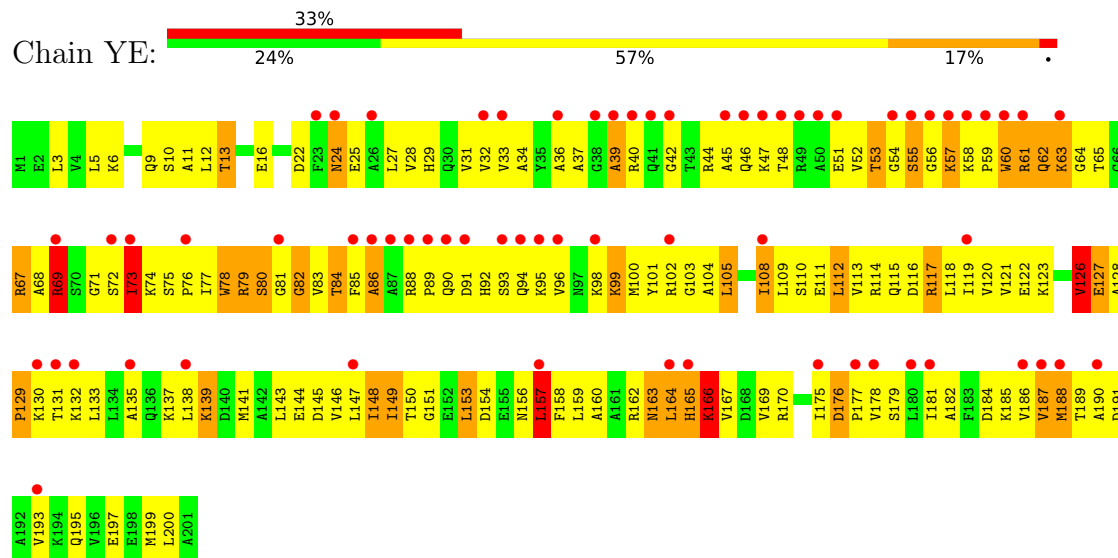
• Molecule 4: 50S ribosomal protein L3



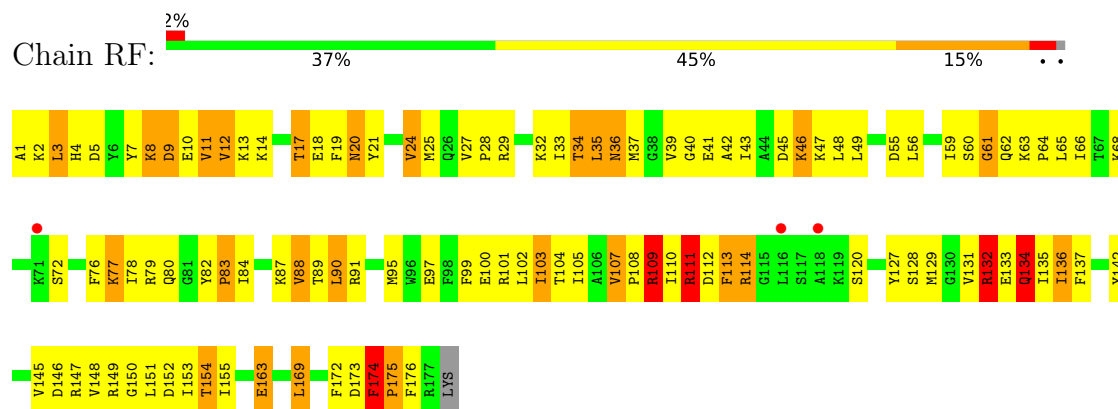
• Molecule 5: 50S ribosomal protein L4



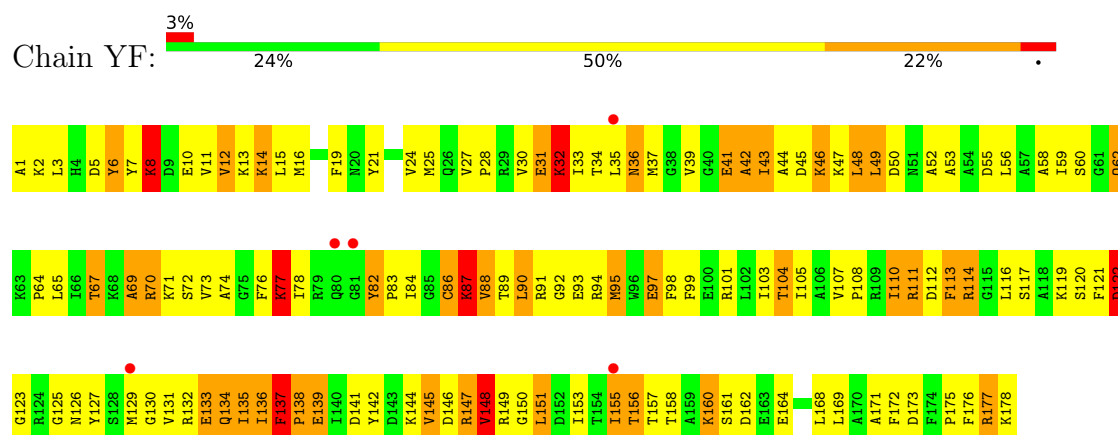
• Molecule 5: 50S ribosomal protein L4



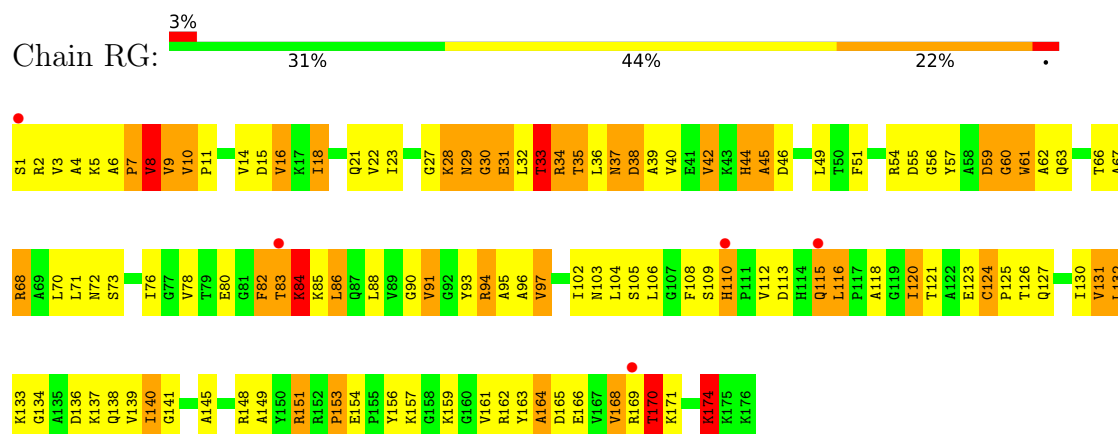
• Molecule 6: 50S ribosomal protein L5



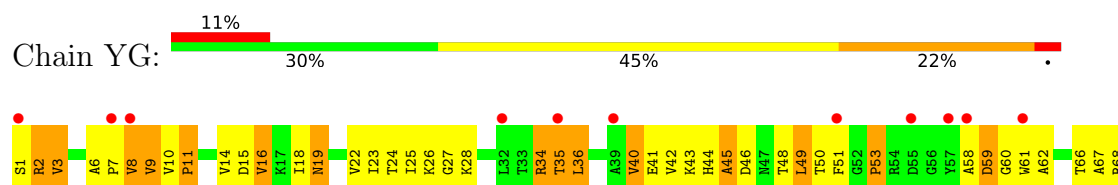
• Molecule 6: 50S ribosomal protein L5

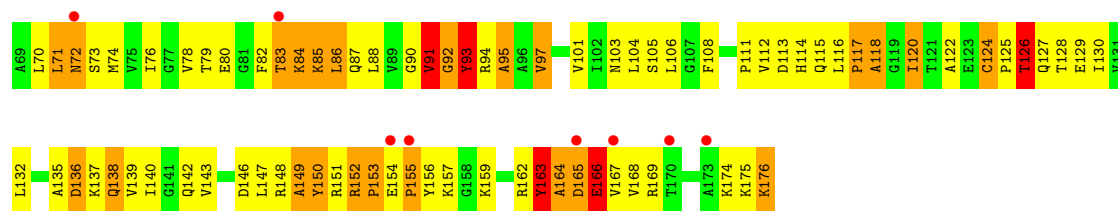


• Molecule 7: 50S ribosomal protein L6

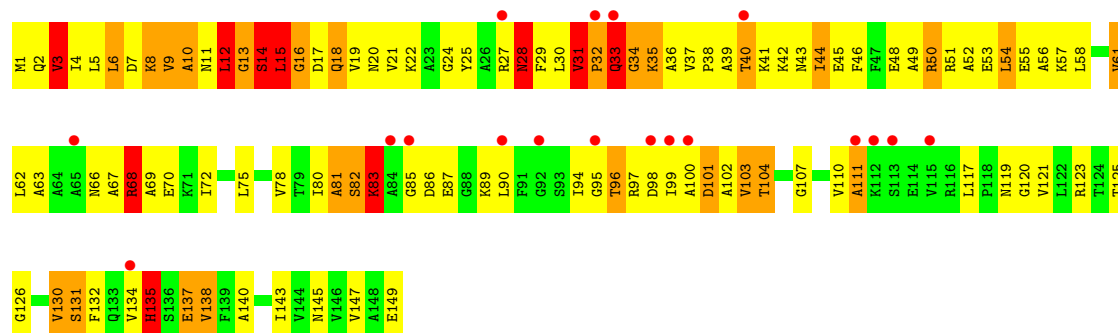


• Molecule 7: 50S ribosomal protein L6

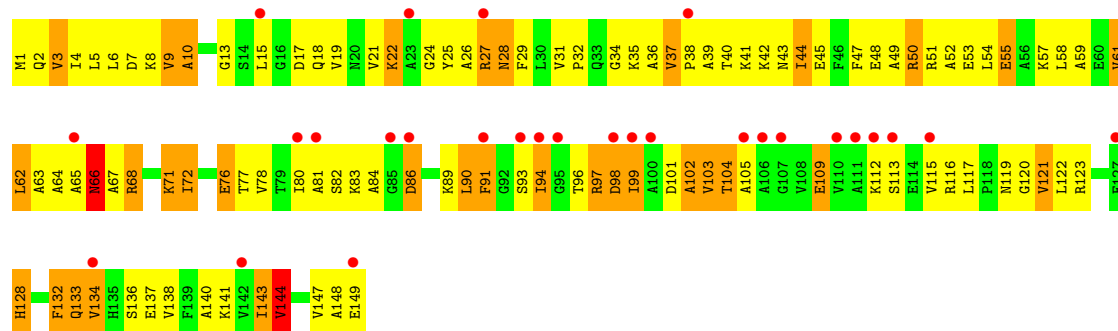




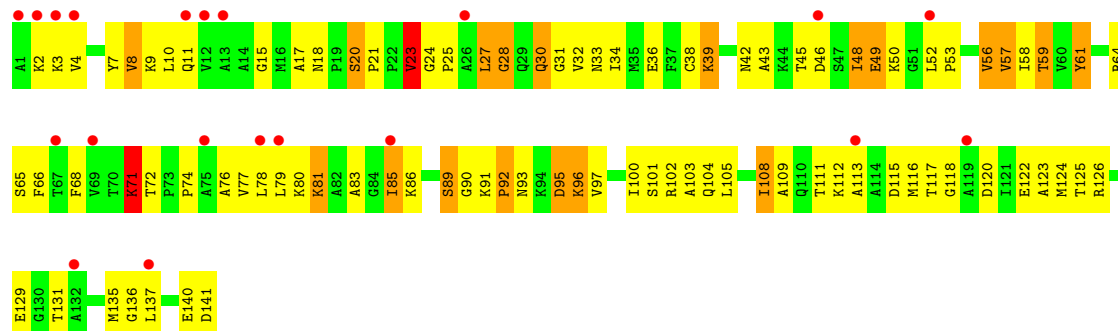
• Molecule 8: 50S ribosomal protein L9



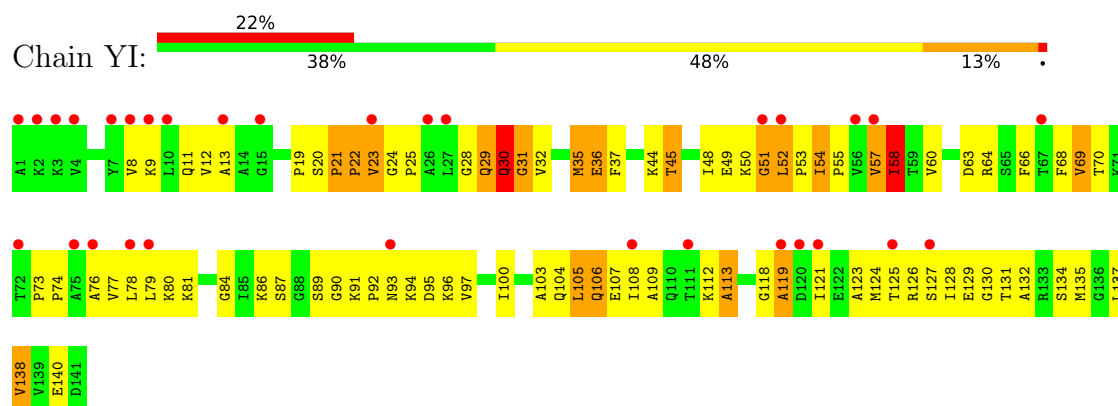
• Molecule 8: 50S ribosomal protein L9



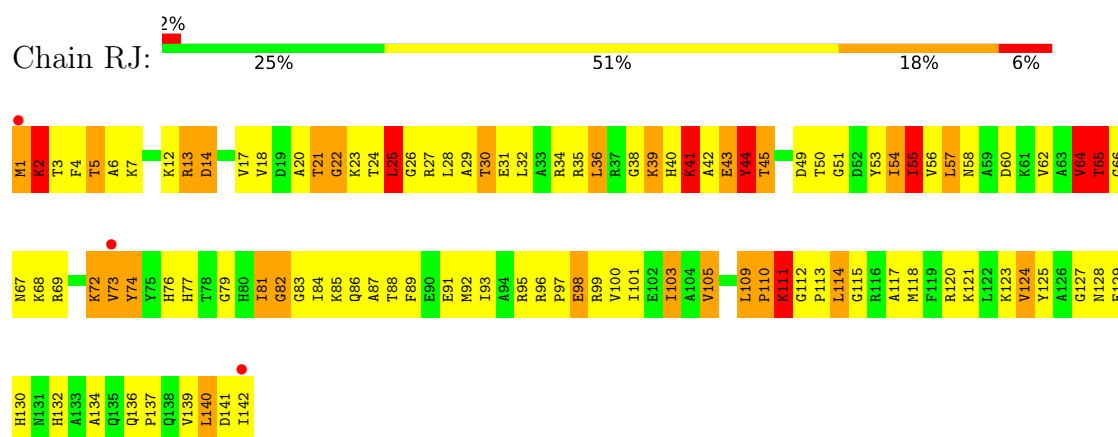
• Molecule 9: 50S ribosomal protein L11



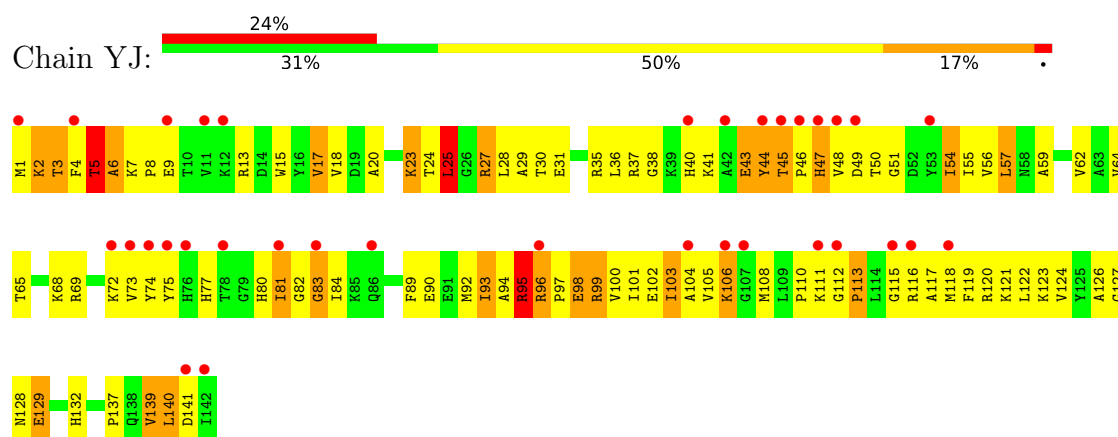
- Molecule 9: 50S ribosomal protein L11



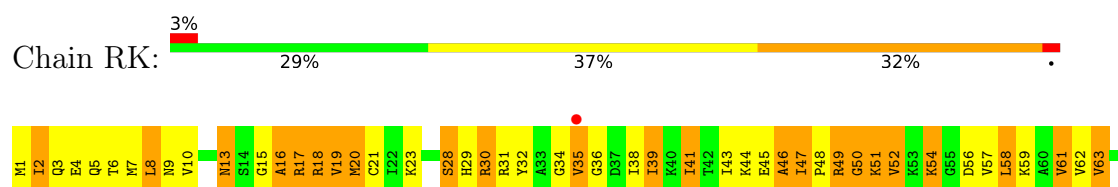
- Molecule 10: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L13

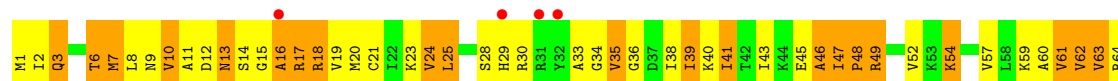


- Molecule 11: 50S ribosomal protein L14

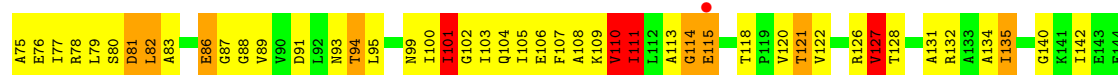
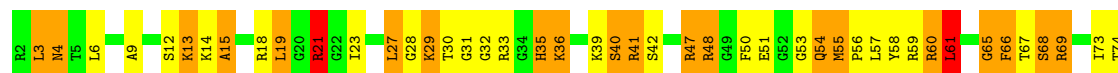




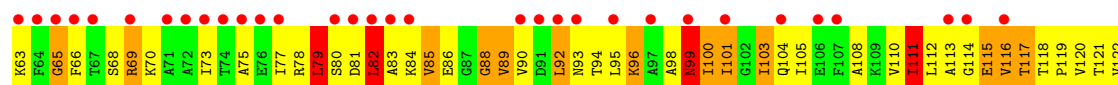
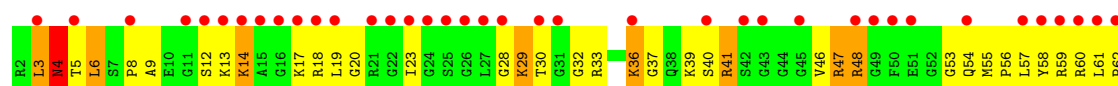
- Molecule 11: 50S ribosomal protein L14



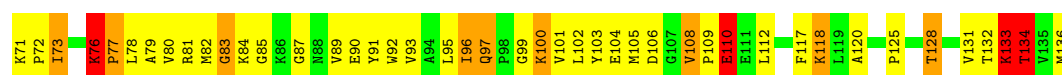
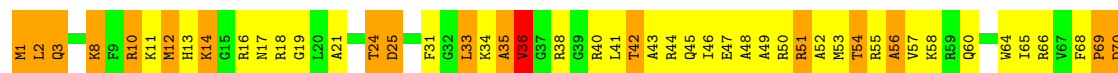
- Molecule 12: 50S ribosomal protein L15



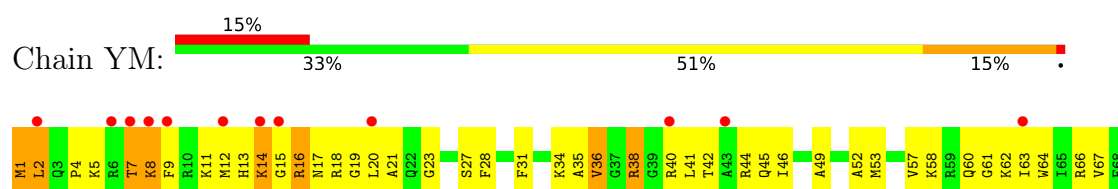
- Molecule 12: 50S ribosomal protein L15



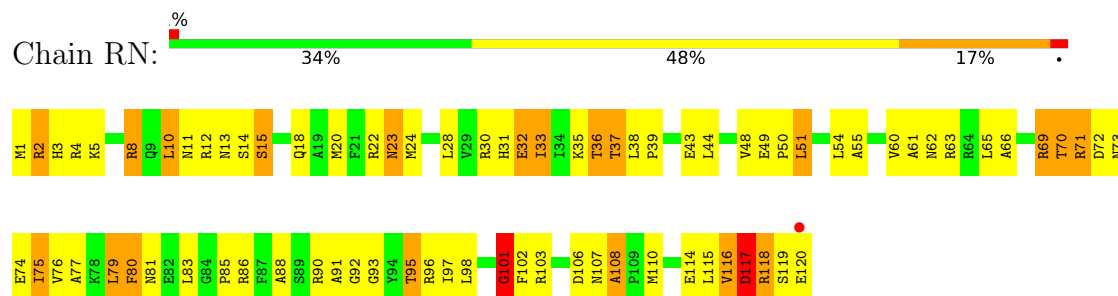
- Molecule 13: 50S ribosomal protein L16



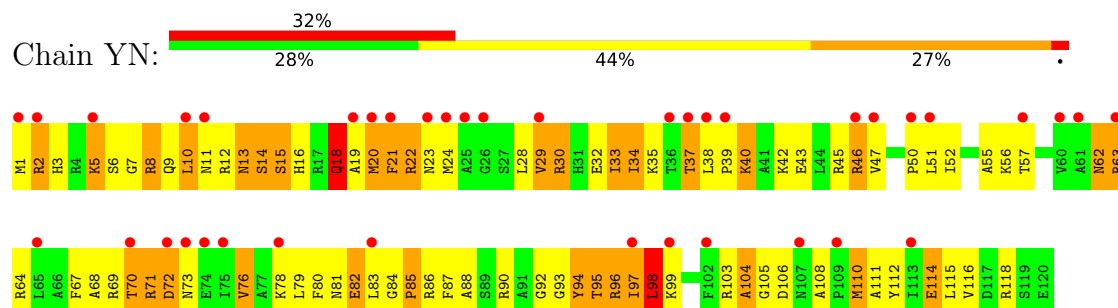
- Molecule 13: 50S ribosomal protein L16



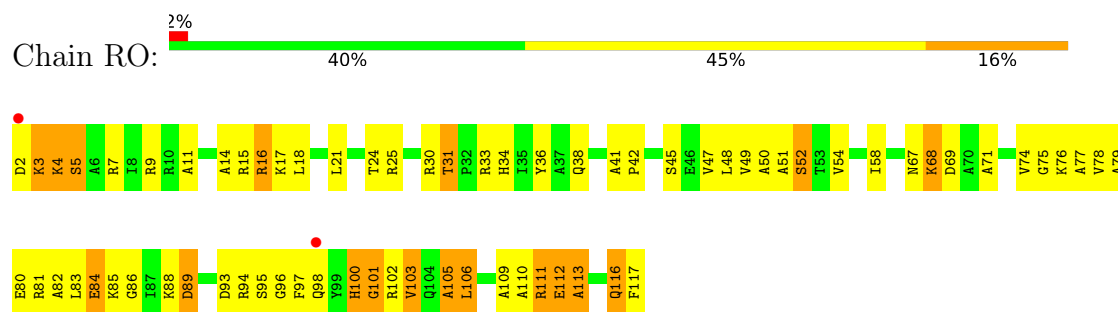
• Molecule 14: 50S ribosomal protein L17



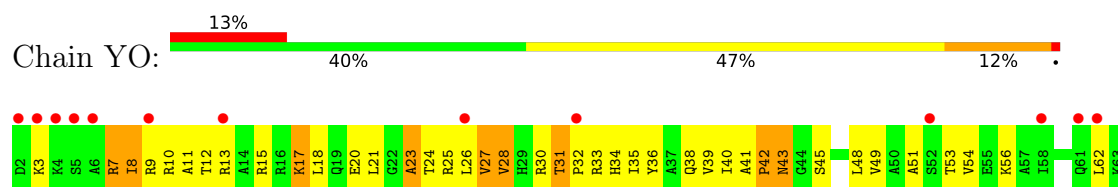
• Molecule 14: 50S ribosomal protein L17

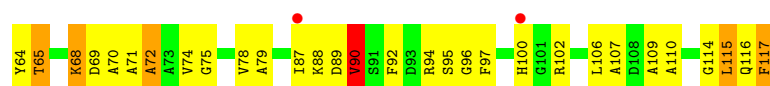


• Molecule 15: 50S ribosomal protein L18



• Molecule 15: 50S ribosomal protein L18

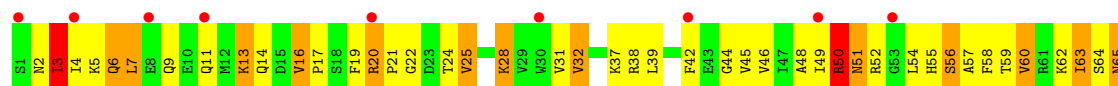




- Molecule 16: 50S ribosomal protein L19



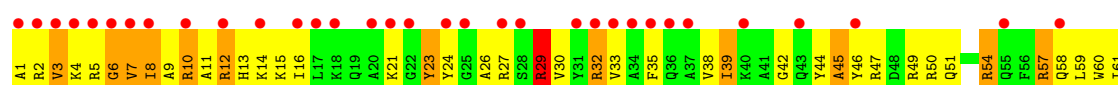
- Molecule 16: 50S ribosomal protein L19



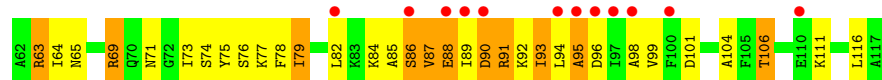
- Molecule 17: 50S ribosomal protein L20

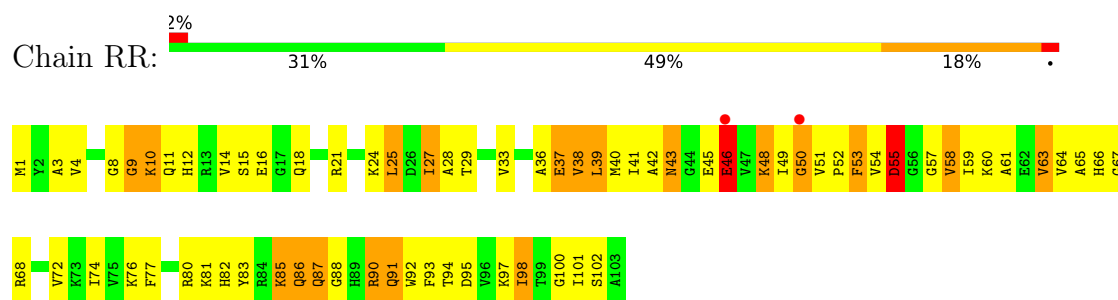


- Molecule 17: 50S ribosomal protein L20

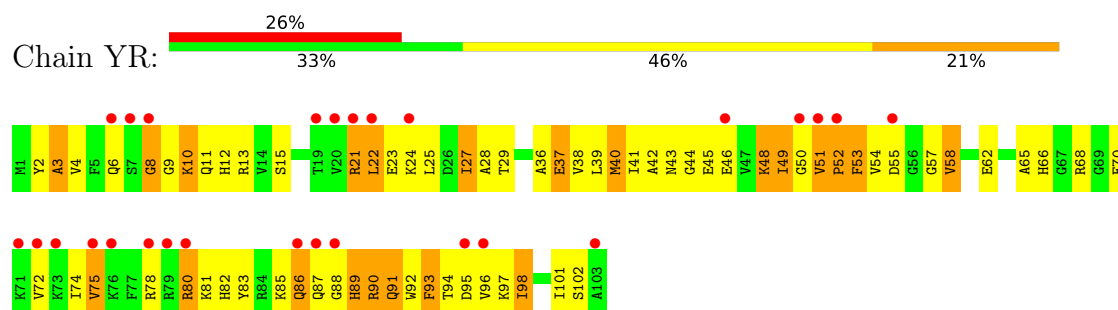


- Molecule 18: 50S ribosomal protein L21

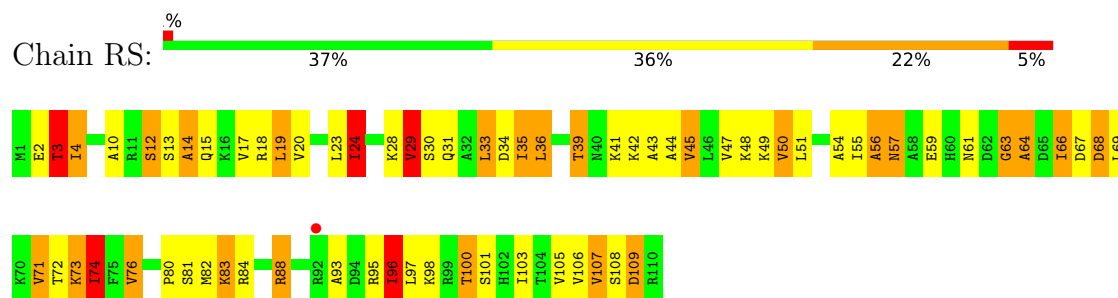




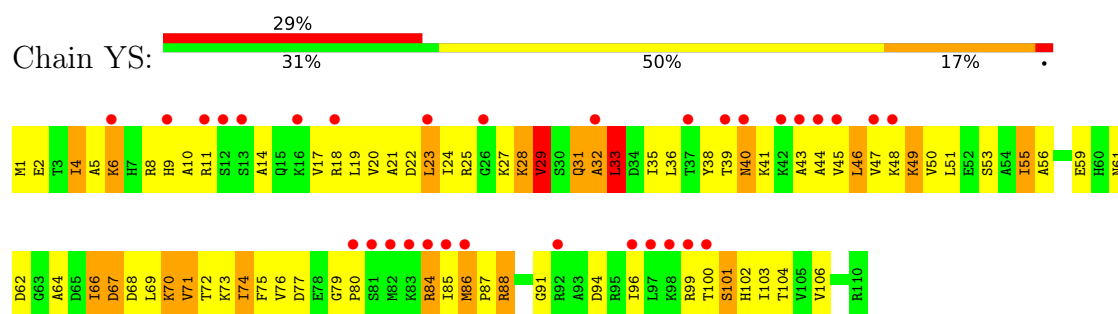
• Molecule 18: 50S ribosomal protein L21



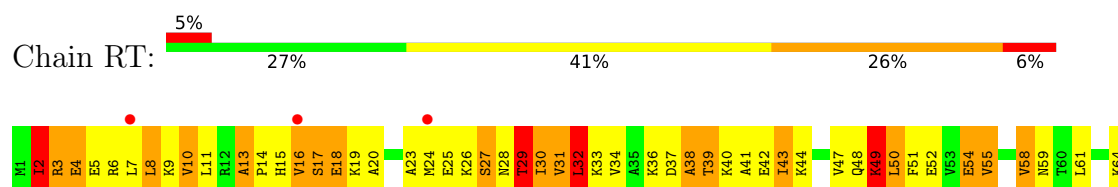
• Molecule 19: 50S ribosomal protein L22



• Molecule 19: 50S ribosomal protein L22

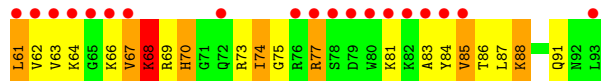
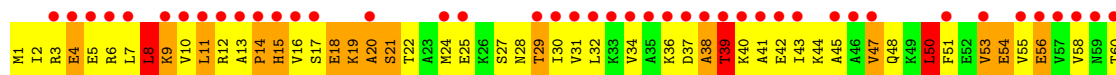


• Molecule 20: 50S ribosomal protein L23

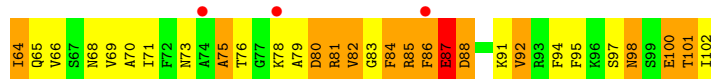




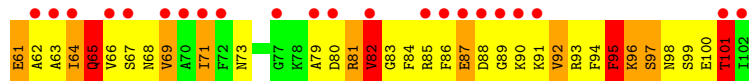
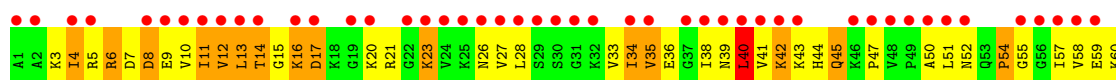
- Molecule 20: 50S ribosomal protein L23



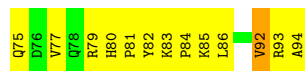
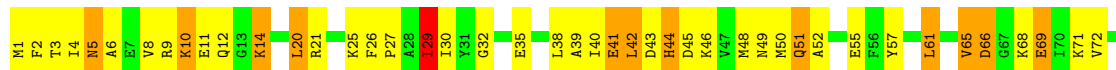
- Molecule 21: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L25

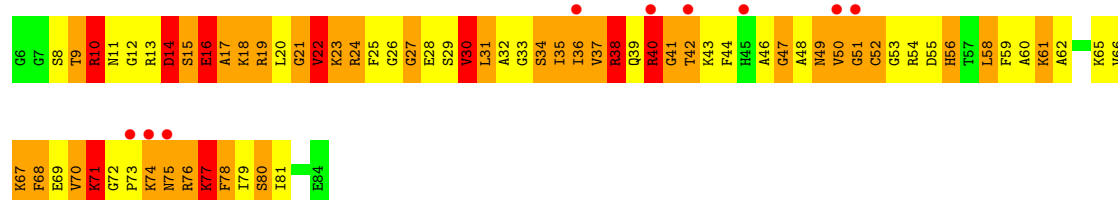


- Molecule 22: 50S ribosomal protein L25

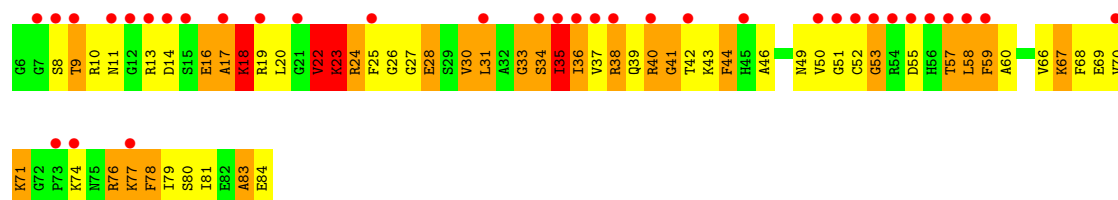




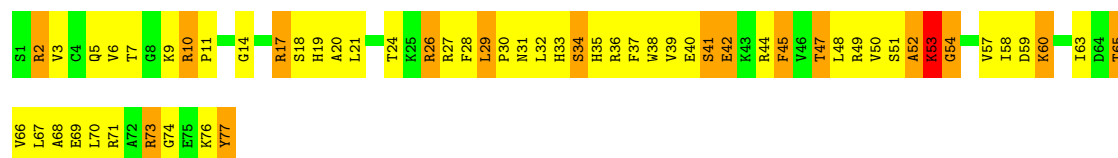
• Molecule 23: 50S ribosomal protein L27



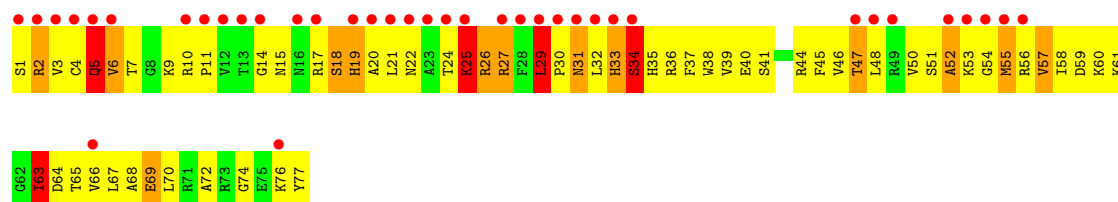
• Molecule 23: 50S ribosomal protein L27



• Molecule 24: 50S ribosomal protein L28



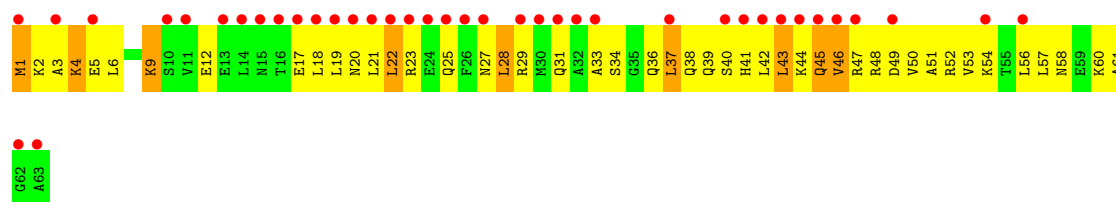
• Molecule 24: 50S ribosomal protein L28



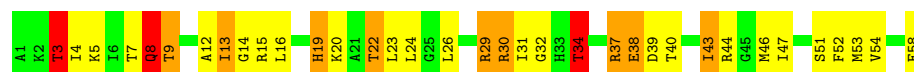
• Molecule 25: 50S ribosomal protein L29



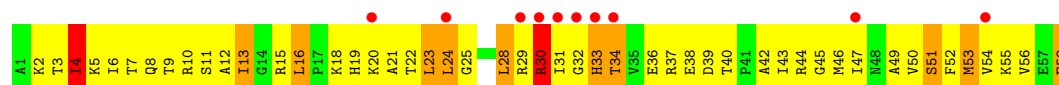
• Molecule 25: 50S ribosomal protein L29



• Molecule 26: 50S ribosomal protein L30



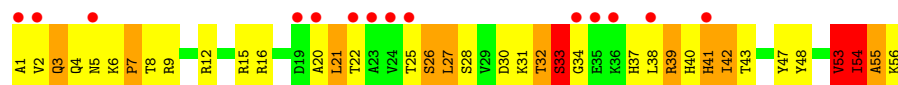
• Molecule 26: 50S ribosomal protein L30



• Molecule 27: 50S ribosomal protein L32

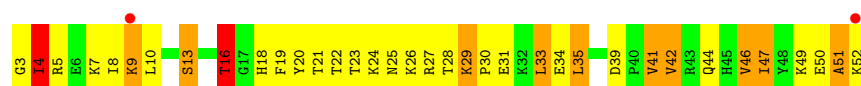


• Molecule 27: 50S ribosomal protein L32

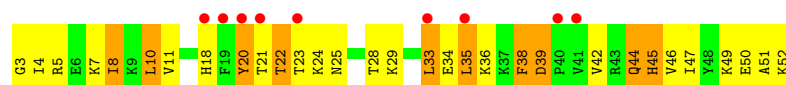


• Molecule 28: 50S ribosomal protein L33

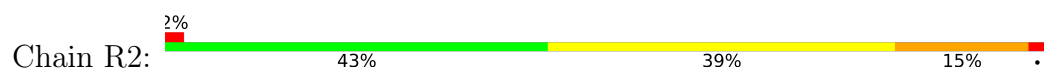




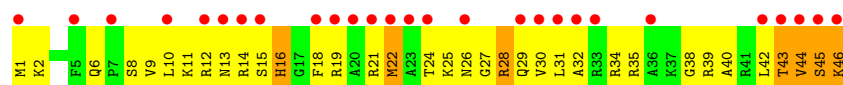
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



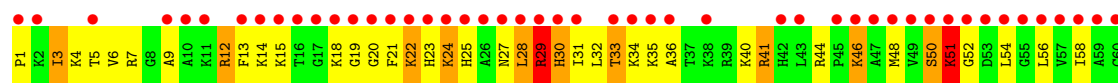
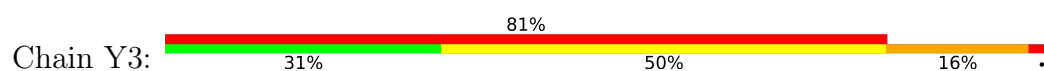
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



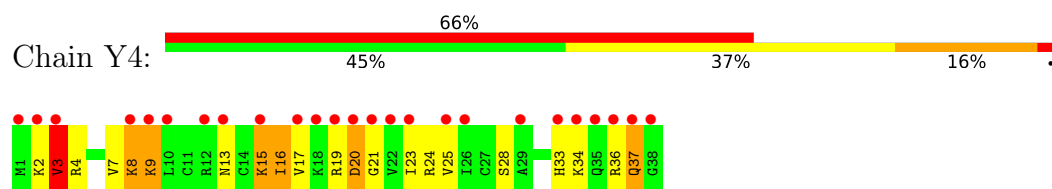
- Molecule 30: 50S ribosomal protein L35



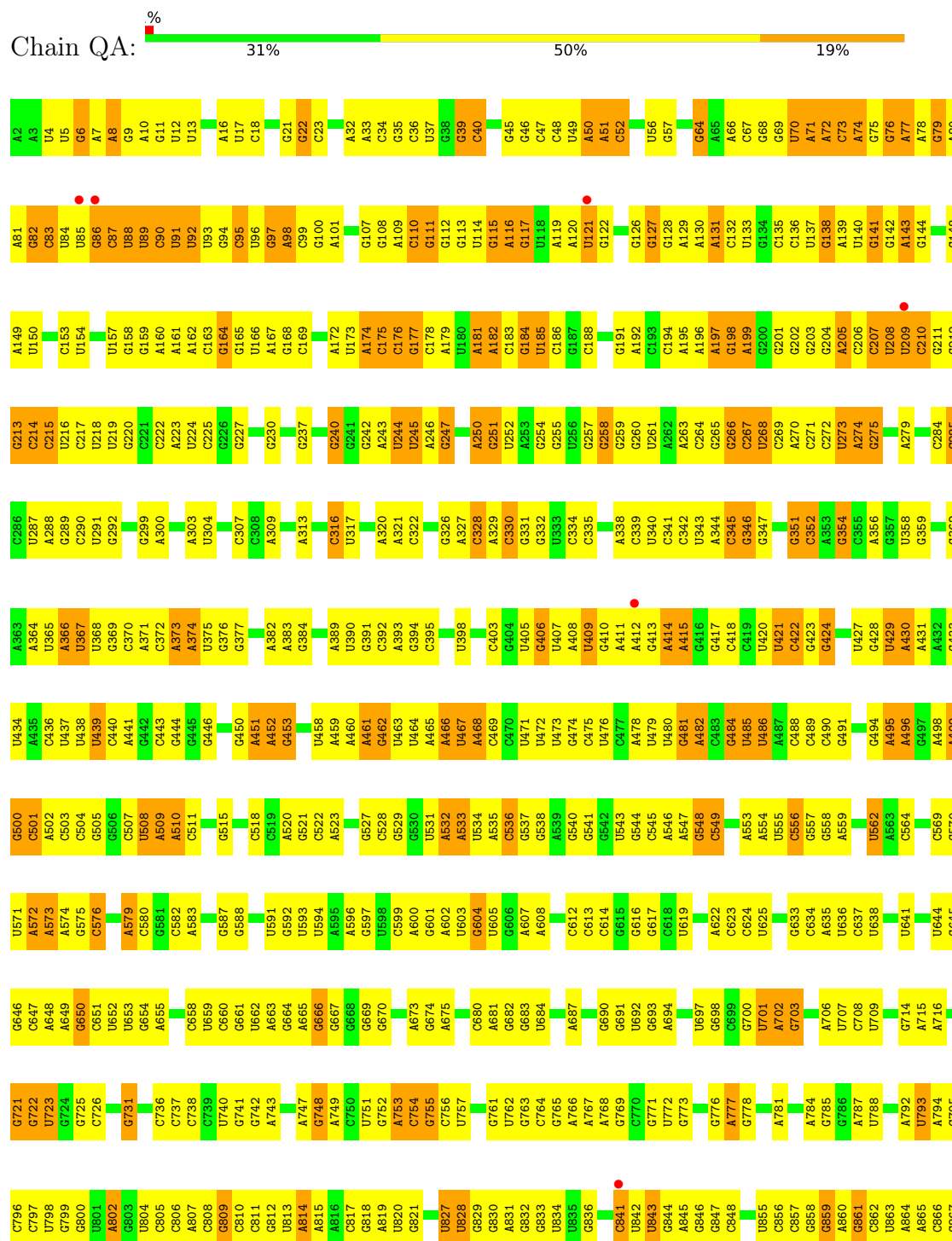
- Molecule 31: 50S ribosomal protein L36

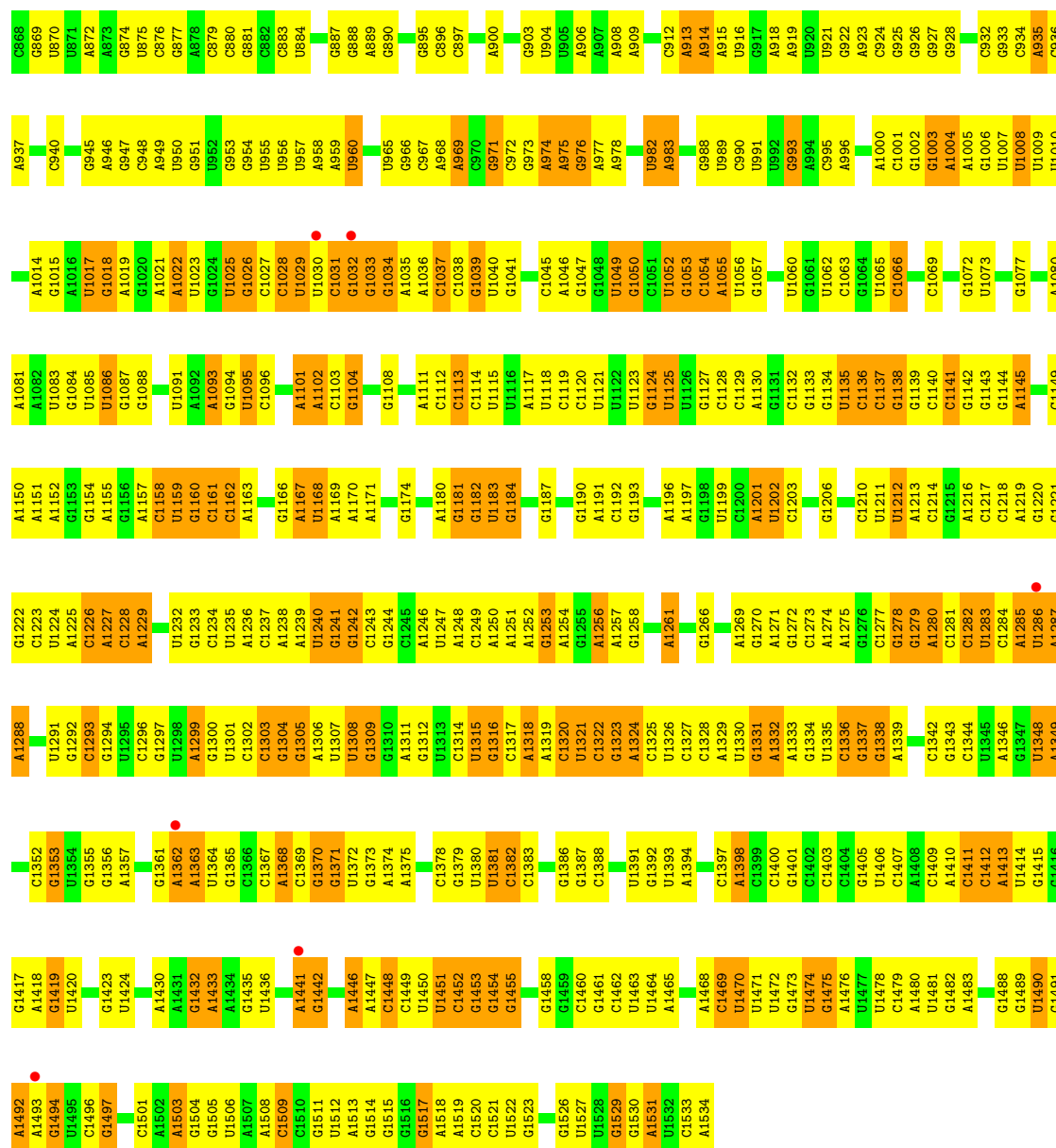


• Molecule 31: 50S ribosomal protein L36

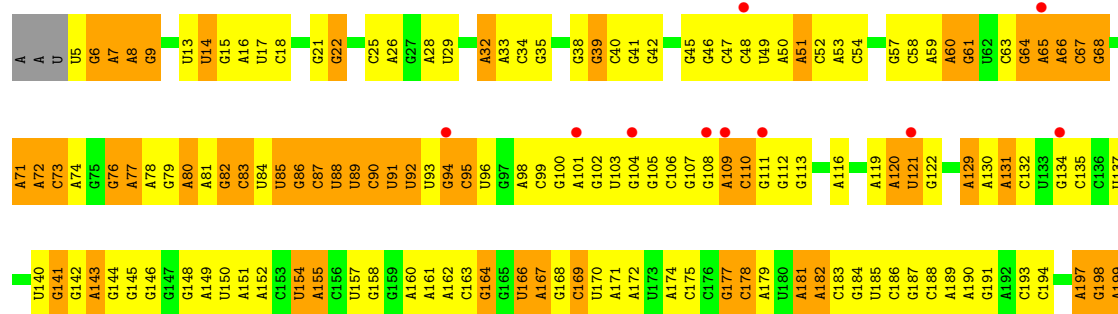


• Molecule 32: 16S rRNA

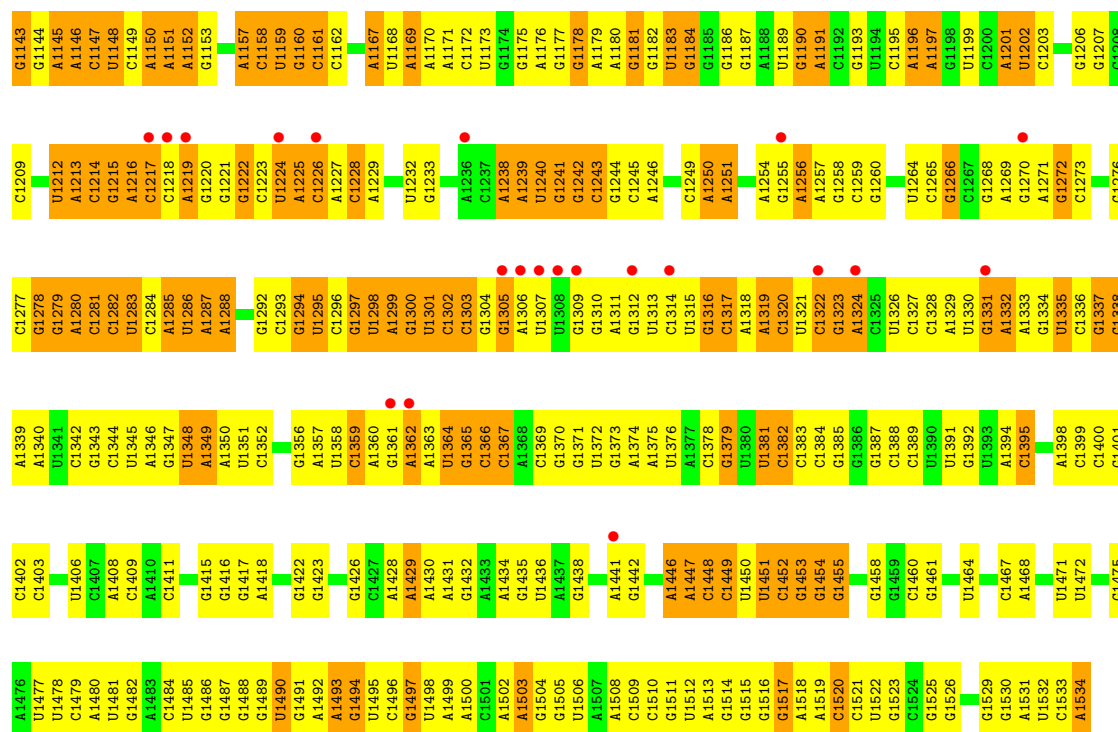




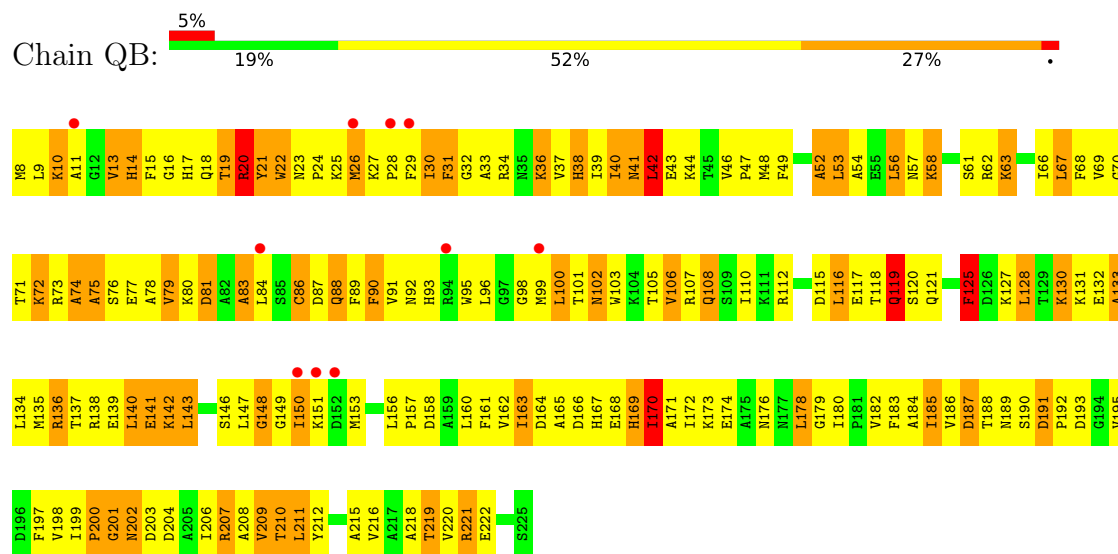
• Molecule 32: 16S rRNA



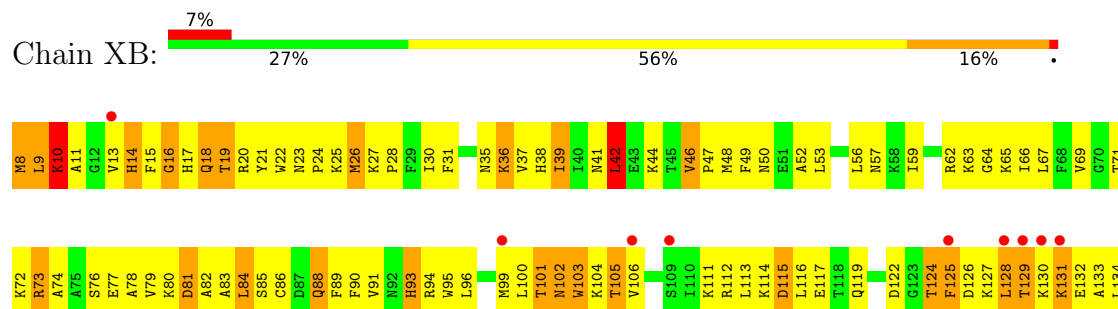
U1078	U1079	A1080	A1081	A1082	U1083	U1084	U1085	U1086	G1087	U1088	G1089	U1090	U1091	A1092	A1093	G1094	U1095	U1096	C1097	C1098	G1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	U1107	G1108	A1111	C1112	C1113	C1114	U1118	C1119	U1123	G1124	U1125	U1126	G1127	C1128	C1129	U1130	G1131	C1132	G1133	U1134	U1135	C1136	C1137	G1138	G1139	U1140	C1141	C1142				
U1017	G1018	A1019	G1020	A1021	A1022	U1023	G1024	U1025	U1026	C1027	C1028	U1029	U1030	C1031	G1032	G1033	G1034	A1035	A1036	C1037	C1038	G1039	U1040	G1041	A1042	G1043	A1046	G1047	U1048	U1049	C1050	C1051	U1052	G1053	C1054	A1055	U1056	G1057	G1058	C1059	U1060	G1061	U1062	C1063	G1064	U1065	C1066	A1067	G1068	C1069	U1070	C1071	G1072	U1073	G1074	U1075	U1076	G1077		
U957	A958	A959	U960	U961	C962	C963	A964	U965	G966	C967	A968	A969	C970	G971	C972	G973	A974	A975	A976	A977	A978	C979	C980	U981	U982	A983	C984	U985	A986	G987	G988	U989	C990	U991	U992	G993	A994	C995	A996	U997	C998	C999	A1000	C1001	G1002	G1003	A1004	A1005	G9945	U9946	G9947	C9948	U9949	U9950	U9951	U9952	G9953	U9954	U9955	U9956
C880	G881	C882	C883	G888	A889	G890	U891	A892	C893	G898	C899	A900	A901	A906	A907	A908	A909	C910	A913	A914	G917	A918	A919	U920	U921	G926	G927	G928	C932	G933	C934	A935	C936	G939	C940	G941	G942	U943	G944	A945	G947	U948	A949	U950	G951	U952	G953	U954	U955	U956										
U813	A814	A815	A816	C817	G818	A819	U820	G821	U822	C823	G824	A825	C826	U827	U828	G829	G830	A831	U834	U835	U836	U837	C841	U842	U843	G844	A845	G846	G847	C848	G849	C853	U854	U855	C856	C857	C858	G861	C862	A865	C866	C867	A872	A873	C874	U875	C876	G877	A878	C879										
C750	U751	G752	A753	C754	G755	C756	U757	A758	A759	G760	G761	G763	C764	G765	A766	G769	C770	G771	U772	G773	G775	G776	A777	G778	C779	A780	A781	A782	G783	A784	G785	G786	A787	A790	G791	A792	U793	A794	C795	C796	U797	U798	G799	U801	A802	G803	U804	C805	C806	A807	C808	C811	G812							
U677	U678	A609	U610	G615	G616	G617	U618	G618	U619	C620	A621	A622	C623	C624	U625	G626	G627	C628	A629	A630	C631	U632	G633	U636	C637	U638	G639	A640	U641	A642	C643	U644	G645	A649	G650	U653	G654	U659	C660	G661	U662	A663	G664	A665	G666	C667	G668	G669	G670	G671	U672	A673	G674	A675	A676					
U531	A532	U534	U535	C536	G537	G542	U543	A546	A547	G550	A554	U555	C556	C557	G558	A559	A560	U561	U562	A563	C564	G567	U568	A569	C570	U571	A572	A573	A574	G575	C576	C577	C578	A579	C580	G581	C582	G587	U590	U591	A595	A596	G597	U598	C599	A602	U603	G604	U605											
A468	C469	C470	U471	U472	U473	G474	C475	U476	C477	A478	U479	U480	G481	G484	U485	U486	A487	C488	C489	C490	C491	C492	A493	G494	A495	U496	C497	A498	A499	G500	C501	A502	C503	C504	G505	A509	A510	C511	U512	C513	C514	G515	U516	G517	C518	C519	A520	G521	C522	A523	G524	C525	U526	G527	C528	G529				
A336	G337	C338	C339	U343	A344	C345	U346	C347	G348	A349	U350	C351	C352	A353	G354	C355	A356	C357	U358	C359	C360	G361	G362	A366	U367	U368	A369	C370	A371	C372	A373	U374	U375	G376	G377	G378	C379	C380	C381	A382	A383	G384	C385	C386	U387	G388	A389	U390	C391	C392	A393	G394	C395	C396	U398	C399				
C403	G404	U405	U406	U407	A408	U409	G410	A411	C412	G413	A414	A415	G416	G417	C418	U421	C422	G423	G424	G425	U426	U427	G428	A430	U431	A435	A436	U437	U438	U439	G442	C443	G444	G445	G446	G447	A448	A451	A452	G453	G454	G455	A456	G457	U458	A459	A460	A461	A462	U463	U464	A465	A466	U467						
C267	U268	C269	A270	C271	A274	C275	U276	C277	U278	G279	C280	G281	A282	U283	C284	C285	C286	U287	A288	C289	C290	U291	G292	G295	U296	G297	A298	C299	A300	C301	G302	G305	A306	C312	A313	C314	C315	C316	U317	G318	G319	A320	C321	C322	G326	C327	A327	C328	A329	G260	U261	A263	C264	G265	G266					

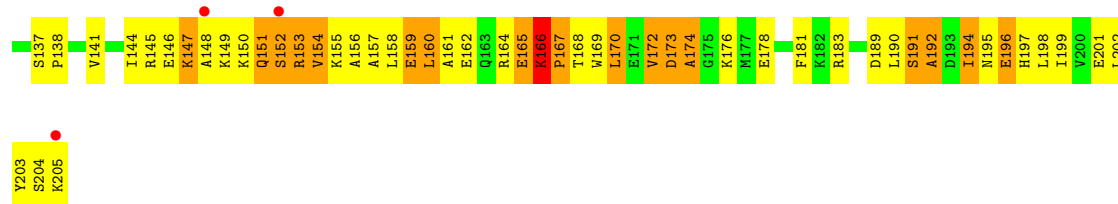


• Molecule 33: 30S ribosomal protein S2

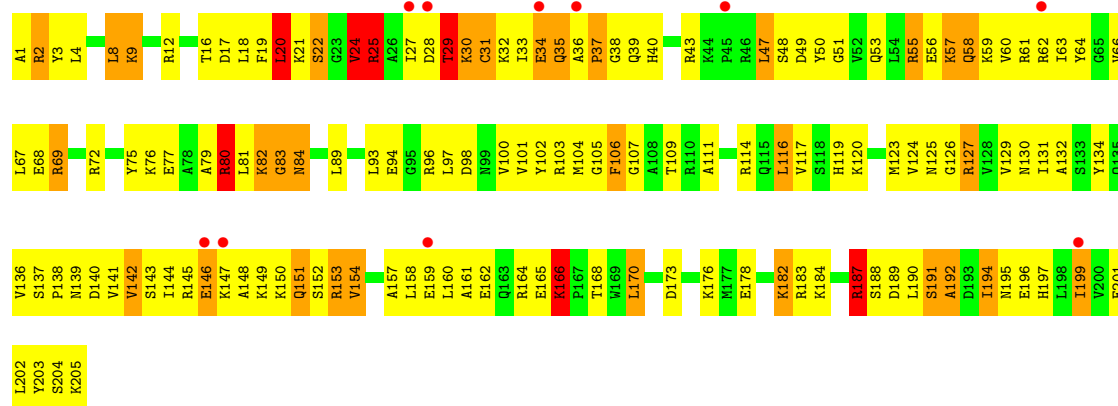


• Molecule 33: 30S ribosomal protein S2

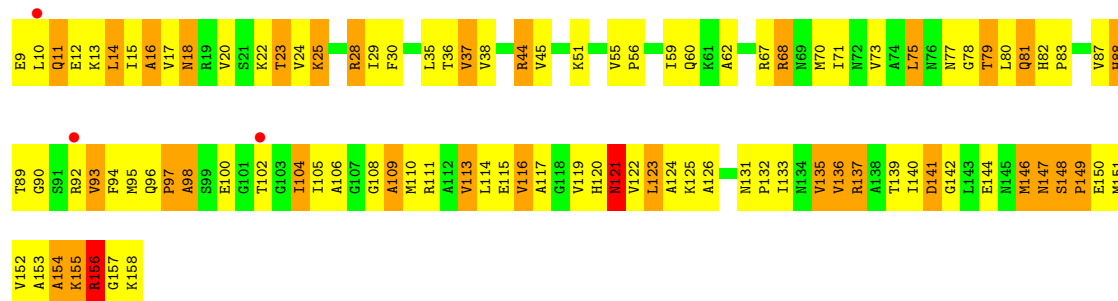




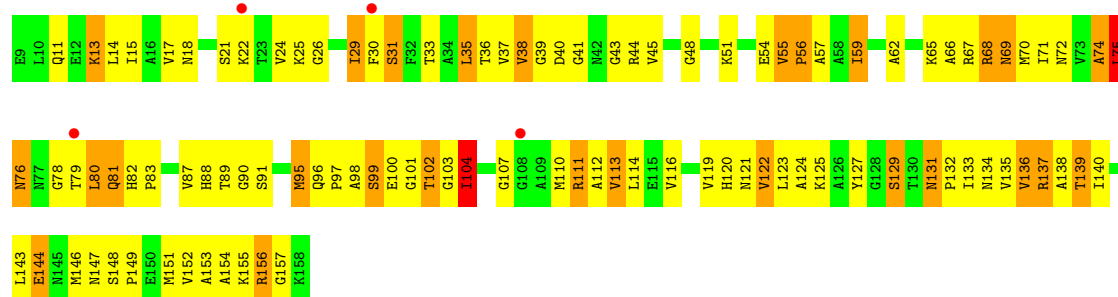
• Molecule 35: 30S ribosomal protein S4



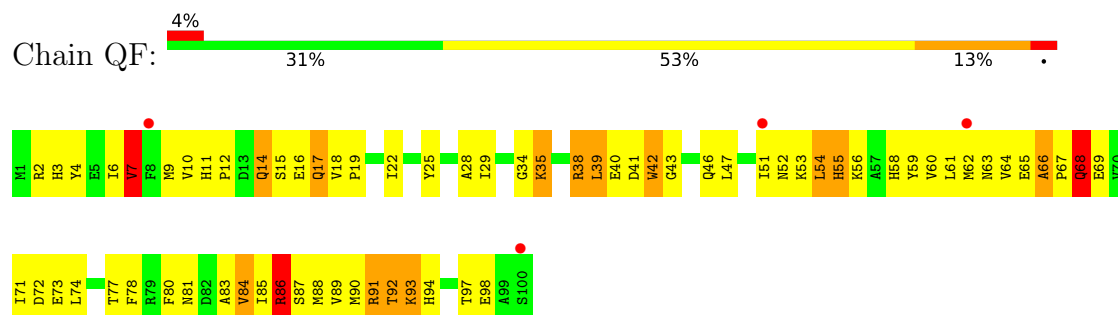
• Molecule 36: 30S ribosomal protein S5



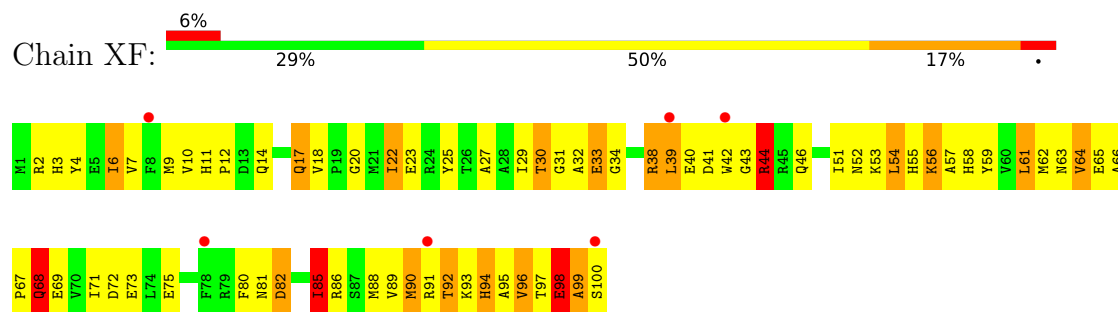
• Molecule 36: 30S ribosomal protein S5



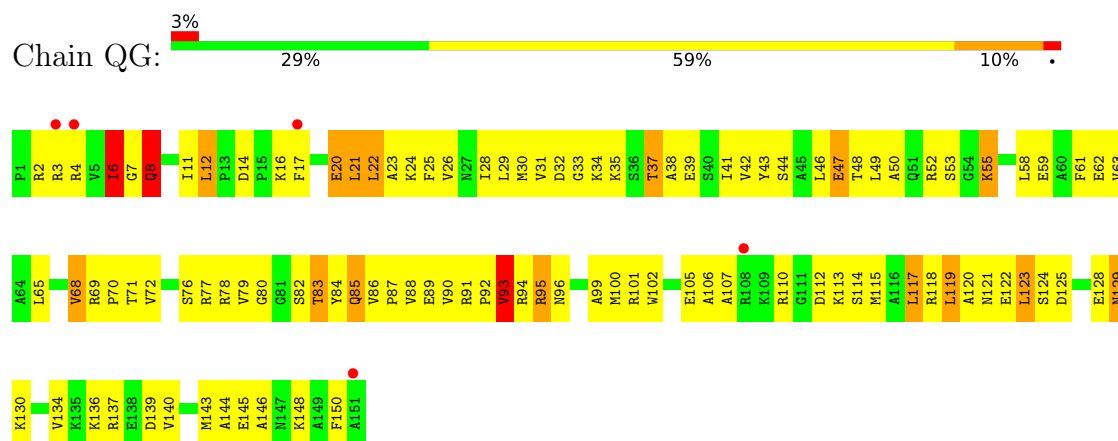
- Molecule 37: 30S ribosomal protein S6



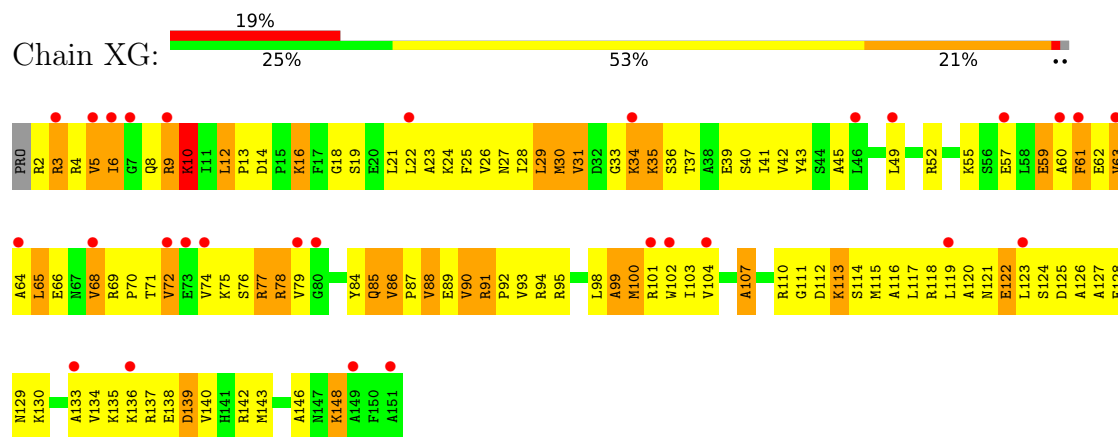
- Molecule 37: 30S ribosomal protein S6



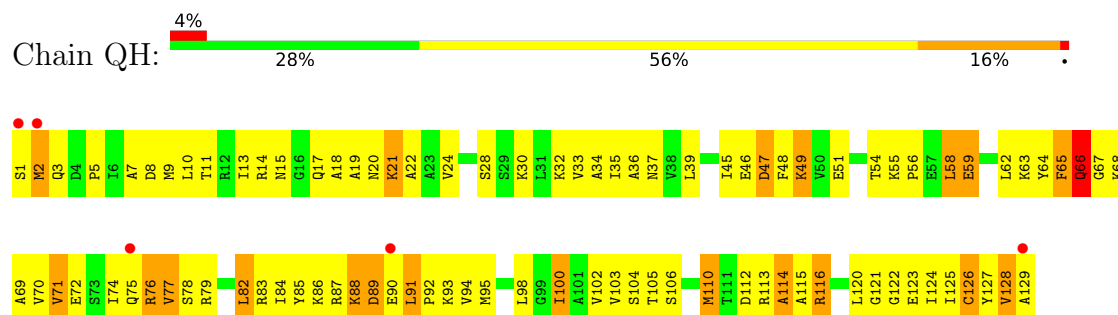
- Molecule 38: 30S ribosomal protein S7



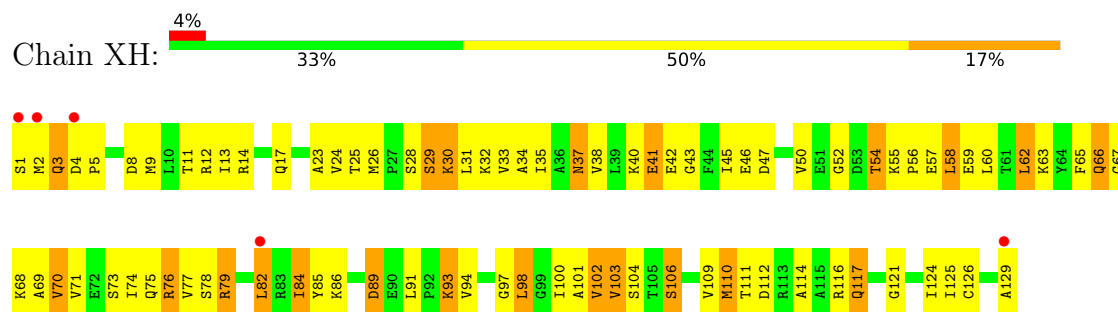
- Molecule 38: 30S ribosomal protein S7



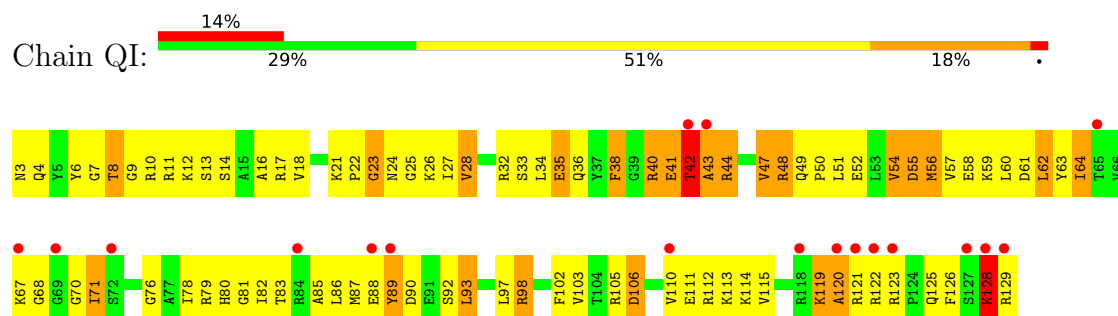
- Molecule 39: 30S ribosomal protein S8



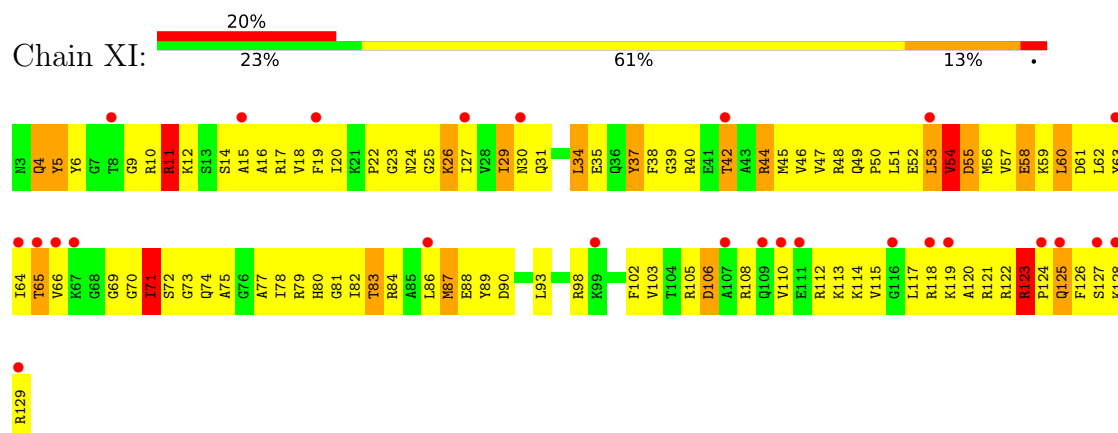
- Molecule 39: 30S ribosomal protein S8



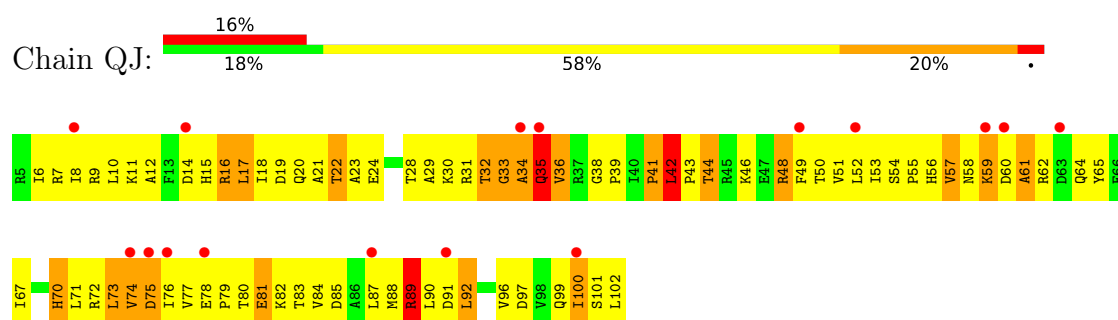
- Molecule 40: 30S ribosomal protein S9



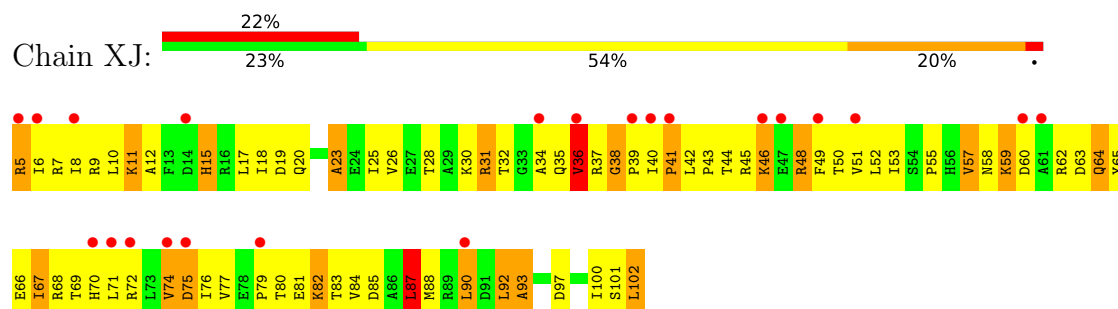
- Molecule 40: 30S ribosomal protein S9



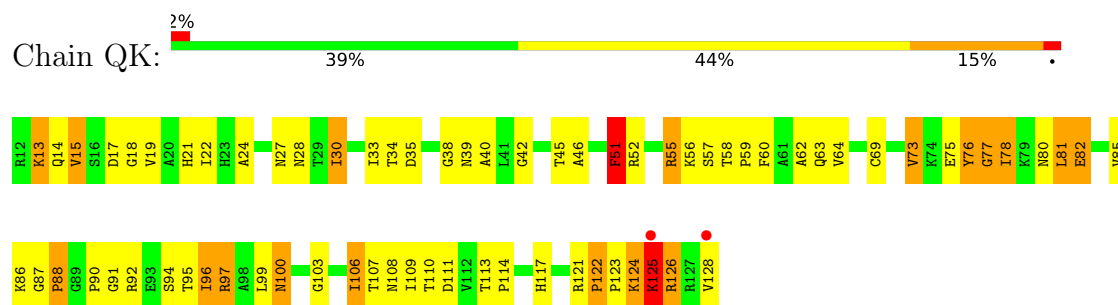
- Molecule 41: 30S ribosomal protein S10



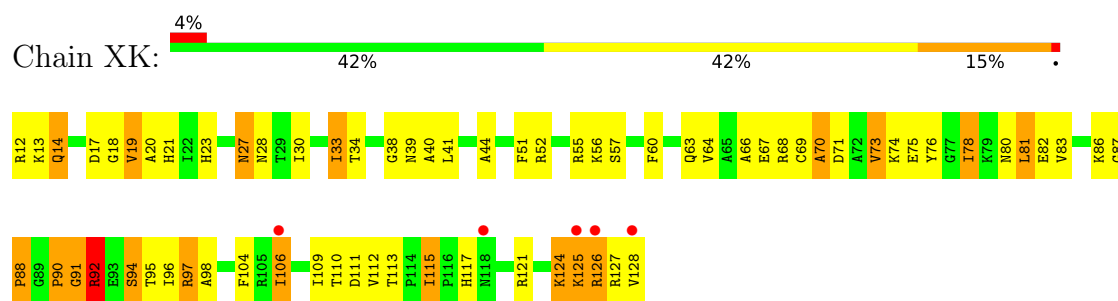
• Molecule 41: 30S ribosomal protein S10



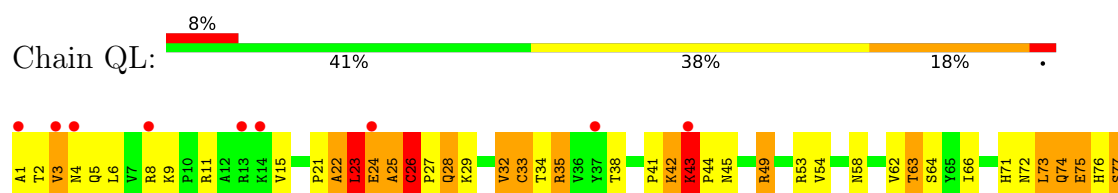
• Molecule 42: 30S ribosomal protein S11



• Molecule 42: 30S ribosomal protein S11

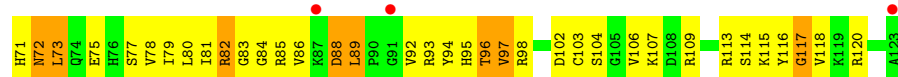
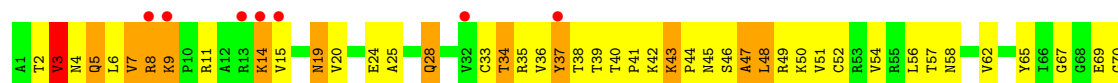


• Molecule 43: 30S ribosomal protein S12

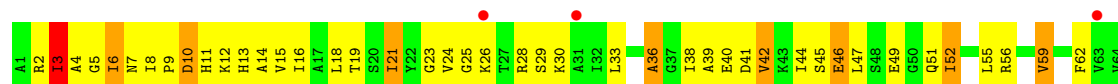




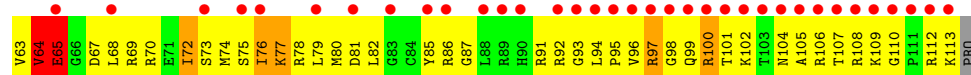
• Molecule 43: 30S ribosomal protein S12



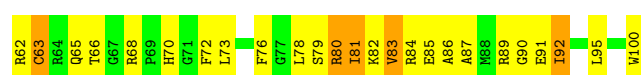
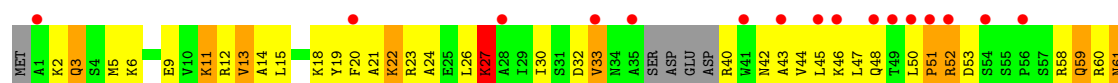
• Molecule 44: 30S ribosomal protein S13



• Molecule 44: 30S ribosomal protein S13

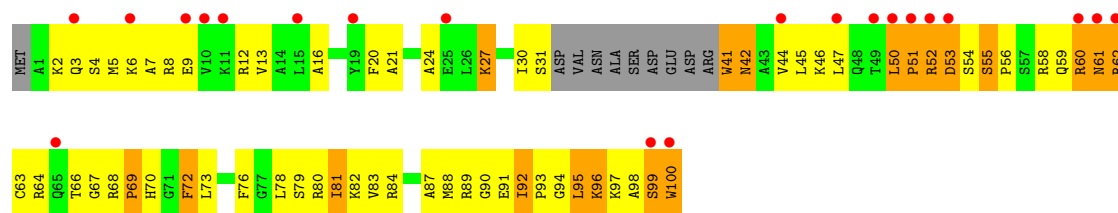


• Molecule 45: 30S ribosomal protein S14

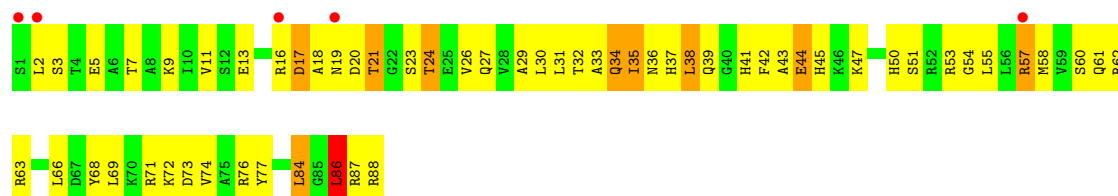


• Molecule 45: 30S ribosomal protein S14

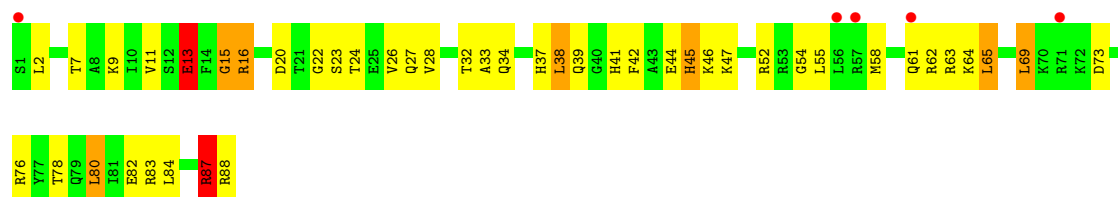




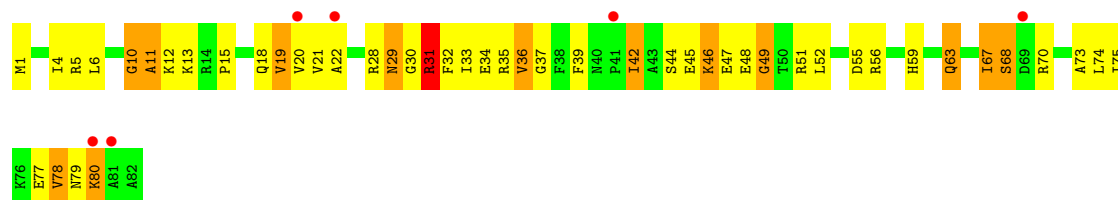
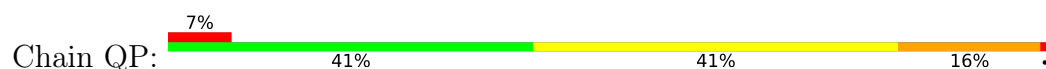
• Molecule 46: 30S ribosomal protein S15



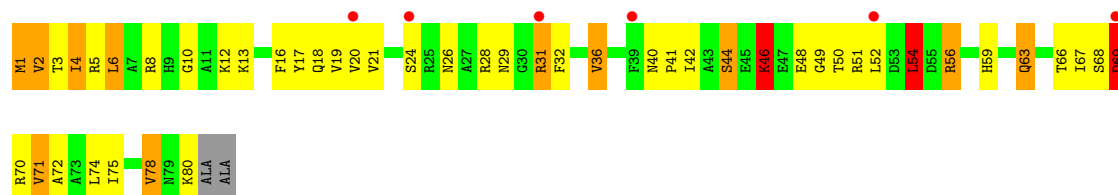
• Molecule 46: 30S ribosomal protein S15



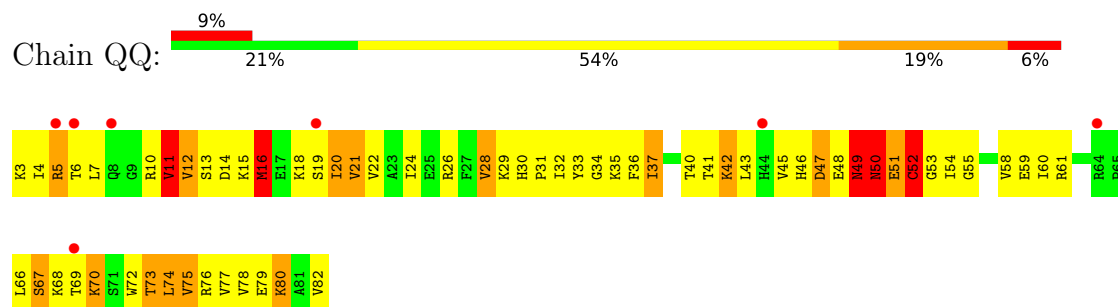
• Molecule 47: 30S ribosomal protein S16



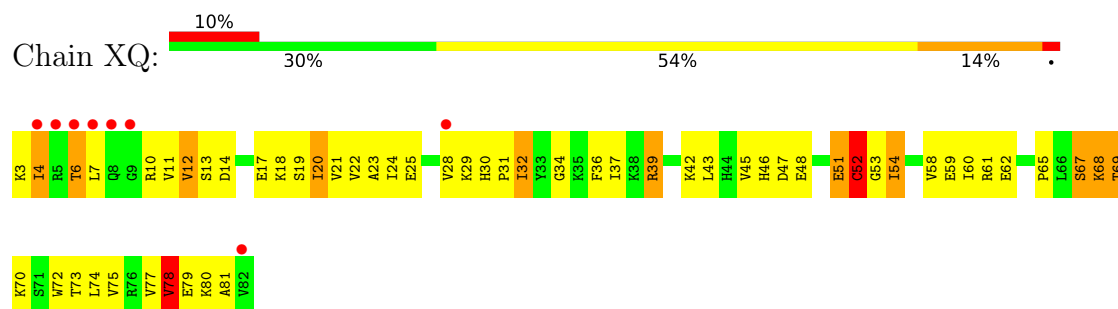
• Molecule 47: 30S ribosomal protein S16



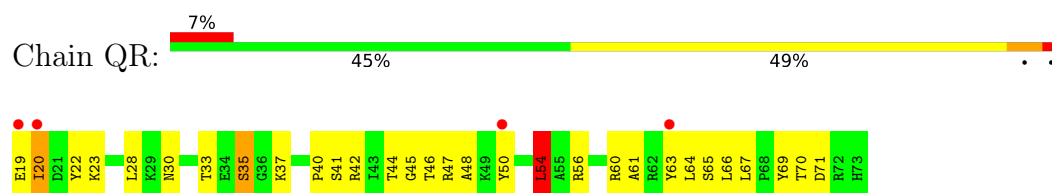
- Molecule 48: 30S ribosomal protein S17



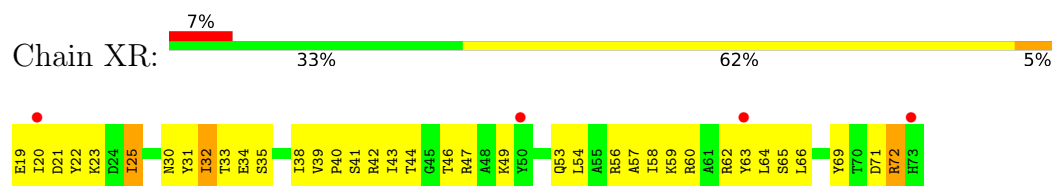
- Molecule 48: 30S ribosomal protein S17



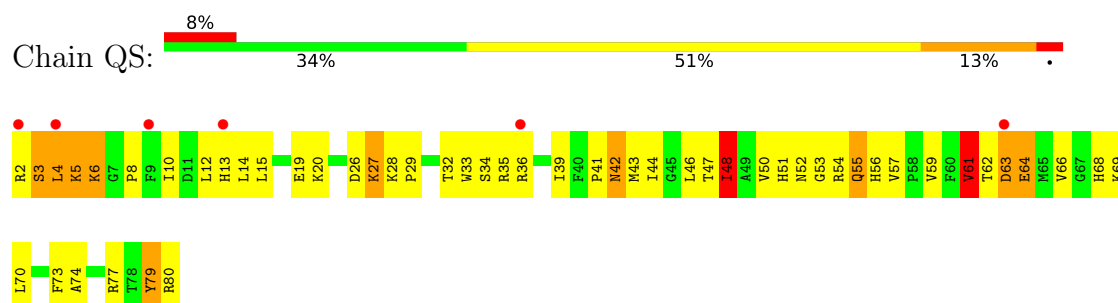
- Molecule 49: 30S ribosomal protein S18



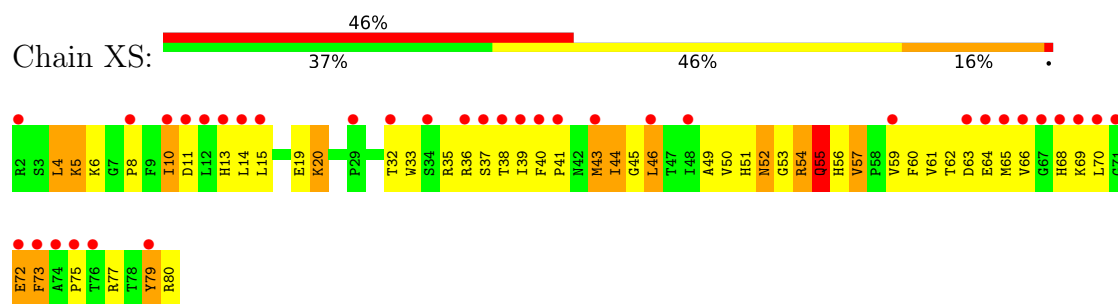
- Molecule 49: 30S ribosomal protein S18



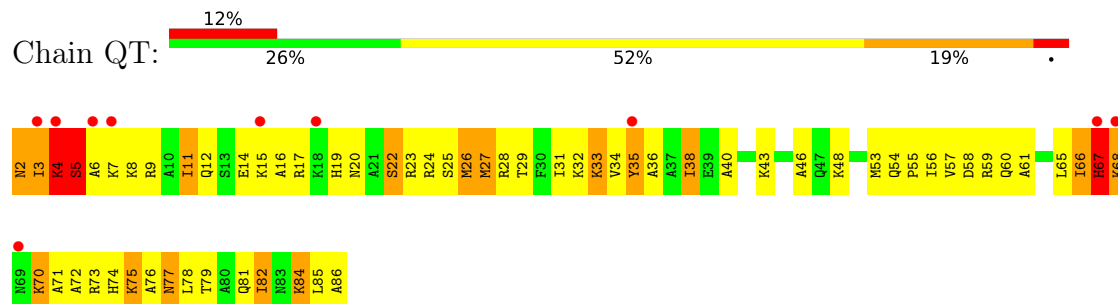
- Molecule 50: 30S ribosomal protein S19



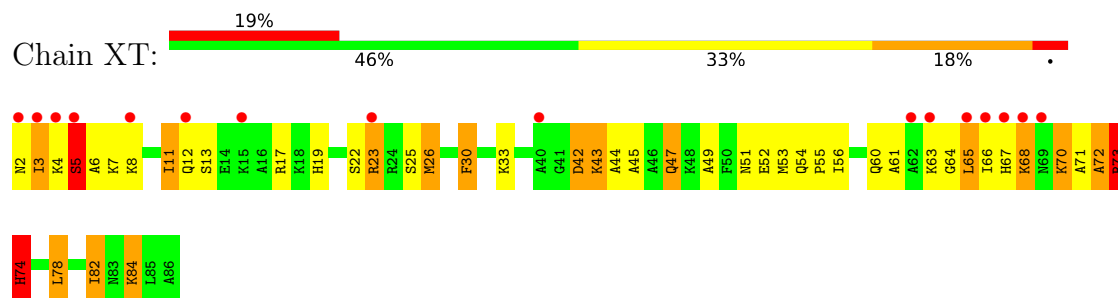
- Molecule 50: 30S ribosomal protein S19



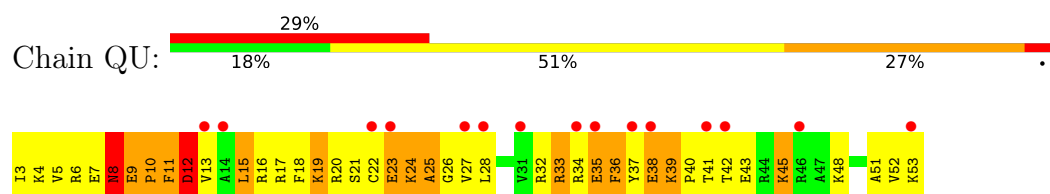
- Molecule 51: 30S ribosomal protein S20



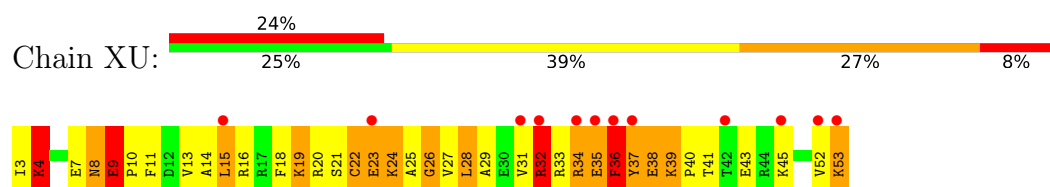
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein S21



- Molecule 52: 30S ribosomal protein S21



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) 95.8 (69.78-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (1.00%)	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)	0.25 , 90.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EM1, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	RA	0.42	0/68626	0.46	0/107056
1	YA	0.23	0/68314	0.46	0/106569
2	RB	0.37	0/2828	0.41	0/4410
2	YB	0.18	0/2803	0.47	0/4371
3	RC	0.60	0/2121	1.15	18/2852 (0.6%)
3	YC	0.42	0/2121	0.92	6/2852 (0.2%)
4	RD	0.75	0/1586	1.18	11/2134 (0.5%)
4	YD	0.40	0/1586	0.90	6/2134 (0.3%)
5	RE	0.57	0/1571	0.99	7/2113 (0.3%)
5	YE	0.35	0/1571	0.85	4/2113 (0.2%)
6	RF	0.41	0/1434	0.87	4/1926 (0.2%)
6	YF	0.33	0/1444	0.84	3/1937 (0.2%)
7	RG	0.54	0/1343	1.01	4/1816 (0.2%)
7	YG	0.33	0/1343	0.84	4/1816 (0.2%)
8	RH	0.44	0/1122	0.91	3/1515 (0.2%)
8	YH	0.41	0/1122	0.84	2/1515 (0.1%)
9	RI	0.35	0/1046	0.90	1/1410 (0.1%)
9	YI	0.36	0/1046	0.90	4/1410 (0.3%)
10	RJ	0.79	1/1152 (0.1%)	1.30	17/1551 (1.1%)
10	YJ	0.40	0/1152	0.89	1/1551 (0.1%)
11	RK	0.69	0/947	1.09	3/1268 (0.2%)
11	YK	0.44	0/947	0.92	2/1268 (0.2%)
12	RL	0.63	1/1054 (0.1%)	1.14	6/1403 (0.4%)
12	YL	0.38	0/1054	0.85	1/1403 (0.1%)
13	RM	0.65	0/1093	1.09	7/1460 (0.5%)
13	YM	0.37	0/1093	0.90	5/1460 (0.3%)
14	RN	0.66	0/973	1.03	3/1301 (0.2%)
14	YN	0.40	0/973	0.92	5/1301 (0.4%)
15	RO	0.56	0/902	0.91	1/1209 (0.1%)
15	YO	0.32	0/902	0.73	0/1209
16	RP	0.63	0/929	1.10	6/1242 (0.5%)
16	YP	0.40	0/929	0.87	5/1242 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	RQ	0.78	0/960	1.06	2/1278 (0.2%)
17	YQ	0.39	0/960	0.79	1/1278 (0.1%)
18	RR	0.70	0/829	1.11	4/1107 (0.4%)
18	YR	0.38	0/829	0.78	0/1107
19	RS	0.74	0/864	1.06	1/1156 (0.1%)
19	YS	0.42	0/864	0.83	1/1156 (0.1%)
20	RT	0.63	0/744	1.11	5/994 (0.5%)
20	YT	0.36	0/744	0.86	1/994 (0.1%)
21	RU	0.56	0/787	1.06	8/1051 (0.8%)
21	YU	0.37	0/787	0.81	0/1051
22	RV	0.57	0/766	0.92	2/1025 (0.2%)
22	YV	0.33	0/766	0.76	0/1025
23	RW	0.88	2/603 (0.3%)	1.26	5/797 (0.6%)
23	YW	0.38	0/603	0.82	0/797
24	RX	0.59	0/635	0.99	2/848 (0.2%)
24	YX	0.39	0/635	0.98	4/848 (0.5%)
25	RY	0.47	0/510	0.87	3/677 (0.4%)
25	YY	0.29	0/510	0.78	0/677
26	RZ	0.86	2/453 (0.4%)	1.14	1/605 (0.2%)
26	YZ	0.38	0/453	0.87	1/605 (0.2%)
27	R0	0.63	0/450	0.96	0/599
27	Y0	0.35	0/450	0.78	0/599
28	R1	0.48	0/416	0.91	0/554
28	Y1	0.39	0/416	0.76	2/554 (0.4%)
29	R2	0.70	0/380	1.05	1/498 (0.2%)
29	Y2	0.39	0/380	0.92	2/498 (0.4%)
30	R3	0.61	0/513	1.04	1/676 (0.1%)
30	Y3	0.39	0/513	0.89	0/676
31	R4	0.75	0/303	1.12	2/397 (0.5%)
31	Y4	0.60	1/303 (0.3%)	0.73	0/397
32	QA	0.26	0/36834	0.43	0/57462
32	XA	0.24	0/36762	0.44	0/57350
33	QB	0.38	0/1735	0.87	6/2338 (0.3%)
33	XB	0.34	0/1735	0.83	3/2338 (0.1%)
34	QC	0.39	0/1651	0.88	5/2225 (0.2%)
34	XC	0.35	0/1651	0.80	0/2225
35	QD	0.39	0/1665	0.84	4/2227 (0.2%)
35	XD	0.51	0/1665	0.93	4/2227 (0.2%)
36	QE	0.49	0/1118	0.95	3/1504 (0.2%)
36	XE	0.47	0/1118	0.99	5/1504 (0.3%)
37	QF	0.40	0/835	0.77	2/1128 (0.2%)
37	XF	0.40	0/835	0.82	1/1128 (0.1%)
38	QG	0.36	0/1195	0.81	0/1602

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	XG	0.32	0/1187	0.87	4/1591 (0.3%)
39	QH	0.45	0/989	0.94	8/1326 (0.6%)
39	XH	0.39	0/989	0.85	3/1326 (0.2%)
40	QI	0.35	0/1034	0.82	1/1375 (0.1%)
40	XI	0.34	0/1034	0.85	2/1375 (0.1%)
41	QJ	0.40	0/796	0.82	0/1077
41	XJ	0.38	0/796	0.86	1/1077 (0.1%)
42	QK	0.40	0/893	0.91	2/1205 (0.2%)
42	XK	0.39	0/893	0.92	1/1205 (0.1%)
43	QL	0.46	0/969	1.00	6/1300 (0.5%)
43	XL	0.44	0/969	0.94	5/1300 (0.4%)
44	QM	0.36	0/892	0.82	1/1193 (0.1%)
44	XM	0.29	0/884	0.73	0/1181
45	QN	0.36	0/785	0.80	2/1043 (0.2%)
45	XN	0.30	0/746	0.79	2/990 (0.2%)
46	QO	0.40	0/722	0.75	0/964
46	XO	0.37	0/722	0.76	0/964
47	QP	0.38	0/659	0.84	0/884
47	XP	0.40	0/648	0.80	0/870
48	QQ	0.47	0/657	0.88	0/881
48	XQ	0.43	0/657	0.85	0/881
49	QR	0.39	0/462	0.84	0/621
49	XR	0.41	0/462	0.81	0/621
50	QS	0.34	0/652	0.78	1/877 (0.1%)
50	XS	0.28	0/652	0.81	1/877 (0.1%)
51	QT	0.47	0/671	0.94	3/888 (0.3%)
51	XT	0.34	0/671	0.92	4/888 (0.5%)
52	QU	0.43	0/430	0.88	0/570
52	XU	0.45	0/430	0.97	0/570
All	All	0.37	7/306703 (0.0%)	0.61	268/458519 (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 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	RZ	19	HIS	CG-ND1	6.69	1.45	1.38
23	RW	32	ALA	CA-CB	6.43	1.64	1.53
10	RJ	55	ILE	CA-CB	6.18	1.61	1.54
31	Y4	33	HIS	CE1-NE2	-6.04	1.26	1.32
26	RZ	19	HIS	ND1-CE1	-6.02	1.26	1.32

The worst 5 of 268 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	QC	204	GLY	N-CA-C	12.13	126.21	110.20
10	RJ	64	VAL	N-CA-C	11.46	121.75	112.12
21	RU	82	VAL	N-CA-C	11.01	122.13	111.67
4	RD	151	THR	CA-C-N	-10.94	108.51	119.56
4	RD	151	THR	C-N-CA	-10.94	108.51	119.56

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 ⓘ

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	3670	0
2	RB	2529	0	1281	58	0
2	YB	2507	0	1270	166	0
3	RC	2082	0	2157	212	0
3	YC	2082	0	2157	232	0
4	RD	1565	0	1616	211	0
4	YD	1565	0	1616	210	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	RE	1552	0	1619	159	0
5	YE	1552	0	1619	197	0
6	RF	1410	0	1447	133	0
6	YF	1420	0	1460	170	0
7	RG	1323	0	1374	144	0
7	YG	1323	0	1374	149	0
8	RH	1111	0	1148	105	0
8	YH	1111	0	1148	128	0
9	RI	1032	0	1088	113	0
9	YI	1032	0	1088	86	0
10	RJ	1129	0	1162	157	0
10	YJ	1129	0	1162	137	0
11	RK	938	0	1012	99	0
11	YK	938	0	1012	112	0
12	RL	1045	0	1117	115	0
12	YL	1045	0	1117	147	0
13	RM	1074	0	1157	101	0
13	YM	1074	0	1157	101	0
14	RN	960	0	1000	81	0
14	YN	960	0	1000	148	0
15	RO	892	0	923	53	0
15	YO	892	0	923	79	0
16	RP	917	0	965	128	0
16	YP	917	0	965	126	0
17	RQ	947	0	1022	145	0
17	YQ	947	0	1022	127	0
18	RR	816	0	839	105	0
18	YR	816	0	839	97	0
19	RS	857	0	922	84	0
19	YS	857	0	922	70	0
20	RT	738	0	807	113	0
20	YT	738	0	807	109	0
21	RU	779	0	834	65	0
21	YU	779	0	834	101	0
22	RV	753	0	780	53	0
22	YV	753	0	780	70	0
23	RW	596	0	610	196	0
23	YW	596	0	610	132	0
24	RX	625	0	655	57	0
24	YX	625	0	655	81	0
25	RY	509	0	543	45	0
25	YY	509	0	543	82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	RZ	449	0	491	37	0
26	YZ	449	0	491	50	0
27	R0	444	0	461	30	0
27	Y0	444	0	461	56	0
28	R1	409	0	440	47	0
28	Y1	409	0	440	41	0
29	R2	377	0	418	28	0
29	Y2	377	0	418	53	0
30	R3	504	0	574	43	0
30	Y3	504	0	574	57	0
31	R4	302	0	340	29	0
31	Y4	302	0	342	24	0
32	QA	32895	0	16553	1244	0
32	XA	32831	0	16521	1591	0
33	QB	1704	0	1732	236	0
33	XB	1704	0	1732	177	0
34	QC	1624	0	1699	117	0
34	XC	1624	0	1699	130	0
35	QD	1643	0	1710	160	0
35	XD	1643	0	1710	162	0
36	QE	1105	0	1148	144	0
36	XE	1105	0	1148	108	0
37	QF	817	0	808	89	0
37	XF	817	0	808	93	0
38	QG	1181	0	1240	101	0
38	XG	1174	0	1230	133	0
39	QH	979	0	1034	96	0
39	XH	979	0	1034	101	0
40	QI	1022	0	1070	107	0
40	XI	1022	0	1070	134	0
41	QJ	786	0	828	99	0
41	XJ	786	0	828	97	0
42	QK	877	0	887	89	0
42	XK	877	0	887	78	0
43	QL	955	0	1019	90	0
43	XL	955	0	1019	91	0
44	QM	883	0	944	71	0
44	XM	876	0	937	109	0
45	QN	774	0	827	83	0
45	XN	735	0	790	102	0
46	QO	714	0	737	59	0
46	XO	714	0	737	47	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	QP	649	0	666	51	0
47	XP	638	0	656	49	0
48	QQ	648	0	691	92	0
48	XQ	648	0	691	54	0
49	QR	455	0	478	25	0
49	XR	455	0	478	43	0
50	QS	637	0	665	61	0
50	XS	637	0	665	88	0
51	QT	665	0	714	87	0
51	XT	665	0	714	47	0
52	QU	425	0	449	82	0
52	XU	425	0	449	82	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

Continued on next page...

Continued from previous page...

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	16909	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 36.

The worst 5 of 16909 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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	RC	269/271 (99%)	198 (74%)	43 (16%)	28 (10%)	0	2
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	2
5	YE	199/201 (99%)	117 (59%)	55 (28%)	27 (14%)	0	1
6	RF	175/178 (98%)	138 (79%)	22 (13%)	15 (9%)	0	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	2
14	RN	118/120 (98%)	96 (81%)	14 (12%)	8 (7%)	1	5
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	5
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	12
17	YQ	115/117 (98%)	77 (67%)	27 (24%)	11 (10%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	RR	101/103 (98%)	82 (81%)	11 (11%)	8 (8%)	1	4
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%)	5	24
22	YV	92/94 (98%)	61 (66%)	23 (25%)	8 (9%)	0	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%)	2	13
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	6
26	RZ	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	2	16
26	YZ	56/58 (97%)	34 (61%)	16 (29%)	6 (11%)	0	2
27	R0	54/56 (96%)	42 (78%)	9 (17%)	3 (6%)	1	8
27	Y0	54/56 (96%)	38 (70%)	7 (13%)	9 (17%)	0	0
28	R1	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	0	4
28	Y1	48/50 (96%)	33 (69%)	10 (21%)	5 (10%)	0	2
29	R2	44/46 (96%)	37 (84%)	5 (11%)	2 (4%)	2	12
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	6
30	Y3	62/64 (97%)	43 (69%)	13 (21%)	6 (10%)	0	3
31	R4	36/38 (95%)	29 (81%)	5 (14%)	2 (6%)	1	8
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

Continued on next page...

Continued from previous page...

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%)	0	3
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%)	0	4
37	XF	98/100 (98%)	59 (60%)	28 (29%)	11 (11%)	0	2
38	QG	149/151 (99%)	108 (72%)	33 (22%)	8 (5%)	1	9
38	XG	148/151 (98%)	86 (58%)	46 (31%)	16 (11%)	0	2
39	QH	127/129 (98%)	95 (75%)	25 (20%)	7 (6%)	1	9
39	XH	127/129 (98%)	92 (72%)	25 (20%)	10 (8%)	1	4
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	5
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%)	0	4
42	XK	115/117 (98%)	87 (76%)	18 (16%)	10 (9%)	0	4
43	QL	121/123 (98%)	87 (72%)	23 (19%)	11 (9%)	0	3
43	XL	121/123 (98%)	90 (74%)	22 (18%)	9 (7%)	1	5
44	QM	112/114 (98%)	83 (74%)	20 (18%)	9 (8%)	1	4
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	8
46	XO	86/88 (98%)	64 (74%)	18 (21%)	4 (5%)	2	11
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	2
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	1
49	QR	53/55 (96%)	41 (77%)	10 (19%)	2 (4%)	2	15
49	XR	53/55 (96%)	37 (70%)	15 (28%)	1 (2%)	6	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	QS	77/79 (98%)	57 (74%)	14 (18%)	6 (8%)	1	4
50	XS	77/79 (98%)	47 (61%)	25 (32%)	5 (6%)	1	6
51	QT	83/85 (98%)	61 (74%)	16 (19%)	6 (7%)	1	5
51	XT	83/85 (98%)	59 (71%)	18 (22%)	6 (7%)	1	5
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	1

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%)	163 (76%)	53 (24%)	1	3
3	YC	216/216 (100%)	182 (84%)	34 (16%)	2	12
4	RD	164/164 (100%)	137 (84%)	27 (16%)	2	11
4	YD	164/164 (100%)	135 (82%)	29 (18%)	2	9
5	RE	165/165 (100%)	120 (73%)	45 (27%)	0	1
5	YE	165/165 (100%)	141 (86%)	24 (14%)	3	14
6	RF	148/149 (99%)	121 (82%)	27 (18%)	2	8
6	YF	149/149 (100%)	118 (79%)	31 (21%)	1	5
7	RG	137/137 (100%)	107 (78%)	30 (22%)	1	4
7	YG	137/137 (100%)	116 (85%)	21 (15%)	3	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	RH	114/114 (100%)	95 (83%)	19 (17%)	2	10
8	YH	114/114 (100%)	89 (78%)	25 (22%)	1	4
9	RI	109/109 (100%)	94 (86%)	15 (14%)	3	15
9	YI	109/109 (100%)	100 (92%)	9 (8%)	10	35
10	RJ	116/116 (100%)	84 (72%)	32 (28%)	0	1
10	YJ	116/116 (100%)	96 (83%)	20 (17%)	2	10
11	RK	103/103 (100%)	71 (69%)	32 (31%)	0	0
11	YK	103/103 (100%)	77 (75%)	26 (25%)	0	2
12	RL	102/102 (100%)	74 (72%)	28 (28%)	0	1
12	YL	102/102 (100%)	85 (83%)	17 (17%)	2	10
13	RM	109/109 (100%)	86 (79%)	23 (21%)	1	5
13	YM	109/109 (100%)	95 (87%)	14 (13%)	4	18
14	RN	100/100 (100%)	79 (79%)	21 (21%)	1	5
14	YN	100/100 (100%)	81 (81%)	19 (19%)	1	7
15	RO	86/86 (100%)	62 (72%)	24 (28%)	0	1
15	YO	86/86 (100%)	77 (90%)	9 (10%)	6	26
16	RP	99/99 (100%)	73 (74%)	26 (26%)	0	2
16	YP	99/99 (100%)	86 (87%)	13 (13%)	4	17
17	RQ	89/89 (100%)	70 (79%)	19 (21%)	1	5
17	YQ	89/89 (100%)	71 (80%)	18 (20%)	1	5
18	RR	84/84 (100%)	67 (80%)	17 (20%)	1	5
18	YR	84/84 (100%)	69 (82%)	15 (18%)	2	9
19	RS	93/93 (100%)	65 (70%)	28 (30%)	0	1
19	YS	93/93 (100%)	71 (76%)	22 (24%)	1	3
20	RT	80/80 (100%)	59 (74%)	21 (26%)	0	2
20	YT	80/80 (100%)	69 (86%)	11 (14%)	3	15
21	RU	83/83 (100%)	59 (71%)	24 (29%)	0	1
21	YU	83/83 (100%)	65 (78%)	18 (22%)	1	5
22	RV	78/78 (100%)	60 (77%)	18 (23%)	1	4
22	YV	78/78 (100%)	68 (87%)	10 (13%)	4	18
23	RW	59/59 (100%)	36 (61%)	23 (39%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	YW	59/59 (100%)	44 (75%)	15 (25%)	0	2
24	RX	67/67 (100%)	50 (75%)	17 (25%)	0	2
24	YX	67/67 (100%)	54 (81%)	13 (19%)	1	7
25	RY	55/55 (100%)	41 (74%)	14 (26%)	0	2
25	YY	55/55 (100%)	49 (89%)	6 (11%)	6	24
26	RZ	48/48 (100%)	32 (67%)	16 (33%)	0	0
26	YZ	48/48 (100%)	35 (73%)	13 (27%)	0	2
27	R0	47/47 (100%)	39 (83%)	8 (17%)	2	10
27	Y0	47/47 (100%)	37 (79%)	10 (21%)	1	5
28	R1	45/45 (100%)	33 (73%)	12 (27%)	0	2
28	Y1	45/45 (100%)	38 (84%)	7 (16%)	2	12
29	R2	38/38 (100%)	29 (76%)	9 (24%)	1	3
29	Y2	38/38 (100%)	33 (87%)	5 (13%)	4	17
30	R3	51/51 (100%)	43 (84%)	8 (16%)	2	12
30	Y3	51/51 (100%)	37 (72%)	14 (28%)	0	1
31	R4	34/34 (100%)	29 (85%)	5 (15%)	3	14
31	Y4	34/34 (100%)	28 (82%)	6 (18%)	2	9
33	QB	180/180 (100%)	141 (78%)	39 (22%)	1	5
33	XB	180/180 (100%)	153 (85%)	27 (15%)	3	13
34	QC	170/170 (100%)	133 (78%)	37 (22%)	1	5
34	XC	170/170 (100%)	142 (84%)	28 (16%)	2	11
35	QD	172/172 (100%)	145 (84%)	27 (16%)	2	12
35	XD	172/172 (100%)	133 (77%)	39 (23%)	1	4
36	QE	113/113 (100%)	87 (77%)	26 (23%)	1	4
36	XE	113/113 (100%)	85 (75%)	28 (25%)	1	2
37	QF	87/87 (100%)	72 (83%)	15 (17%)	2	10
37	XF	87/87 (100%)	70 (80%)	17 (20%)	1	6
38	QG	124/124 (100%)	106 (86%)	18 (14%)	3	14
38	XG	123/124 (99%)	95 (77%)	28 (23%)	1	4
39	QH	104/104 (100%)	84 (81%)	20 (19%)	1	7
39	XH	104/104 (100%)	85 (82%)	19 (18%)	2	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	QI	105/105 (100%)	84 (80%)	21 (20%)	1	6
40	XI	105/105 (100%)	84 (80%)	21 (20%)	1	6
41	QJ	86/86 (100%)	68 (79%)	18 (21%)	1	5
41	XJ	86/86 (100%)	67 (78%)	19 (22%)	1	4
42	QK	90/90 (100%)	74 (82%)	16 (18%)	2	9
42	XK	90/90 (100%)	77 (86%)	13 (14%)	3	14
43	QL	103/103 (100%)	82 (80%)	21 (20%)	1	5
43	XL	103/103 (100%)	85 (82%)	18 (18%)	2	9
44	QM	92/92 (100%)	82 (89%)	10 (11%)	6	24
44	XM	91/92 (99%)	79 (87%)	12 (13%)	4	17
45	QN	79/84 (94%)	72 (91%)	7 (9%)	9	33
45	XN	75/84 (89%)	65 (87%)	10 (13%)	4	17
46	QO	76/76 (100%)	64 (84%)	12 (16%)	2	12
46	XO	76/76 (100%)	67 (88%)	9 (12%)	5	21
47	QP	65/65 (100%)	54 (83%)	11 (17%)	2	10
47	XP	65/65 (100%)	50 (77%)	15 (23%)	1	4
48	QQ	74/74 (100%)	55 (74%)	19 (26%)	0	2
48	XQ	74/74 (100%)	58 (78%)	16 (22%)	1	5
49	QR	48/48 (100%)	44 (92%)	4 (8%)	10	35
49	XR	48/48 (100%)	42 (88%)	6 (12%)	4	19
50	QS	70/70 (100%)	59 (84%)	11 (16%)	2	12
50	XS	70/70 (100%)	60 (86%)	10 (14%)	3	14
51	QT	65/65 (100%)	46 (71%)	19 (29%)	0	1
51	XT	65/65 (100%)	49 (75%)	16 (25%)	1	3
52	QU	44/44 (100%)	33 (75%)	11 (25%)	0	2
52	XU	44/44 (100%)	34 (77%)	10 (23%)	1	4
All	All	9327/9344 (100%)	7489 (80%)	1838 (20%)	1	6

5 of 1838 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	QO	84	LEU
24	YX	46	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	XG	9	ARG
23	YW	31	LEU
12	YL	143	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 342 such sidechains are listed below:

Mol	Chain	Res	Type
46	XO	19	ASN
12	YL	4	ASN
47	XP	63	GLN
4	YD	49	GLN
16	YP	6	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	RA	2850/2904 (98%)	556 (19%)	74 (2%)
1	YA	2837/2904 (97%)	878 (30%)	153 (5%)
2	RB	117/118 (99%)	22 (18%)	0
2	YB	116/118 (98%)	33 (28%)	6 (5%)
32	QA	1532/1533 (99%)	378 (24%)	56 (3%)
32	XA	1529/1533 (99%)	448 (29%)	70 (4%)
All	All	8981/9110 (98%)	2315 (25%)	359 (3%)

5 of 2315 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	YA	1775	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	60,64,64	2.08	15 (25%)	78,97,97	2.90	30 (38%)

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	-	-	10/75/112/112	0/4/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	RA	3135	EM1	C76-C78	-6.68	1.37	1.47
54	RA	3135	EM1	N80-N81	-5.67	1.25	1.34
54	RA	3135	EM1	C21-C15	-4.70	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	RA	3135	EM1	C77-C72	-4.60	1.32	1.39
54	RA	3135	EM1	C21-C26	-4.07	1.50	1.54

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	RA	3135	EM1	C8-C4-C2	-11.37	99.56	115.23
54	RA	3135	EM1	N80-N81-N82	8.27	114.46	107.02
54	RA	3135	EM1	C76-C77-C72	-6.26	115.50	120.66
54	RA	3135	EM1	O20-C15-C21	-5.35	117.22	123.36
54	RA	3135	EM1	O9-C15-C21	5.31	117.70	110.87

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

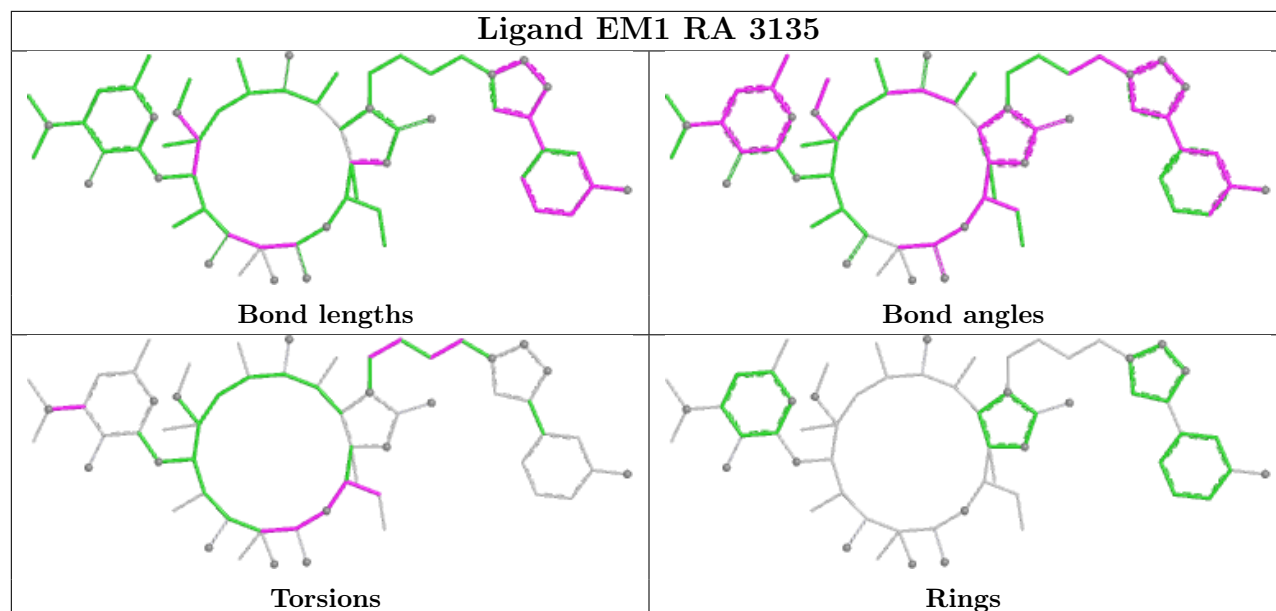
Mol	Chain	Res	Type	Atoms
54	RA	3135	EM1	O9-C4-C8-C14
54	RA	3135	EM1	C21-C15-O9-C4
54	RA	3135	EM1	O9-C15-C21-C26
54	RA	3135	EM1	O20-C15-C21-C26
54	RA	3135	EM1	O20-C15-O9-C4

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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	RA	2853/2904 (98%)	-0.81	38 (1%) 75 56	19, 47, 175, 400	0
1	YA	2841/2904 (97%)	0.90	327 (11%) 9 5	64, 140, 260, 408	0
2	RB	118/118 (100%)	-0.83	0 100 100	32, 61, 95, 115	0
2	YB	117/118 (99%)	0.33	1 (0%) 81 63	111, 185, 242, 277	0
3	RC	271/271 (100%)	-0.03	14 (5%) 33 17	25, 57, 97, 202	0
3	YC	271/271 (100%)	1.24	58 (21%) 2 1	64, 107, 154, 181	0
4	RD	209/209 (100%)	-0.38	3 (1%) 73 53	19, 41, 90, 149	0
4	YD	209/209 (100%)	1.30	46 (22%) 2 1	71, 122, 174, 236	0
5	RE	201/201 (100%)	-0.35	0 100 100	23, 58, 116, 177	0
5	YE	201/201 (100%)	1.75	66 (32%) 1 0	91, 214, 335, 378	0
6	RF	177/178 (99%)	0.09	3 (1%) 69 48	52, 93, 166, 225	0
6	YF	178/178 (100%)	0.59	5 (2%) 55 34	154, 229, 270, 299	0
7	RG	176/176 (100%)	-0.03	5 (2%) 55 34	41, 75, 129, 161	0
7	YG	176/176 (100%)	0.89	19 (10%) 11 6	129, 198, 270, 312	0
8	RH	149/149 (100%)	0.92	18 (12%) 8 5	59, 178, 260, 278	0
8	YH	149/149 (100%)	1.18	28 (18%) 3 1	100, 197, 252, 272	0
9	RI	141/141 (100%)	1.15	20 (14%) 6 3	149, 241, 292, 339	0
9	YI	141/141 (100%)	1.44	31 (21%) 2 1	231, 317, 353, 360	0
10	RJ	142/142 (100%)	-0.34	3 (2%) 63 42	21, 40, 76, 139	0
10	YJ	142/142 (100%)	1.28	34 (23%) 2 1	75, 126, 168, 193	0
11	RK	122/122 (100%)	-0.28	4 (3%) 49 29	23, 45, 94, 191	0
11	YK	122/122 (100%)	0.68	8 (6%) 24 13	66, 107, 155, 228	0
12	RL	143/143 (100%)	-0.15	1 (0%) 84 68	18, 55, 93, 123	0
12	YL	143/143 (100%)	2.10	70 (48%) 0 0	86, 169, 242, 284	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	RM	136/136 (100%)	-0.47	0 100 100	17, 45, 85, 146	0
13	YM	136/136 (100%)	0.96	20 (14%) 6 3	78, 131, 175, 208	0
14	RN	120/120 (100%)	-0.36	1 (0%) 82 65	18, 41, 63, 132	0
14	YN	120/120 (100%)	1.72	39 (32%) 1 0	88, 136, 190, 237	0
15	RO	116/116 (100%)	-0.29	2 (1%) 69 48	40, 64, 97, 124	0
15	YO	116/116 (100%)	0.90	15 (12%) 7 4	134, 182, 227, 252	0
16	RP	114/114 (100%)	-0.28	3 (2%) 57 36	29, 53, 104, 149	0
16	YP	114/114 (100%)	1.04	16 (14%) 6 4	82, 121, 160, 197	0
17	RQ	117/117 (100%)	-0.45	3 (2%) 57 36	19, 34, 63, 108	0
17	YQ	117/117 (100%)	1.86	45 (38%) 1 0	88, 126, 203, 287	0
18	RR	103/103 (100%)	-0.25	2 (1%) 66 45	20, 48, 92, 115	0
18	YR	103/103 (100%)	1.45	27 (26%) 1 1	98, 154, 219, 274	0
19	RS	110/110 (100%)	-0.42	1 (0%) 81 63	20, 38, 83, 143	0
19	YS	110/110 (100%)	1.67	32 (29%) 1 1	86, 141, 208, 266	0
20	RT	93/93 (100%)	0.42	5 (5%) 31 17	35, 69, 134, 207	0
20	YT	93/93 (100%)	2.81	62 (66%) 0 0	133, 215, 282, 315	0
21	RU	102/102 (100%)	0.29	7 (6%) 23 12	38, 72, 160, 192	0
21	YU	102/102 (100%)	2.76	69 (67%) 0 0	151, 251, 347, 416	0
22	RV	94/94 (100%)	-0.35	0 100 100	31, 61, 102, 114	0
22	YV	94/94 (100%)	0.62	5 (5%) 32 17	107, 157, 199, 222	0
23	RW	79/79 (100%)	0.46	9 (11%) 10 5	22, 53, 114, 195	0
23	YW	79/79 (100%)	1.92	35 (44%) 0 0	108, 163, 232, 250	0
24	RX	77/77 (100%)	-0.07	0 100 100	32, 58, 110, 124	0
24	YX	77/77 (100%)	2.40	38 (49%) 0 0	88, 134, 182, 237	0
25	RY	63/63 (100%)	0.36	3 (4%) 35 19	53, 90, 153, 175	0
25	YY	63/63 (100%)	2.71	39 (61%) 0 0	167, 286, 366, 383	0
26	RZ	58/58 (100%)	-0.23	0 100 100	19, 40, 87, 117	0
26	YZ	58/58 (100%)	1.27	10 (17%) 4 2	104, 143, 200, 247	0
27	R0	56/56 (100%)	-0.36	1 (1%) 67 47	17, 42, 85, 150	0
27	Y0	56/56 (100%)	1.41	14 (25%) 2 1	87, 161, 210, 255	0
28	R1	50/50 (100%)	0.00	2 (4%) 42 23	45, 65, 111, 143	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	Y1	50/50 (100%)	1.30	9 (18%) 3 1	106, 161, 203, 255	0
29	R2	46/46 (100%)	-0.22	1 (2%) 62 41	30, 42, 69, 166	0
29	Y2	46/46 (100%)	2.24	27 (58%) 0 0	95, 128, 162, 176	0
30	R3	64/64 (100%)	-0.31	0 100 100	25, 44, 64, 91	0
30	Y3	64/64 (100%)	3.22	52 (81%) 0 0	96, 140, 173, 212	0
31	R4	38/38 (100%)	-0.02	0 100 100	40, 58, 98, 108	0
31	Y4	38/38 (100%)	2.59	25 (65%) 0 0	94, 155, 195, 203	0
32	QA	1533/1533 (100%)	-0.21	12 (0%) 82 65	46, 97, 198, 345	0
32	XA	1530/1533 (99%)	0.25	55 (3%) 46 26	55, 113, 259, 356	0
33	QB	218/218 (100%)	0.53	10 (4%) 37 20	82, 141, 198, 243	0
33	XB	218/218 (100%)	0.55	16 (7%) 21 11	93, 145, 201, 251	0
34	QC	206/206 (100%)	0.32	8 (3%) 43 24	71, 107, 156, 198	0
34	XC	206/206 (100%)	0.52	16 (7%) 19 10	86, 136, 185, 215	0
35	QD	205/205 (100%)	0.79	22 (10%) 11 6	57, 114, 174, 236	0
35	XD	205/205 (100%)	0.35	10 (4%) 35 18	41, 78, 132, 212	0
36	QE	150/150 (100%)	0.31	3 (2%) 65 44	59, 90, 147, 217	0
36	XE	150/150 (100%)	0.54	4 (2%) 56 35	55, 92, 141, 191	0
37	QF	100/100 (100%)	0.40	4 (4%) 42 23	80, 126, 168, 190	0
37	XF	100/100 (100%)	0.54	6 (6%) 27 15	82, 119, 176, 211	0
38	QG	151/151 (100%)	0.49	5 (3%) 49 29	98, 138, 186, 203	0
38	XG	150/151 (99%)	1.28	29 (19%) 3 1	121, 195, 245, 277	0
39	QH	129/129 (100%)	0.48	5 (3%) 43 24	62, 101, 142, 189	0
39	XH	129/129 (100%)	0.53	5 (3%) 43 24	77, 115, 152, 209	0
40	QI	127/127 (100%)	0.98	18 (14%) 6 3	82, 137, 209, 250	0
40	XI	127/127 (100%)	1.30	26 (20%) 2 1	114, 158, 225, 259	0
41	QJ	98/98 (100%)	1.00	16 (16%) 4 2	71, 121, 175, 200	0
41	XJ	98/98 (100%)	1.48	22 (22%) 2 1	117, 166, 211, 238	0
42	QK	117/117 (100%)	0.50	2 (1%) 69 48	54, 123, 177, 206	0
42	XK	117/117 (100%)	0.49	5 (4%) 40 22	67, 115, 162, 186	0
43	QL	123/123 (100%)	0.42	10 (8%) 18 10	50, 79, 123, 189	0
43	XL	123/123 (100%)	0.57	10 (8%) 18 10	61, 89, 142, 202	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	QM	114/114 (100%)	0.61	5 (4%) 39 21	94, 142, 198, 217	0
44	XM	113/114 (99%)	2.72	58 (51%) 0 0	218, 370, 442, 470	0
45	QN	96/101 (95%)	1.05	16 (16%) 4 2	80, 116, 187, 224	0
45	XN	91/101 (90%)	1.34	21 (23%) 2 1	107, 180, 260, 287	0
46	QO	88/88 (100%)	0.45	5 (5%) 29 16	64, 102, 139, 188	0
46	XO	88/88 (100%)	0.61	5 (5%) 29 16	76, 116, 160, 209	0
47	QP	82/82 (100%)	0.86	6 (7%) 21 11	78, 99, 166, 223	0
47	XP	80/82 (97%)	1.01	6 (7%) 20 11	72, 107, 158, 222	0
48	QQ	80/80 (100%)	0.80	7 (8%) 15 9	62, 96, 136, 164	0
48	XQ	80/80 (100%)	0.75	8 (10%) 12 6	78, 115, 144, 155	0
49	QR	55/55 (100%)	0.74	4 (7%) 21 11	90, 110, 168, 218	0
49	XR	55/55 (100%)	0.45	4 (7%) 21 11	74, 103, 171, 243	0
50	QS	79/79 (100%)	0.83	6 (7%) 20 11	110, 143, 197, 208	0
50	XS	79/79 (100%)	1.99	36 (45%) 0 0	205, 346, 411, 424	0
51	QT	85/85 (100%)	0.99	10 (11%) 9 5	74, 103, 147, 179	0
51	XT	85/85 (100%)	1.24	16 (18%) 3 1	91, 134, 190, 216	0
52	QU	51/51 (100%)	1.36	15 (29%) 1 1	96, 139, 187, 225	0
52	XU	51/51 (100%)	1.32	12 (23%) 2 1	83, 120, 184, 224	0
All	All	20426/20564 (99%)	0.42	1980 (9%) 13 7	17, 111, 252, 470	0

The worst 5 of 1980 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	XM	97	ARG	14.7
44	XM	98	GLY	12.4
24	YX	2	ARG	9.8
51	QT	3	ILE	9.7
44	XM	93	GLY	9.1

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
53	MG	YA	3130	1/1	0.32	0.29	271,271,271,271	0
53	MG	YA	3125	1/1	0.40	0.19	200,200,200,200	0
53	MG	YA	3003	1/1	0.47	0.34	238,238,238,238	0
53	MG	YA	3049	1/1	0.49	0.10	243,243,243,243	0
53	MG	YA	3108	1/1	0.53	0.19	217,217,217,217	0
53	MG	YA	3019	1/1	0.55	0.22	278,278,278,278	0
53	MG	YA	3058	1/1	0.56	0.18	249,249,249,249	0
53	MG	YJ	201	1/1	0.57	0.38	319,319,319,319	0
53	MG	YA	3062	1/1	0.58	0.32	190,190,190,190	0
53	MG	YA	3045	1/1	0.59	0.17	206,206,206,206	0
53	MG	YA	3109	1/1	0.63	0.30	227,227,227,227	0
53	MG	XA	1636	1/1	0.63	0.31	224,224,224,224	0
53	MG	YA	3006	1/1	0.65	0.12	237,237,237,237	0
53	MG	YA	3028	1/1	0.66	0.27	222,222,222,222	0
53	MG	QA	1619	1/1	0.67	0.30	230,230,230,230	0
53	MG	YA	3005	1/1	0.69	0.28	282,282,282,282	0
53	MG	YA	3007	1/1	0.70	0.21	232,232,232,232	0
53	MG	RA	3068	1/1	0.70	0.13	175,175,175,175	0
53	MG	RA	3024	1/1	0.70	0.37	210,210,210,210	0
53	MG	YA	3002	1/1	0.71	0.19	231,231,231,231	0
53	MG	YA	3026	1/1	0.71	0.50	242,242,242,242	0
53	MG	YE	301	1/1	0.71	0.23	199,199,199,199	0
53	MG	YA	3017	1/1	0.71	0.13	185,185,185,185	0
53	MG	YA	3088	1/1	0.73	0.19	222,222,222,222	0
53	MG	YA	3015	1/1	0.74	0.15	219,219,219,219	0
53	MG	YA	3010	1/1	0.74	0.28	272,272,272,272	0
53	MG	YA	3128	1/1	0.75	0.34	163,163,163,163	0
53	MG	YA	3079	1/1	0.75	0.19	225,225,225,225	0
53	MG	YA	3082	1/1	0.76	0.14	164,164,164,164	0
53	MG	YA	3132	1/1	0.76	0.22	240,240,240,240	0
53	MG	XA	1619	1/1	0.76	0.14	212,212,212,212	0
53	MG	XA	1615	1/1	0.76	0.12	187,187,187,187	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	YA	3025	1/1	0.77	0.24	162,162,162,162	0
53	MG	YA	3105	1/1	0.77	0.16	97,97,97,97	0
53	MG	XA	1616	1/1	0.77	0.15	195,195,195,195	0
53	MG	RA	3046	1/1	0.77	0.12	176,176,176,176	0
53	MG	YA	3083	1/1	0.77	0.12	214,214,214,214	0
53	MG	YA	3074	1/1	0.78	0.28	260,260,260,260	0
53	MG	XA	1614	1/1	0.78	0.20	236,236,236,236	0
53	MG	YA	3123	1/1	0.78	0.27	217,217,217,217	0
53	MG	YA	3064	1/1	0.79	0.33	256,256,256,256	0
53	MG	YA	3013	1/1	0.79	0.27	241,241,241,241	0
53	MG	YA	3033	1/1	0.79	0.20	151,151,151,151	0
53	MG	YA	3009	1/1	0.79	0.18	157,157,157,157	0
53	MG	YA	3069	1/1	0.80	0.22	267,267,267,267	0
53	MG	RB	201	1/1	0.80	0.14	255,255,255,255	0
53	MG	YA	3133	1/1	0.80	0.16	220,220,220,220	0
53	MG	XA	1617	1/1	0.80	0.12	202,202,202,202	0
53	MG	YA	3129	1/1	0.80	0.36	261,261,261,261	0
53	MG	YA	3127	1/1	0.81	0.57	248,248,248,248	0
53	MG	YA	3097	1/1	0.81	0.12	159,159,159,159	0
53	MG	RA	3129	1/1	0.81	0.43	285,285,285,285	0
53	MG	YA	3076	1/1	0.81	0.21	195,195,195,195	0
53	MG	XA	1622	1/1	0.82	0.10	187,187,187,187	0
53	MG	YA	3085	1/1	0.82	0.17	158,158,158,158	0
53	MG	YA	3022	1/1	0.82	0.12	149,149,149,149	0
53	MG	YA	3091	1/1	0.82	0.14	184,184,184,184	0
53	MG	QA	1630	1/1	0.82	0.11	196,196,196,196	0
53	MG	RA	3069	1/1	0.82	0.17	197,197,197,197	0
53	MG	YA	3041	1/1	0.83	0.10	119,119,119,119	0
53	MG	YA	3087	1/1	0.83	0.10	199,199,199,199	0
53	MG	XA	1602	1/1	0.83	0.11	139,139,139,139	0
53	MG	RA	3131	1/1	0.84	0.30	187,187,187,187	0
53	MG	YA	3011	1/1	0.84	0.17	150,150,150,150	0
53	MG	RA	3113	1/1	0.84	0.12	190,190,190,190	0
53	MG	YA	3100	1/1	0.84	0.12	124,124,124,124	0
53	MG	YA	3036	1/1	0.84	0.11	205,205,205,205	0
53	MG	RA	3096	1/1	0.84	0.18	169,169,169,169	0
53	MG	YA	3066	1/1	0.84	0.14	105,105,105,105	0
53	MG	YA	3120	1/1	0.84	0.13	124,124,124,124	0
53	MG	YA	3043	1/1	0.84	0.13	155,155,155,155	0
53	MG	YA	3073	1/1	0.85	0.08	193,193,193,193	0
53	MG	QA	1610	1/1	0.85	0.14	197,197,197,197	0
53	MG	XA	1610	1/1	0.85	0.10	168,168,168,168	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	YA	3092	1/1	0.85	0.22	169,169,169,169	0
53	MG	XA	1634	1/1	0.85	0.09	165,165,165,165	0
53	MG	YA	3018	1/1	0.85	0.14	185,185,185,185	0
53	MG	YA	3101	1/1	0.85	0.13	96,96,96,96	0
53	MG	QA	1636	1/1	0.85	0.12	218,218,218,218	0
53	MG	YA	3084	1/1	0.85	0.13	168,168,168,168	0
53	MG	YA	3072	1/1	0.85	0.11	183,183,183,183	0
53	MG	YA	3115	1/1	0.85	0.17	176,176,176,176	0
53	MG	YA	3021	1/1	0.86	0.18	183,183,183,183	0
53	MG	YA	3038	1/1	0.86	0.10	234,234,234,234	0
53	MG	XA	1612	1/1	0.86	0.13	125,125,125,125	0
53	MG	YA	3059	1/1	0.86	0.22	232,232,232,232	0
53	MG	RA	3004	1/1	0.86	0.16	184,184,184,184	0
53	MG	YA	3134	1/1	0.86	0.15	201,201,201,201	0
53	MG	YA	3063	1/1	0.86	1.13	273,273,273,273	0
53	MG	YA	3075	1/1	0.86	0.25	209,209,209,209	0
53	MG	YA	3114	1/1	0.87	0.13	182,182,182,182	0
53	MG	YA	3057	1/1	0.87	0.20	205,205,205,205	0
53	MG	YA	3093	1/1	0.88	0.12	188,188,188,188	0
53	MG	RA	3085	1/1	0.88	0.16	133,133,133,133	0
53	MG	YA	3098	1/1	0.88	0.14	183,183,183,183	0
53	MG	YA	3027	1/1	0.88	0.15	194,194,194,194	0
53	MG	QA	1627	1/1	0.88	0.15	132,132,132,132	0
53	MG	XA	1620	1/1	0.88	0.12	182,182,182,182	0
53	MG	YA	3106	1/1	0.88	0.15	218,218,218,218	0
53	MG	YA	3024	1/1	0.88	0.13	102,102,102,102	0
53	MG	YA	3078	1/1	0.88	0.18	214,214,214,214	0
53	MG	XA	1638	1/1	0.88	0.13	204,204,204,204	0
53	MG	YA	3080	1/1	0.88	0.17	154,154,154,154	0
53	MG	YA	3118	1/1	0.88	0.12	100,100,100,100	0
53	MG	YA	3047	1/1	0.89	0.15	174,174,174,174	0
53	MG	XA	1629	1/1	0.89	0.09	190,190,190,190	0
53	MG	YA	3001	1/1	0.89	0.11	141,141,141,141	0
53	MG	XA	1624	1/1	0.89	0.18	146,146,146,146	0
53	MG	YA	3099	1/1	0.89	0.10	188,188,188,188	0
53	MG	YA	3111	1/1	0.89	0.10	202,202,202,202	0
53	MG	XA	1627	1/1	0.89	0.16	197,197,197,197	0
53	MG	QA	1631	1/1	0.90	0.14	228,228,228,228	0
53	MG	YA	3034	1/1	0.90	0.12	88,88,88,88	0
53	MG	YA	3050	1/1	0.90	0.10	154,154,154,154	0
53	MG	RA	3122	1/1	0.90	0.24	164,164,164,164	0
53	MG	XA	1625	1/1	0.90	0.11	111,111,111,111	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	QA	1639	1/1	0.90	0.10	118,118,118,118	0
53	MG	YA	3060	1/1	0.90	0.30	235,235,235,235	0
53	MG	XA	1628	1/1	0.90	0.16	224,224,224,224	0
53	MG	RA	3089	1/1	0.90	0.10	127,127,127,127	0
53	MG	YA	3008	1/1	0.91	0.10	147,147,147,147	0
53	MG	XA	1632	1/1	0.91	0.10	122,122,122,122	0
53	MG	YA	3095	1/1	0.91	0.11	138,138,138,138	0
53	MG	RA	3090	1/1	0.91	0.12	135,135,135,135	0
53	MG	XA	1640	1/1	0.91	0.11	137,137,137,137	0
53	MG	YA	3030	1/1	0.91	0.14	130,130,130,130	0
53	MG	YA	3053	1/1	0.91	0.17	127,127,127,127	0
53	MG	YA	3086	1/1	0.92	0.16	109,109,109,109	0
53	MG	YA	3122	1/1	0.92	0.08	104,104,104,104	0
53	MG	YA	3023	1/1	0.92	0.07	130,130,130,130	0
53	MG	XA	1623	1/1	0.92	0.13	108,108,108,108	0
53	MG	XA	1630	1/1	0.92	0.09	160,160,160,160	0
53	MG	YA	3107	1/1	0.92	0.12	91,91,91,91	0
53	MG	QA	1641	1/1	0.92	0.18	171,171,171,171	0
53	MG	YA	3039	1/1	0.92	0.10	105,105,105,105	0
53	MG	YA	3110	1/1	0.92	0.06	120,120,120,120	0
53	MG	YA	3071	1/1	0.92	0.10	102,102,102,102	0
53	MG	RA	3117	1/1	0.92	0.18	162,162,162,162	0
53	MG	XA	1607	1/1	0.92	0.10	167,167,167,167	0
53	MG	RA	3058	1/1	0.92	0.18	100,100,100,100	0
53	MG	XA	1637	1/1	0.93	0.11	94,94,94,94	0
53	MG	QA	1629	1/1	0.93	0.06	97,97,97,97	0
53	MG	RA	3020	1/1	0.93	0.15	200,200,200,200	0
53	MG	RA	3047	1/1	0.93	0.09	122,122,122,122	0
53	MG	YA	3102	1/1	0.93	0.09	118,118,118,118	0
53	MG	YA	3126	1/1	0.93	0.14	120,120,120,120	0
53	MG	QA	1614	1/1	0.93	0.12	159,159,159,159	0
53	MG	QA	1638	1/1	0.93	0.10	67,67,67,67	0
53	MG	RA	3130	1/1	0.93	0.15	118,118,118,118	0
53	MG	XA	1618	1/1	0.93	0.08	136,136,136,136	0
53	MG	QA	1620	1/1	0.93	0.07	116,116,116,116	0
53	MG	QA	1624	1/1	0.93	0.10	143,143,143,143	0
53	MG	YA	3094	1/1	0.93	0.09	145,145,145,145	0
53	MG	RA	3055	1/1	0.93	0.28	252,252,252,252	0
53	MG	YA	3042	1/1	0.93	0.09	81,81,81,81	0
54	EM1	RA	3135	60/60	0.93	0.14	0,23,85,88	0
53	MG	YA	3004	1/1	0.94	0.10	134,134,134,134	0
53	MG	YA	3121	1/1	0.94	0.11	168,168,168,168	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	RA	3033	1/1	0.94	0.15	159,159,159,159	0
53	MG	XA	1635	1/1	0.94	0.05	76,76,76,76	0
53	MG	XA	1601	1/1	0.94	0.07	106,106,106,106	0
53	MG	RA	3086	1/1	0.94	0.11	151,151,151,151	0
53	MG	QA	1604	1/1	0.94	0.06	139,139,139,139	0
53	MG	XA	1639	1/1	0.94	0.06	159,159,159,159	0
53	MG	RA	3035	1/1	0.94	0.20	189,189,189,189	0
53	MG	XA	1642	1/1	0.94	0.09	139,139,139,139	0
53	MG	YA	3029	1/1	0.94	0.21	178,178,178,178	0
53	MG	XA	1611	1/1	0.94	0.09	110,110,110,110	0
53	MG	YA	3031	1/1	0.94	0.10	80,80,80,80	0
53	MG	YB	201	1/1	0.94	0.07	111,111,111,111	0
53	MG	RA	3114	1/1	0.94	0.12	28,28,28,28	0
53	MG	YA	3096	1/1	0.94	0.10	127,127,127,127	0
53	MG	XA	1613	1/1	0.94	0.08	147,147,147,147	0
53	MG	QA	1602	1/1	0.95	0.12	177,177,177,177	0
53	MG	YA	3032	1/1	0.95	0.09	162,162,162,162	0
53	MG	RA	3120	1/1	0.95	0.20	45,45,45,45	0
53	MG	RA	3011	1/1	0.95	0.10	129,129,129,129	0
53	MG	QA	1612	1/1	0.95	0.09	113,113,113,113	0
53	MG	QA	1637	1/1	0.95	0.08	131,131,131,131	0
53	MG	YA	3103	1/1	0.95	0.09	86,86,86,86	0
53	MG	RA	3126	1/1	0.95	0.07	40,40,40,40	0
53	MG	QA	1617	1/1	0.95	0.09	129,129,129,129	0
53	MG	RA	3110	1/1	0.95	0.08	84,84,84,84	0
53	MG	YA	3131	1/1	0.95	0.08	94,94,94,94	0
53	MG	RA	3030	1/1	0.95	0.05	56,56,56,56	0
53	MG	RA	3007	1/1	0.95	0.07	112,112,112,112	0
53	MG	XA	1606	1/1	0.95	0.07	93,93,93,93	0
53	MG	RA	3054	1/1	0.95	0.20	198,198,198,198	0
53	MG	QA	1628	1/1	0.95	0.18	142,142,142,142	0
53	MG	YA	3014	1/1	0.95	0.11	113,113,113,113	0
53	MG	YA	3077	1/1	0.95	0.06	109,109,109,109	0
53	MG	RA	3070	1/1	0.96	0.18	137,137,137,137	0
53	MG	XA	1603	1/1	0.96	0.09	136,136,136,136	0
53	MG	RA	3081	1/1	0.96	0.06	99,99,99,99	0
53	MG	YA	3112	1/1	0.96	0.07	79,79,79,79	0
53	MG	YA	3113	1/1	0.96	0.05	128,128,128,128	0
53	MG	QA	1623	1/1	0.96	0.08	77,77,77,77	0
53	MG	XA	1609	1/1	0.96	0.07	98,98,98,98	0
53	MG	YA	3090	1/1	0.96	0.08	112,112,112,112	0
53	MG	YA	3119	1/1	0.96	0.10	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	RA	3083	1/1	0.96	0.06	53,53,53,53	0
53	MG	XA	1631	1/1	0.96	0.08	82,82,82,82	0
53	MG	RA	3059	1/1	0.96	0.23	207,207,207,207	0
53	MG	RB	202	1/1	0.96	0.07	82,82,82,82	0
53	MG	YA	3035	1/1	0.96	0.09	90,90,90,90	0
53	MG	RA	3060	1/1	0.96	0.31	236,236,236,236	0
53	MG	RA	3056	1/1	0.96	0.16	148,148,148,148	0
53	MG	QA	1606	1/1	0.96	0.07	80,80,80,80	0
53	MG	QA	1607	1/1	0.96	0.06	136,136,136,136	0
53	MG	QA	1609	1/1	0.96	0.07	77,77,77,77	0
53	MG	RA	3121	1/1	0.96	0.09	45,45,45,45	0
53	MG	RA	3026	1/1	0.96	0.10	143,143,143,143	0
53	MG	RA	3124	1/1	0.96	0.12	63,63,63,63	0
53	MG	YA	3104	1/1	0.96	0.11	52,52,52,52	0
53	MG	YA	3048	1/1	0.96	0.07	103,103,103,103	0
53	MG	QA	1643	1/1	0.96	0.06	67,67,67,67	0
53	MG	RA	3095	1/1	0.96	0.12	139,139,139,139	0
53	MG	YA	3051	1/1	0.96	0.06	88,88,88,88	0
53	MG	RA	3076	1/1	0.97	0.08	107,107,107,107	0
53	MG	YA	3081	1/1	0.97	0.09	83,83,83,83	0
53	MG	QA	1632	1/1	0.97	0.07	85,85,85,85	0
53	MG	QA	1634	1/1	0.97	0.08	94,94,94,94	0
53	MG	RA	3091	1/1	0.97	0.06	84,84,84,84	0
53	MG	RA	3022	1/1	0.97	0.05	27,27,27,27	0
53	MG	RA	3082	1/1	0.97	0.08	86,86,86,86	0
53	MG	YA	3054	1/1	0.97	0.06	86,86,86,86	0
53	MG	RA	3100	1/1	0.97	0.13	119,119,119,119	0
53	MG	YA	3089	1/1	0.97	0.09	101,101,101,101	0
53	MG	QA	1616	1/1	0.97	0.11	98,98,98,98	0
53	MG	RA	3103	1/1	0.97	0.06	30,30,30,30	0
53	MG	QA	1618	1/1	0.97	0.06	78,78,78,78	0
53	MG	RA	3105	1/1	0.97	0.15	66,66,66,66	0
53	MG	YA	3124	1/1	0.97	0.06	82,82,82,82	0
53	MG	RA	3133	1/1	0.97	0.15	116,116,116,116	0
53	MG	QA	1621	1/1	0.97	0.08	131,131,131,131	0
53	MG	YA	3065	1/1	0.97	0.06	88,88,88,88	0
53	MG	RA	3014	1/1	0.97	0.06	38,38,38,38	0
53	MG	RA	3051	1/1	0.97	0.06	70,70,70,70	0
53	MG	QA	1625	1/1	0.97	0.05	101,101,101,101	0
53	MG	YA	3037	1/1	0.97	0.07	81,81,81,81	0
53	MG	XA	1633	1/1	0.97	0.07	79,79,79,79	0
53	MG	RA	3003	1/1	0.97	0.08	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	YA	3040	1/1	0.97	0.05	72,72,72,72	0
53	MG	YA	3016	1/1	0.97	0.06	60,60,60,60	0
53	MG	RA	3088	1/1	0.97	0.04	59,59,59,59	0
53	MG	QA	1605	1/1	0.97	0.09	72,72,72,72	0
53	MG	RA	3074	1/1	0.97	0.06	93,93,93,93	0
55	ZN	Y4	101	1/1	0.97	0.06	169,169,169,169	0
53	MG	RA	3136	1/1	0.98	0.05	61,61,61,61	0
53	MG	YA	3012	1/1	0.98	0.05	72,72,72,72	0
53	MG	RA	3031	1/1	0.98	0.06	37,37,37,37	0
53	MG	RA	3002	1/1	0.98	0.05	75,75,75,75	0
53	MG	XA	1604	1/1	0.98	0.05	96,96,96,96	0
53	MG	RB	203	1/1	0.98	0.06	58,58,58,58	0
53	MG	RA	3118	1/1	0.98	0.05	48,48,48,48	0
53	MG	YA	3046	1/1	0.98	0.11	73,73,73,73	0
53	MG	XA	1608	1/1	0.98	0.14	46,46,46,46	0
53	MG	RA	3119	1/1	0.98	0.05	56,56,56,56	0
53	MG	YA	3116	1/1	0.98	0.08	84,84,84,84	0
53	MG	YA	3117	1/1	0.98	0.06	73,73,73,73	0
53	MG	YA	3020	1/1	0.98	0.11	53,53,53,53	0
53	MG	RA	3097	1/1	0.98	0.08	54,54,54,54	0
53	MG	RA	3027	1/1	0.98	0.05	33,33,33,33	0
53	MG	YA	3052	1/1	0.98	0.04	72,72,72,72	0
53	MG	RA	3045	1/1	0.98	0.07	25,25,25,25	0
53	MG	QA	1608	1/1	0.98	0.12	61,61,61,61	0
53	MG	YA	3056	1/1	0.98	0.09	85,85,85,85	0
53	MG	RA	3028	1/1	0.98	0.15	92,92,92,92	0
53	MG	XA	1641	1/1	0.98	0.09	116,116,116,116	0
53	MG	RA	3108	1/1	0.98	0.08	95,95,95,95	0
53	MG	RA	3109	1/1	0.98	0.07	46,46,46,46	0
53	MG	YA	3061	1/1	0.98	0.08	110,110,110,110	0
53	MG	QA	1635	1/1	0.98	0.04	87,87,87,87	0
53	MG	QA	1613	1/1	0.98	0.04	76,76,76,76	0
53	MG	RA	3005	1/1	0.98	0.05	74,74,74,74	0
53	MG	QA	1615	1/1	0.98	0.04	152,152,152,152	0
53	MG	RA	3112	1/1	0.98	0.04	49,49,49,49	0
53	MG	QA	1640	1/1	0.98	0.04	79,79,79,79	0
53	MG	YA	3070	1/1	0.98	0.05	91,91,91,91	0
53	MG	RA	3050	1/1	0.98	0.06	39,39,39,39	0
53	MG	QA	1642	1/1	0.98	0.05	79,79,79,79	0
53	MG	RA	3134	1/1	0.98	0.21	210,210,210,210	0
53	MG	RB	204	1/1	0.99	0.05	45,45,45,45	0
53	MG	QA	1601	1/1	0.99	0.03	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	RA	3010	1/1	0.99	0.04	31,31,31,31	0
53	MG	QA	1603	1/1	0.99	0.03	65,65,65,65	0
53	MG	RA	3025	1/1	0.99	0.06	40,40,40,40	0
53	MG	RA	3087	1/1	0.99	0.02	47,47,47,47	0
53	MG	RA	3048	1/1	0.99	0.03	25,25,25,25	0
53	MG	RA	3049	1/1	0.99	0.05	76,76,76,76	0
53	MG	RA	3006	1/1	0.99	0.07	54,54,54,54	0
53	MG	RA	3012	1/1	0.99	0.04	20,20,20,20	0
53	MG	XA	1621	1/1	0.99	0.09	57,57,57,57	0
53	MG	RA	3093	1/1	0.99	0.07	45,45,45,45	0
53	MG	QA	1611	1/1	0.99	0.04	57,57,57,57	0
53	MG	RA	3053	1/1	0.99	0.05	55,55,55,55	0
53	MG	RA	3001	1/1	0.99	0.05	98,98,98,98	0
53	MG	RA	3029	1/1	0.99	0.09	14,14,14,14	0
53	MG	RA	3098	1/1	0.99	0.03	49,49,49,49	0
53	MG	RA	3099	1/1	0.99	0.07	34,34,34,34	0
53	MG	RA	3015	1/1	0.99	0.05	65,65,65,65	0
53	MG	RA	3101	1/1	0.99	0.05	48,48,48,48	0
53	MG	YA	3044	1/1	0.99	0.07	87,87,87,87	0
53	MG	RA	3057	1/1	0.99	0.04	71,71,71,71	0
53	MG	RA	3104	1/1	0.99	0.07	23,23,23,23	0
53	MG	RA	3018	1/1	0.99	0.18	32,32,32,32	0
53	MG	QA	1622	1/1	0.99	0.10	54,54,54,54	0
53	MG	RA	3106	1/1	0.99	0.07	13,13,13,13	0
53	MG	RA	3107	1/1	0.99	0.07	17,17,17,17	0
53	MG	RA	3032	1/1	0.99	0.05	23,23,23,23	0
53	MG	RA	3019	1/1	0.99	0.06	34,34,34,34	0
53	MG	RA	3061	1/1	0.99	0.03	18,18,18,18	0
53	MG	RA	3111	1/1	0.99	0.04	31,31,31,31	0
53	MG	YA	3055	1/1	0.99	0.06	103,103,103,103	0
53	MG	RA	3062	1/1	0.99	0.05	19,19,19,19	0
53	MG	RA	3063	1/1	0.99	0.04	26,26,26,26	0
53	MG	RA	3065	1/1	0.99	0.04	35,35,35,35	0
53	MG	QA	1633	1/1	0.99	0.07	70,70,70,70	0
53	MG	RA	3116	1/1	0.99	0.07	72,72,72,72	0
53	MG	RA	3066	1/1	0.99	0.04	32,32,32,32	0
53	MG	RA	3067	1/1	0.99	0.04	28,28,28,28	0
53	MG	RA	3008	1/1	0.99	0.05	45,45,45,45	0
53	MG	RA	3036	1/1	0.99	0.05	23,23,23,23	0
53	MG	RA	3037	1/1	0.99	0.03	30,30,30,30	0
53	MG	RA	3072	1/1	0.99	0.06	61,61,61,61	0
53	MG	YA	3067	1/1	0.99	0.04	72,72,72,72	0

Continued on next page...

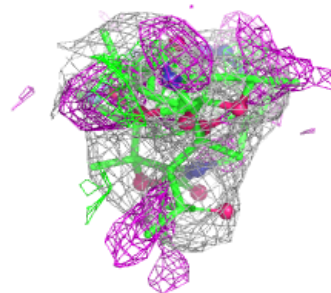
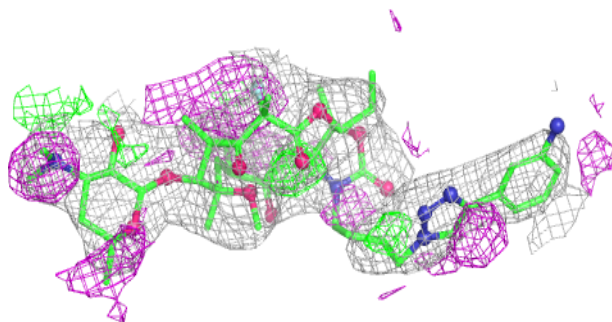
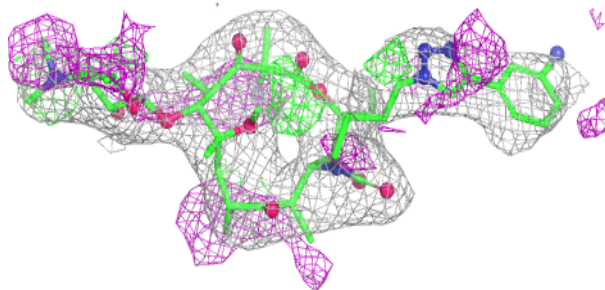
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	YA	3068	1/1	0.99	0.04	98,98,98,98	0
53	MG	RA	3123	1/1	0.99	0.02	24,24,24,24	0
53	MG	RA	3073	1/1	0.99	0.07	43,43,43,43	0
53	MG	RA	3040	1/1	0.99	0.05	47,47,47,47	0
53	MG	RA	3075	1/1	0.99	0.03	43,43,43,43	0
53	MG	RA	3041	1/1	0.99	0.03	38,38,38,38	0
53	MG	RA	3077	1/1	0.99	0.06	63,63,63,63	0
53	MG	RA	3078	1/1	0.99	0.03	58,58,58,58	0
53	MG	XA	1605	1/1	0.99	0.06	54,54,54,54	0
53	MG	RA	3080	1/1	0.99	0.05	60,60,60,60	0
53	MG	RA	3042	1/1	0.99	0.06	60,60,60,60	0
53	MG	RA	3044	1/1	0.99	0.05	34,34,34,34	0
53	MG	RA	3009	1/1	0.99	0.05	38,38,38,38	0
55	ZN	R4	101	1/1	0.99	0.07	108,108,108,108	0
53	MG	RA	3084	1/1	0.99	0.05	26,26,26,26	0
53	MG	RA	3034	1/1	1.00	0.02	11,11,11,11	0
53	MG	RA	3102	1/1	1.00	0.08	24,24,24,24	0
53	MG	RA	3052	1/1	1.00	0.04	34,34,34,34	0
53	MG	RA	3043	1/1	1.00	0.12	11,11,11,11	0
53	MG	XA	1626	1/1	1.00	0.11	20,20,20,20	0
53	MG	RA	3064	1/1	1.00	0.03	28,28,28,28	0
53	MG	QA	1626	1/1	1.00	0.08	29,29,29,29	0
53	MG	RA	3016	1/1	1.00	0.02	22,22,22,22	0
53	MG	RA	3017	1/1	1.00	0.04	57,57,57,57	0
53	MG	RA	3125	1/1	1.00	0.04	40,40,40,40	0
53	MG	RA	3092	1/1	1.00	0.04	68,68,68,68	0
53	MG	RA	3127	1/1	1.00	0.03	8,8,8,8	0
53	MG	RA	3128	1/1	1.00	0.04	33,33,33,33	0
53	MG	RA	3079	1/1	1.00	0.05	32,32,32,32	0
53	MG	RA	3094	1/1	1.00	0.02	32,32,32,32	0
53	MG	RA	3021	1/1	1.00	0.03	24,24,24,24	0
53	MG	RA	3132	1/1	1.00	0.02	20,20,20,20	0
53	MG	RA	3038	1/1	1.00	0.02	19,19,19,19	0
53	MG	RA	3039	1/1	1.00	0.08	7,7,7,7	0
53	MG	RA	3013	1/1	1.00	0.05	18,18,18,18	0
53	MG	RA	3115	1/1	1.00	0.04	22,22,22,22	0
53	MG	RA	3071	1/1	1.00	0.02	16,16,16,16	0
53	MG	RA	3023	1/1	1.00	0.03	22,22,22,22	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 [i](#)

There are no such residues in this entry.