



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:33 PM GMT

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

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

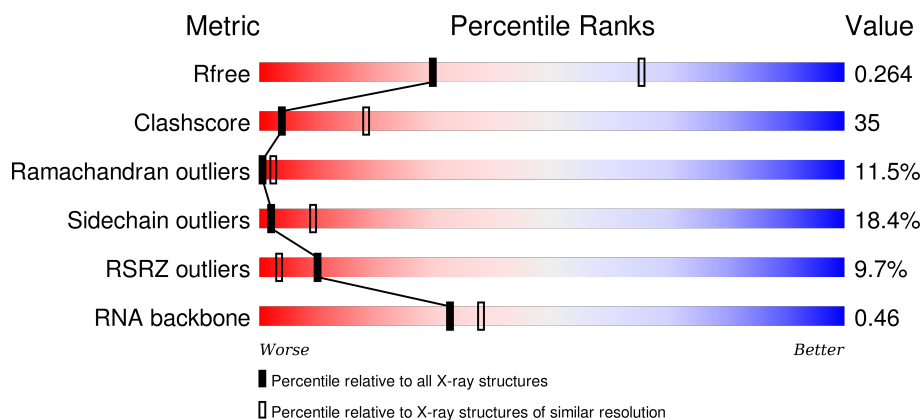
1 Overall quality at a glance

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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>39% 43% 15% ..</div> </div>
1	YA	2904	<div> <div>3%</div> <div>19% 52% 26% ..</div> </div>
2	RB	118	<div> <div>43% 47% 10%</div> </div>
2	YB	118	<div> <div>21% 54% 24% .</div> </div>

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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	

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

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Mol	Chain	Length	Quality of chain
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	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MG	RA	3020	-	-	-	X
53	MG	RA	3035	-	-	-	X
53	MG	RA	3039	-	-	-	X
53	MG	RA	3070	-	-	-	X
53	MG	RA	3081	-	-	-	X
53	MG	RA	3099	-	-	-	X
53	MG	RA	3105	-	-	-	X
53	MG	RA	3107	-	-	-	X
53	MG	RA	3134	-	-	-	X
53	MG	XA	1616	-	-	-	X
53	MG	XA	1625	-	-	-	X
53	MG	XA	1628	-	-	-	X
53	MG	XA	1640	-	-	-	X
53	MG	YA	3002	-	-	-	X
53	MG	YA	3033	-	-	-	X
53	MG	YA	3075	-	-	-	X
53	MG	YA	3079	-	-	-	X
53	MG	YA	3108	-	-	-	X
53	MG	YA	3115	-	-	-	X
53	MG	YA	3128	-	-	-	X
54	EM1	RA	3135	-	-	-	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			

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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			

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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			

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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			

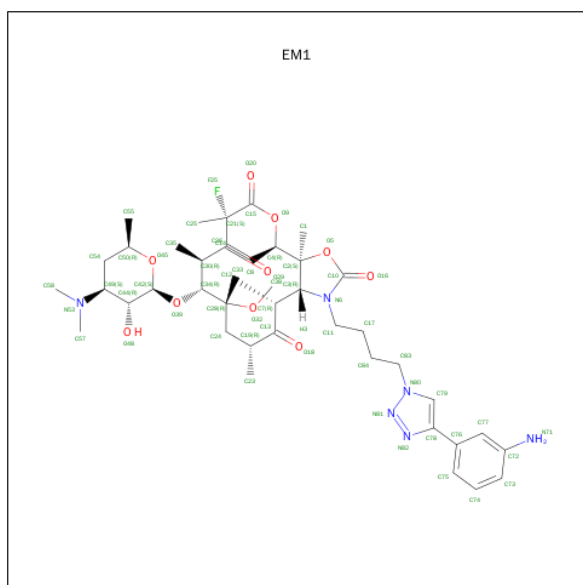
- Molecule 52 is a protein called 30S ribosomal protein S21.

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 (three-letter code: MG) (formula: Mg).

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

- 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 (three-letter code: EM1) (formula: C₄₃H₆₅FN₆O₁₀).



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

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

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

- Molecule 56 is water.

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

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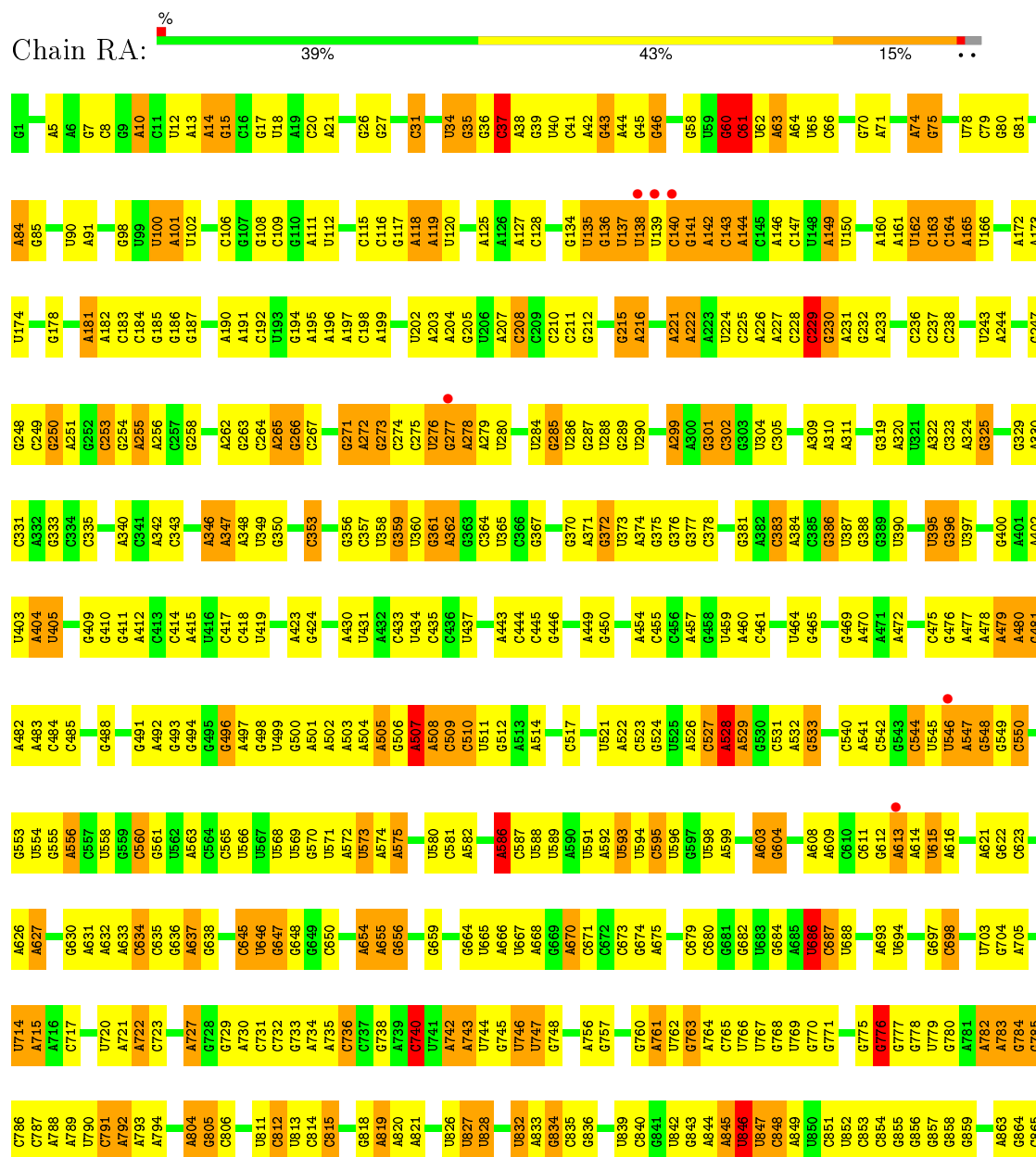
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	XL	1	Total 1	O 1	0	0
56	XN	3	Total 3	O 3	0	0
56	XT	2	Total 2	O 2	0	0
56	XU	1	Total 1	O 1	0	0
56	YA	605	Total 605	O 605	0	0
56	YB	4	Total 4	O 4	0	0
56	YC	8	Total 8	O 8	0	0
56	YD	3	Total 3	O 3	0	0
56	YE	3	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

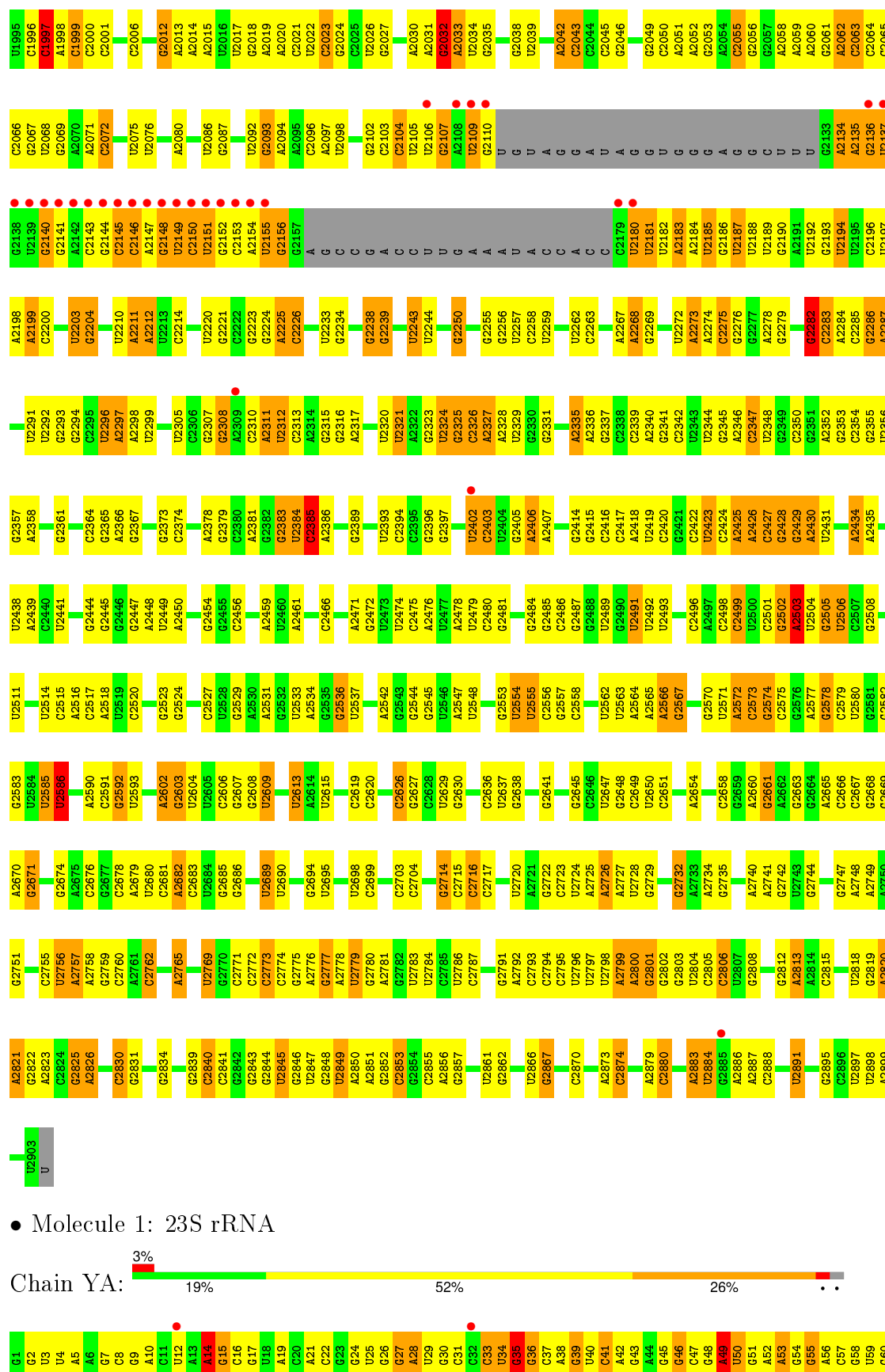
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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



A1927	G1849	A1783	U1716	A1626	G1546	U1467	A1392	G1309	G1229	A1151	U1082	G1011	A936	A866
A1928	G1850	A1784	A1717	G1627	G1546	U1468	A1393	G1310	C1229	C1152	U1083	U1012	C937	C867
G1930	U1851	A1785	U1720	G1628	U1554	A1469	A1394	G1311	U1230	C1153	A1084	C1013	U868	U869
U1931	A1853	A1786	U1721	U1635	G1555	A1470	A1395	C1315	G1232	G1154	A1085	A1014	A941	G869
A1932	A1854	A1789	A1722	U1636	C1558	U1474	C1399	U1316	C1233	A1155	A1086	U1015	G946	U870
G1933	U1855	C1790	G1723	A1637	C1558	U1475	U1402	G1317	U1234	A1156	A1087	U1019	A947	U871
C1934	G1856	A1791	G1724	C1638	U1562	U1476	U1403	U1318	G1235	U1160	A1088	A1020	C943	G875
G1935	U1857	G1792	U1725	C1644	U1563	A1477	A1404	C1319	G1238	C1161	A1089	A1021	G949	C876
A1936	A1858	C1793	G1726	C1644	U1564	A1478	A1405	G1320	G1239	G1165	A1090	G1022	A950	C877
A1937	U1859	A1794	C1727	U1647	C1565	G1479	U1405	A1321	G1238	C1161	G1091	U1023	A877	A878
A1938	C1795	A1796	G1728	U1648	C1565	G1479	U1405	A1322	G1239	A1165	G1092	G1024	C951	G879
U1939	U1796	U1797	U1729	U1648	C1566	U1479	U1405	C1323	U1242	A1166	G1093	G1025	G954	
U1940	U1865	G1797	C1730	G1649	G1567	G1482	G1408	G1324	C1243	C1167	U1094	G1026	U884	U885
C1941	A1866	U1798	G1731	A1650	G1568	U1483	U1409	U1325	A1244	G1168	A1095	A1027	U958	A
G1942	G1867	G1799	C1732	G1651	A1569	U1484	G1410	U1326	G1245	A1169	A1096	A1028	A959	U
U1943	C1868	C1800	G1733	A1652	A1570	U1485	U1411	A1327	A1246	C1170	A1098	U1032	C961	C
U1944	G1869	A1801	G1734	G1653	A1571	U1486	U1412	A1328	A1247	C1171	G1099	U1033	C	C
G1945	A1870	A1802	A1735	A1654	A1572	U1487	A1413	G1333	U1248	C1172			G962	C
A1871	A1871	A1805	U1736	A1655	G1573	C1488	C1414	U1334	U1249	U1173	A1103	U1037	G969	G
U1946	A1872	A1806	G1737	C1656	U1576	C1489	U1415	G1335	C1250	U1174	C1104	G1037	U970	
G1948	G1873	A1807	G1738	G1663	U1576	C1493	G1416	U1336	C1251	U1175	U1105	A1040	G971	C893
A1952	C1874	A1808	A1739	A1664	U1578	U1494	G1417	A1337	G1252	U1176	G1106	A1040	A972	C894
A1953	G1875	A1809	G1743	A1665	U1578	A1495	G1418	G1338	A1253	G1177	U1107	G1042	A973	U894
G1954	A1876	G1811	A1744	G1666	C1581	A1496	A1420	G1339	U1255	G1178	C1109	C1043	A896	U895
U1955	C1881	U1812	A1745	G1667	C1582	U1497	G1421	U1340	G1256	U1180	G1110	C1044	G975	A897
U1956	U1882	G1813	A1746	A1668	A1583	U1498	G1422	G1341	U1257	U1181	G1111	C1045	C898	C899
C1957	U1883	A1814	U1747	A1669	U1584	C1499	G1423	U1342	U1258	G1182	G1112	A1046	G977	A899
G1958	G1884	A1815	G1748	C1670	C1585	G1500	G1423	U1347	U1258	U1183	U1113	G1047	G978	A900
A1959	A1885	C1816	C1748	C1670	C1585	G1500	G1423	A1347	U1258	U1184	C1114	A1048	A979	C901
U1960	U1886	U1817	A1749	G1674	G1587	G1501	A1427	C1348	C1261	U1185	G1115	C1049	A980	
C1961	U1887	U1818	A1754	G1675	G1587	A1502	C1428	C1351	A1262	G1186		A1050	A981	U906
G1962	A1889	A1819	A1755	C1675	G1588	A1503	G1429	U1352	G1266	G1187	U1119	G1056	C982	C907
U1963	U1890	U1820	G1756	A1677	U1589	A1504	A1430	U1353	U1267	U1188	G1122	A1057	C983	C908
G1964	A1821	A1821	A1757	U1607	A1590	A1505	A1431	A1354	A1268	A1189	C1123	U1058	A984	A909
C1965	C1822	C1822	U1758	U1680	C1592	U1506	G1432	G1355	A1269	G1190	G1124	G1059	C985	A910
A1966	U1898	A1759	A1759	G1681	A1593	A1507	A1433	G1356	C1270	G1193	G1128	G1063	C986	A911
C1967	A1899	G1826	C1760	G1682	U1594	A1508	A1434	C1357	G1271	G1193	A1129	C1064	C987	C912
G1968	A1900	U1827	C1761	U1683	U1599	A1509	G1435	G1358	U1272	U1198	U1130	U1065	A988	U913
A1969	A1901	G1828	A1762	G1684	C1599	C1510	C1437	A1359	U1273	U1199	G1131	U1066	C989	G914
U1970	C1902	A1829	G1763	G1684	C1600	C1512	U1438	G1360	U1274	C1205	G1136	A1070	G922	G923
U1971	U1971	C1830	C1764	U1688	A1603	U1513	A1439		A1275	G1206	G1137	G1071	A1000	G924
G1972	G1906	G1831	G1764	U1688	A1603	G1514	U1440	A1365	G1277	C1207	U1132	C1072	A1001	
G1973	G1907	C1832	G1767	U1692	C1604	A1515	G1441		G1278	C1207	U1133	C1072	A927	A928
		C1833	C1768	U1693	C1605	A1516	U1442	G1368	G1279	U1203	A1134	A1073	C994	A918
A1977	A1913	U1834	U1769	C1694	C1606	G1516	U1443		G1279	A1204	G1135	G1068	C995	U919
G1983	U1915	G1835	G1770	G1695	C1607	U1520	G1444	U1371	G1280	C1205	G1136	C1075	C996	A920
C1984	A1916	C1837	C1771	G1696	A1608	U1520	G1444	U1372	G1281	A1205	U1137	G1076	C997	C921
G1985	U1917	C1838	A1772	G1697	A1609	A1528	G1450		G1281	G1206	G1137	C1077	C998	G922
C1986	A1918	G1839	A1773	U1700	A1610	G1529	C1451	G1377	A1287	C1207	U1138	G1078	U999	G923
A1987	U1919	U1840	U1775	A1701	C1612	U1533	C1452	A1378	G1288	G1212	G1139	A1002	A1001	G924
G1988	C1920	U1841	C1776	A1705	G1613	U1534	C1454	U1379	G1289	G1206	C1140	G1003	A927	A928
C1989	G1921	G1842	U1777	A1705	A1614	U1535	G1455	G1380	C1290	G1220	C1141	G1004	U929	U929
G1990	G1922	C1843	U1778	C1706	A1614	C1536	G1456	G1383	C1295	G1221	A1143	C1076	G1005	G930
U1991	U1923	C1844	U1779	G1707	A1618	U1537	U1457	A1384	C1295	G1221	A1143	C1077	G1006	U931
G1992	C1924	A1847	A1781	U1714	G1622	U1538	U1458	A1385	U1300	U1222	A1144	U1078	C1007	U932
U1993	C1925	A1848	U1781	U1715	G1622	U1539	G1459	A1386	A1301	G1223		C1079	A1008	A933
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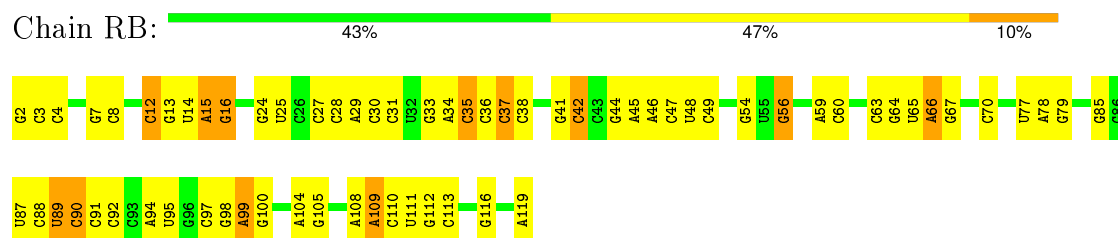


A928	G864	U803	U741	C671	C610	G549	G498	U427	C366	U206	U243	A182	G121	C61
U929	C865	A804	A742	C672	C611	C550	G489	A428	G367	G307	A244	C183	G122	U62
G930	A866	G805	G612	C673	G612	G551	G490	A429	A368	G308	C245	C184	G123	A63
U931	C867	C806	A743	G674	A613	U552	G491	A430	U369	A309	C246	G185	G124	A64
U932	U868	U807	G745	A675	A614	G553	G492	U431	G370	A310	G247	G186	A125	U65
A933	G869	G808	U746	A676	U615	U554	G493	A432	A371	A311	G248	G187	A126	C66
U934	U870	C809	U747	A677	A616	G555	G494	C433	G372	G312	C249	G188	A127	U67
C935	U871	U810	G748		G617		G495	U434	U373	G313	C250	G189	C128	G68
A936	U872	U811	A749	G682	G618	U558	G496	U435	A374	C314	A251	A190	C129	G69
A941	C873	C812	A750	U683	G619	G559	A497	C436	G375	G315	G252	C192	C130	A71
G942	G874	U813	A751	G684	G620	C560	G498	U437	G376	G316	C253	C192	A131	U71
A943	G875	C814	A752	A685	A621	G561	G499	G438	G377	G317	G254	U193	G132	U72
C944	C876	C815	A753	U686	G622	U562	G500	A439	C378	C318	A255	G194	U133	A73
	A877	C816	U754	C687	C623	A563	A501		G379	G319		A195	G134	A74
A945	A878	C817	U755	C564	C624	G565	A502	G442	G380	G75	G259	A196	G135	A75
C946	G	G818	A756	C565	G625	C566	A503	A443	G381	U321	G260	A197	U136	C76
A947	G	A819	G757	C682	A626	U566	A504	C444	A382	A322	C198	C198	U137	C77
C948	C	A820	C758	A693	G627	U567	A505	C445	C383	A323	A262	A199	U138	C78
G949	G	A821	G759	U694	G628	U568	G506	C446	A384	A324	G263	U200	U139	C79
G950	U	G822	G760	G695	G629	U569	A507	A447	C385	G325	C264	C201	C140	G80
C951	C		U761	G696	G630	G570	A508	U448	G386	G326	A265	U202	G141	G81
G952	A		G762	C697	A631	U571	C509	A449	U387	G327	G266	A203	A142	U82
G953	C		G763	C698	A632	A572	C510	G450	G388	U328	C267	A204	C143	A83
G954	U		A764	A699	A633	U573	U511	U451	G389	G329		G205	A144	A84
U955	C	U827		A699	G634	A574	G512	U452	U390	A330		U206	C145	G85
G956	C	U828		G701	C635	A575	A513	A453	A391	C331	G271	A207	A146	G86
C957	C	A829	U767		G636	U576	A514			A332	A272		C147	U87
U958	G	G830	G768	A705	A637	C567	A515	A454	C394	A333	G273	C210	U148	G88
A959	A	U832	G769	U706	G637	G577	C516	A455	U395	C334	C274	C211	A149	A89
A960	C	A833	G770	G707	G638	G578		A456	G396	C335	C275	G212	U150	U90
G961	U	G834	G771	G708	U639	G579	U519	A457	U397	C336	U276	A213	C151	A91
G962	U	C835	G772	U709	U640	C581	G520	U458	C398	G337	G277	G214	C152	U92
U963	A	G836	G773	U710	U642	A582	G521	A460	U399	G338	A278	G215	U153	G93
C964	C	C837	G774	U711	A643	G583	A522	C461	G400	U339	A279	A216	U154	A94
G965	A899	U838	G775	G712	A644	C584	C523	C462	A401	A340	U280	A217	A155	A95
U967		U839	G776	G713	G645	G585	G524	G463	A402	C341	C281	A218	A156	C96
C968		C840	G777		U646	A586	U525	U464	U403	A342	A282	A219	C157	C97
G969	C902	G841	G778	A715	U646	C587	A526	G465	A404	C343	G283	G220	U158	G98
U970	G903	U842	G779	A716	G647	U588	C527	A466	U405	A344	U284	A221	A159	U99
G971	C904	G843	A781	C717	U648	U589	A528	G467	G406	A345	G285	A222	A160	U100
A972	A905	A844	G782	U718	G649	A590	G529	G468	G407	A346	U286	A223		A101
A973		A845	G783	C719	C650	U591	G530	G469	G408	A347	G287	U224	C163	U102
G974		U846	G784	U720		A592	C531	A470	G409	A348	U288	C225	A164	A103
A975	C912	U847	G785	A721	U653	U593	A532	A471	G410	U349	G289	A226	A165	A104
G976	U913	C848	C786		A654	U594	A533	A472	G411	G350	U290	A227	U166	C105
G977	G913	G849	G787	U724	A655	C595	U534	G473	A412	C351	G291	C228	A167	C106
G978	U850	U850	A788	G725	G656	U596	G535	G474	C413	A352	U292	C229	G168	G107
A979	C915	C851	G789	G726	U657	G597	G536	C475	C414	C353	U293	G230	G169	G108
G980	G916	U852	C791	A727	U658	G598	G537	G476	A415	A354	A294	A231	U170	C109
A981	C917	C853	G792	G728	G659	U598	A538	A477	U416	U355	G295	G232	U171	G110
G982	A918	C854	A793	G729	A660	A599	G539	A478	C417	G356	U296	A233	A172	A111
C983	U919	G855	A794	G731	G662	G601	C540	A479	C418	C357	G297	U234	A173	U112
A984	A920	G856	C795	A602	G663	A602	A541	A480	U419	U358	G298	U235	U174	U113
C985	C921	C857	G796	A603	G664	C542	G481	G481	C420	G359	A299	C236	G175	U114
	G922	G858	G797	G604	U665	G605	G543	A482	C421	U360	A300	C237	A176	G115
G986	G923	G859	G798	G605	A666	G606	C544	A483	A422	G361	G301	C238	G177	C116
G987	G924	U860	G799	U667	U667	U606	U545	C484	A423	A362	C302	C239	G178	G117
A989	A925	A861	G799	G737	A668	U546	U546	C485	A424	G363	G303	C240	C179	A118
C990	C926	G862	A800	G738	A669	U607	A547	C486	G425	C364	U304	A241	G180	A119
G991	A927	A863	A802	C740	A670	A609	G548	C487	C426	U365	C305	G242	A181	U120

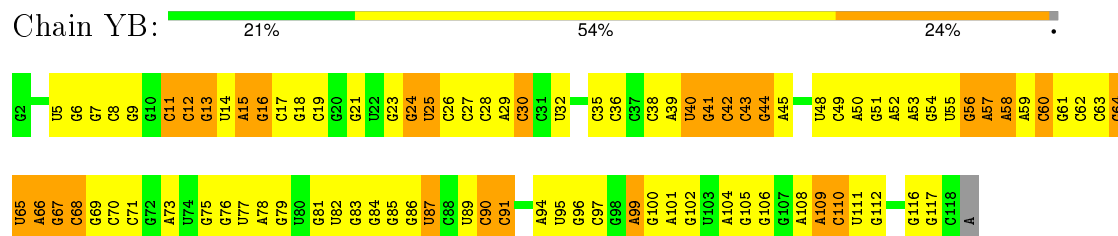
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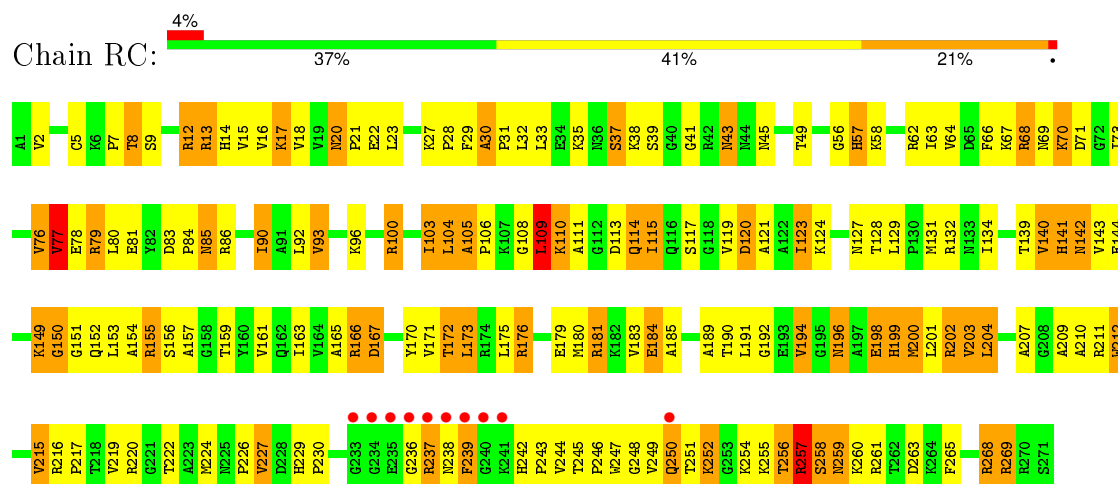
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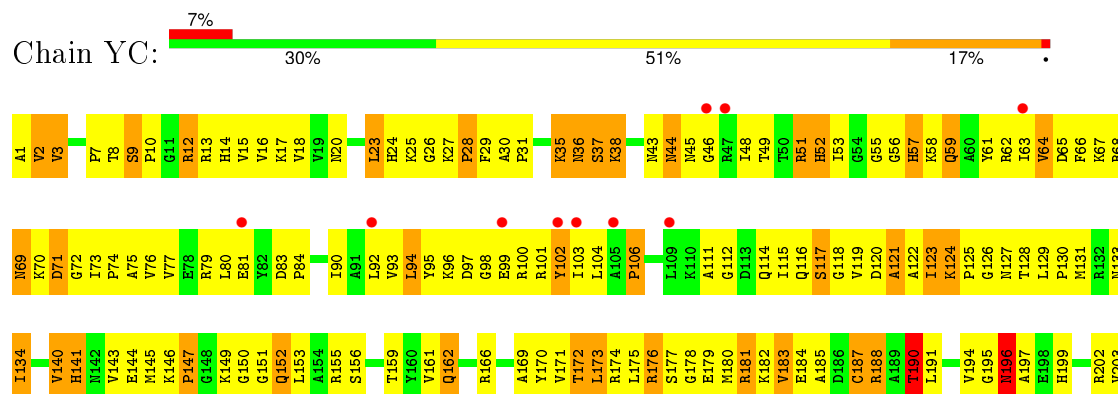
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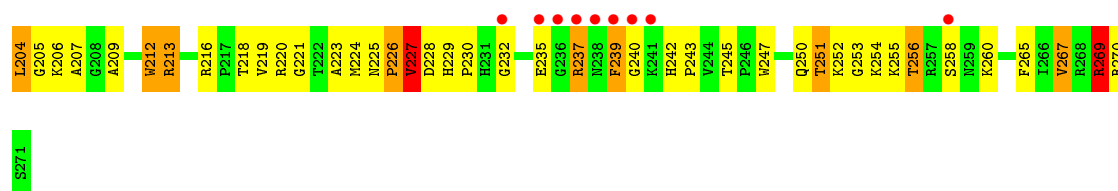


- Molecule 3: 50S ribosomal protein L2

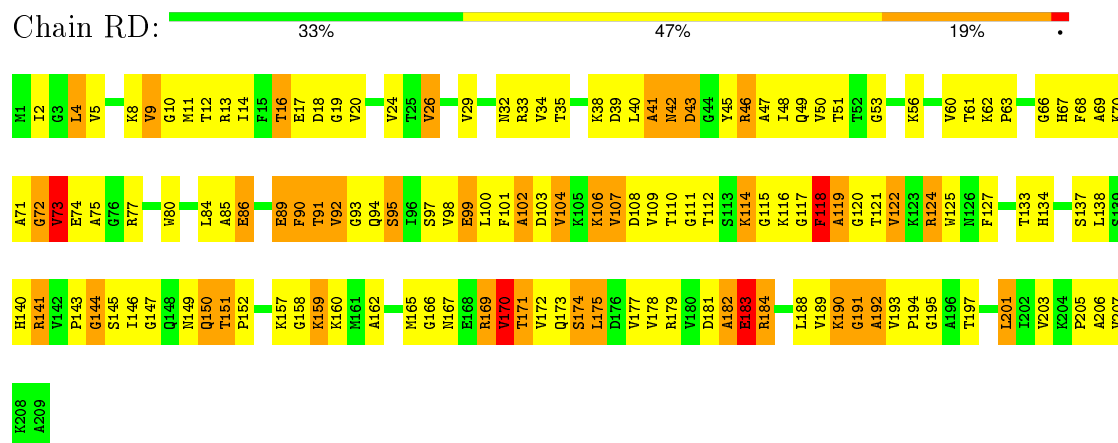


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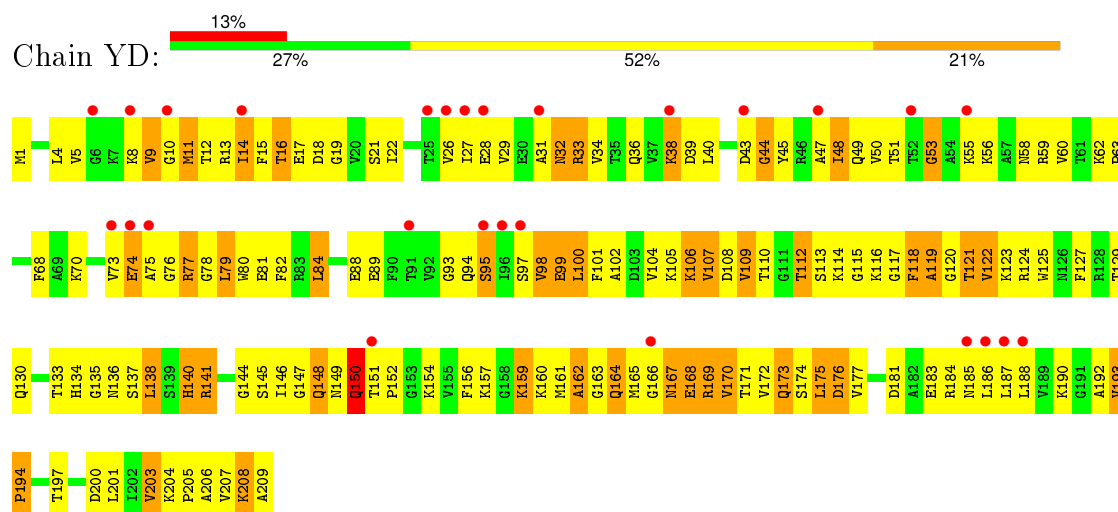




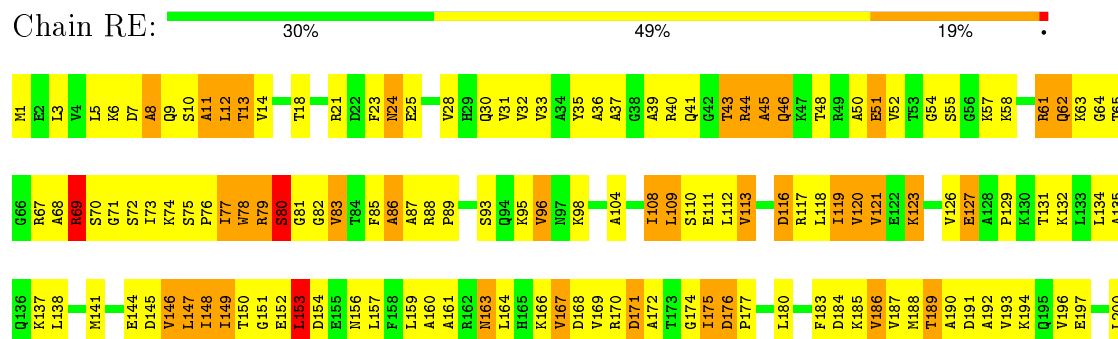
- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3

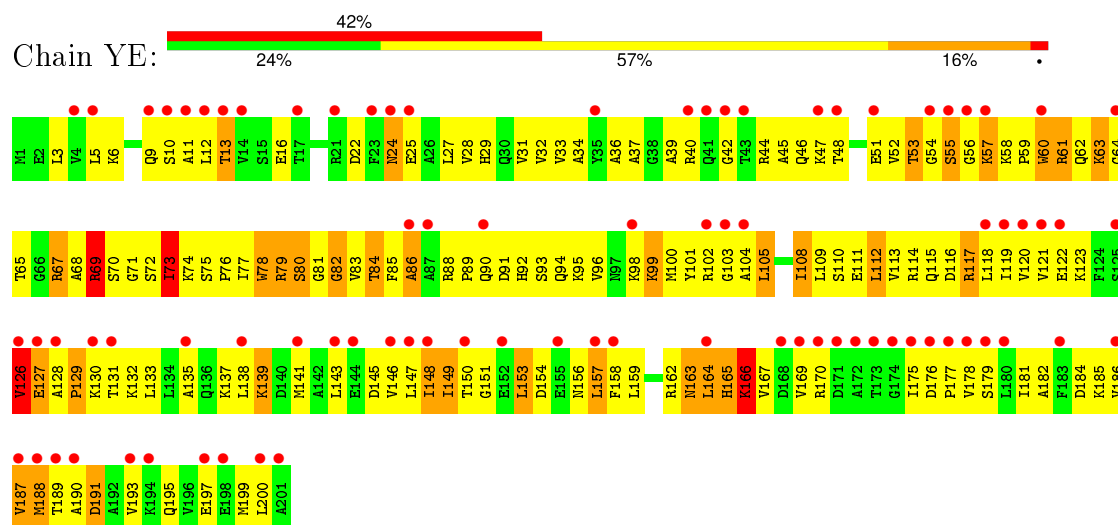


- Molecule 5: 50S ribosomal protein L4

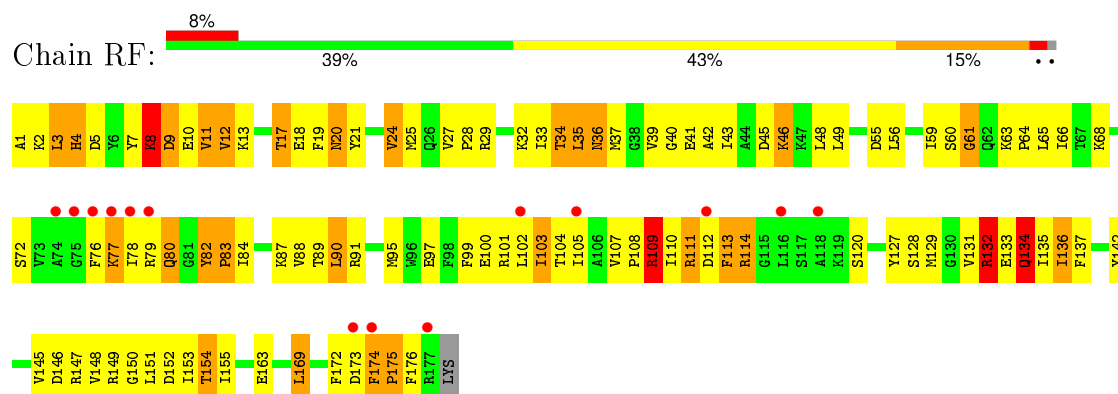


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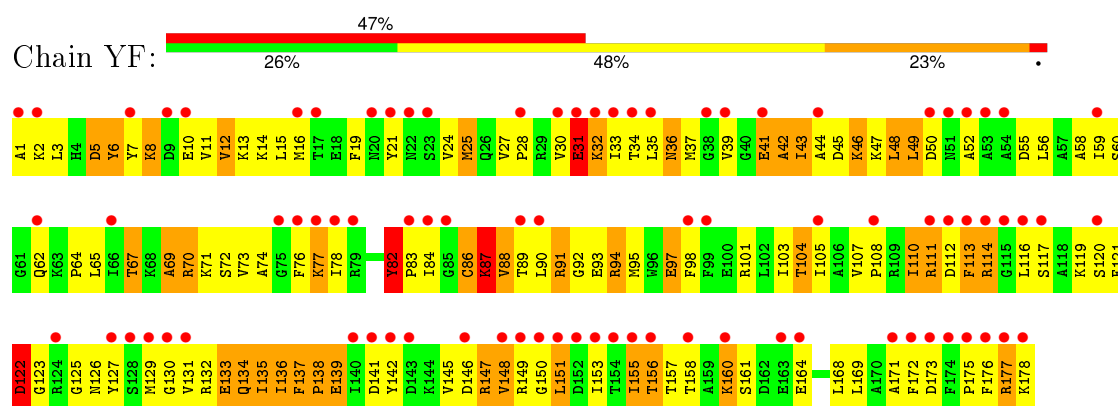
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5

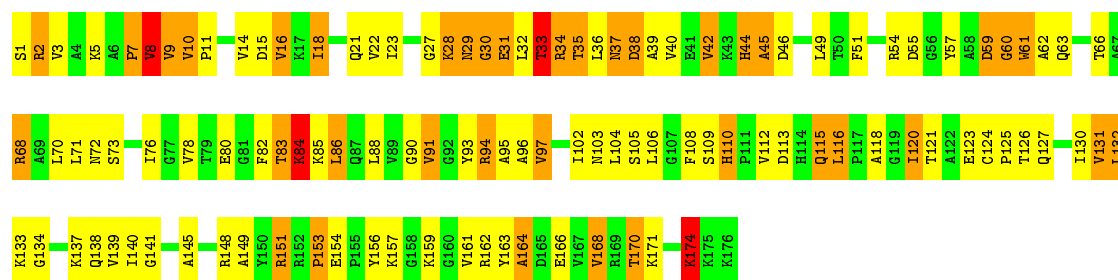


- Molecule 6: 50S ribosomal protein L5

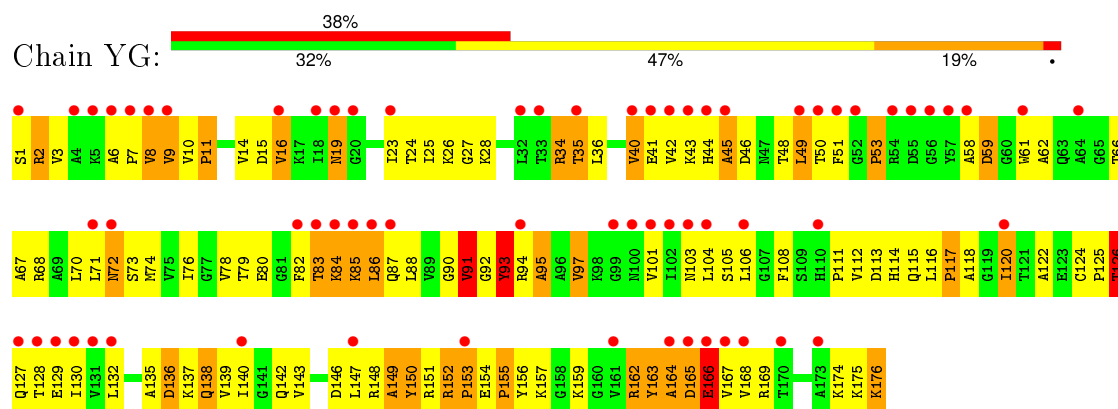


- Molecule 7: 50S ribosomal protein L6

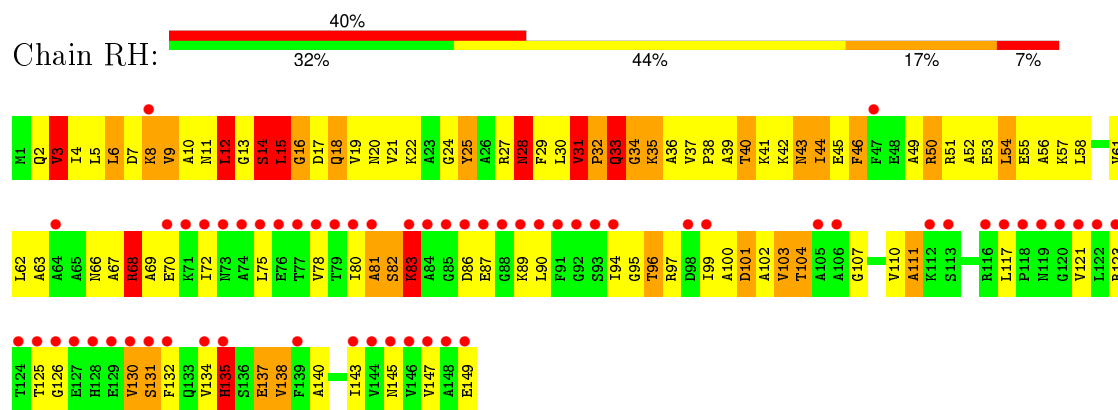




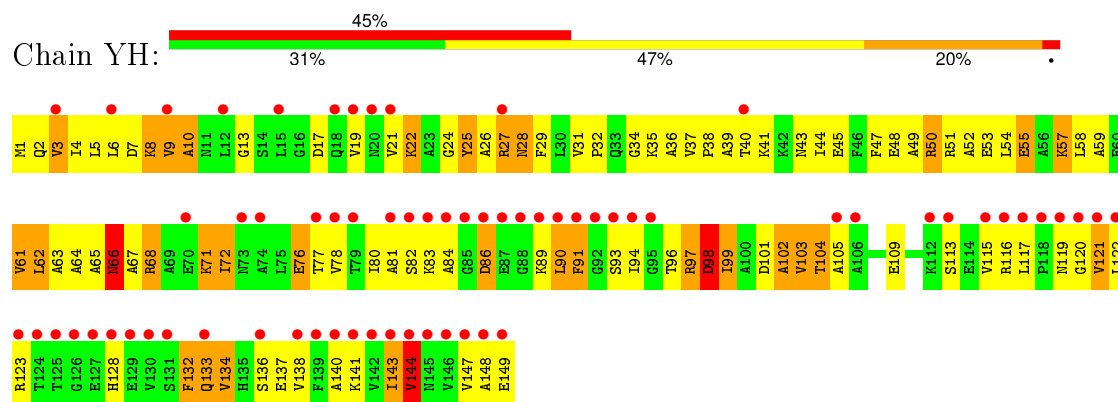
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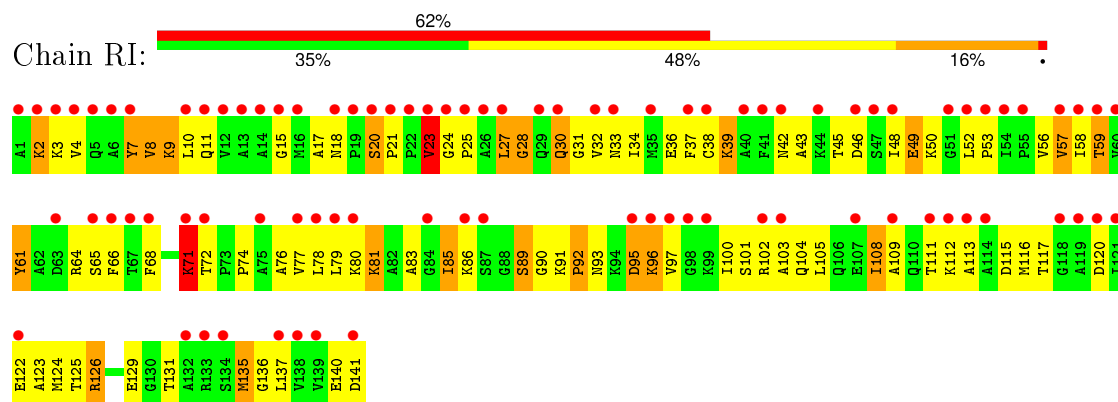
• Molecule 8: 50S ribosomal protein L9



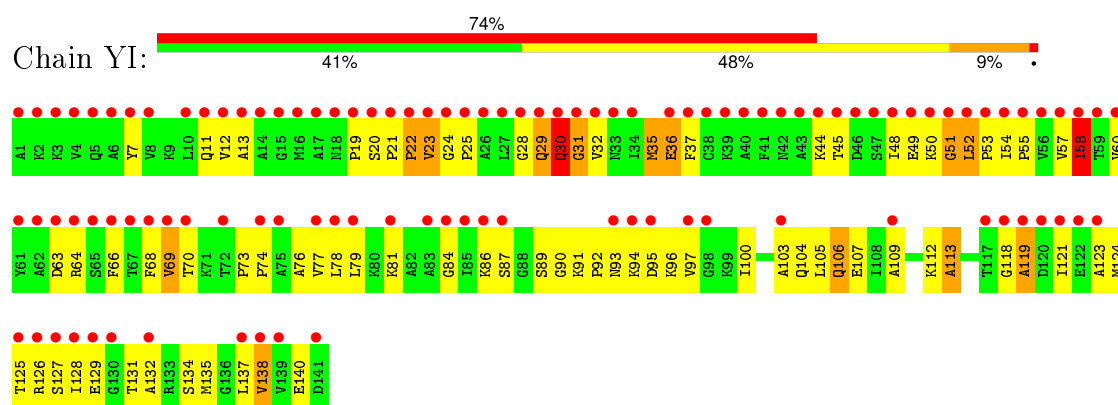
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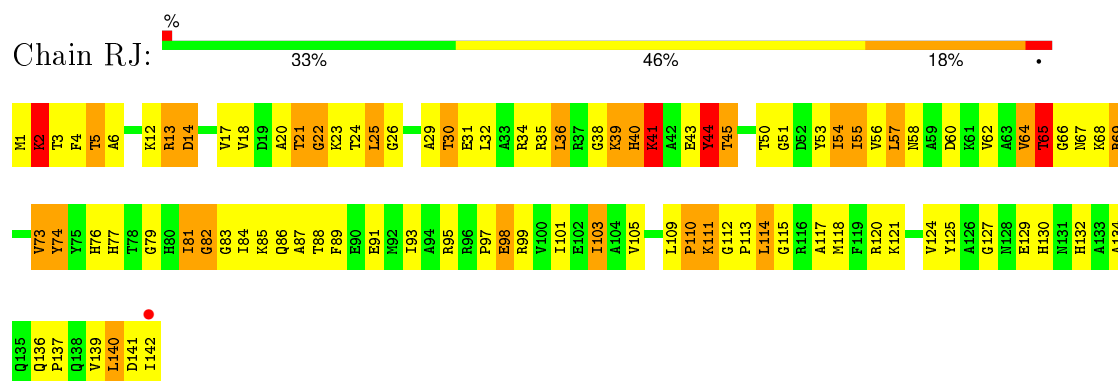
- Molecule 9: 50S ribosomal protein L11



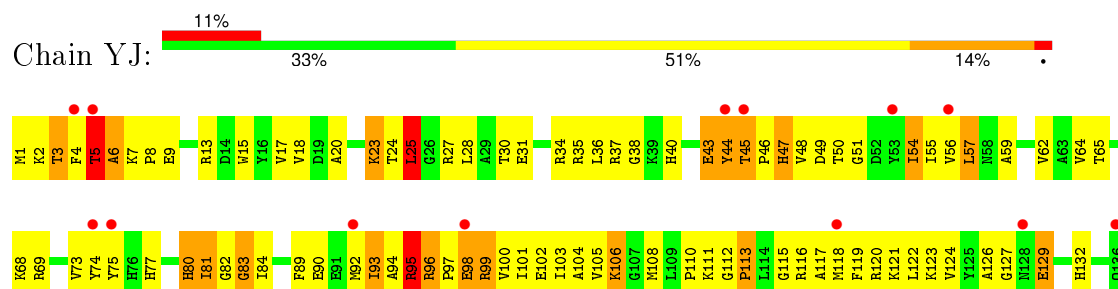
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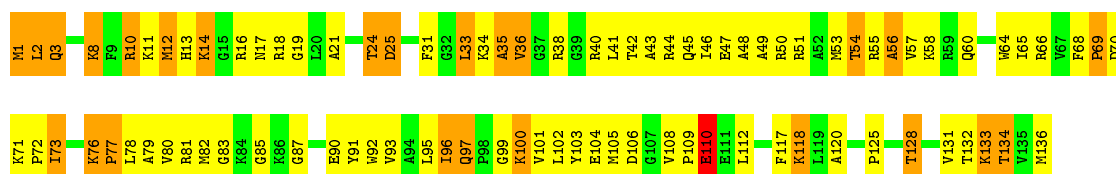


- Molecule 10: 50S ribosomal protein L13

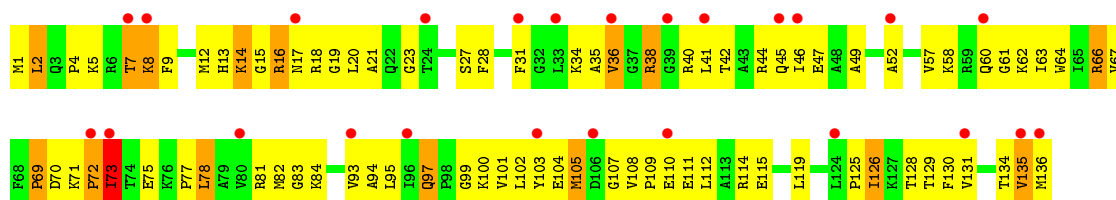


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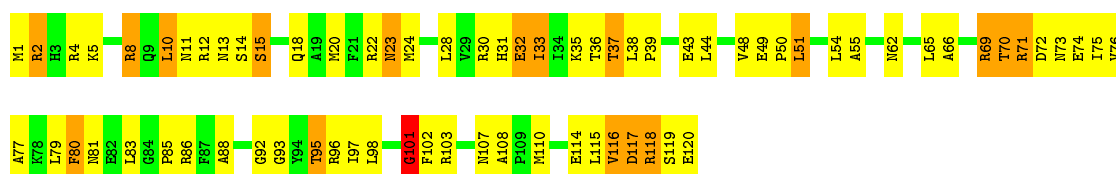




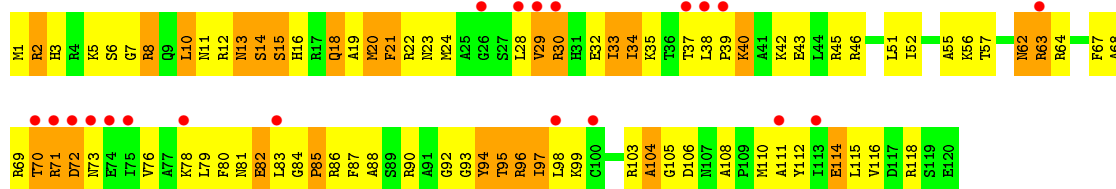
• Molecule 13: 50S ribosomal protein L16



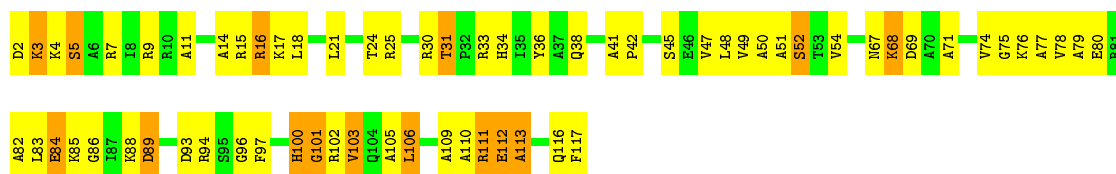
• Molecule 14: 50S ribosomal protein L17



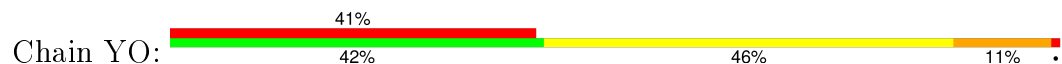
• Molecule 14: 50S ribosomal protein L17

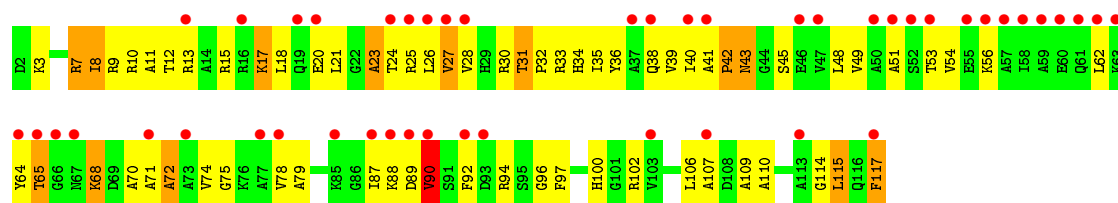


• Molecule 15: 50S ribosomal protein L18



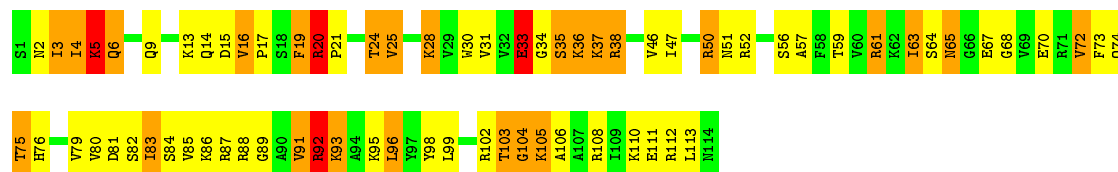
• Molecule 15: 50S ribosomal protein L18





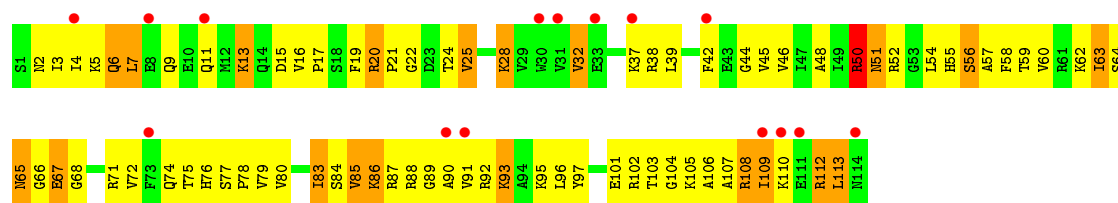
• Molecule 16: 50S ribosomal protein L19

Chain RP: 36% 39% 22%



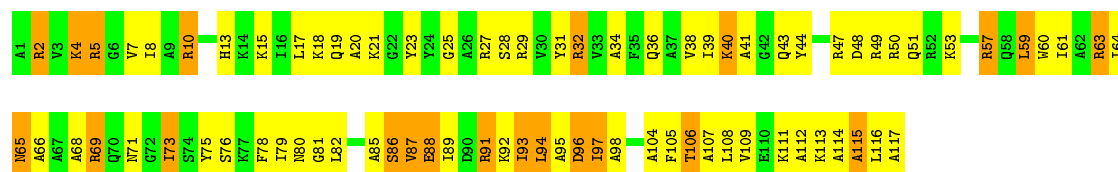
• Molecule 16: 50S ribosomal protein L19

Chain YP: 13% 30% 52% 18%



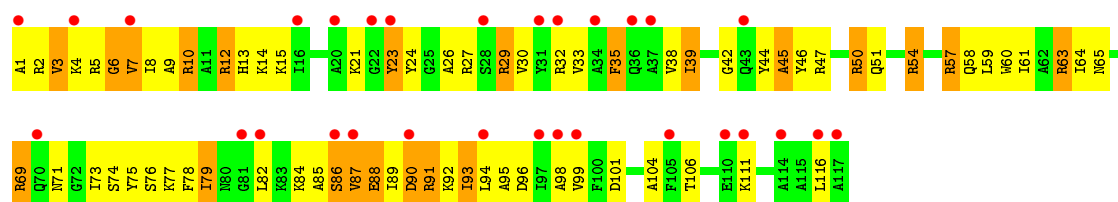
• Molecule 17: 50S ribosomal protein L20

Chain RQ: 32% 49% 19%



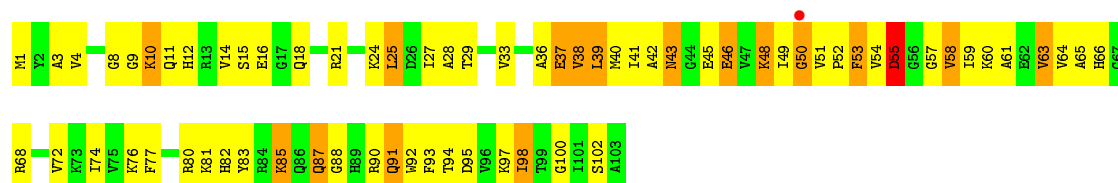
• Molecule 17: 50S ribosomal protein L20

Chain YQ: 26% 38% 43% 19%

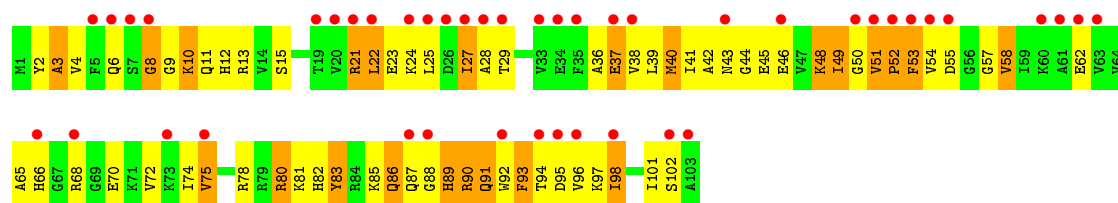


• Molecule 18: 50S ribosomal protein L21

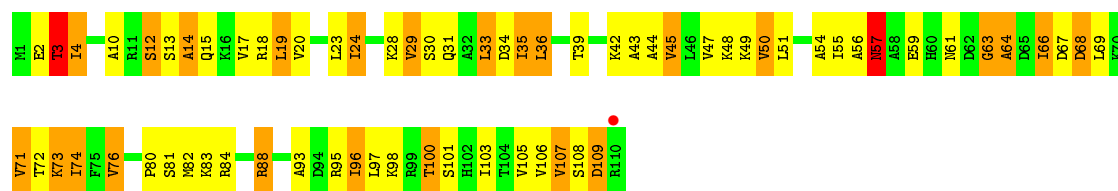
Chain RR: 34% 50% 16%



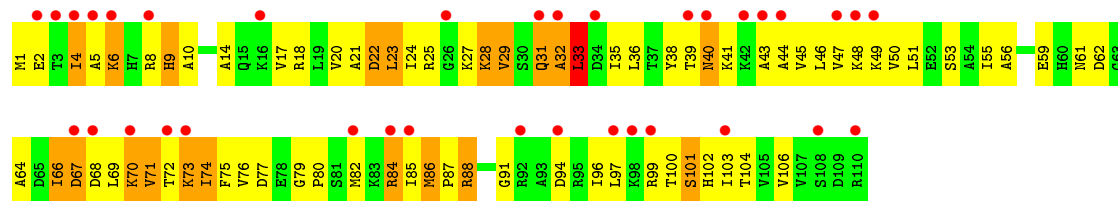
• Molecule 18: 50S ribosomal protein L21



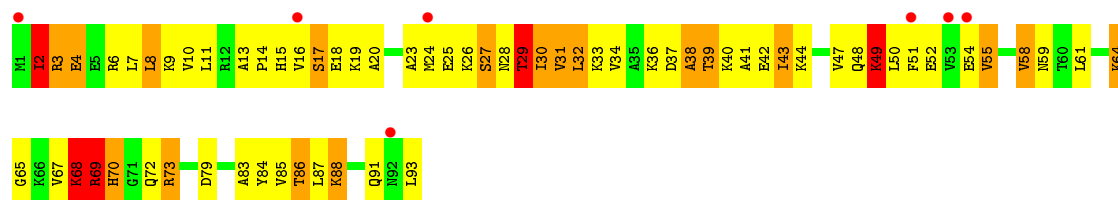
• Molecule 19: 50S ribosomal protein L22



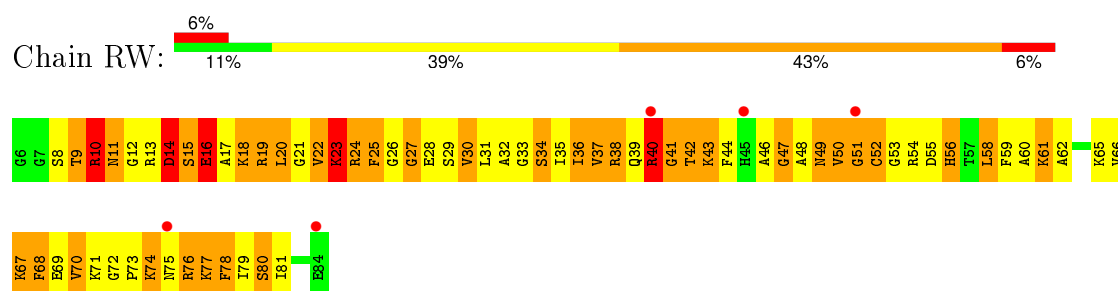
• Molecule 19: 50S ribosomal protein L22



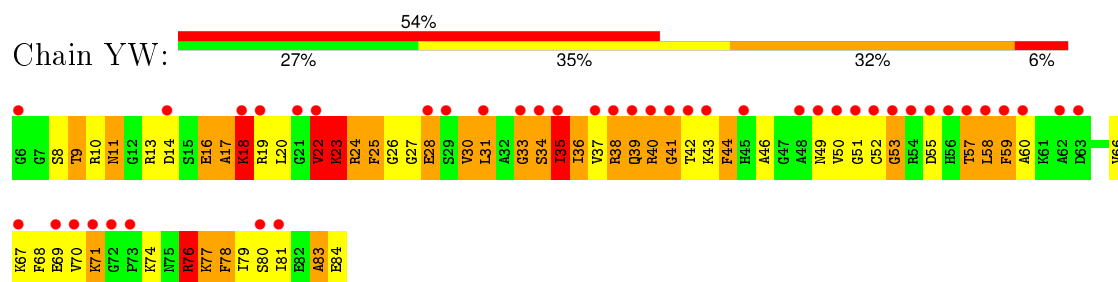
• Molecule 20: 50S ribosomal protein L23



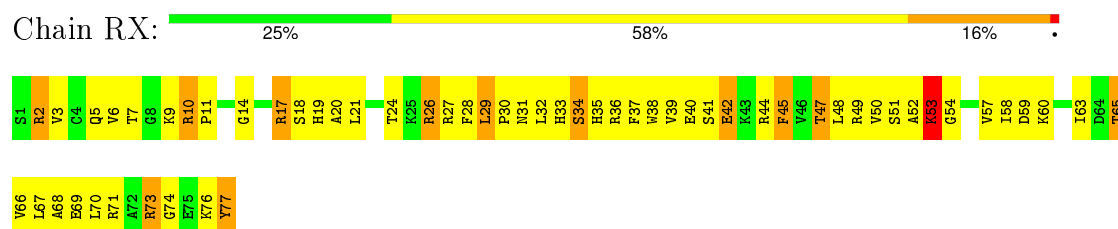
• Molecule 20: 50S ribosomal protein L23



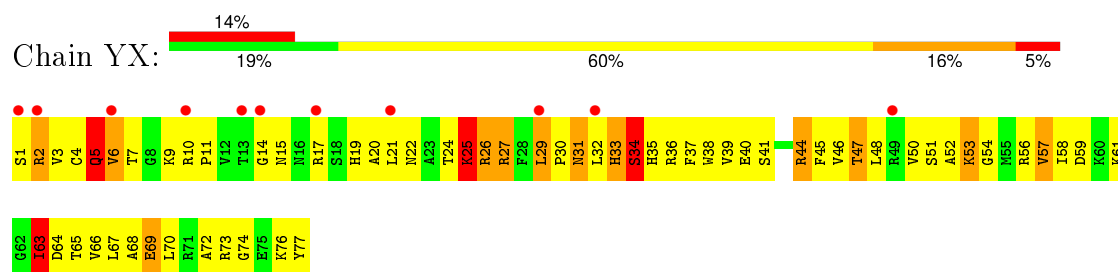
- Molecule 23: 50S ribosomal protein L27



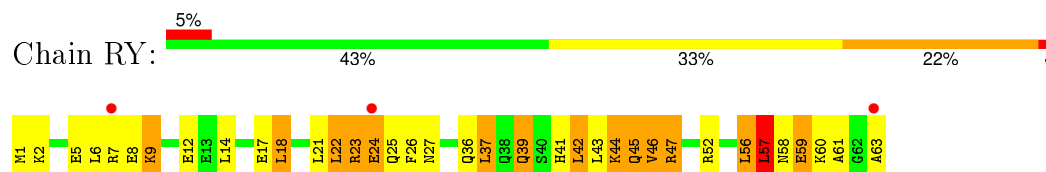
- Molecule 24: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L28

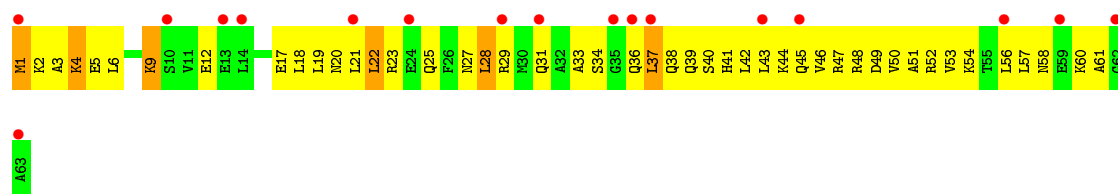


- Molecule 25: 50S ribosomal protein L29



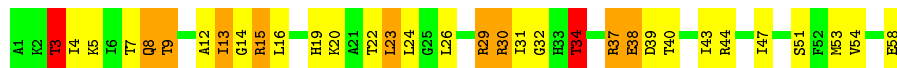
- Molecule 25: 50S ribosomal protein L29





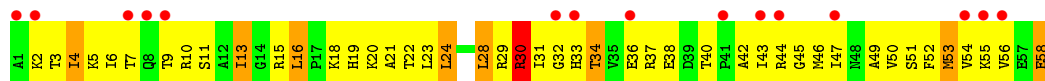
- Molecule 26: 50S ribosomal protein L30

Chain RZ: 43% 38% 16%



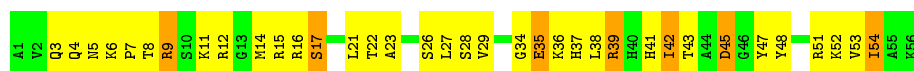
- Molecule 26: 50S ribosomal protein L30

Chain YZ: 22% 62% 14%



- Molecule 27: 50S ribosomal protein L32

Chain R0: 36% 52% 13%



- Molecule 27: 50S ribosomal protein L32

Chain Y0: 34% 39% 21% 5%



- Molecule 28: 50S ribosomal protein L33

Chain R1: 2% 34% 44% 18%



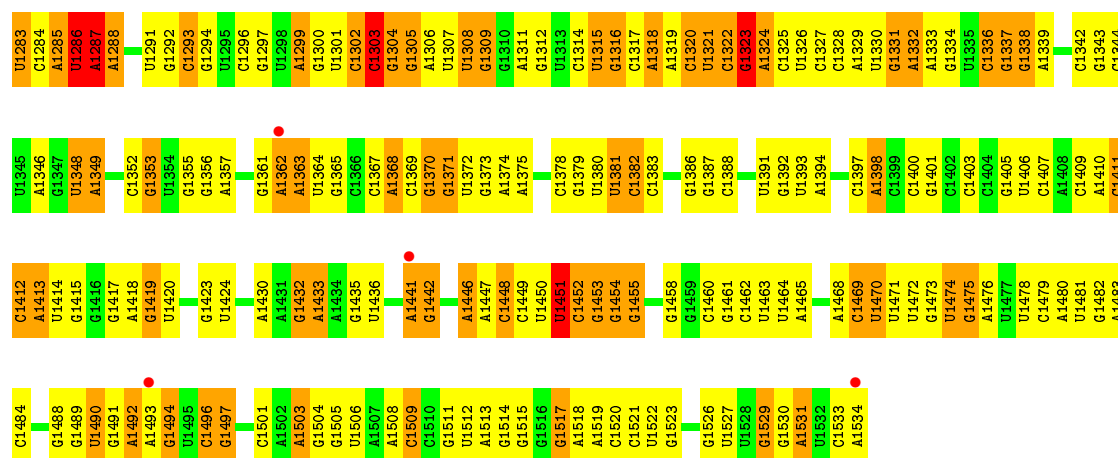
- Molecule 28: 50S ribosomal protein L33

Chain Y1: 32% 42% 46% 12%

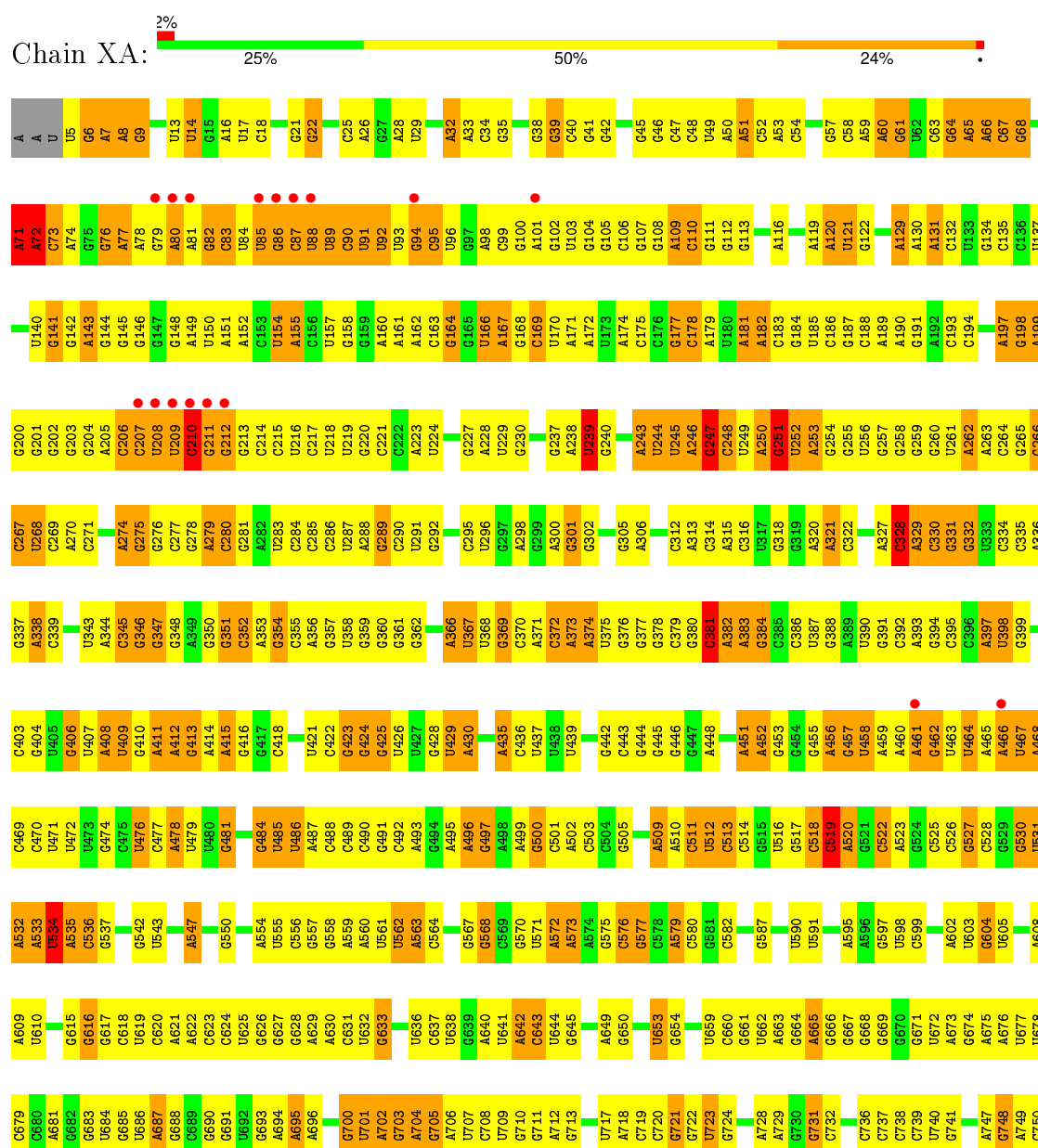


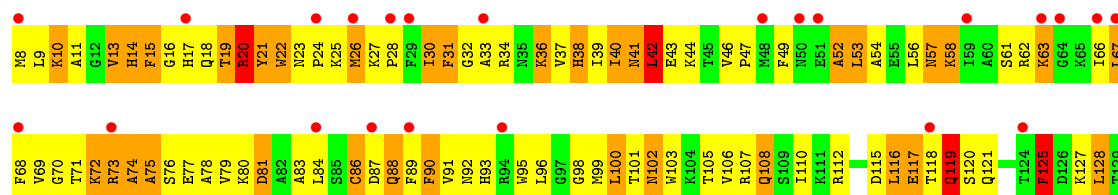
- Molecule 29: 50S ribosomal protein L34

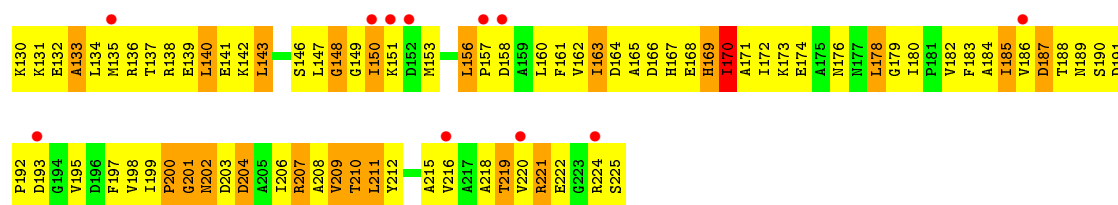
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C1218	A1145	U1008	C934	C866	A794	C647	A572	C501	A435	A364	U287	C214	U150
A1219	A1146	U1009	A935	C867	C795	A649	A573	A502	C436	U365	A288	C215	C153
G1220	C936	U1010	C936	C868	C796	A649	A574	C503	U437	A366	G289	U216	U154
G1221	C1149	A1082	A937	C869	C797	G650	G575	C504	U438	U367	C290	C217	
G1222	A1150	U1083	C940	U870	U798	C651	C576	C505	U439	U368	U291	U218	
G1223	A1151	U1084	C940	U871	G799	U852	C726	C507	C440	C369	G292	U219	
U1224	A1152	G1084	C945	A872	U800	G653		C507	C441	C370	U220		
G1225	G1153	U1017	G945	A873	U801	G654	G731	U508	G442	A371	G221	G158	
C1226	A1154	G1018	A946	C874	A802	A655	G581	U509	C443	C372	A300	G159	
A1227	A1155	U1087	G947	U875	G803		C582	A510	C444	A373	A222	A161	
C1228	G1156	G1088	C948	C876	U804	C658	A583	C511	G445	A374	U224	A162	
A1229	A1157	A1021	A949	G877	U805	U659			G446	U375	C225	C163	
	C1158	A1022	U950	A878	C806	C660	G587	G515		G376	G226	G164	
	U1159	U1023	G951	C879	C807	G661	G588		G450	G377	G227	U166	
G1233	G1160	A1093	U952	C880	C808	U662		C518	A451	A382	G230	A167	
C1234	C1161	G1094	G953	C881	G809	A663	U591	A520	A452	A383		G168	
U1235	C1162	G1095	G954	C882	C810	G664	G592	G521	G453	A384		C169	
A1236	A1163	C1096	U955	C883	C811	A665	U593	C522					
			U956	U884	G812	G666	U594	C522	U458		A313		
G1237			U957		U813	G667	U595	A523	U459	A389	C316	A172	
A1238	G1166	A1101	U958	C887	A814	A747	A596		A460	U390	U317	U173	
A1239	A1167	A1102	A958	C888	A815	G748	G597		A461	G391	G241	A174	
U1240	A1168	C1103	A959	C889	A816	A749	U598	C528	G462	C392	G242	C175	
G1241	A1170	G1032	U960	A890	C817	C750	C599	G529	U463	A393	A243	C176	
C1243	A1171	G1033	U960	G890	C817	U751	A600	G530	U464	G394	C322	G177	
			U965		G818	G752	G601	U531		A465	A321	U245	
G1244			U966	C895	A819	A673	A600	G530	U466	C395	C326	C178	
C1245	G1174	A1035	G966	C896	U820	G674	G601	U532	A466		A327	A179	
U1246	C1112	A1036	C967	C897	A815	A675	G597	A533	U467	U398	G328	U180	
A1248	C1113	C1037	A968	C898	A816	G676	U598	A534	A468	A403	C328	A181	
C1249	C1114	G1038	A969	C899	U827	G680	G605	A535	C469	C404	A329	A182	
A1250	U1115	U1040	C971	A900	U828	G681	G606	C536	C470	U471	C330	C183	
A1251	U1116	G1041	C972		G829	G682	A607	G537	U472	G405	G331	U252	
A1252	U1117		C973	G903	G829	G683	A608	G538	U473	A406	G332	A184	
G1253	C1118	C1046	A974	U904	A831	U684		A539	G474	U407	U334	U185	
A1254	C1119	A1046	A975	U905	G832	U685	C612	G540	G475	A408	C334	C186	
G1255	C1120	G1047	G976	A906	G833	A687	C613	G541	C475	U409	G335	G187	
	U1121	G1048	A977	A907	U834	G765	C614	G542	U476	G410		C188	
A1256	U1122	U1049	A978	A908	U835	G690	G615	U543	C477	A411	A338	G191	
A1257	U1123	G1050	U982	A909	G836	G691	G616	G544	A478	A412	C339	A192	
G1258	G1124	C1051	U982			U692	G617	C545	U479	G413	U340	C193	
	U1125	U1052	U983	C912	C841	G693	C618	A546	U480	A414	C341	C194	
A1261	U1126	G1053	A983	A913	U842	A694	U619	A547	G481	A415	C342	A195	
	G1127	C1054	G988	A914	U843			G548	A482	G416	U343	A196	
G1266	C1128	A1055	U989	A915	G844	U697	A622	C549	C483	G417	A344	A197	
	U1129	U1056	C990	U916	A845	G698	C623		G484	C418	C345	G198	
A1269	C1200	G1057	U991	G917	G846	C699	C624	A553	U485	C419	G346	A199	
G1270	A1201		U992	A918	G847	G700	U625	A554	U486	U420	G347	G200	
A1271	U1202	G1131	G993	A919	C848	U701	G633	U555	A487	U421	C269	G201	
C1272	C1203	G1133	A994	U920		A702	C634	C556	C488	C422	A270	G202	
			C995	U921	U855	G703	C634	G557	C489	G423	C271	G203	
A1273	G1206	U1135	A996	G922	C856		A635	G558	C490	G424	C272	G204	
A1275	C1210	C1136		A923	C857	U706	U636	A559	G491	U427	U273	C206	
G1277	C1137	U1065	A1000	C924	G858	A707	C637				A355	A274	
U1212	G1138	C1066	C1001	G925	G859	G708	U638	U562	G494	U428	A356	G275	
G1278	U1212		G1002	G926	A860	U709	U641	A563		U429	G357	U208	
A1213	C1140	C1069	G1003	G927	G861		U644	C564	A495	U430	U358	U209	
C1214	C1141		A1004	G928	G862	G714	U644		A496	A431	G359	C210	
G1215	G1142	G1072	A1005	G928	U863	A715	U644	C569	G497	A432		C284	
C1282	A1216	U1073	G1006	C932	A864	A716	G645	G570	A499	G433	G362	C285	



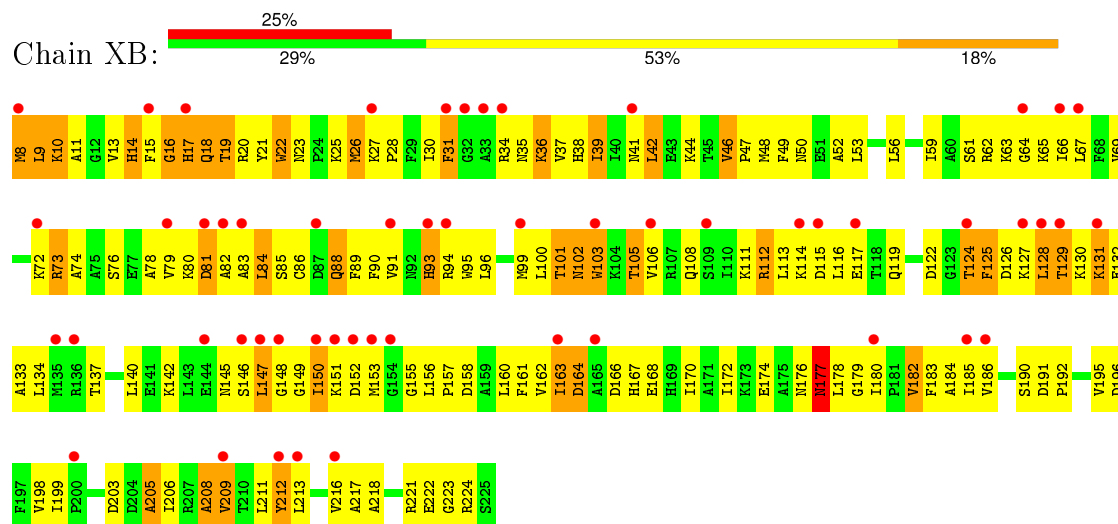
Molecule 32: 16S rRNA



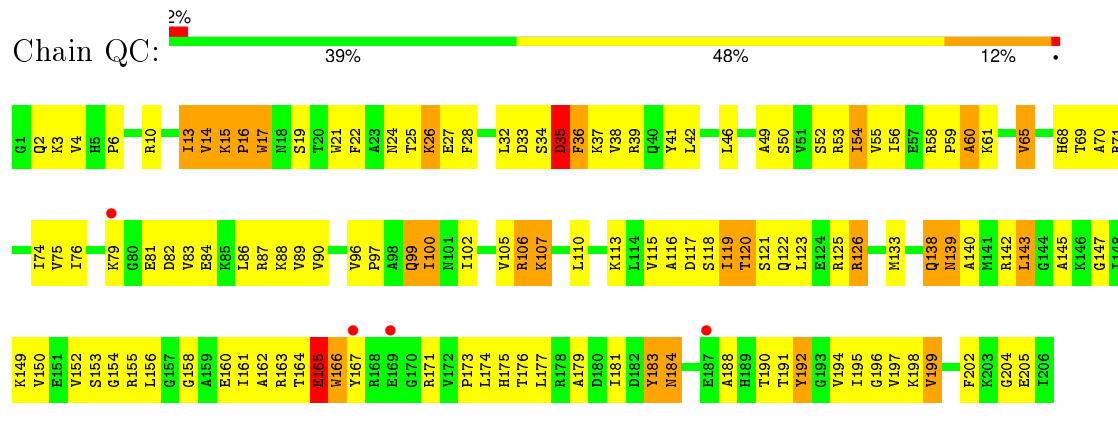




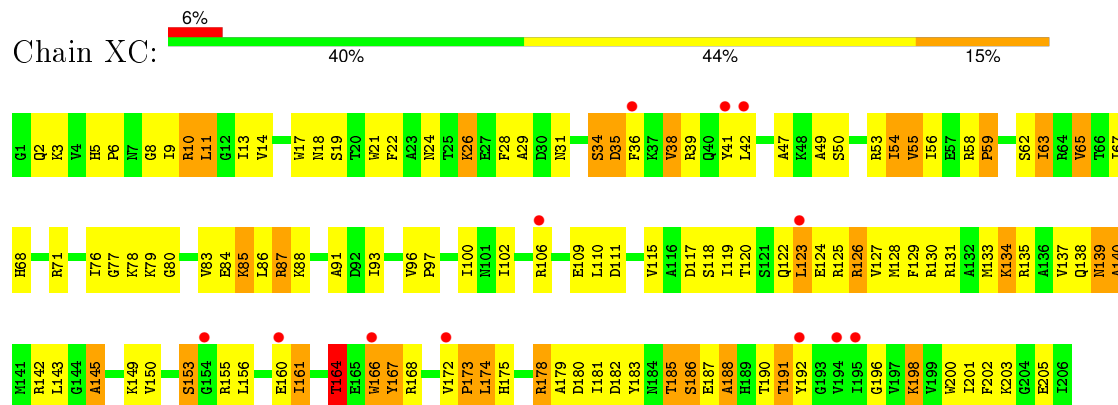
• Molecule 33: 30S ribosomal protein S2



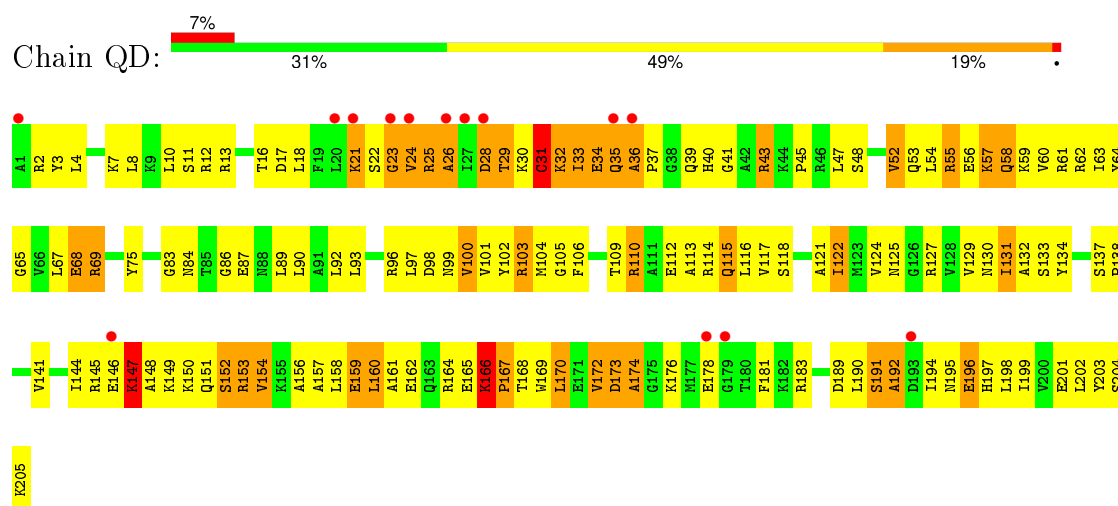
• Molecule 34: 30S ribosomal protein S3



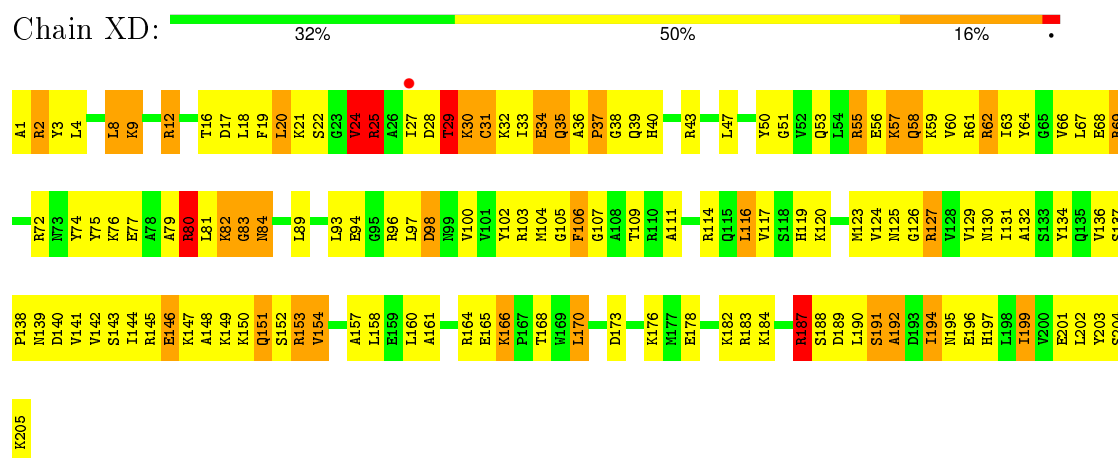
• Molecule 34: 30S ribosomal protein S3



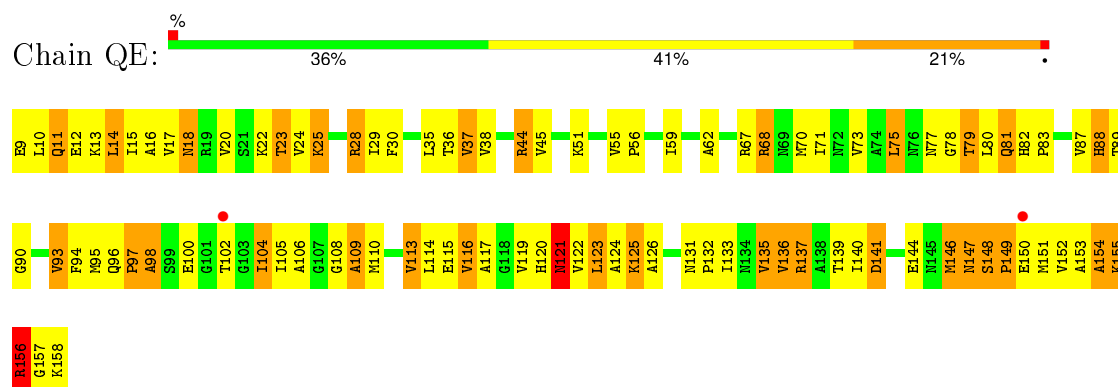
- Molecule 35: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S4

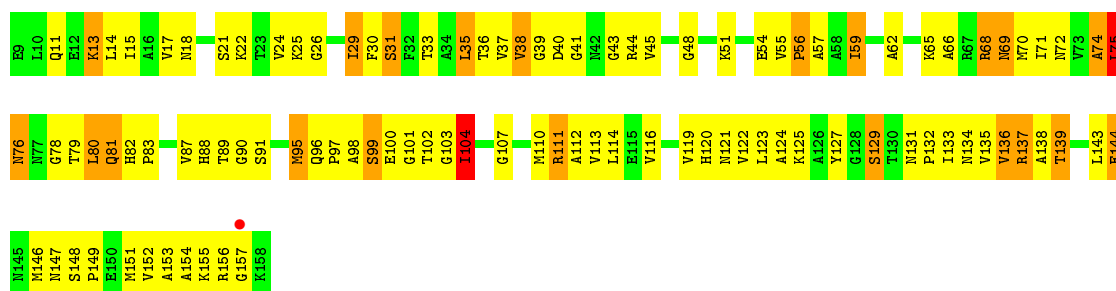


- Molecule 36: 30S ribosomal protein S5

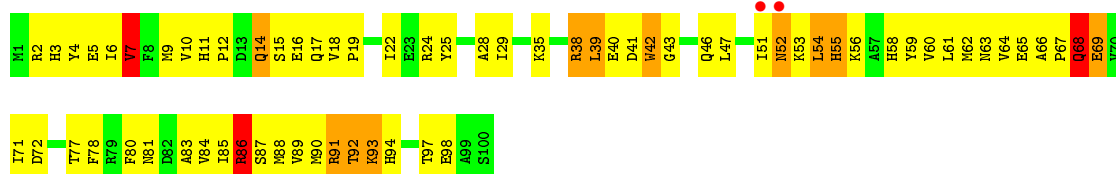


- Molecule 36: 30S ribosomal protein S5

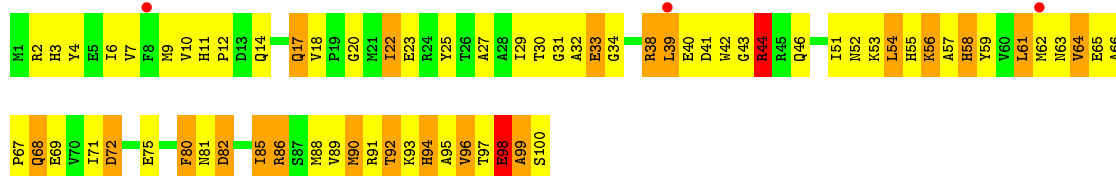




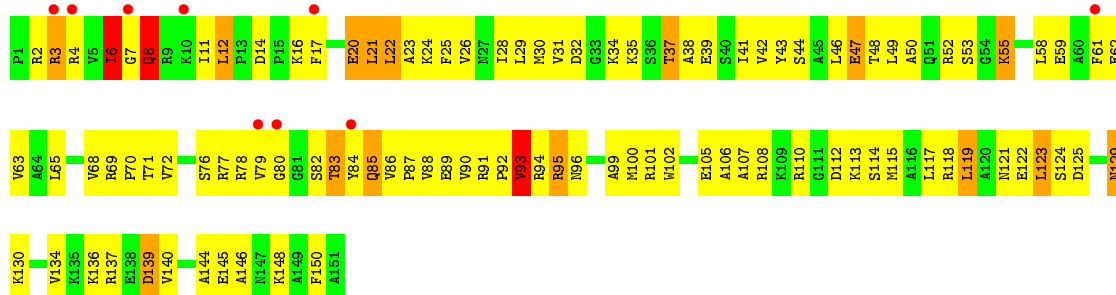
- Molecule 37: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S6

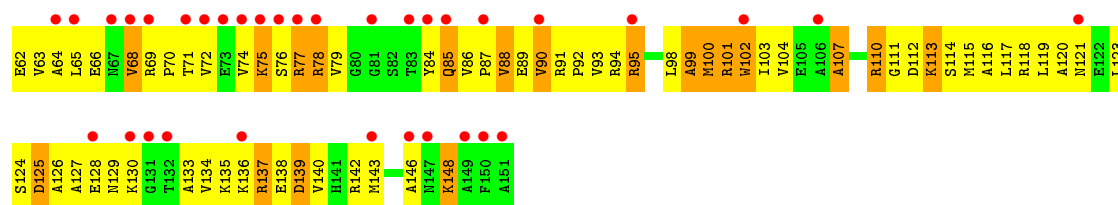


- Molecule 38: 30S ribosomal protein S7

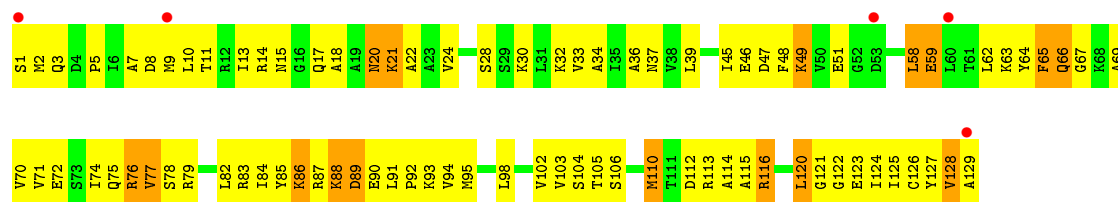


- Molecule 38: 30S ribosomal protein S7

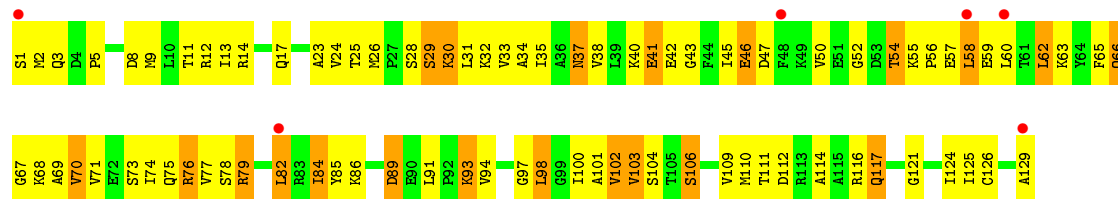




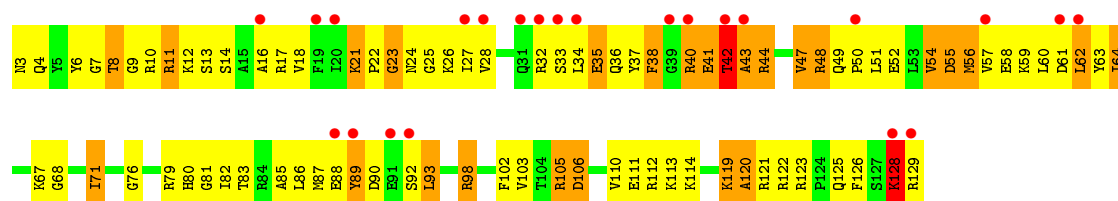
• Molecule 39: 30S ribosomal protein S8



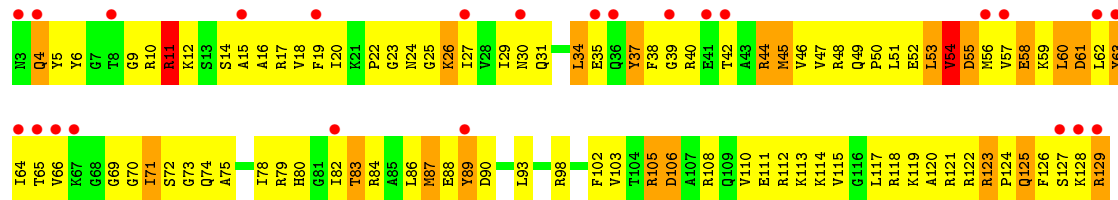
• Molecule 39: 30S ribosomal protein S8



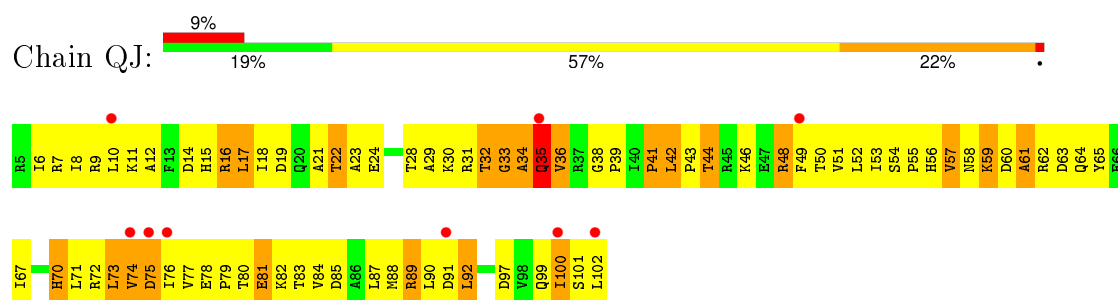
• Molecule 40: 30S ribosomal protein S9



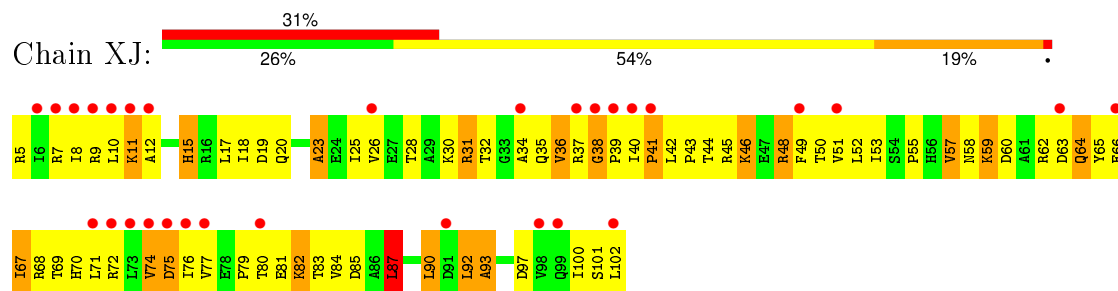
• Molecule 40: 30S ribosomal protein S9



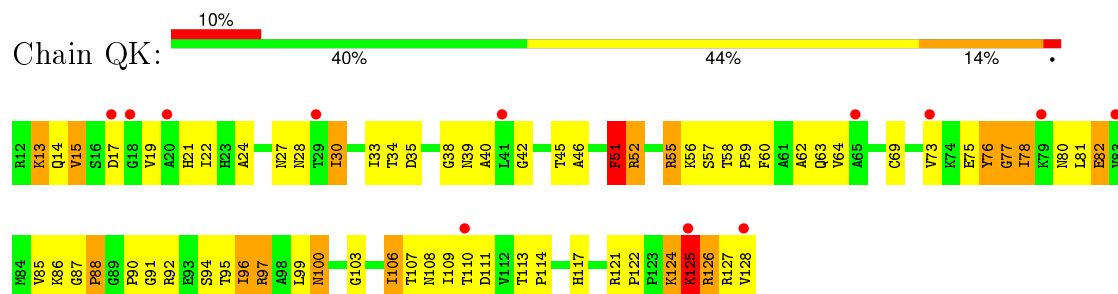
• Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10



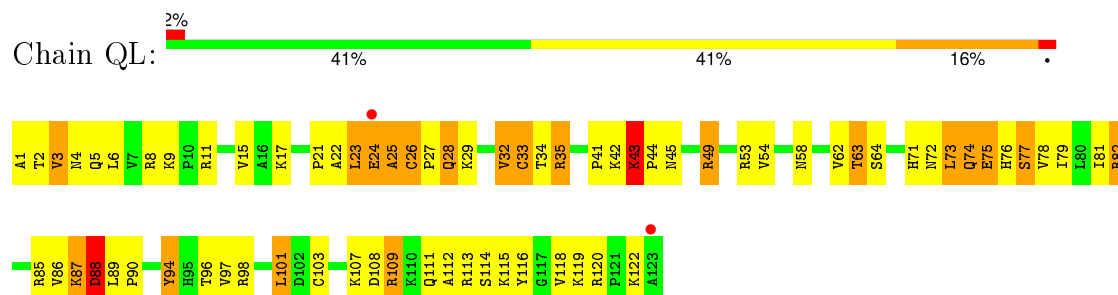
- Molecule 42: 30S ribosomal protein S11



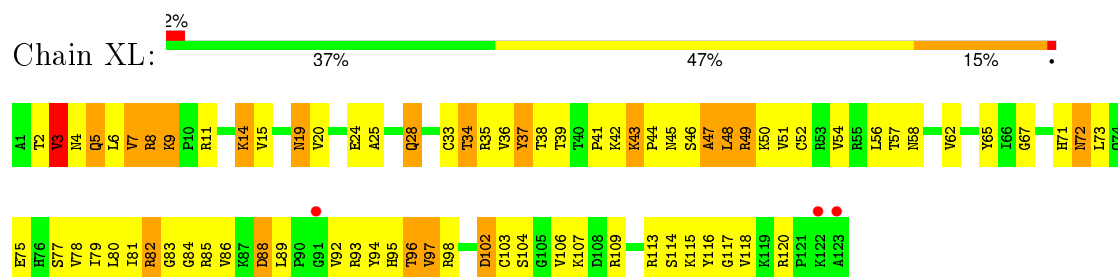
- Molecule 42: 30S ribosomal protein S11



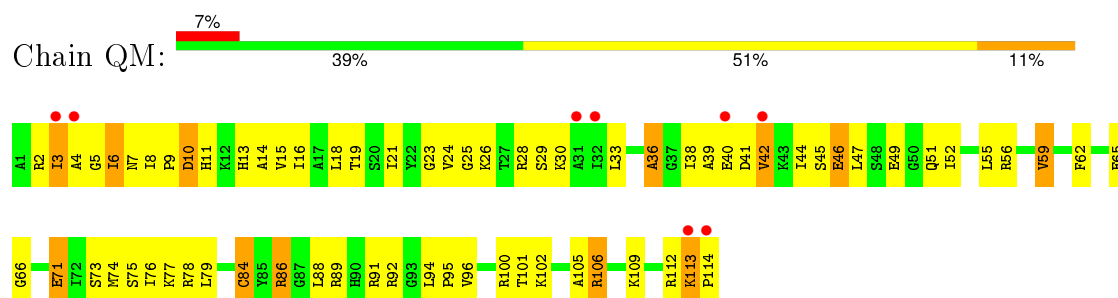
- Molecule 43: 30S ribosomal protein S12



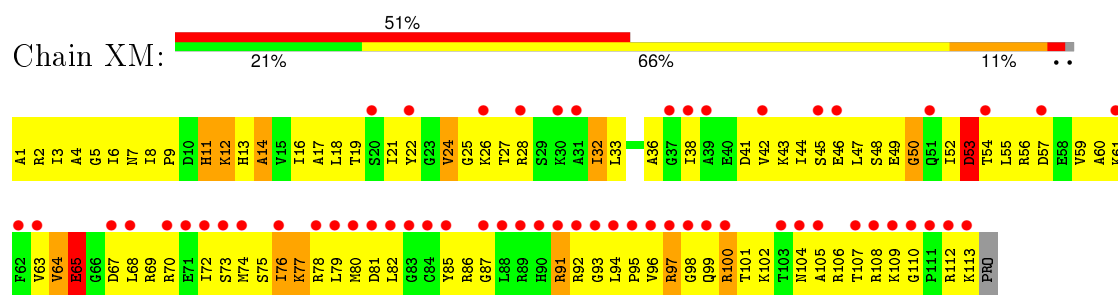
- Molecule 43: 30S ribosomal protein S12



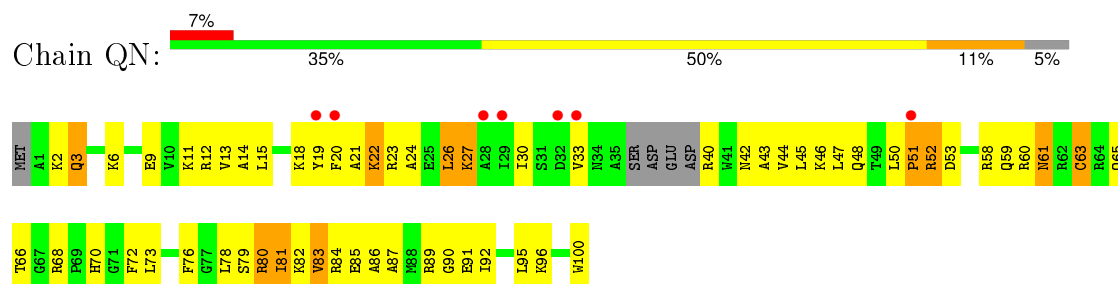
- Molecule 44: 30S ribosomal protein S13



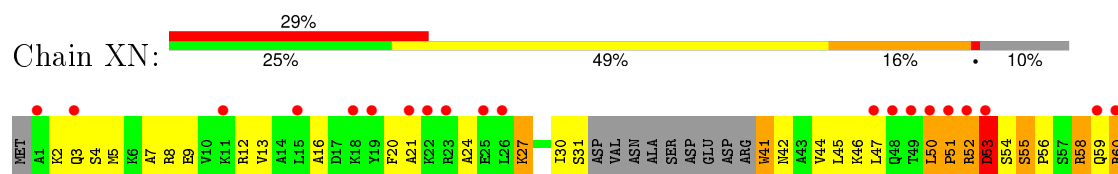
- Molecule 44: 30S ribosomal protein S13

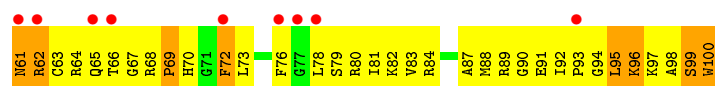


- Molecule 45: 30S ribosomal protein S14

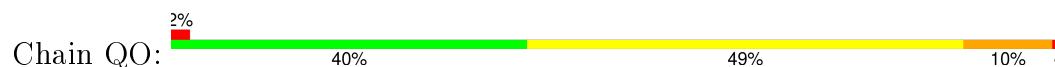


- Molecule 45: 30S ribosomal protein S14





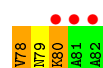
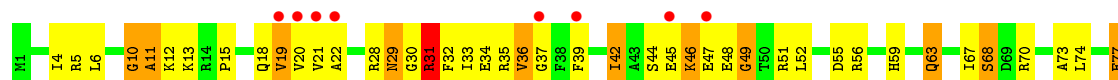
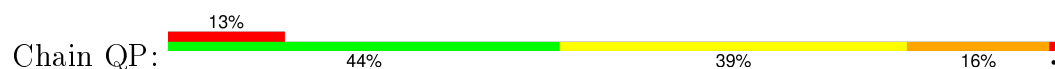
• Molecule 46: 30S ribosomal protein S15



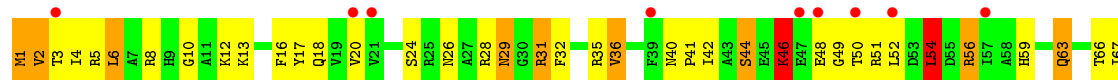
• Molecule 46: 30S ribosomal protein S15



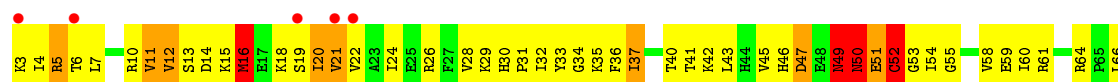
• Molecule 47: 30S ribosomal protein S16

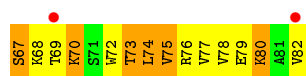


• Molecule 47: 30S ribosomal protein S16

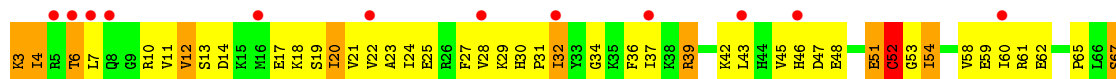


• Molecule 48: 30S ribosomal protein S17





• Molecule 48: 30S ribosomal protein S17



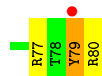
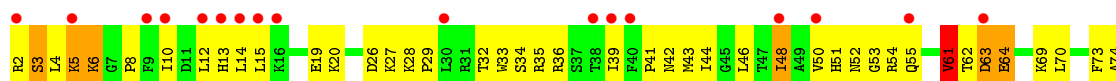
• Molecule 49: 30S ribosomal protein S18



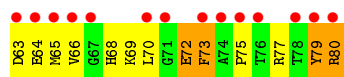
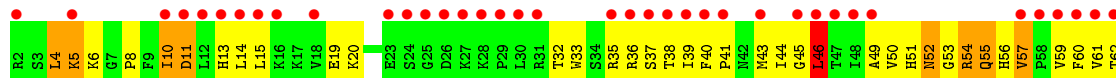
• Molecule 49: 30S ribosomal protein S18



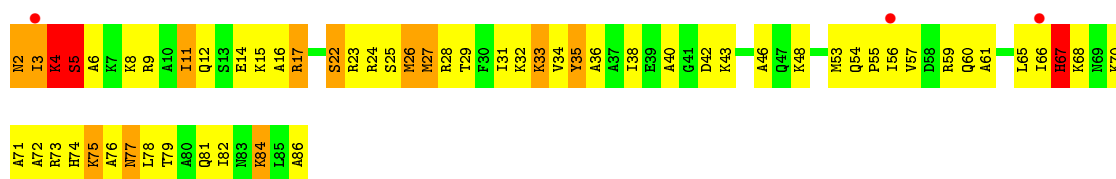
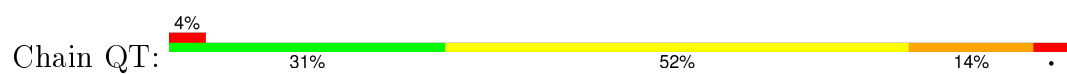
• Molecule 50: 30S ribosomal protein S19



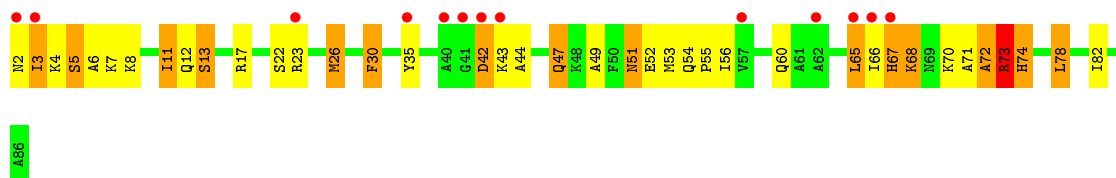
• Molecule 50: 30S ribosomal protein S19



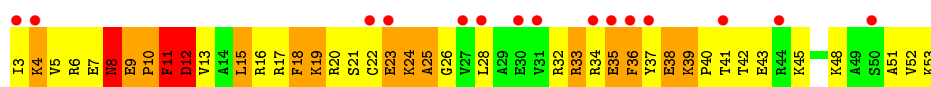
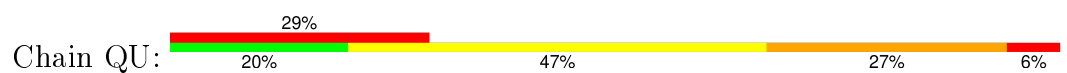
• Molecule 51: 30S ribosomal protein S20



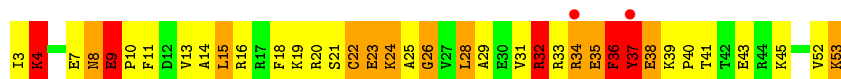
- Molecule 51: 30S ribosomal protein S20



- 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) 95.9 (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 0.214 , 0.264	Depositor DCC
R_{free} test set	19579 reflections (2.06%)	DCC
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 91.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 971020 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284464	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, EM1, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	RA	0.73	7/68626 (0.0%)	1.08	288/107056 (0.3%)
1	YA	0.38	0/68314	0.83	60/106569 (0.1%)
2	RB	0.64	0/2828	0.94	1/4410 (0.0%)
2	YB	0.30	0/2803	0.76	1/4371 (0.0%)
3	RC	0.47	0/2121	0.72	1/2852 (0.0%)
3	YC	0.32	0/2121	0.55	0/2852
4	RD	0.56	0/1586	0.80	1/2134 (0.0%)
4	YD	0.31	0/1586	0.57	0/2134
5	RE	0.43	0/1571	0.66	0/2113
5	YE	0.27	0/1571	0.51	0/2113
6	RF	0.32	0/1434	0.53	0/1926
6	YF	0.24	0/1444	0.50	0/1937
7	RG	0.40	0/1343	0.65	0/1816
7	YG	0.24	0/1343	0.50	0/1816
8	RH	0.32	0/1122	0.56	0/1515
8	YH	0.29	0/1122	0.52	0/1515
9	RI	0.23	0/1046	0.48	0/1410
9	YI	0.22	0/1046	0.47	0/1410
10	RJ	0.57	0/1152	0.82	1/1551 (0.1%)
10	YJ	0.29	0/1152	0.60	1/1551 (0.1%)
11	RK	0.54	0/947	0.80	0/1268
11	YK	0.34	0/947	0.58	0/1268
12	RL	0.44	0/1054	0.75	1/1403 (0.1%)
12	YL	0.28	0/1054	0.56	0/1403
13	RM	0.50	0/1093	0.71	0/1460
13	YM	0.29	0/1093	0.50	0/1460
14	RN	0.49	0/973	0.72	0/1301
14	YN	0.30	0/973	0.53	0/1301
15	RO	0.41	0/902	0.63	0/1209
15	YO	0.24	0/902	0.45	0/1209
16	RP	0.48	0/929	0.73	0/1242
16	YP	0.32	0/929	0.52	0/1242

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

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

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

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

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

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

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

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

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

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

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

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

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

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

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

The worst 5 of 16435 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:RQ:63:ARG:NH1	17:RQ:96:ASP:HA	1.42	1.33
43:XL:43:LYS:HB3	43:XL:44:PRO:HD2	1.18	1.17
1:RA:1073:A:H3'	1:RA:1074:G:H5''	1.20	1.17
32:XA:120:A:C3'	32:XA:121:U:H5''	1.75	1.17
37:QF:16:GLU:HG2	35:XD:191:SER:HB2	1.20	1.17

There are no symmetry-related clashes.

5.3 Torsion angles [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%)	1	3
3	YC	269/271 (99%)	180 (67%)	60 (22%)	29 (11%)	0	3
4	RD	207/209 (99%)	147 (71%)	31 (15%)	29 (14%)	0	1
4	YD	207/209 (99%)	128 (62%)	45 (22%)	34 (16%)	0	0
5	RE	199/201 (99%)	146 (73%)	32 (16%)	21 (11%)	0	3
5	YE	199/201 (99%)	117 (59%)	55 (28%)	27 (14%)	0	1
6	RF	175/178 (98%)	138 (79%)	22 (13%)	15 (9%)	1	5
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%)	1	4
9	RI	139/141 (99%)	84 (60%)	42 (30%)	13 (9%)	1	4
9	YI	139/141 (99%)	85 (61%)	37 (27%)	17 (12%)	0	2
10	RJ	140/142 (99%)	107 (76%)	19 (14%)	14 (10%)	1	4
10	YJ	140/142 (99%)	98 (70%)	28 (20%)	14 (10%)	1	4
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	3
13	YM	134/136 (98%)	92 (69%)	28 (21%)	14 (10%)	1	3
14	RN	118/120 (98%)	96 (81%)	14 (12%)	8 (7%)	1	8
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	8
15	YO	114/116 (98%)	74 (65%)	29 (25%)	11 (10%)	1	4
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%)	3	19
17	YQ	115/117 (98%)	77 (67%)	27 (24%)	11 (10%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	RR	101/103 (98%)	82 (81%)	11 (11%)	8 (8%)	1	6
18	YR	101/103 (98%)	66 (65%)	22 (22%)	13 (13%)	0	1
19	RS	108/110 (98%)	88 (82%)	10 (9%)	10 (9%)	1	4
19	YS	108/110 (98%)	75 (69%)	22 (20%)	11 (10%)	1	4
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%)	8	36
22	YV	92/94 (98%)	61 (66%)	23 (25%)	8 (9%)	1	5
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%)	4	21
24	YX	75/77 (97%)	45 (60%)	22 (29%)	8 (11%)	0	3
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	9
26	RZ	56/58 (97%)	46 (82%)	8 (14%)	2 (4%)	4	24
26	YZ	56/58 (97%)	34 (61%)	16 (29%)	6 (11%)	0	3
27	R0	54/56 (96%)	42 (78%)	9 (17%)	3 (6%)	2	13
27	Y0	54/56 (96%)	38 (70%)	7 (13%)	9 (17%)	0	0
28	R1	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	1	6
28	Y1	48/50 (96%)	33 (69%)	10 (21%)	5 (10%)	1	3
29	R2	44/46 (96%)	37 (84%)	5 (11%)	2 (4%)	3	17
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	9
30	Y3	62/64 (97%)	43 (69%)	13 (21%)	6 (10%)	1	4
31	R4	36/38 (95%)	29 (81%)	5 (14%)	2 (6%)	2	13
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%)	1	4
34	QC	204/206 (99%)	159 (78%)	26 (13%)	19 (9%)	1	4

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	QS	77/79 (98%)	57 (74%)	14 (18%)	6 (8%)	1	6
50	XS	77/79 (98%)	47 (61%)	25 (32%)	5 (6%)	1	9
51	QT	83/85 (98%)	61 (74%)	16 (19%)	6 (7%)	1	7
51	XT	83/85 (98%)	59 (71%)	18 (22%)	6 (7%)	1	7
52	QU	49/51 (96%)	25 (51%)	14 (29%)	10 (20%)	0	0
52	XU	49/51 (96%)	21 (43%)	12 (24%)	16 (33%)	0	0
All	All	11234/11454 (98%)	7596 (68%)	2346 (21%)	1292 (12%)	0	2

5 of 1292 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	RC	216/216 (100%)	164 (76%)	52 (24%)	1	3
3	YC	216/216 (100%)	181 (84%)	35 (16%)	3	12
4	RD	164/164 (100%)	138 (84%)	26 (16%)	3	13
4	YD	164/164 (100%)	142 (87%)	22 (13%)	5	20
5	RE	165/165 (100%)	126 (76%)	39 (24%)	1	3
5	YE	165/165 (100%)	140 (85%)	25 (15%)	3	14
6	RF	148/149 (99%)	121 (82%)	27 (18%)	2	9
6	YF	149/149 (100%)	120 (80%)	29 (20%)	2	7
7	RG	137/137 (100%)	108 (79%)	29 (21%)	1	6
7	YG	137/137 (100%)	119 (87%)	18 (13%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	RH	114/114 (100%)	93 (82%)	21 (18%)	2	9
8	YH	114/114 (100%)	91 (80%)	23 (20%)	1	7
9	RI	109/109 (100%)	89 (82%)	20 (18%)	2	9
9	YI	109/109 (100%)	102 (94%)	7 (6%)	22	57
10	RJ	116/116 (100%)	86 (74%)	30 (26%)	0	2
10	YJ	116/116 (100%)	99 (85%)	17 (15%)	4	16
11	RK	103/103 (100%)	81 (79%)	22 (21%)	1	5
11	YK	103/103 (100%)	84 (82%)	19 (18%)	2	9
12	RL	102/102 (100%)	80 (78%)	22 (22%)	1	5
12	YL	102/102 (100%)	85 (83%)	17 (17%)	3	11
13	RM	109/109 (100%)	89 (82%)	20 (18%)	2	9
13	YM	109/109 (100%)	98 (90%)	11 (10%)	9	33
14	RN	100/100 (100%)	82 (82%)	18 (18%)	2	10
14	YN	100/100 (100%)	85 (85%)	15 (15%)	3	15
15	RO	86/86 (100%)	67 (78%)	19 (22%)	1	5
15	YO	86/86 (100%)	79 (92%)	7 (8%)	15	47
16	RP	99/99 (100%)	76 (77%)	23 (23%)	1	4
16	YP	99/99 (100%)	89 (90%)	10 (10%)	9	33
17	RQ	89/89 (100%)	69 (78%)	20 (22%)	1	4
17	YQ	89/89 (100%)	75 (84%)	14 (16%)	3	13
18	RR	84/84 (100%)	70 (83%)	14 (17%)	3	11
18	YR	84/84 (100%)	67 (80%)	17 (20%)	1	7
19	RS	93/93 (100%)	70 (75%)	23 (25%)	1	3
19	YS	93/93 (100%)	73 (78%)	20 (22%)	1	5
20	RT	80/80 (100%)	62 (78%)	18 (22%)	1	4
20	YT	80/80 (100%)	71 (89%)	9 (11%)	7	28
21	RU	83/83 (100%)	63 (76%)	20 (24%)	1	3
21	YU	83/83 (100%)	68 (82%)	15 (18%)	2	9
22	RV	78/78 (100%)	62 (80%)	16 (20%)	1	6
22	YV	78/78 (100%)	67 (86%)	11 (14%)	4	18
23	RW	59/59 (100%)	37 (63%)	22 (37%)	0	0

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	QI	105/105 (100%)	82 (78%)	23 (22%)	1	5
40	XI	105/105 (100%)	82 (78%)	23 (22%)	1	5
41	QJ	86/86 (100%)	69 (80%)	17 (20%)	1	7
41	XJ	86/86 (100%)	70 (81%)	16 (19%)	2	9
42	QK	90/90 (100%)	73 (81%)	17 (19%)	2	8
42	XK	90/90 (100%)	76 (84%)	14 (16%)	3	14
43	QL	103/103 (100%)	85 (82%)	18 (18%)	2	10
43	XL	103/103 (100%)	84 (82%)	19 (18%)	2	9
44	QM	92/92 (100%)	85 (92%)	7 (8%)	16	51
44	XM	91/92 (99%)	81 (89%)	10 (11%)	8	30
45	QN	79/84 (94%)	74 (94%)	5 (6%)	22	58
45	XN	75/84 (89%)	64 (85%)	11 (15%)	4	16
46	QO	76/76 (100%)	66 (87%)	10 (13%)	5	20
46	XO	76/76 (100%)	69 (91%)	7 (9%)	11	40
47	QP	65/65 (100%)	55 (85%)	10 (15%)	3	14
47	XP	65/65 (100%)	51 (78%)	14 (22%)	1	5
48	QQ	74/74 (100%)	57 (77%)	17 (23%)	1	4
48	XQ	74/74 (100%)	57 (77%)	17 (23%)	1	4
49	QR	48/48 (100%)	44 (92%)	4 (8%)	14	46
49	XR	48/48 (100%)	42 (88%)	6 (12%)	6	22
50	QS	70/70 (100%)	61 (87%)	9 (13%)	5	21
50	XS	70/70 (100%)	60 (86%)	10 (14%)	4	17
51	QT	65/65 (100%)	48 (74%)	17 (26%)	0	2
51	XT	65/65 (100%)	48 (74%)	17 (26%)	0	2
52	QU	44/44 (100%)	32 (73%)	12 (27%)	0	1
52	XU	44/44 (100%)	36 (82%)	8 (18%)	2	9
All	All	9327/9344 (100%)	7607 (82%)	1720 (18%)	2	9

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

Mol	Chain	Res	Type
40	QI	64	ILE
33	XB	209	VAL

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Mol	Chain	Res	Type
19	YS	84	ARG
41	QJ	70	HIS
48	QQ	3	LYS

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

Mol	Chain	Res	Type
40	QI	80	HIS
33	XB	38	HIS
19	YS	9	HIS
41	QJ	56	HIS
47	QP	9	HIS

5.3.3 RNA ⓘ

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

5 of 2284 RNA backbone outliers are listed below:

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

5 of 359 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	XA	451	A
1	YA	14	A
1	YA	2497	A
32	XA	519	C

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Mol	Chain	Res	Type
32	XA	1101	A

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 carbohydrates 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	-	57,64,64	1.95	13 (22%)	74,97,97	2.81	22 (29%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	RA	3135	EM1	C76-C78	-7.34	1.37	1.48
54	RA	3135	EM1	N82-N81	-5.43	1.26	1.34
54	RA	3135	EM1	C77-C72	-4.71	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	RA	3135	EM1	N81-N80	-4.50	1.25	1.34
54	RA	3135	EM1	O5-C2	-3.80	1.41	1.47

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	RA	3135	EM1	C8-C4-C2	-10.64	99.56	115.25
54	RA	3135	EM1	C84-C83-N80	-7.70	97.44	112.34
54	RA	3135	EM1	C76-C77-C72	-5.67	115.50	120.61
54	RA	3135	EM1	O45-C42-C44	-4.67	100.70	110.28
54	RA	3135	EM1	C2-O5-C10	-4.66	105.41	109.28

There are no chirality outliers.

There are no torsion outliers.

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

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	2854/2904 (98%)	-0.42	41 (1%) 78 60	19, 47, 175, 400	0
1	YA	2841/2904 (97%)	0.18	96 (3%) 49 24	64, 141, 260, 408	0
2	RB	118/118 (100%)	-0.62	0 100 100	32, 61, 95, 115	0
2	YB	117/118 (99%)	-0.16	0 100 100	111, 185, 242, 277	0
3	RC	271/271 (100%)	-0.23	10 (3%) 45 22	25, 57, 97, 202	0
3	YC	271/271 (100%)	0.46	19 (7%) 19 7	64, 107, 154, 181	0
4	RD	209/209 (100%)	-0.35	0 100 100	19, 41, 90, 149	0
4	YD	209/209 (100%)	0.87	27 (12%) 5 2	71, 122, 174, 236	0
5	RE	201/201 (100%)	-0.23	0 100 100	23, 58, 116, 177	0
5	YE	201/201 (100%)	1.92	84 (41%) 0 0	91, 214, 335, 378	0
6	RF	177/178 (99%)	0.25	14 (7%) 15 5	52, 93, 166, 225	0
6	YF	178/178 (100%)	2.10	84 (47%) 0 0	154, 229, 270, 299	0
7	RG	176/176 (100%)	-0.03	0 100 100	41, 75, 129, 161	0
7	YG	176/176 (100%)	1.95	67 (38%) 0 0	129, 198, 270, 312	0
8	RH	149/149 (100%)	2.64	60 (40%) 0 0	59, 178, 260, 278	0
8	YH	149/149 (100%)	2.50	67 (44%) 0 0	100, 197, 252, 272	0
9	RI	141/141 (100%)	3.40	87 (61%) 0 0	149, 241, 292, 339	0
9	YI	141/141 (100%)	4.43	105 (74%) 0 0	231, 317, 353, 360	0
10	RJ	142/142 (100%)	-0.47	1 (0%) 89 78	21, 40, 76, 139	0
10	YJ	142/142 (100%)	0.51	15 (10%) 8 3	75, 127, 168, 193	0
11	RK	122/122 (100%)	-0.34	1 (0%) 87 75	23, 45, 94, 191	0
11	YK	122/122 (100%)	0.58	13 (10%) 8 3	66, 107, 155, 228	0
12	RL	143/143 (100%)	-0.40	0 100 100	18, 55, 93, 123	0
12	YL	143/143 (100%)	1.42	44 (30%) 1 0	86, 169, 242, 284	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	RM	136/136 (100%)	-0.41	0 100 100	17, 45, 85, 146	0
13	YM	136/136 (100%)	1.09	25 (18%) 2 1	78, 131, 175, 208	0
14	RN	120/120 (100%)	-0.45	0 100 100	18, 41, 63, 132	0
14	YN	120/120 (100%)	0.93	20 (16%) 2 1	88, 136, 190, 237	0
15	RO	116/116 (100%)	-0.22	0 100 100	40, 64, 97, 124	0
15	YO	116/116 (100%)	1.95	47 (40%) 0 0	134, 182, 227, 252	0
16	RP	114/114 (100%)	-0.31	0 100 100	29, 53, 104, 149	0
16	YP	114/114 (100%)	0.69	15 (13%) 4 2	82, 121, 160, 197	0
17	RQ	117/117 (100%)	-0.53	0 100 100	19, 34, 63, 108	0
17	YQ	117/117 (100%)	1.22	30 (25%) 1 0	88, 126, 203, 287	0
18	RR	103/103 (100%)	-0.41	1 (0%) 84 69	20, 48, 92, 115	0
18	YR	103/103 (100%)	2.16	44 (42%) 0 0	98, 154, 219, 274	0
19	RS	110/110 (100%)	-0.41	1 (0%) 85 72	20, 38, 83, 143	0
19	YS	110/110 (100%)	1.61	35 (31%) 1 0	86, 141, 208, 266	0
20	RT	93/93 (100%)	0.37	7 (7%) 17 6	35, 69, 134, 207	0
20	YT	93/93 (100%)	2.38	46 (49%) 0 0	133, 215, 282, 315	0
21	RU	102/102 (100%)	0.04	2 (1%) 68 46	38, 72, 160, 192	0
21	YU	102/102 (100%)	3.37	63 (61%) 0 0	151, 251, 347, 416	0
22	RV	94/94 (100%)	-0.19	0 100 100	31, 61, 102, 114	0
22	YV	94/94 (100%)	1.13	22 (23%) 1 0	107, 157, 199, 222	0
23	RW	79/79 (100%)	0.13	5 (6%) 23 9	22, 53, 114, 195	0
23	YW	79/79 (100%)	2.32	43 (54%) 0 0	108, 163, 232, 250	0
24	RX	77/77 (100%)	-0.14	0 100 100	32, 58, 110, 124	0
24	YX	77/77 (100%)	0.89	11 (14%) 4 2	88, 134, 182, 237	0
25	RY	63/63 (100%)	0.25	3 (4%) 34 15	53, 90, 153, 175	0
25	YY	63/63 (100%)	1.50	17 (26%) 1 0	167, 286, 366, 383	0
26	RZ	58/58 (100%)	-0.34	0 100 100	19, 40, 87, 117	0
26	YZ	58/58 (100%)	1.07	15 (25%) 1 0	104, 143, 200, 247	0
27	R0	56/56 (100%)	-0.50	0 100 100	17, 42, 85, 150	0
27	Y0	56/56 (100%)	1.25	14 (25%) 1 0	87, 161, 210, 255	0
28	R1	50/50 (100%)	0.27	1 (2%) 68 46	45, 65, 111, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	Y1	50/50 (100%)	1.64	16 (32%) 1 0	106, 161, 203, 255	0
29	R2	46/46 (100%)	-0.37	1 (2%) 65 42	30, 42, 69, 166	0
29	Y2	46/46 (100%)	1.15	8 (17%) 2 1	95, 128, 162, 176	0
30	R3	64/64 (100%)	-0.44	0 100 100	25, 44, 64, 91	0
30	Y3	64/64 (100%)	1.82	21 (32%) 0 0	96, 140, 173, 212	0
31	R4	38/38 (100%)	0.09	0 100 100	40, 58, 98, 108	0
31	Y4	38/38 (100%)	2.59	20 (52%) 0 0	94, 155, 195, 203	0
32	QA	1533/1533 (100%)	-0.45	19 (1%) 81 64	46, 97, 198, 345	0
32	XA	1530/1533 (99%)	-0.15	34 (2%) 65 42	55, 113, 259, 356	0
33	QB	218/218 (100%)	0.88	34 (15%) 3 1	82, 141, 198, 243	0
33	XB	218/218 (100%)	1.24	54 (24%) 1 0	93, 145, 201, 251	0
34	QC	206/206 (100%)	0.13	4 (1%) 70 48	71, 107, 156, 198	0
34	XC	206/206 (100%)	0.51	12 (5%) 26 11	86, 136, 185, 215	0
35	QD	205/205 (100%)	0.36	14 (6%) 20 7	57, 114, 174, 236	0
35	XD	205/205 (100%)	-0.18	1 (0%) 91 83	41, 78, 132, 212	0
36	QE	150/150 (100%)	-0.10	2 (1%) 79 62	59, 90, 147, 217	0
36	XE	150/150 (100%)	-0.17	1 (0%) 89 78	55, 92, 141, 191	0
37	QF	100/100 (100%)	0.05	2 (2%) 68 46	80, 126, 168, 190	0
37	XF	100/100 (100%)	0.17	3 (3%) 54 29	82, 119, 176, 211	0
38	QG	151/151 (100%)	0.37	9 (5%) 25 10	98, 138, 186, 203	0
38	XG	150/151 (99%)	1.75	57 (38%) 0 0	121, 195, 245, 277	0
39	QH	129/129 (100%)	0.25	5 (3%) 43 21	62, 101, 142, 189	0
39	XH	129/129 (100%)	0.13	6 (4%) 35 16	77, 115, 152, 209	0
40	QI	127/127 (100%)	0.97	23 (18%) 2 1	82, 137, 209, 250	0
40	XI	127/127 (100%)	1.24	25 (19%) 1 0	114, 158, 225, 259	0
41	QJ	98/98 (100%)	0.44	9 (9%) 11 4	71, 121, 175, 200	0
41	XJ	98/98 (100%)	1.63	30 (30%) 1 0	117, 166, 211, 238	0
42	QK	117/117 (100%)	0.89	12 (10%) 9 3	54, 123, 177, 206	0
42	XK	117/117 (100%)	0.04	3 (2%) 59 35	67, 115, 162, 186	0
43	QL	123/123 (100%)	0.08	2 (1%) 74 55	50, 79, 123, 189	0
43	XL	123/123 (100%)	0.30	3 (2%) 62 39	61, 89, 142, 202	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	QM	114/114 (100%)	0.38	8 (7%) 19 7	94, 142, 198, 217	0
44	XM	113/114 (99%)	2.58	58 (51%) 0 0	218, 370, 442, 470	0
45	QN	96/101 (95%)	0.48	7 (7%) 18 6	80, 116, 187, 224	0
45	XN	91/101 (90%)	1.52	29 (31%) 1 0	107, 180, 260, 287	0
46	QO	88/88 (100%)	0.08	2 (2%) 64 40	64, 102, 139, 188	0
46	XO	88/88 (100%)	-0.10	1 (1%) 82 66	76, 116, 160, 209	0
47	QP	82/82 (100%)	0.89	11 (13%) 4 2	78, 99, 166, 223	0
47	XP	80/82 (97%)	0.83	9 (11%) 7 2	72, 107, 158, 222	0
48	QQ	80/80 (100%)	0.68	7 (8%) 12 4	62, 96, 136, 164	0
48	XQ	80/80 (100%)	1.23	14 (17%) 2 1	78, 115, 144, 155	0
49	QR	55/55 (100%)	0.54	4 (7%) 18 6	90, 110, 168, 218	0
49	XR	55/55 (100%)	0.10	2 (3%) 46 23	74, 103, 171, 243	0
50	QS	79/79 (100%)	1.11	18 (22%) 1 0	110, 143, 197, 208	0
50	XS	79/79 (100%)	3.89	52 (65%) 0 0	205, 346, 411, 424	0
51	QT	85/85 (100%)	0.38	3 (3%) 48 23	74, 103, 147, 179	0
51	XT	85/85 (100%)	1.08	13 (15%) 3 1	91, 134, 190, 216	0
52	QU	51/51 (100%)	1.17	15 (29%) 1 0	96, 139, 187, 225	0
52	XU	51/51 (100%)	0.25	2 (3%) 43 21	83, 120, 184, 224	0
All	All	20427/20564 (99%)	0.34	1987 (9%) 10 3	17, 111, 252, 470	0

The worst 5 of 1987 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	YH	91	PHE	20.0
9	RI	52	LEU	17.6
8	RH	92	GLY	16.8
6	YF	129	MET	16.7
9	YI	57	VAL	16.6

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
53	MG	YA	3079	1/1	0.83	0.80	29.89	225,225,225,225	0
53	MG	YA	3108	1/1	-0.03	0.81	24.66	217,217,217,217	0
53	MG	YA	3002	1/1	0.42	0.52	13.12	231,231,231,231	0
53	MG	YA	3075	1/1	0.94	0.54	12.20	209,209,209,209	0
53	MG	RA	3020	1/1	0.85	0.38	8.48	200,200,200,200	0
53	MG	RA	3035	1/1	0.89	0.33	6.26	189,189,189,189	0
53	MG	RA	3081	1/1	0.97	0.17	5.82	99,99,99,99	0
53	MG	RA	3070	1/1	0.89	0.33	5.38	137,137,137,137	0
53	MG	YA	3115	1/1	0.92	0.26	5.03	176,176,176,176	0
53	MG	XA	1628	1/1	0.91	0.45	4.54	224,224,224,224	0
53	MG	RA	3099	1/1	0.96	0.19	4.47	34,34,34,34	0
53	MG	RA	3134	1/1	0.75	0.27	4.40	210,210,210,210	0
54	EM1	RA	3135	60/60	0.93	0.26	4.32	0,23,85,88	0
53	MG	RA	3039	1/1	0.98	0.24	4.26	7,7,7,7	0
53	MG	XA	1625	1/1	0.92	0.23	4.21	111,111,111,111	0
53	MG	XA	1640	1/1	0.92	0.17	3.10	137,137,137,137	0
53	MG	RA	3105	1/1	0.96	0.21	2.96	66,66,66,66	0
53	MG	XA	1616	1/1	0.80	0.60	2.82	195,195,195,195	0
53	MG	YA	3033	1/1	0.71	0.29	2.71	151,151,151,151	0
53	MG	RA	3107	1/1	0.98	0.21	2.37	17,17,17,17	0
53	MG	YA	3128	1/1	0.84	0.80	2.07	163,163,163,163	0
53	MG	YA	3022	1/1	0.87	0.23	1.96	149,149,149,149	0
53	MG	XA	1610	1/1	0.80	0.13	1.90	168,168,168,168	0
53	MG	RA	3114	1/1	0.97	0.19	1.90	28,28,28,28	0
53	MG	RA	3106	1/1	0.98	0.19	1.85	13,13,13,13	0
53	MG	QA	1631	1/1	0.96	0.19	1.71	228,228,228,228	0
53	MG	YA	3104	1/1	0.91	0.22	1.49	52,52,52,52	0
53	MG	YA	3133	1/1	0.63	0.30	1.48	220,220,220,220	0
53	MG	QA	1641	1/1	0.87	0.16	1.24	171,171,171,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	YA	3105	1/1	0.97	0.19	1.20	97,97,97,97	0
53	MG	XA	1631	1/1	0.95	0.22	1.15	82,82,82,82	0
53	MG	RA	3102	1/1	0.98	0.17	1.03	24,24,24,24	0
53	MG	RA	3026	1/1	0.98	0.17	1.01	143,143,143,143	0
53	MG	YA	3097	1/1	0.72	0.21	0.83	159,159,159,159	0
53	MG	YA	3027	1/1	0.89	0.22	0.72	194,194,194,194	0
53	MG	QA	1622	1/1	0.97	0.17	0.57	54,54,54,54	0
53	MG	YA	3069	1/1	0.91	0.23	0.53	267,267,267,267	0
53	MG	XA	1641	1/1	0.98	0.15	0.50	116,116,116,116	0
53	MG	RA	3048	1/1	0.96	0.17	0.11	25,25,25,25	0
53	MG	RA	3128	1/1	0.99	0.16	0.11	33,33,33,33	0
53	MG	QA	1634	1/1	0.94	0.15	0.00	94,94,94,94	0
53	MG	RA	3005	1/1	0.96	0.12	-0.22	74,74,74,74	0
53	MG	YA	3101	1/1	0.80	0.20	-0.25	96,96,96,96	0
53	MG	QA	1617	1/1	0.98	0.17	-0.28	129,129,129,129	0
53	MG	QA	1633	1/1	0.98	0.12	-0.29	70,70,70,70	0
53	MG	QA	1616	1/1	0.92	0.18	-0.36	98,98,98,98	0
53	MG	RA	3130	1/1	0.90	0.24	-0.38	118,118,118,118	0
53	MG	RA	3062	1/1	1.00	0.15	-0.53	19,19,19,19	0
53	MG	RA	3049	1/1	0.96	0.14	-0.56	76,76,76,76	0
53	MG	RA	3118	1/1	0.94	0.15	-0.63	48,48,48,48	0
53	MG	QA	1642	1/1	0.97	0.13	-0.69	79,79,79,79	0
53	MG	YA	3066	1/1	0.95	0.17	-0.74	105,105,105,105	0
53	MG	RA	3013	1/1	0.99	0.16	-0.78	18,18,18,18	0
53	MG	RA	3064	1/1	0.97	0.14	-0.82	28,28,28,28	0
53	MG	RA	3103	1/1	0.89	0.15	-0.85	30,30,30,30	0
53	MG	RA	3110	1/1	0.92	0.15	-0.85	84,84,84,84	0
53	MG	RA	3119	1/1	0.92	0.08	-0.89	56,56,56,56	0
53	MG	RA	3008	1/1	0.96	0.14	-0.92	45,45,45,45	0
53	MG	YA	3084	1/1	0.82	0.16	-0.99	168,168,168,168	0
53	MG	YA	3106	1/1	0.84	0.17	-1.04	218,218,218,218	0
53	MG	YA	3042	1/1	0.90	0.17	-1.05	81,81,81,81	0
53	MG	YA	3095	1/1	0.96	0.14	-1.06	138,138,138,138	0
53	MG	RB	202	1/1	0.80	0.11	-1.07	82,82,82,82	0
53	MG	QA	1606	1/1	0.92	0.12	-1.09	80,80,80,80	0
53	MG	XA	1617	1/1	0.49	0.12	-1.09	202,202,202,202	0
53	MG	YA	3083	1/1	0.79	0.10	-1.16	214,214,214,214	0
53	MG	YA	3055	1/1	0.98	0.16	-1.18	103,103,103,103	0
53	MG	XA	1629	1/1	0.80	0.15	-1.20	190,190,190,190	0
53	MG	YA	3025	1/1	0.87	0.15	-1.24	162,162,162,162	0
53	MG	YA	3070	1/1	0.89	0.13	-1.25	91,91,91,91	0
53	MG	YA	3024	1/1	0.97	0.15	-1.29	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	YA	3061	1/1	0.97	0.14	-1.35	110,110,110,110	0
53	MG	XA	1613	1/1	0.94	0.17	-1.37	147,147,147,147	0
53	MG	RA	3017	1/1	0.94	0.09	-1.41	57,57,57,57	0
53	MG	RA	3095	1/1	0.96	0.16	-1.43	139,139,139,139	0
53	MG	YA	3037	1/1	0.95	0.13	-1.44	81,81,81,81	0
53	MG	YA	3131	1/1	0.95	0.14	-1.45	94,94,94,94	0
53	MG	YA	3110	1/1	0.77	0.07	-1.46	120,120,120,120	0
53	MG	YB	201	1/1	0.97	0.09	-1.48	111,111,111,111	0
53	MG	XA	1621	1/1	0.95	0.13	-1.54	57,57,57,57	0
53	MG	RA	3045	1/1	0.94	0.14	-1.59	25,25,25,25	0
55	ZN	Y4	101	1/1	0.96	0.07	-1.67	169,169,169,169	0
53	MG	XA	1618	1/1	0.90	0.11	-1.72	136,136,136,136	0
53	MG	XA	1637	1/1	0.94	0.13	-1.72	94,94,94,94	0
53	MG	YA	3040	1/1	0.94	0.17	-1.72	72,72,72,72	0
53	MG	XA	1609	1/1	0.97	0.16	-1.92	98,98,98,98	0
53	MG	RA	3132	1/1	0.97	0.12	-1.94	20,20,20,20	0
53	MG	QA	1618	1/1	0.94	0.12	-2.01	78,78,78,78	0
55	ZN	R4	101	1/1	0.99	0.10	-2.01	108,108,108,108	0
53	MG	XA	1642	1/1	0.93	0.10	-2.04	139,139,139,139	0
53	MG	RA	3112	1/1	0.96	0.10	-2.04	49,49,49,49	0
53	MG	YA	3072	1/1	0.86	0.12	-2.05	183,183,183,183	0
53	MG	XA	1606	1/1	0.89	0.13	-2.12	93,93,93,93	0
53	MG	RA	3022	1/1	0.98	0.12	-2.12	27,27,27,27	0
53	MG	YA	3065	1/1	0.95	0.13	-2.13	88,88,88,88	0
53	MG	QA	1635	1/1	0.95	0.10	-2.13	87,87,87,87	0
53	MG	YA	3112	1/1	0.95	0.09	-2.15	79,79,79,79	0
53	MG	XA	1604	1/1	0.93	0.10	-2.30	96,96,96,96	0
53	MG	YA	3068	1/1	0.98	0.07	-2.36	98,98,98,98	0
53	MG	YA	3051	1/1	0.92	0.14	-2.47	88,88,88,88	0
53	MG	QA	1607	1/1	0.94	0.13	-2.54	136,136,136,136	0
53	MG	YA	3124	1/1	0.92	0.16	-2.55	82,82,82,82	0
53	MG	YA	3103	1/1	0.92	0.13	-2.60	86,86,86,86	0
53	MG	RA	3077	1/1	0.97	0.10	-2.80	63,63,63,63	0
53	MG	RA	3052	1/1	0.95	0.14	-2.82	34,34,34,34	0
53	MG	QA	1611	1/1	0.97	0.14	-2.86	57,57,57,57	0
53	MG	RA	3108	1/1	0.97	0.13	-2.90	95,95,95,95	0
53	MG	RA	3021	1/1	0.99	0.12	-2.92	24,24,24,24	0
53	MG	YA	3100	1/1	0.88	0.13	-3.00	124,124,124,124	0
53	MG	RA	3023	1/1	0.99	0.12	-3.16	22,22,22,22	0
53	MG	RA	3027	1/1	0.98	0.12	-3.16	33,33,33,33	0
53	MG	XA	1607	1/1	0.95	0.13	-3.18	167,167,167,167	0
53	MG	RA	3046	1/1	0.93	0.08	-3.24	176,176,176,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	QA	1625	1/1	0.90	0.14	-3.64	101,101,101,101	0
53	MG	RA	3002	1/1	0.95	0.11	-3.71	75,75,75,75	0
53	MG	YA	3023	1/1	0.62	0.09	-3.82	130,130,130,130	0
53	MG	RA	3056	1/1	0.86	0.12	-4.05	148,148,148,148	0
53	MG	RA	3061	1/1	0.94	0.12	-4.05	18,18,18,18	0
53	MG	YA	3044	1/1	0.92	0.15	-4.09	87,87,87,87	0
53	MG	YA	3048	1/1	0.95	0.10	-4.18	103,103,103,103	0
53	MG	YA	3052	1/1	0.98	0.07	-4.49	72,72,72,72	0
53	MG	YA	3012	1/1	0.96	0.09	-4.56	72,72,72,72	0
53	MG	QA	1643	1/1	0.91	0.11	-4.68	67,67,67,67	0
53	MG	RA	3067	1/1	0.97	0.14	-4.78	28,28,28,28	0
53	MG	RA	3016	1/1	0.97	0.11	-5.04	22,22,22,22	0
53	MG	YA	3016	1/1	0.92	0.10	-5.26	60,60,60,60	0
53	MG	RA	3116	1/1	0.97	0.10	-5.36	72,72,72,72	0
53	MG	QA	1613	1/1	0.95	0.07	-5.48	76,76,76,76	0
53	MG	RA	3012	1/1	0.97	0.12	-5.66	20,20,20,20	0
53	MG	XA	1639	1/1	0.94	0.05	-5.95	159,159,159,159	0
53	MG	RA	3091	1/1	0.89	0.10	-5.97	84,84,84,84	0
53	MG	QA	1629	1/1	0.95	0.06	-6.06	97,97,97,97	0
53	MG	RA	3094	1/1	0.98	0.10	-6.42	32,32,32,32	0
53	MG	RA	3057	1/1	0.94	0.07	-6.76	71,71,71,71	0
53	MG	QA	1604	1/1	0.96	0.04	-7.77	139,139,139,139	0
53	MG	RA	3127	1/1	0.97	0.09	-8.86	8,8,8,8	0
53	MG	QA	1609	1/1	0.92	0.08	-9.61	77,77,77,77	0
53	MG	QA	1637	1/1	0.69	0.16	-	131,131,131,131	0
53	MG	RA	3125	1/1	0.98	0.14	-	40,40,40,40	0
53	MG	YA	3020	1/1	0.85	0.21	-	53,53,53,53	0
53	MG	YA	3035	1/1	0.93	0.09	-	90,90,90,90	0
53	MG	RA	3109	1/1	0.97	0.16	-	46,46,46,46	0
53	MG	RA	3068	1/1	0.78	0.12	-	175,175,175,175	0
53	MG	XA	1612	1/1	0.93	0.19	-	125,125,125,125	0
53	MG	RA	3097	1/1	0.97	0.13	-	54,54,54,54	0
53	MG	YA	3102	1/1	0.96	0.10	-	118,118,118,118	0
53	MG	XA	1619	1/1	0.74	0.12	-	212,212,212,212	0
53	MG	RA	3090	1/1	0.84	0.17	-	135,135,135,135	0
53	MG	QA	1626	1/1	0.99	0.20	-	29,29,29,29	0
53	MG	RA	3060	1/1	0.82	0.48	-	236,236,236,236	0
53	MG	YA	3088	1/1	0.79	0.35	-	222,222,222,222	0
53	MG	RA	3007	1/1	0.97	0.13	-	112,112,112,112	0
53	MG	RA	3133	1/1	0.94	0.28	-	116,116,116,116	0
53	MG	RA	3032	1/1	0.98	0.14	-	23,23,23,23	0
53	MG	RA	3040	1/1	0.98	0.13	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	YA	3121	1/1	0.97	0.17	-	168,168,168,168	0
53	MG	YA	3081	1/1	0.92	0.10	-	83,83,83,83	0
53	MG	YA	3134	1/1	0.95	0.33	-	201,201,201,201	0
53	MG	QA	1610	1/1	0.84	0.11	-	197,197,197,197	0
53	MG	RA	3015	1/1	0.98	0.06	-	65,65,65,65	0
53	MG	YA	3018	1/1	0.95	0.10	-	185,185,185,185	0
53	MG	YA	3015	1/1	0.89	0.19	-	219,219,219,219	0
53	MG	RA	3014	1/1	0.91	0.18	-	38,38,38,38	0
53	MG	XA	1623	1/1	0.90	0.11	-	108,108,108,108	0
53	MG	YA	3091	1/1	0.51	0.22	-	184,184,184,184	0
53	MG	RA	3072	1/1	0.94	0.05	-	61,61,61,61	0
53	MG	YA	3116	1/1	0.92	0.12	-	84,84,84,84	0
53	MG	RA	3043	1/1	0.99	0.26	-	11,11,11,11	0
53	MG	XA	1615	1/1	0.92	0.20	-	187,187,187,187	0
53	MG	RB	201	1/1	0.91	0.33	-	255,255,255,255	0
53	MG	YA	3111	1/1	0.91	0.14	-	202,202,202,202	0
53	MG	YA	3089	1/1	0.92	0.21	-	101,101,101,101	0
53	MG	YA	3031	1/1	0.77	0.21	-	80,80,80,80	0
53	MG	QA	1602	1/1	0.73	0.12	-	177,177,177,177	0
53	MG	RA	3034	1/1	0.99	0.10	-	11,11,11,11	0
53	MG	RA	3098	1/1	0.97	0.07	-	49,49,49,49	0
53	MG	YA	3060	1/1	0.85	0.76	-	235,235,235,235	0
53	MG	QA	1608	1/1	0.96	0.25	-	61,61,61,61	0
53	MG	QA	1614	1/1	0.97	0.15	-	159,159,159,159	0
53	MG	RA	3018	1/1	0.94	0.33	-	32,32,32,32	0
53	MG	RA	3100	1/1	0.92	0.27	-	119,119,119,119	0
53	MG	XA	1624	1/1	0.83	0.37	-	146,146,146,146	0
53	MG	RA	3082	1/1	0.83	0.14	-	86,86,86,86	0
53	MG	RA	3136	1/1	0.98	0.07	-	61,61,61,61	0
53	MG	XA	1635	1/1	0.84	0.11	-	76,76,76,76	0
53	MG	RA	3063	1/1	0.97	0.13	-	26,26,26,26	0
53	MG	RA	3074	1/1	0.96	0.10	-	93,93,93,93	0
53	MG	RA	3033	1/1	0.98	0.15	-	159,159,159,159	0
53	MG	RA	3055	1/1	0.90	0.33	-	252,252,252,252	0
53	MG	YA	3056	1/1	0.96	0.07	-	85,85,85,85	0
53	MG	YA	3029	1/1	0.91	0.22	-	178,178,178,178	0
53	MG	YA	3001	1/1	0.89	0.15	-	141,141,141,141	0
53	MG	RB	204	1/1	0.96	0.14	-	45,45,45,45	0
53	MG	RA	3036	1/1	0.97	0.18	-	23,23,23,23	0
53	MG	RA	3096	1/1	0.81	0.18	-	169,169,169,169	0
53	MG	YA	3127	1/1	0.67	1.28	-	248,248,248,248	0
53	MG	QA	1624	1/1	0.89	0.14	-	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	YA	3120	1/1	0.33	0.21	-	124,124,124,124	0
53	MG	YA	3094	1/1	0.91	0.14	-	145,145,145,145	0
53	MG	XA	1626	1/1	0.98	0.24	-	20,20,20,20	0
53	MG	RA	3117	1/1	0.93	0.17	-	162,162,162,162	0
53	MG	RA	3050	1/1	0.93	0.18	-	39,39,39,39	0
53	MG	RA	3086	1/1	0.82	0.09	-	151,151,151,151	0
53	MG	RA	3011	1/1	0.82	0.18	-	129,129,129,129	0
53	MG	YA	3086	1/1	0.95	0.13	-	109,109,109,109	0
53	MG	YA	3043	1/1	0.85	0.23	-	155,155,155,155	0
53	MG	YA	3003	1/1	0.40	1.58	-	238,238,238,238	0
53	MG	QA	1636	1/1	0.93	0.38	-	218,218,218,218	0
53	MG	RA	3047	1/1	0.70	0.13	-	122,122,122,122	0
53	MG	YA	3010	1/1	0.80	1.07	-	272,272,272,272	0
53	MG	YA	3078	1/1	0.66	0.26	-	214,214,214,214	0
53	MG	RA	3065	1/1	0.96	0.15	-	35,35,35,35	0
53	MG	YA	3046	1/1	0.97	0.22	-	73,73,73,73	0
53	MG	YA	3039	1/1	0.79	0.19	-	105,105,105,105	0
53	MG	RA	3121	1/1	0.95	0.17	-	45,45,45,45	0
53	MG	QA	1628	1/1	0.96	0.24	-	142,142,142,142	0
53	MG	XA	1611	1/1	0.89	0.11	-	110,110,110,110	0
53	MG	XA	1601	1/1	0.86	0.08	-	106,106,106,106	0
53	MG	RA	3029	1/1	0.96	0.19	-	14,14,14,14	0
53	MG	YA	3132	1/1	0.88	0.50	-	240,240,240,240	0
53	MG	RA	3038	1/1	0.98	0.17	-	19,19,19,19	0
53	MG	YA	3082	1/1	0.82	0.19	-	164,164,164,164	0
53	MG	YA	3045	1/1	0.72	0.22	-	206,206,206,206	0
53	MG	YA	3026	1/1	0.86	0.76	-	242,242,242,242	0
53	MG	RA	3093	1/1	0.98	0.08	-	45,45,45,45	0
53	MG	QA	1619	1/1	0.66	0.53	-	230,230,230,230	0
53	MG	YA	3067	1/1	0.93	0.11	-	72,72,72,72	0
53	MG	XA	1620	1/1	0.81	0.19	-	182,182,182,182	0
53	MG	YA	3099	1/1	0.96	0.17	-	188,188,188,188	0
53	MG	YA	3096	1/1	0.91	0.14	-	127,127,127,127	0
53	MG	YA	3113	1/1	0.93	0.07	-	128,128,128,128	0
53	MG	RA	3131	1/1	0.89	0.60	-	187,187,187,187	0
53	MG	QA	1623	1/1	0.96	0.11	-	77,77,77,77	0
53	MG	RA	3080	1/1	0.97	0.07	-	60,60,60,60	0
53	MG	RA	3089	1/1	0.80	0.16	-	127,127,127,127	0
53	MG	RA	3124	1/1	0.97	0.20	-	63,63,63,63	0
53	MG	YA	3071	1/1	0.84	0.20	-	102,102,102,102	0
53	MG	RA	3044	1/1	0.98	0.14	-	34,34,34,34	0
53	MG	RA	3037	1/1	0.97	0.14	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	RA	3004	1/1	0.86	0.19	-	184,184,184,184	0
53	MG	YA	3028	1/1	0.67	0.33	-	222,222,222,222	0
53	MG	XA	1627	1/1	0.92	0.23	-	197,197,197,197	0
53	MG	RA	3111	1/1	0.98	0.15	-	31,31,31,31	0
53	MG	YA	3064	1/1	0.72	0.87	-	256,256,256,256	0
53	MG	RA	3031	1/1	0.93	0.14	-	37,37,37,37	0
53	MG	YA	3125	1/1	0.51	0.35	-	200,200,200,200	0
53	MG	YA	3123	1/1	0.80	0.36	-	217,217,217,217	0
53	MG	QA	1639	1/1	0.97	0.18	-	118,118,118,118	0
53	MG	YA	3014	1/1	0.98	0.20	-	113,113,113,113	0
53	MG	RA	3088	1/1	0.95	0.08	-	59,59,59,59	0
53	MG	YA	3107	1/1	0.95	0.20	-	91,91,91,91	0
53	MG	RA	3059	1/1	0.96	0.43	-	207,207,207,207	0
53	MG	YA	3053	1/1	0.96	0.18	-	127,127,127,127	0
53	MG	QA	1605	1/1	0.90	0.18	-	72,72,72,72	0
53	MG	XA	1614	1/1	0.74	0.64	-	236,236,236,236	0
53	MG	YA	3054	1/1	0.90	0.12	-	86,86,86,86	0
53	MG	RA	3122	1/1	0.94	0.70	-	164,164,164,164	0
53	MG	YA	3087	1/1	0.58	0.10	-	199,199,199,199	0
53	MG	YA	3059	1/1	0.74	0.18	-	232,232,232,232	0
53	MG	YA	3019	1/1	0.48	0.66	-	278,278,278,278	0
53	MG	YA	3119	1/1	0.94	0.11	-	60,60,60,60	0
53	MG	RA	3058	1/1	0.68	0.22	-	100,100,100,100	0
53	MG	YA	3122	1/1	0.72	0.15	-	104,104,104,104	0
53	MG	YJ	201	1/1	0.20	2.55	-	319,319,319,319	0
53	MG	RA	3053	1/1	0.97	0.17	-	55,55,55,55	0
53	MG	YA	3080	1/1	0.90	0.18	-	154,154,154,154	0
53	MG	RA	3030	1/1	0.95	0.11	-	56,56,56,56	0
53	MG	YA	3118	1/1	0.94	0.17	-	100,100,100,100	0
53	MG	RA	3028	1/1	0.96	0.14	-	92,92,92,92	0
53	MG	XA	1634	1/1	0.78	0.13	-	165,165,165,165	0
53	MG	RA	3087	1/1	0.98	0.08	-	47,47,47,47	0
53	MG	QA	1632	1/1	0.85	0.15	-	85,85,85,85	0
53	MG	RA	3009	1/1	0.98	0.14	-	38,38,38,38	0
53	MG	QA	1603	1/1	0.98	0.09	-	65,65,65,65	0
53	MG	RA	3024	1/1	0.81	0.46	-	210,210,210,210	0
53	MG	RA	3104	1/1	0.98	0.17	-	23,23,23,23	0
53	MG	RA	3084	1/1	0.95	0.15	-	26,26,26,26	0
53	MG	RA	3083	1/1	0.93	0.16	-	53,53,53,53	0
53	MG	RA	3010	1/1	0.97	0.12	-	31,31,31,31	0
53	MG	YA	3063	1/1	0.58	1.61	-	273,273,273,273	0
53	MG	XA	1636	1/1	0.27	0.37	-	224,224,224,224	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	YA	3008	1/1	0.77	0.24	-	147,147,147,147	0
53	MG	RA	3042	1/1	0.98	0.07	-	60,60,60,60	0
53	MG	RA	3041	1/1	0.95	0.14	-	38,38,38,38	0
53	MG	YA	3109	1/1	0.37	1.51	-	227,227,227,227	0
53	MG	YA	3013	1/1	0.92	0.39	-	241,241,241,241	0
53	MG	YA	3057	1/1	0.67	0.30	-	205,205,205,205	0
53	MG	YA	3050	1/1	0.80	0.16	-	154,154,154,154	0
53	MG	QA	1638	1/1	0.88	0.13	-	67,67,67,67	0
53	MG	YA	3085	1/1	0.71	0.23	-	158,158,158,158	0
53	MG	YA	3017	1/1	0.80	0.13	-	185,185,185,185	0
53	MG	YA	3030	1/1	0.91	0.13	-	130,130,130,130	0
53	MG	XA	1622	1/1	0.58	0.09	-	187,187,187,187	0
53	MG	YA	3077	1/1	0.89	0.07	-	109,109,109,109	0
53	MG	RA	3019	1/1	0.97	0.06	-	34,34,34,34	0
53	MG	RA	3113	1/1	0.93	0.15	-	190,190,190,190	0
53	MG	RA	3051	1/1	0.91	0.16	-	70,70,70,70	0
53	MG	YA	3021	1/1	0.92	0.29	-	183,183,183,183	0
53	MG	RA	3079	1/1	0.97	0.15	-	32,32,32,32	0
53	MG	YA	3058	1/1	0.90	0.38	-	249,249,249,249	0
53	MG	YA	3117	1/1	0.97	0.17	-	73,73,73,73	0
53	MG	YA	3073	1/1	0.68	0.18	-	193,193,193,193	0
53	MG	XA	1632	1/1	0.84	0.10	-	122,122,122,122	0
53	MG	RA	3101	1/1	0.97	0.11	-	48,48,48,48	0
53	MG	RA	3006	1/1	0.97	0.13	-	54,54,54,54	0
53	MG	RA	3076	1/1	0.99	0.07	-	107,107,107,107	0
53	MG	YA	3005	1/1	0.66	0.87	-	282,282,282,282	0
53	MG	YA	3047	1/1	0.83	0.18	-	174,174,174,174	0
53	MG	QA	1630	1/1	0.86	0.14	-	196,196,196,196	0
53	MG	RA	3092	1/1	0.99	0.09	-	68,68,68,68	0
53	MG	RA	3066	1/1	0.98	0.16	-	32,32,32,32	0
53	MG	YA	3074	1/1	0.71	0.56	-	260,260,260,260	0
53	MG	XA	1638	1/1	0.89	0.15	-	204,204,204,204	0
53	MG	RA	3054	1/1	0.76	0.36	-	198,198,198,198	0
53	MG	RA	3071	1/1	0.95	0.11	-	16,16,16,16	0
53	MG	YA	3032	1/1	0.95	0.13	-	162,162,162,162	0
53	MG	QA	1620	1/1	0.97	0.08	-	116,116,116,116	0
53	MG	XA	1608	1/1	0.98	0.27	-	46,46,46,46	0
53	MG	YA	3129	1/1	0.53	0.73	-	261,261,261,261	0
53	MG	YA	3036	1/1	0.79	0.15	-	205,205,205,205	0
53	MG	XA	1633	1/1	0.96	0.10	-	79,79,79,79	0
53	MG	RA	3003	1/1	0.90	0.14	-	77,77,77,77	0
53	MG	YA	3092	1/1	0.89	0.15	-	169,169,169,169	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	RA	3075	1/1	0.96	0.05	-	43,43,43,43	0
53	MG	YA	3076	1/1	0.60	0.19	-	195,195,195,195	0
53	MG	QA	1601	1/1	0.98	0.07	-	94,94,94,94	0
53	MG	YA	3007	1/1	0.83	0.45	-	232,232,232,232	0
53	MG	YA	3114	1/1	0.90	0.12	-	182,182,182,182	0
53	MG	YA	3004	1/1	0.86	0.17	-	134,134,134,134	0
53	MG	RB	203	1/1	0.93	0.12	-	58,58,58,58	0
53	MG	QA	1640	1/1	0.92	0.05	-	79,79,79,79	0
53	MG	RA	3115	1/1	0.98	0.07	-	22,22,22,22	0
53	MG	QA	1615	1/1	0.98	0.11	-	152,152,152,152	0
53	MG	QA	1627	1/1	0.54	0.16	-	132,132,132,132	0
53	MG	RA	3129	1/1	0.71	1.06	-	285,285,285,285	0
53	MG	YA	3098	1/1	0.85	0.21	-	183,183,183,183	0
53	MG	YA	3038	1/1	0.83	0.07	-	234,234,234,234	0
53	MG	QA	1612	1/1	0.97	0.17	-	113,113,113,113	0
53	MG	RA	3123	1/1	0.98	0.10	-	24,24,24,24	0
53	MG	XA	1603	1/1	0.97	0.09	-	136,136,136,136	0
53	MG	QA	1621	1/1	0.93	0.13	-	131,131,131,131	0
53	MG	XA	1605	1/1	0.97	0.19	-	54,54,54,54	0
53	MG	XA	1602	1/1	0.77	0.13	-	139,139,139,139	0
53	MG	YA	3062	1/1	0.69	0.55	-	190,190,190,190	0
53	MG	RA	3085	1/1	0.83	0.17	-	133,133,133,133	0
53	MG	RA	3069	1/1	0.80	0.24	-	197,197,197,197	0
53	MG	YA	3130	1/1	0.69	1.79	-	271,271,271,271	0
53	MG	RA	3120	1/1	0.96	0.31	-	45,45,45,45	0
53	MG	YA	3006	1/1	0.55	0.10	-	237,237,237,237	0
53	MG	YE	301	1/1	0.84	0.29	-	199,199,199,199	0
53	MG	YA	3093	1/1	0.87	0.37	-	188,188,188,188	0
53	MG	RA	3078	1/1	0.98	0.13	-	58,58,58,58	0
53	MG	XA	1630	1/1	0.96	0.16	-	160,160,160,160	0
53	MG	YA	3011	1/1	0.91	0.21	-	150,150,150,150	0
53	MG	RA	3073	1/1	0.97	0.24	-	43,43,43,43	0
53	MG	RA	3025	1/1	0.97	0.06	-	40,40,40,40	0
53	MG	YA	3049	1/1	-0.02	0.45	-	243,243,243,243	0
53	MG	YA	3126	1/1	0.91	0.19	-	120,120,120,120	0
53	MG	RA	3001	1/1	0.94	0.09	-	98,98,98,98	0
53	MG	YA	3034	1/1	0.91	0.09	-	88,88,88,88	0
53	MG	RA	3126	1/1	0.97	0.14	-	40,40,40,40	0
53	MG	YA	3090	1/1	0.98	0.10	-	112,112,112,112	0
53	MG	YA	3009	1/1	0.93	0.28	-	157,157,157,157	0
53	MG	YA	3041	1/1	0.93	0.15	-	119,119,119,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.