



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 01:41 am BST

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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

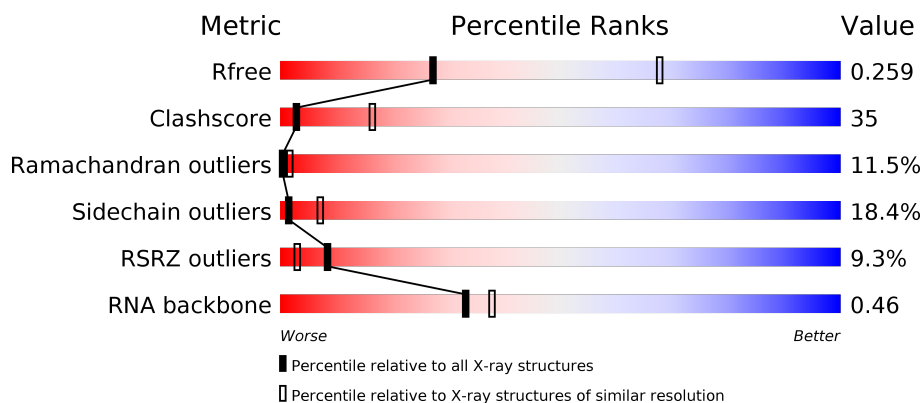
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	RA	2904	 3% 39% 43% 15% ..
1	YA	2904	 3% 19% 52% 26% ..
2	RB	118	 43% 47% 10%
2	YB	118	 21% 54% 24% .

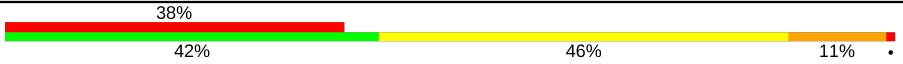
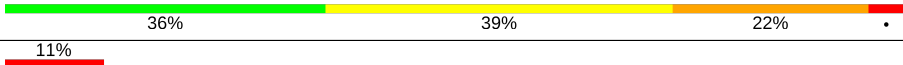

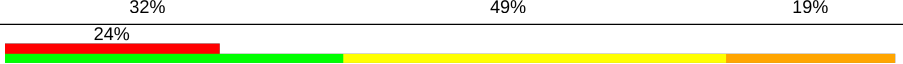
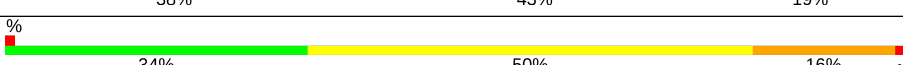
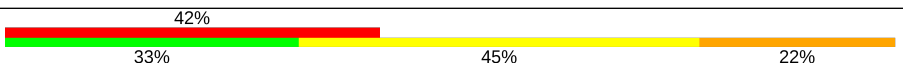

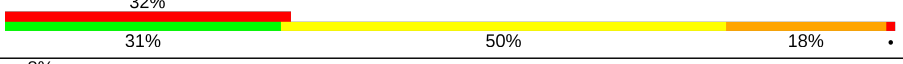
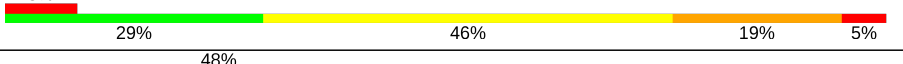
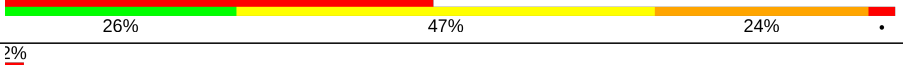

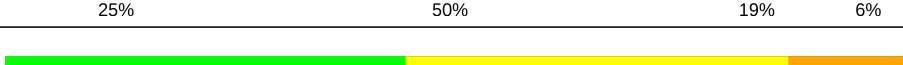
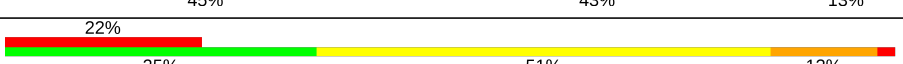


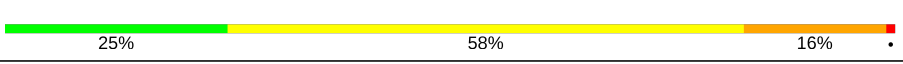
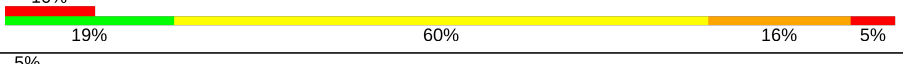


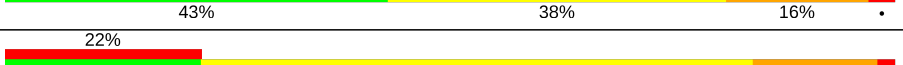
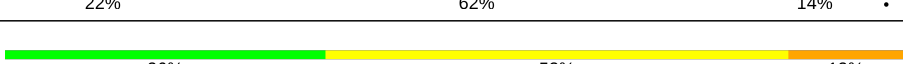
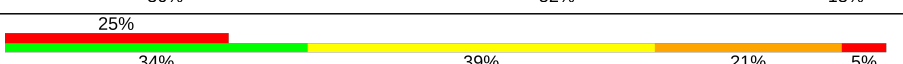



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Mol	Chain	Length	Quality of chain
3	RC	271	
3	YC	271	
4	RD	209	
4	YD	209	
5	RE	201	
5	YE	201	
6	RF	178	
6	YF	178	
7	RG	176	
7	YG	176	
8	RH	149	
8	YH	149	
9	RI	141	
9	YI	141	
10	RJ	142	
10	YJ	142	
11	RK	122	
11	YK	122	
12	RL	143	
12	YL	143	
13	RM	136	
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	QA	1619	-	-	-	X
53	MG	RA	3129	-	-	-	X
53	MG	XA	1614	-	-	-	X
53	MG	XA	1616	-	-	-	X
53	MG	YA	3002	-	-	-	X
53	MG	YA	3003	-	-	-	X
53	MG	YA	3005	-	-	-	X
53	MG	YA	3019	-	-	-	X
53	MG	YA	3049	-	-	-	X
53	MG	YA	3062	-	-	-	X
53	MG	YA	3063	-	-	-	X
53	MG	YA	3064	-	-	-	X
53	MG	YA	3074	-	-	-	X
53	MG	YA	3108	-	-	-	X
53	MG	YA	3109	-	-	-	X
53	MG	YA	3127	-	-	-	X
53	MG	YA	3129	-	-	-	X
53	MG	YA	3130	-	-	-	X
53	MG	YJ	201	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284464 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

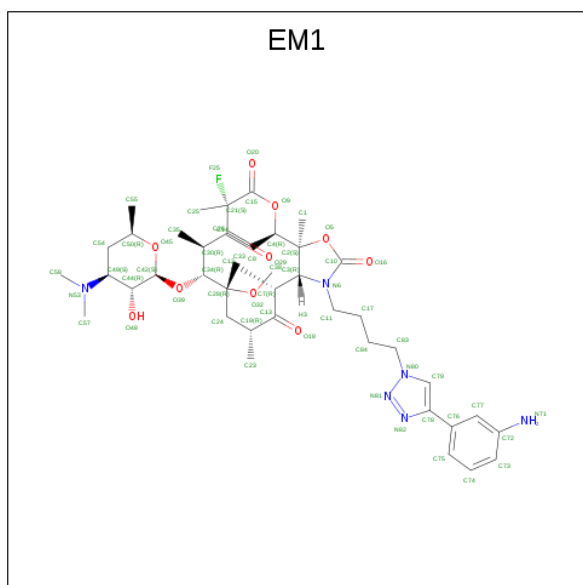
- Molecule 52 is a protein called 30S ribosomal protein S21.

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 (3aS,4R,7S,9R,10R,11R,13R,15R,15aR)-1-{4-[4-(3-aminophenyl)-1H-1,2,3-triazol-1-yl]butyl}-4-ethyl-7-fluoro-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,8,14-tetraoxotetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-10-yl 3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranoside (three-letter code: EM1) (formula: 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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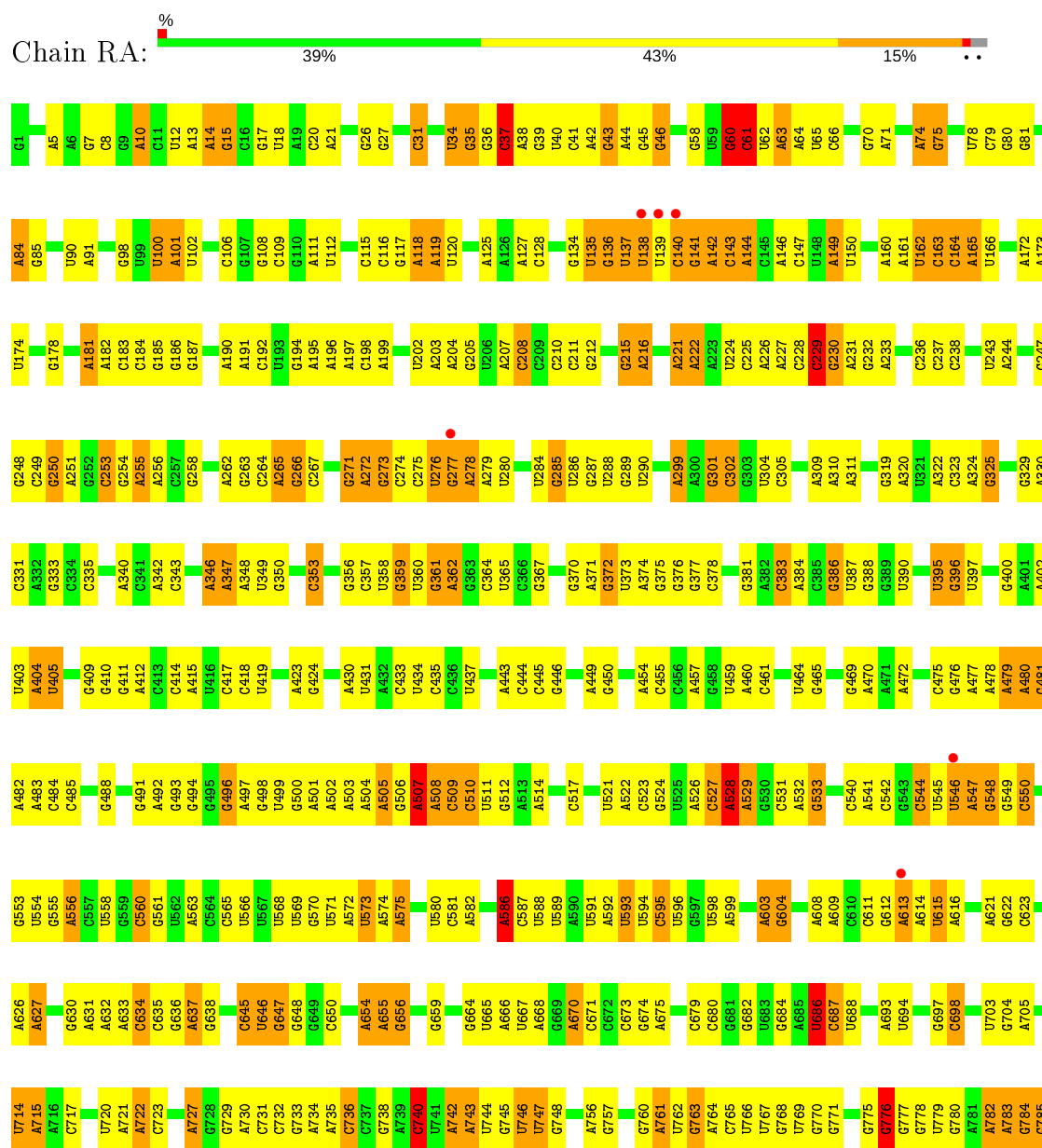
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	XL	1	Total 1	O 1	0	0
56	XN	3	Total 3	O 3	0	0
56	XT	2	Total 2	O 2	0	0
56	XU	1	Total 1	O 1	0	0
56	YA	605	Total 605	O 605	0	0
56	YB	4	Total 4	O 4	0	0
56	YC	8	Total 8	O 8	0	0
56	YD	3	Total 3	O 3	0	0
56	YE	3	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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S rRNA

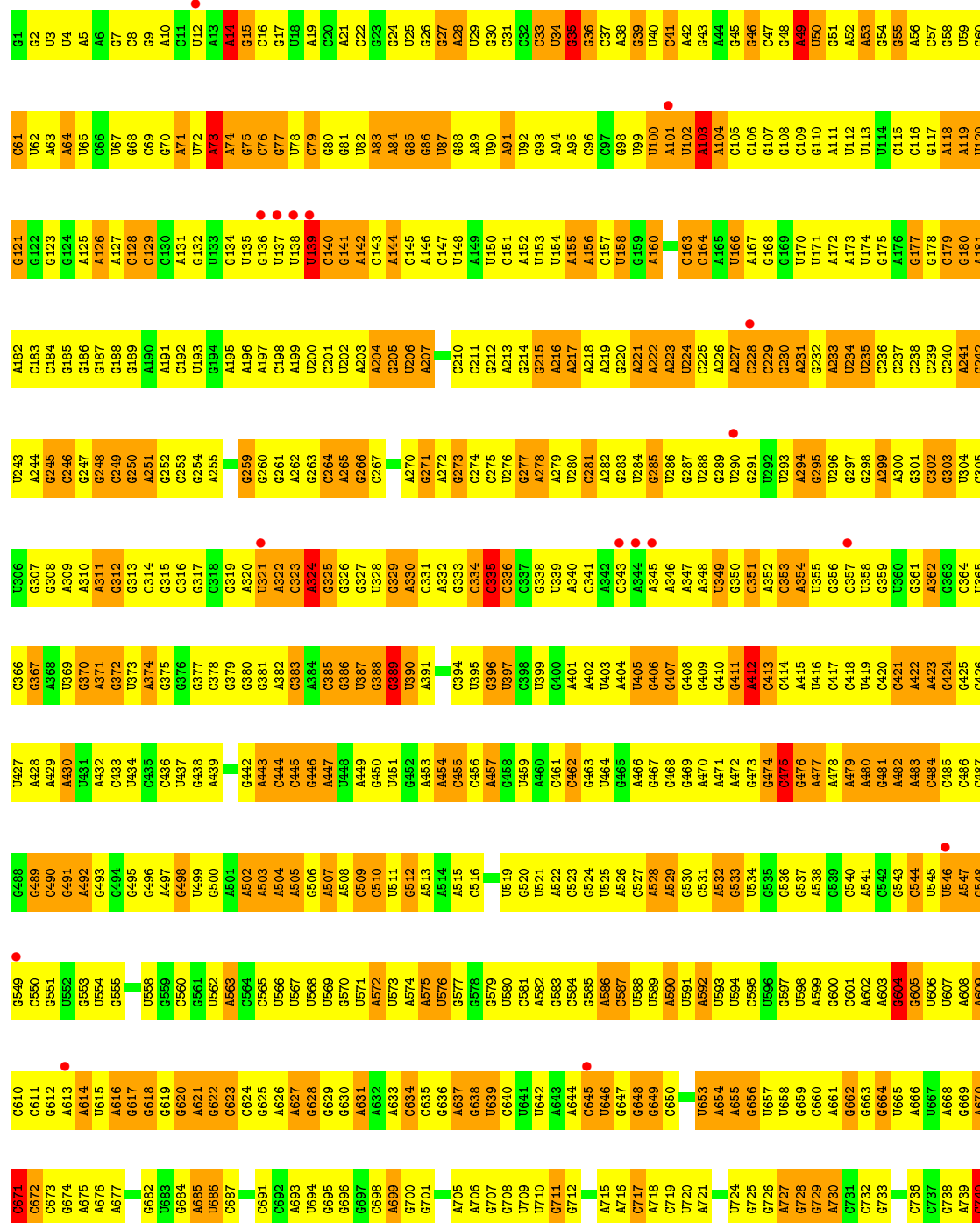
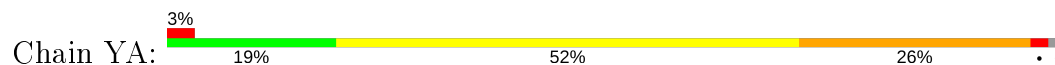


A1783	A1626	G1546	U1467	A1392	G1309	G1229	A1151	U1082	G1011	A936	A866	C786
A1784	G1627	G1547	U1468	A1393	G1310	C1230	C1152	U1083	U1012	C937	C867	C787
A1785	G1628	U1554	A1469	U1394	G1311	U1231	G1153	A1084	C1013	A941	U868	A788
A1786	A1635	G1555	A1470	A1395	C1315	G1232	A1155	A1085	A1014		G869	A789
A1789	U1636	C1558	U1474	C1399	U1316	C1233	A1156	A1086	U1015	C946	U870	C791
C1790	A1637		G1475	U1402	G1317	U1234	G1157	A1088	U1019	A947	A792	A792
A1791	C1638		G1476	C1403	U1318	G1235	G1160	A1089	A1020	C948	A793	A793
G1792		U1562	A1477	A1404	C1319	G1238	C1161	A1090	A1021	C949	C876	A794
C1793	C1644	U1563	G1478	C1403	A1320	G1239	G1166	A1091	G1022	G950	A877	A804
A1794		C1564	G1479	U1405	A1321	G1239	G1167	G1092	U1023	C951	A878	G805
C1795	U1647	G1565		U1408	A1322	U1242	A1165	G1093	G1024	G954	G879	C806
U1796	U1648	C1566	G1482	U1409	C1323	U1243	G1166	U1094	G1025		U884	
G1797	G1649	G1567	G1483	U1410	G1324	C1243	C1167	A1095	G1026		C885	U811
U1798	A1650	U1568	U1484	U1411	U1325	A1244	A1168	A1096	A1027	U958	A	C812
G1799	G1651	A1569	U1485	C1410	U1326	G1245	A1169	U1097	A1028	C959	U	U813
C1800	A1652	A1570	U1486	U1412	A1327	A1246	C1170	A1098	C1092	C961	C	C814
A1801	G1653	A1571	U1487	A1413	A1328	A1247	G1171	A1099	G1023	G962	C	C815
A1802	A1654	A1572	U1487	C1414	A1329	U1248	C1172		A1032		C	
	G1655	G1573	C1488	C1414	G1333	U1249	U1173	A1103	U1033		G	
A1805	C1656		C1489	U1415	G1334	G1250	U1174	C1104	G1037	G969	G818	
		U1576		C1416	C1335	C1251	A1175	U1105	A1040	U970	A892	A819
A1808	G1663	C1577	C1493	C1417	A1336	G1252	U1176	G1106	U1041	C893	C897	A820
A1809	A1664	U1578	A1494	G1418	G1337	A1253	G1177	G1107	G1042	A972	U894	A821
A1810	A1665		A1495	A1419	U1338	U1254	C1178	U1108	C1043	A973	U895	
G1811	G1666	G1581	A1496	A1420	G1339	U1255	G1179	C1109	C1044	C874	A896	U826
U1812	G1667	C1582	U1497	G1421	U1340	G1256	U1180	G1110	C1045	A975	C897	U827
A1813	G1668	A1583	C1498	G1422	G1341	U1257	U1181	A1111	G1046	C898	C898	U828
G1814	A1669	U1584	C1499	G1423	G1342	U1258	G1182	G1112	A1047	A999	A900	U832
A1815	C1670	C1585	G1500	G1427	A1347		U1183	U1113	G1047	G978	U901	A833
C1816		G1586	G1501	A1428	C1348	C1261	U1184	C1114	A1048	A979	C834	A834
G1817	G1674	U1587	A1502	C1429		A1262	G1185	G1115	C1049	A980	U906	G835
U1818	C1675	G1588	A1503	G1428	C1351	U1266	G1186	U1119	A1050	C982	G907	C836
A1819	A1676	U1589	U1504	G1430	A1352	U1267	U1187	G1122	G1056	A984	C908	U839
U1820	A1677	A1590	A1505	A1431	A1353	A1268	U1188	C1123	A1057	C985	A910	C840
A1821		A1591	U1506	G1432	G1354	A1269	A1189	G1124	U1058	C986	A911	C841
C1822	U1680	C1592	C1507	A1433	G1355	G1270	G1190	G1125	U1059	C987	U842	U842
	G1681	A1593	A1508	A1434	G1356			G1128	U1060	A988	U913	A844
G1826	G1682	U1594	A1509	G1435	C1357	G1271	G1193	A1129	G1063	A990	C915	A845
U1827	U1683		G1510	G1436	G1358	A1272	A1194	U1130	U1064		U846	U846
A1828	G1684	U1599	G1511	C1437	G1359	U1273	G1197	U1131	U1065	C994	U847	U847
A1829		C1600	C1512	U1438	G1360	A1274	U1198	U1132	U1066	C995	C848	C848
C1830	U1688		U1513	A1439	A1365	A1276	U1199	U1133	A1067	A996	A920	A849
G1831		A1603	G1514	U1440		G1277	C1200	A1134	G1068	G997	U850	U850
C1832	U1692	C1604	A1515	G1441	G1368	C1278	U1203	C1135	A1069	C998	C921	C851
C1833	U1693	C1605	G1516	U1442		G1279	A1204	G1136	A1070	U999	U852	U852
U1834	C1694	C1606		U1443	U1371	G1280	A1205	G1137	G1071	A1000	C924	C853
G1835	G1695	C1607	U1520	G1444	G1372	G1281	G1206	G1138	C1072	A1001	A927	C854
C1836	G1696	A1608		G1445	U1373		C1207	G1139	A1073	G1002	G855	G855
C1837	G1697	A1609	A1528	G1450	G1377	A1287	C1207	C1140	G1074	G1003	U929	G856
C1838		G1610	G1529	C1451	A1378	G1288	G1212	U1141	C1075	U1004	G930	G857
G1839	A1700	C1611	C1533	A1452	U1379	C1290	G1221	A1142	C1076	C1005	U931	G858
U1840	A1701	C1612	C1534	C1453	G1380	C1295	U1222	A1144	C1077	C1006	U932	G859
U1841		G1613	A1454	G1455		G1300	G1223		U1078	C1007	A933	A863
G1842	A1705	A1614	A1535	G1456	A1383	A1301	U1224	G1149	C1079	A1008	U934	G864
C1843	U1778		C1536	U1457	A1384		G1225		U1081	A1010	C935	C865
C1844	G1707	A1618	G1537	U1458	A1385							
	U1780	G1622	U1538	G1459	A1386							
A1847	U1714		U1539	U1460	A1387							
A1848	G1715		G1540									

A2821	G2751	A2670	G2583	U2511	U2438	G2357	A2198	G2138	C2066	U1985	A1927	G1849
A2822	G2755	G2671	U2585	U2514	C2440	A2358	A2199	U2139	C2067	C1996	A1928	G1850
A2823	G2756	G2675	U2586	C2515	U2441	G2361	C2200	G2140	U2068	C1997	G1929	U1851
G2824	A2757	A2676	G2586	A2516	U2444	G2364	U2203	A2142	G2070	A1998	G1930	U1852
A2826	A2758	G2678	A2590	C2517	G2444	C2364	G2204	C2143	A2071	U1999	U1931	A1853
C2830	G2759	G2677	C2591	C2518	G2445	G2365	U2210	C2144	C2072	C2001	A1932	A1854
G2831	G2760	C2678	G2592	U2519	G2446	A2366	A2211	C2145	G1934	C1934	U1855	U1856
G2832	A2761	A2679	U2593	C2520	G2447	G2367	A2212	C2146	U2075	G1935	G1857	U1857
G2833	G2762	U2680	G2602	G2523	A2448	G2373	U2213	A2147	U2076	A1936	A1858	A1858
G2834	A2765	C2681	G2603	G2524	U2449	C2374	C2214	C2148	U2080	A1937	U1859	U1859
G2839	G2769	G2682	U2604	C2527	A2450	G2378	U2305	U2149	A2080	A1938	U1864	U1864
C2840	U2770	U2683	U2605	C2528	G2454	A2378	C2306	C2150	A2014	U1939	U1865	U1865
C2841	G2770	G2684	G2606	U2528	G2455	C2379	U2220	U2151	A2015	A1940	A1866	A1866
G2842	G2771	G2685	G2607	G2529	C2456	G2380	G2221	G2152	U2016	C1941	G1941	G1941
G2843	C2772	G2686	G2608	C2530	U2456	C2381	C2222	G2153	C1942	C1942	G1942	G1942
G2844	G2773	U2689	U2609	A2531	A2459	G2382	G2223	A2154	U2092	U1943	U1943	C1868
G2845	C2774	U2690	U2610	G2532	U2460	G2383	G2224	U2155	G2093	U1944	U1944	G1869
G2846	G2775	U2691	U2611	U2533	A2461	U2384	A2225	G2156	A2094	C1945	G1945	C1870
U2847	A2776	G2694	A2614	A2534	A2462	G2385	U2226	A	A2095	C2021	U1946	A1871
G2848	G2777	U2695	U2615	G2535	C2466	C2386	U2233	G	C2096	U2022	C1947	A1872
U2849	A2778	U2698	G2619	G2536	U2466	A2386	G2234	C	C2023	G1948	G1948	G1873
A2850	U2779	G2699	C2620	U2537	A2471	G2389	U2234	C	G2024			C1874
A2851	G2780	G2699	G2621	G2538	G2472	G2390	G2238	G	C2025	A1952		G1875
G2852	A2781	G2703	C2626	A2542	G2473	U2393	G2239	A	U2026	A1953		A1876
G2853	G2782	C2703	G2627	G2543	U2474	U2394	G2240	C	G2027	G1954	U1955	C1881
G2854	C2704	G2704	C2628	G2544	A2475	C2395	U2243	C	A2030	U1956	U1956	U1882
G2855	U2784	G2629	G2629	G2545	A2476	G2396	U2244	U	A2031	C1957	U1883	U1883
A2856	G2785	G2714	U2629	U2546	U2477	G2397	G2250	G	G2032	C1958	G1884	G1884
G2857	U2786	C2715	G2630	A2547	A2478	C2398	U2251	G	A2033	A1959	U1885	U1885
G2858	C2716	G2716	G2631	U2548	U2479	C2399	G2252	A	U2034	A1960	U1886	U1886
U2861	G2717	C2717	C2636	U2549	A2480	U2402	G2253	C	G2035	C1961		
G2791	U2720	C2637	U2637	G2553	G2481	U2403	G2255	A	U	C1962	A1889	A1889
A2792	G2721	G2721	G2638	U2554	C2482	C2404	U2257	A	G	U1963	A1890	A1890
C2793	G2722	A2722	U2555	U2555	G2484	A2406	U2258	C	U	C1964		
G2866	G2723	C2485	G2641	C2556	G2485	A2407	U2259	C	A	C1965	G1897	G1897
G2867	U2724	G2486	G2642	G2557	C2486	G2415	U2262	C	G	A1966	U1898	U1898
C2870	G2725	G2487	G2643	C2558	G2487	G2416	C2263	C	A	C1967	A1966	A1966
A2873	A2726	U2488	G2644	U2562	G2488	C2417	G2264	C	A	A1968	A1900	A1900
G2874	G2727	G2489	G2645	U2563	U2489	C2417	U2267	C	U	A1969	A1901	A1901
A2879	A2728	U2491	C2649	A2564	G2490	C2417	A2268	A	A	C1970		
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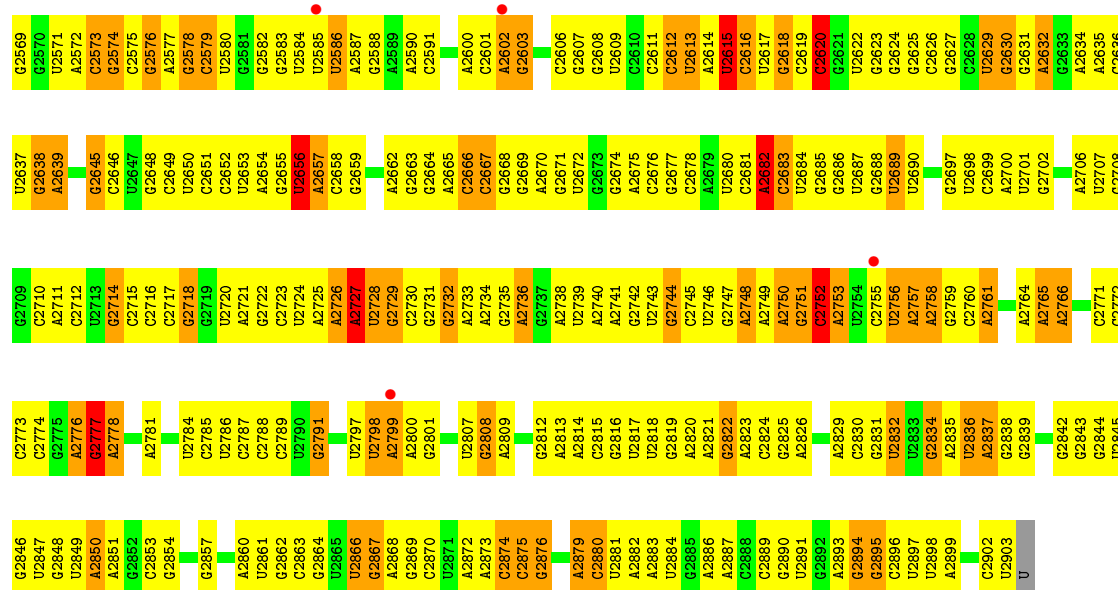


● Molecule 1: 23S rRNA



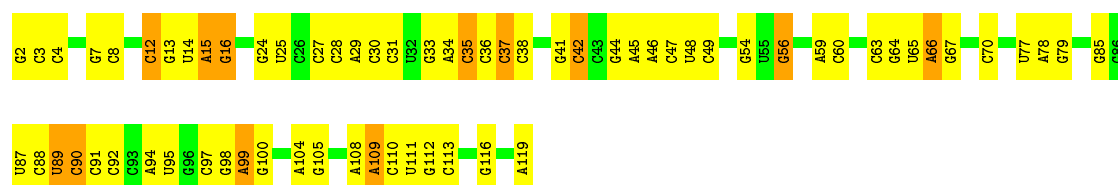


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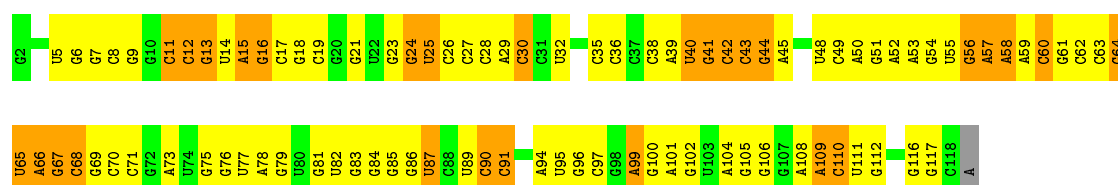
• Molecule 2: 5S rRNA

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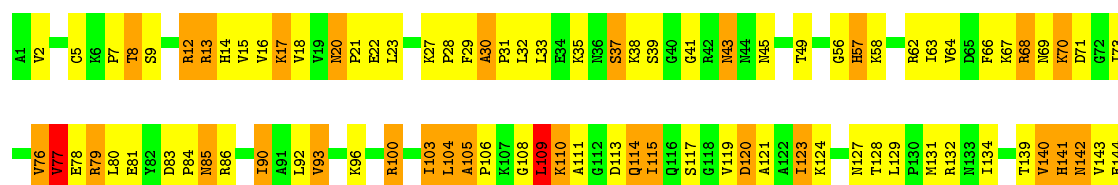
• Molecule 2: 5S rRNA

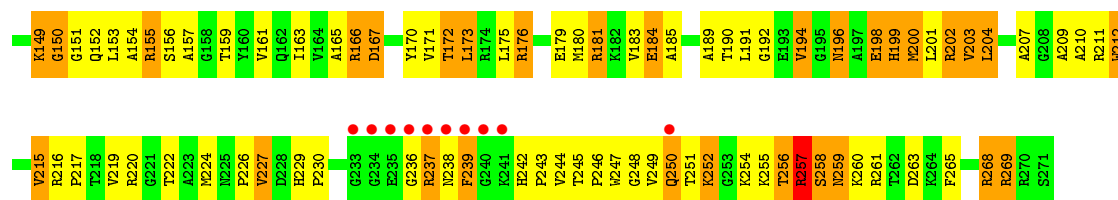
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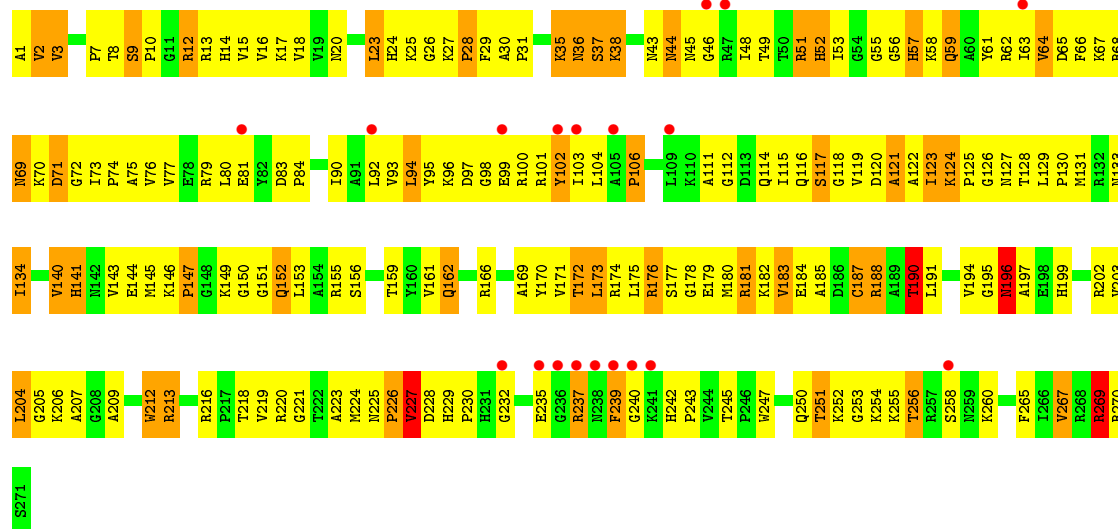
• Molecule 3: 50S ribosomal protein L2

Chain RC:

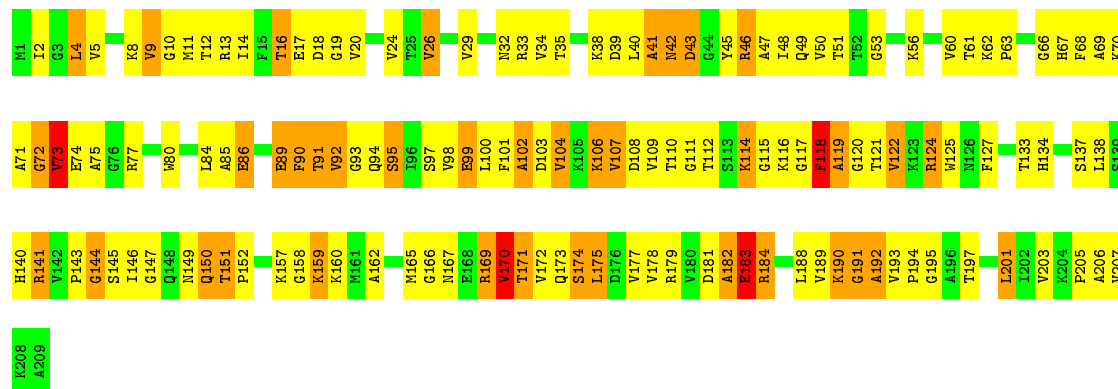
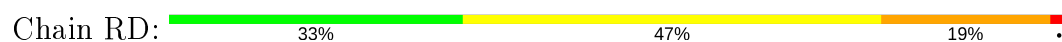




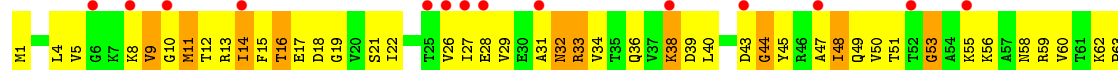
• Molecule 3: 50S ribosomal protein L2

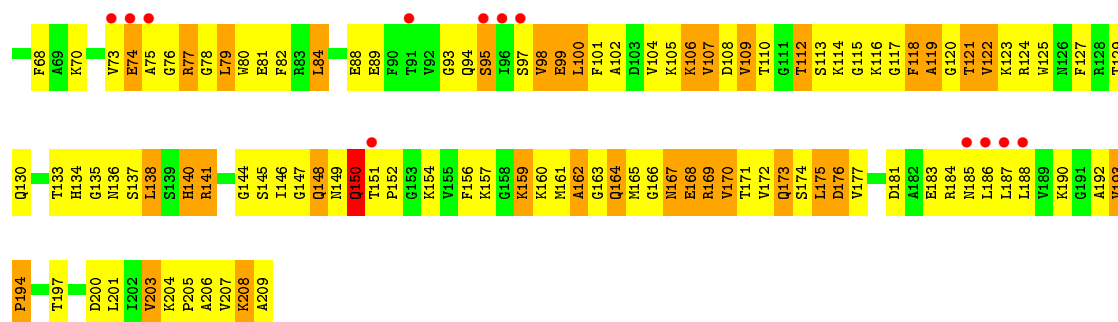


• Molecule 4: 50S ribosomal protein L3

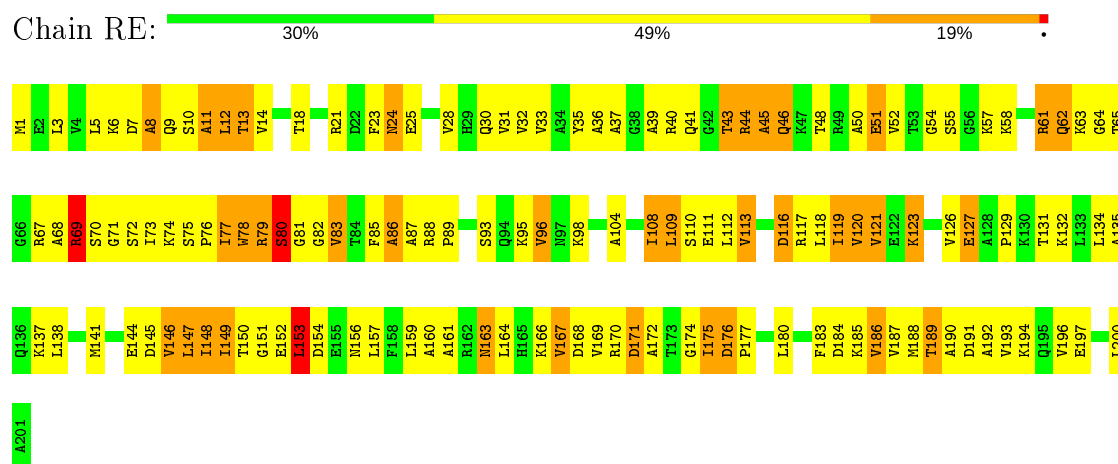


• Molecule 4: 50S ribosomal protein L3

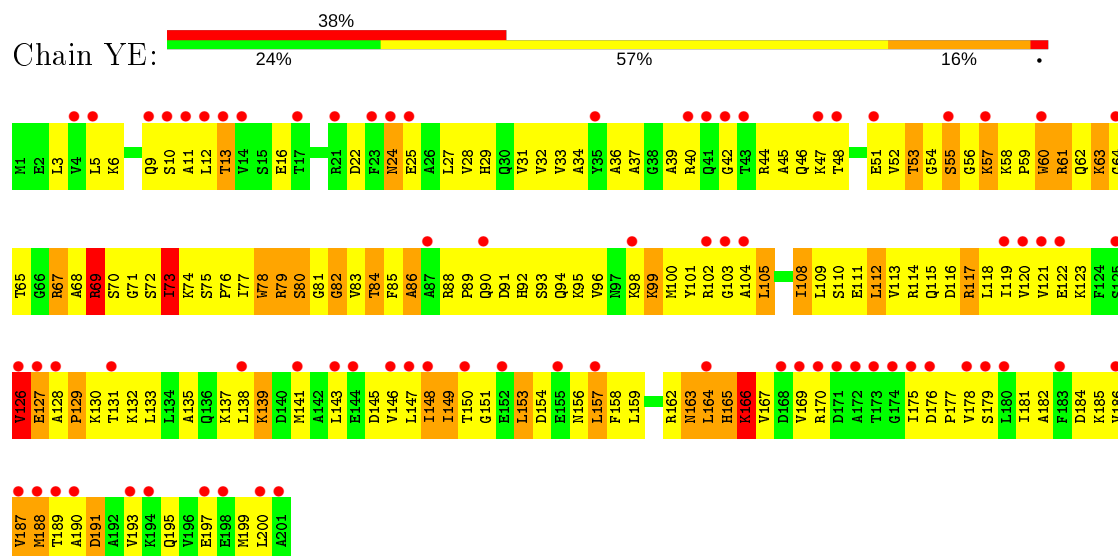




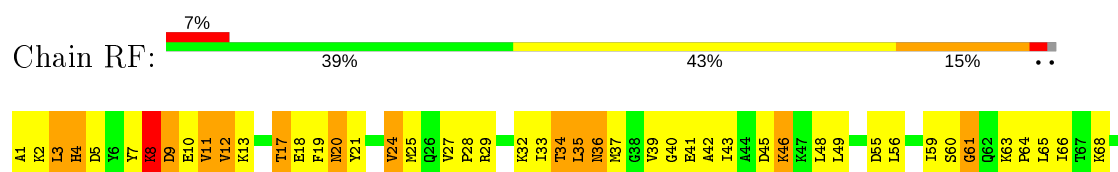
• Molecule 5: 50S ribosomal protein L4

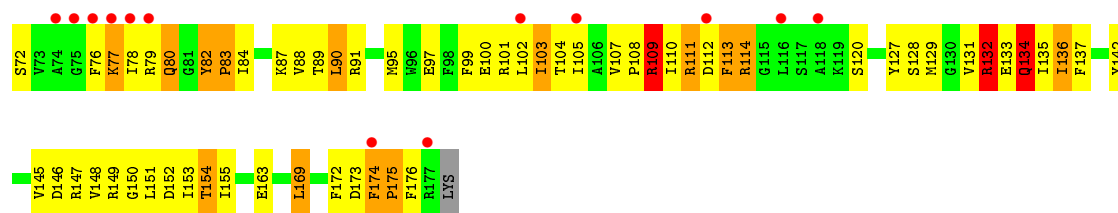


• Molecule 5: 50S ribosomal protein L4

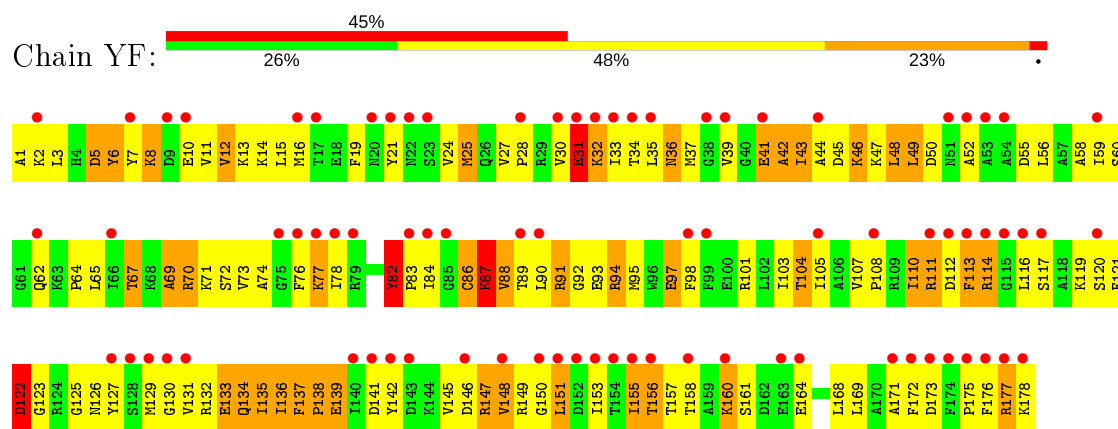


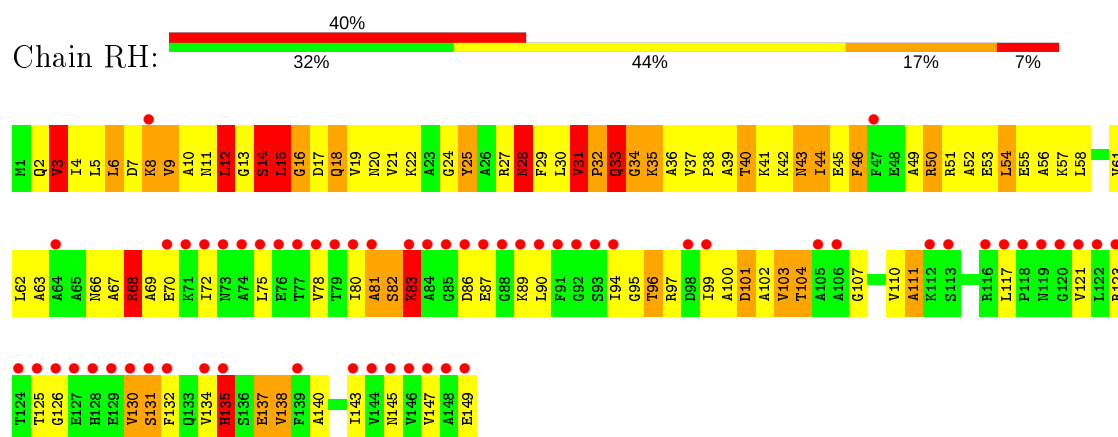
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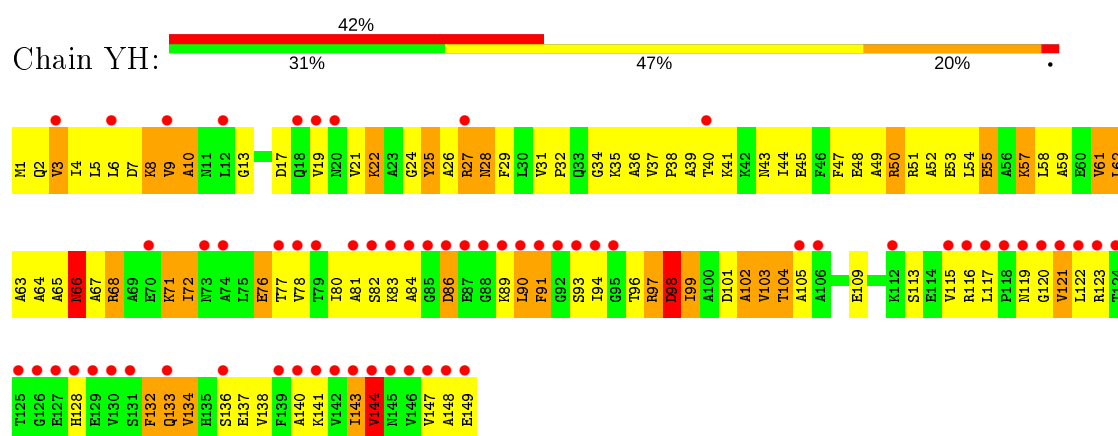


• Molecule 6: 50S ribosomal protein L5

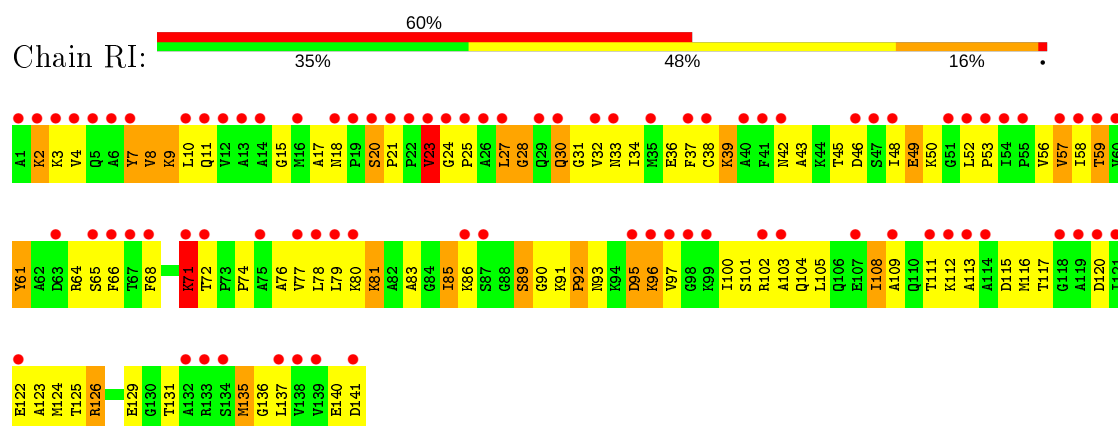




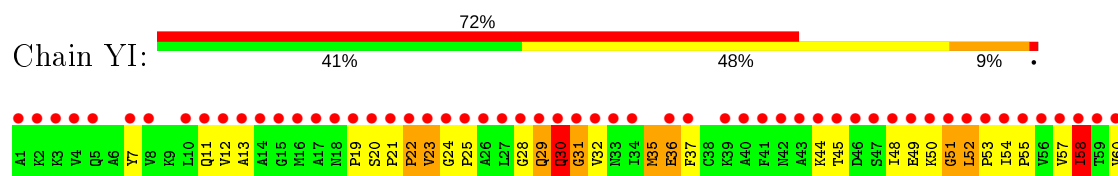
• Molecule 8: 50S ribosomal protein L9

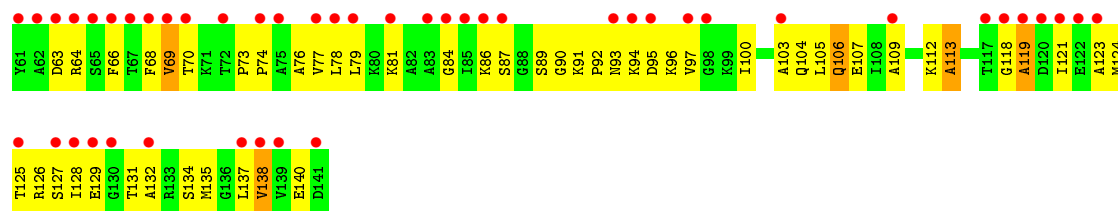


• Molecule 9: 50S ribosomal protein L11

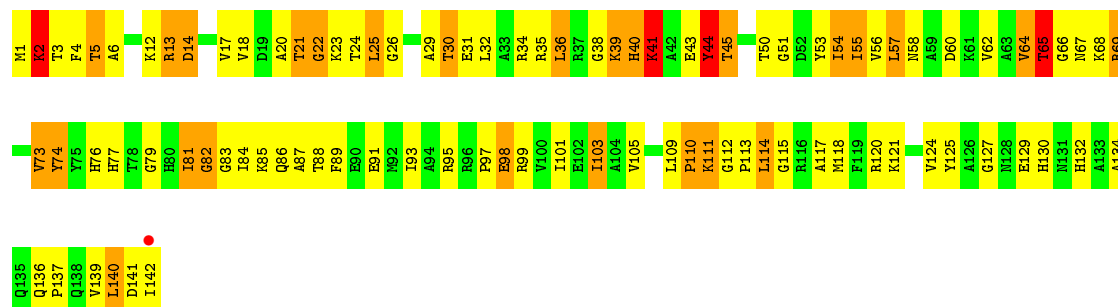


• Molecule 9: 50S ribosomal protein L11

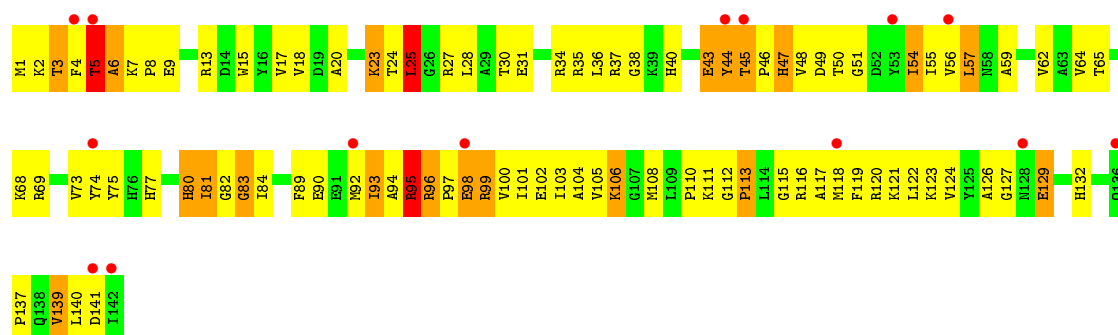




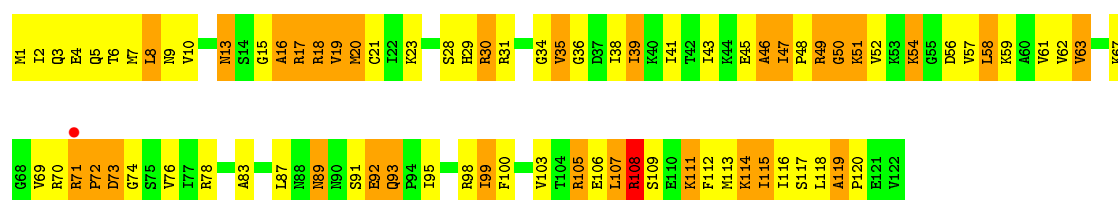
• Molecule 10: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L13

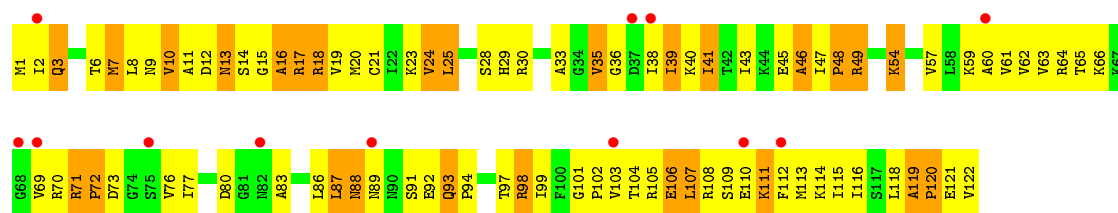


• Molecule 11: 50S ribosomal protein L14

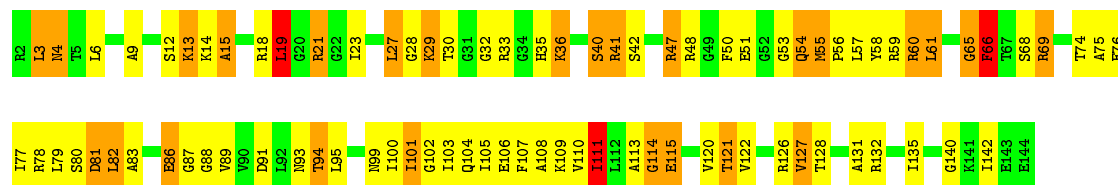


• Molecule 11: 50S ribosomal protein L14

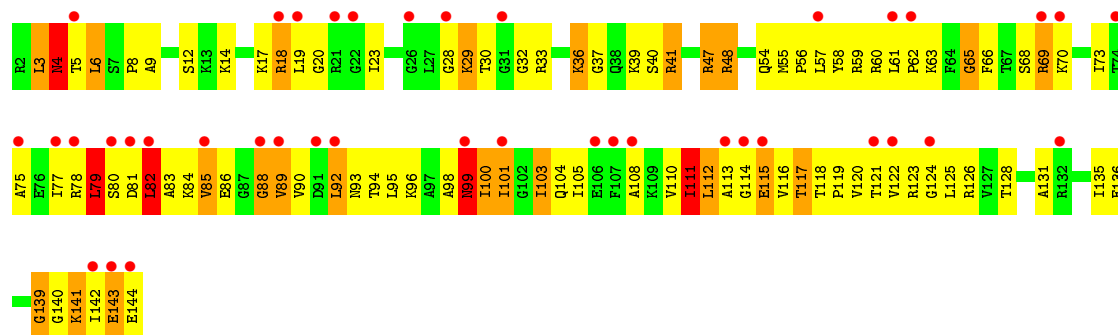




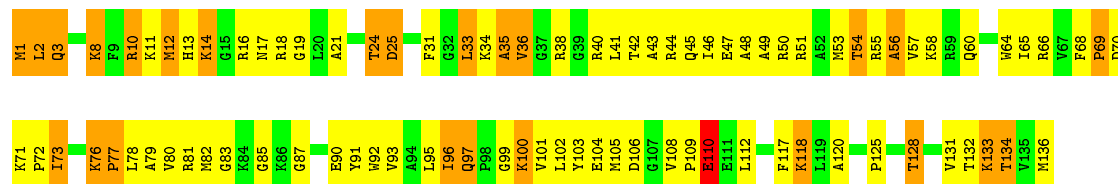
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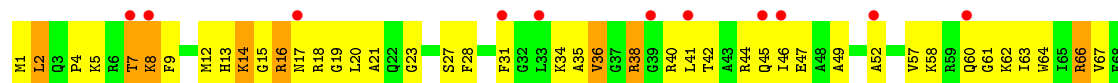
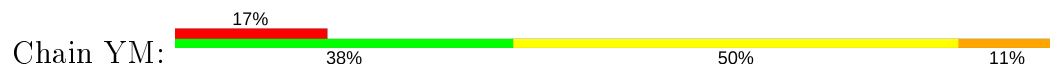
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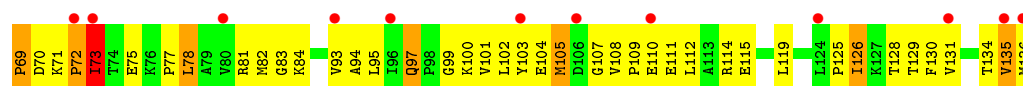


• Molecule 13: 50S ribosomal protein L16

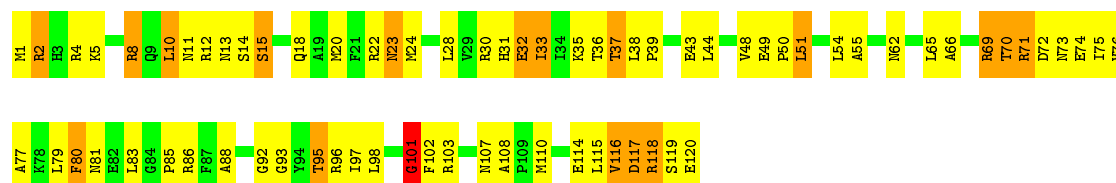


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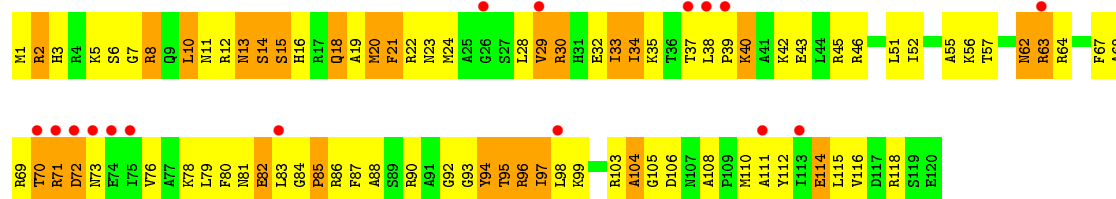




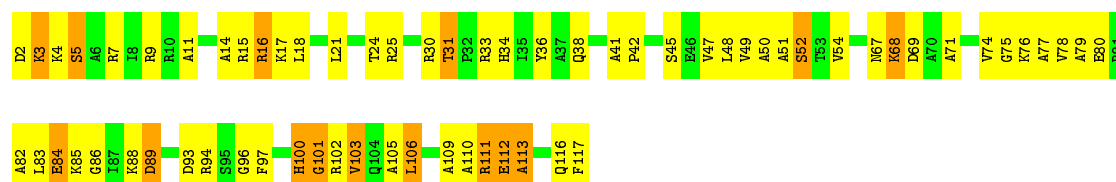
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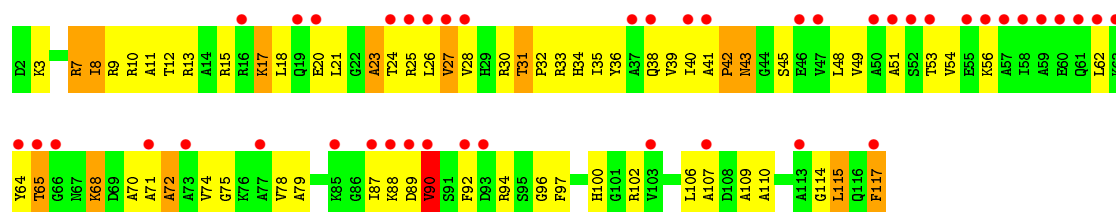
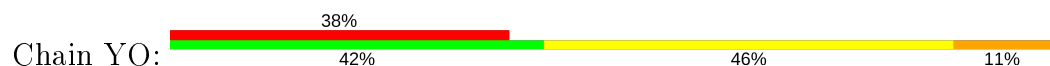
- Molecule 14: 50S ribosomal protein L17



- Molecule 15: 50S ribosomal protein L18

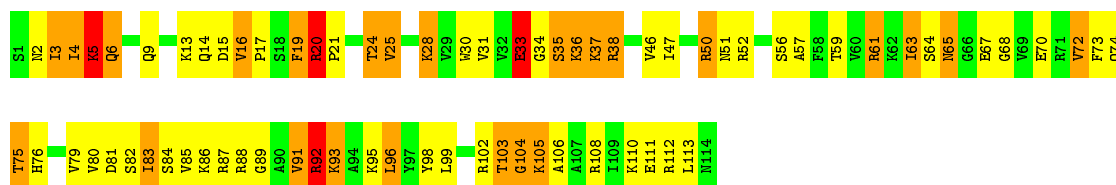


- Molecule 15: 50S ribosomal protein L18

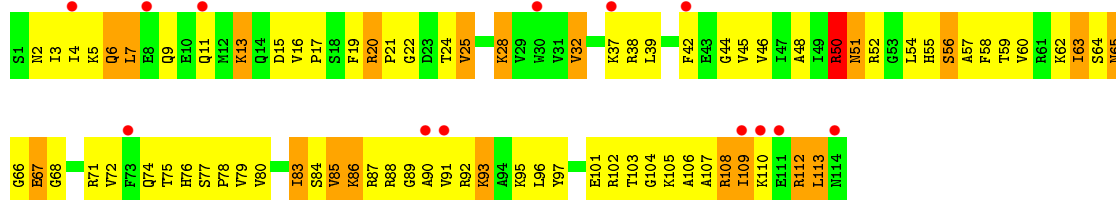


- Molecule 16: 50S ribosomal protein L19

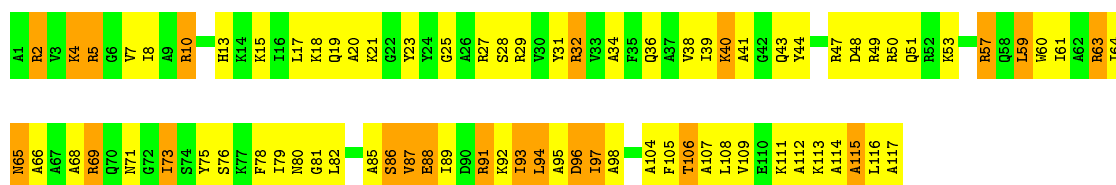




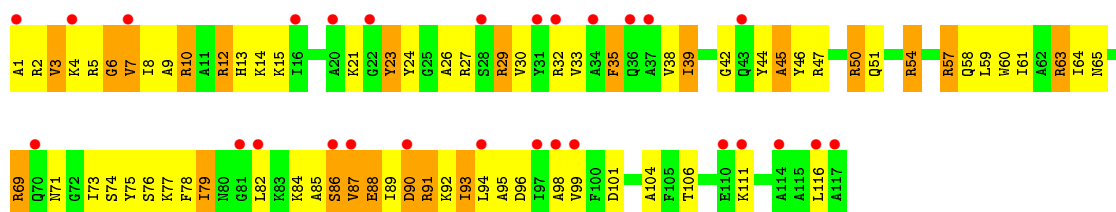
- Molecule 16: 50S ribosomal protein L19



- Molecule 17: 50S ribosomal protein L20



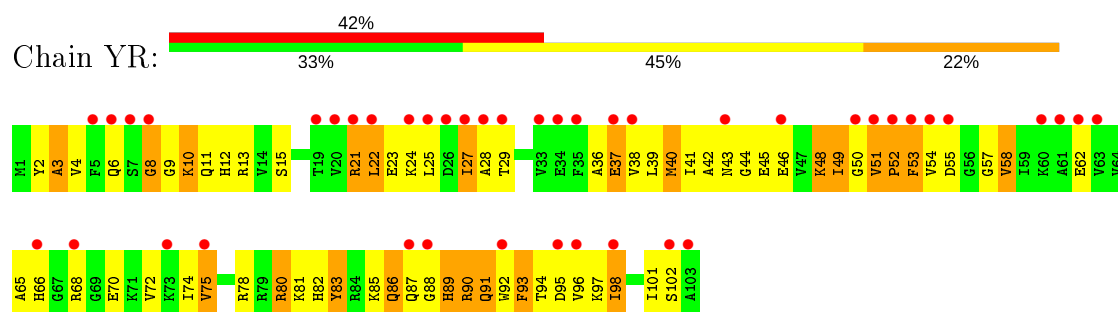
- Molecule 17: 50S ribosomal protein L20



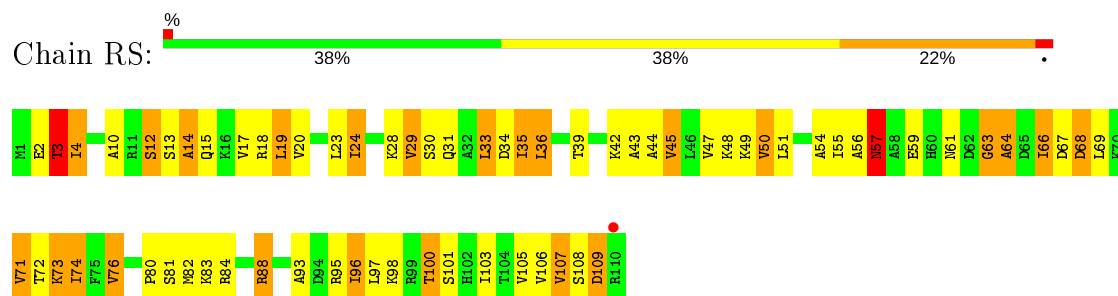
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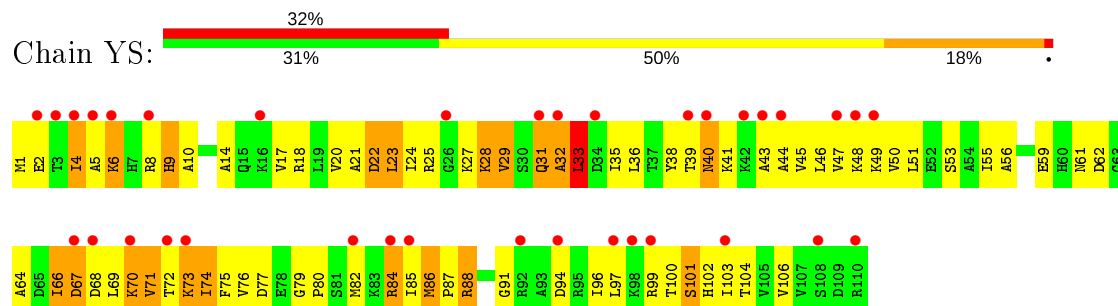
- Molecule 18: 50S ribosomal protein L21



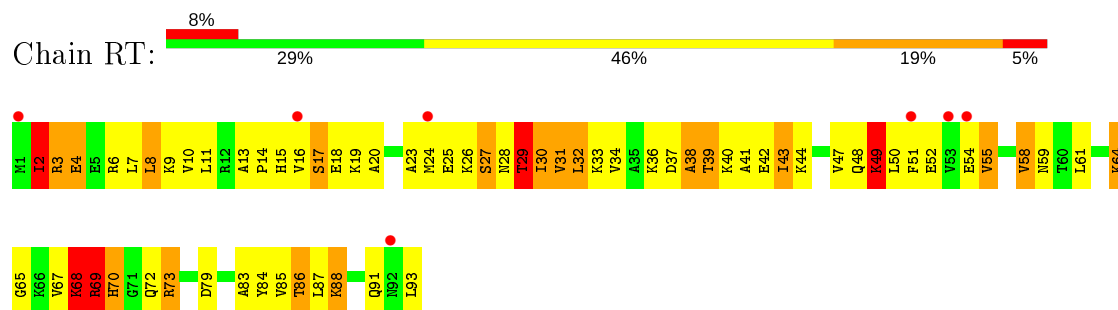
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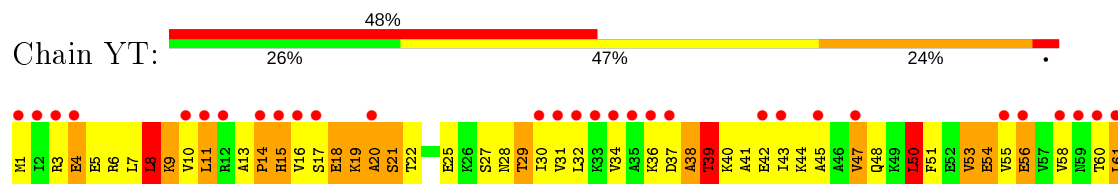
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- Molecule 20: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L23

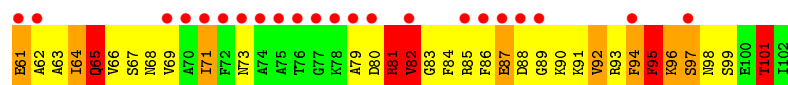
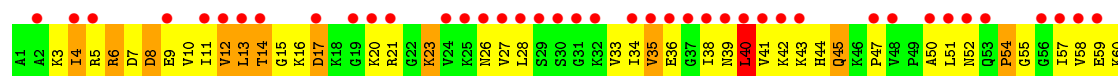




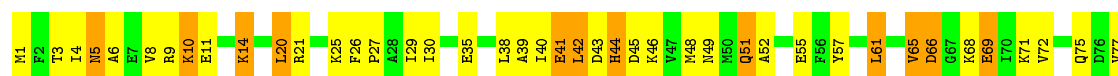
- Molecule 21: 50S ribosomal protein L24



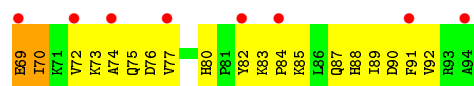
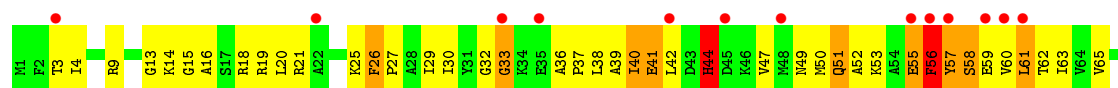
- Molecule 21: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L25

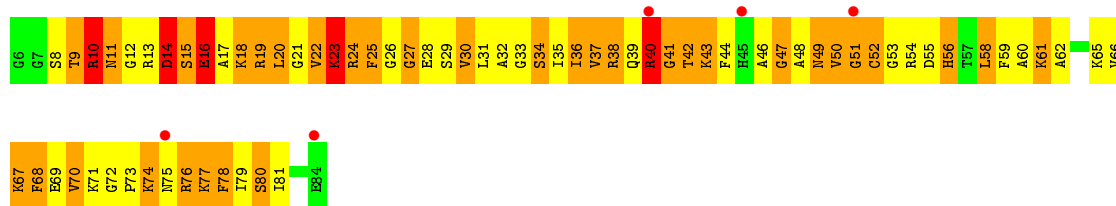


- Molecule 22: 50S ribosomal protein L25

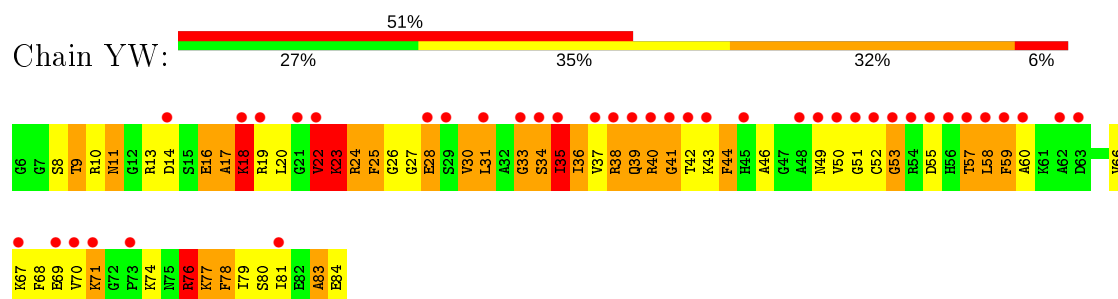


- Molecule 23: 50S ribosomal protein L27

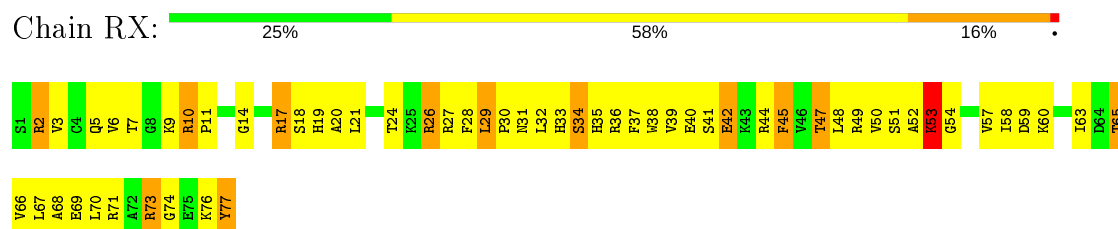




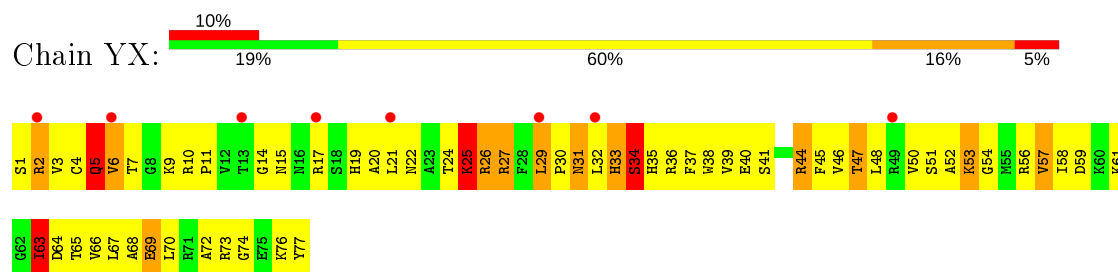
• Molecule 23: 50S ribosomal protein L27



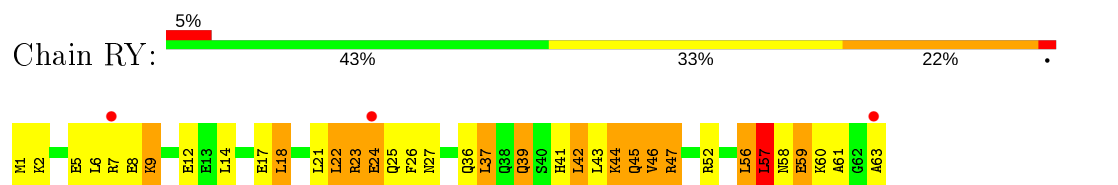
• Molecule 24: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L28

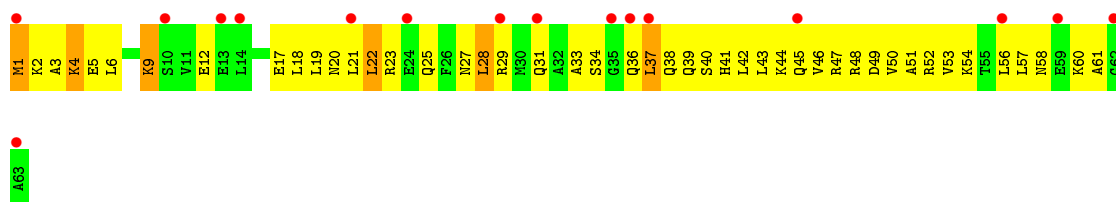


• Molecule 25: 50S ribosomal protein L29



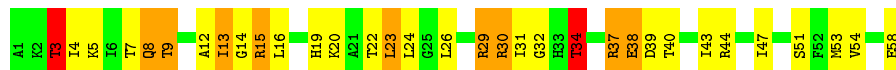
• Molecule 25: 50S ribosomal protein L29





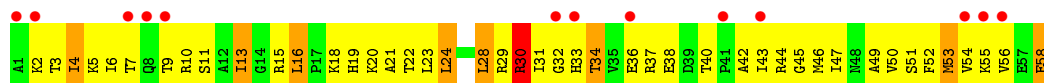
- Molecule 26: 50S ribosomal protein L30

Chain RZ: 43% 38% 16%



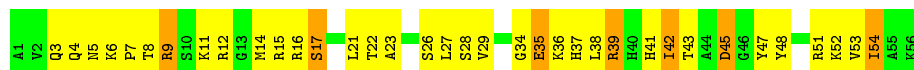
- Molecule 26: 50S ribosomal protein L30

Chain YZ: 22% 62% 14%



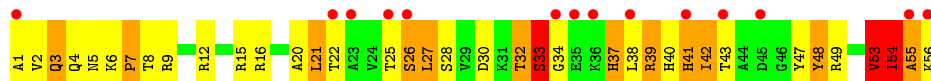
- Molecule 27: 50S ribosomal protein L32

Chain R0: 36% 52% 13%



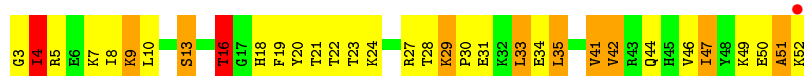
- Molecule 27: 50S ribosomal protein L32

Chain Y0: 25% 34% 39% 21% 5%



- Molecule 28: 50S ribosomal protein L33

Chain R1: 2% 34% 44% 18%

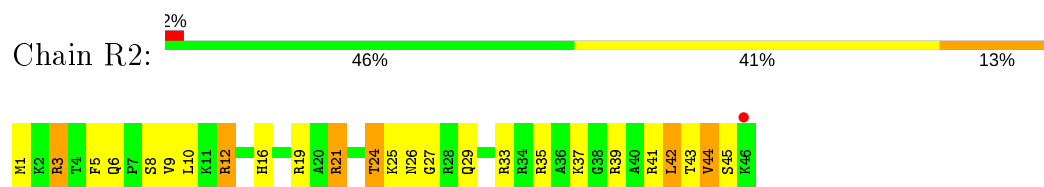


- Molecule 28: 50S ribosomal protein L33

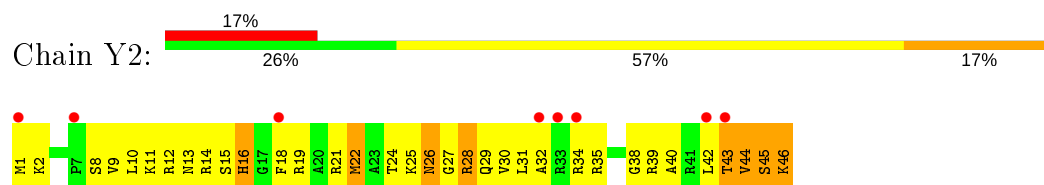
Chain Y1: 32% 42% 46% 12%



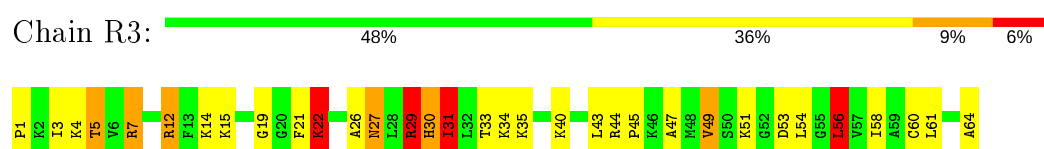
- Molecule 29: 50S ribosomal protein L34



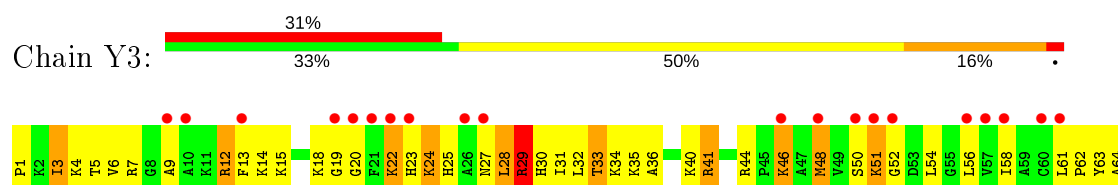
- Molecule 29: 50S ribosomal protein L34



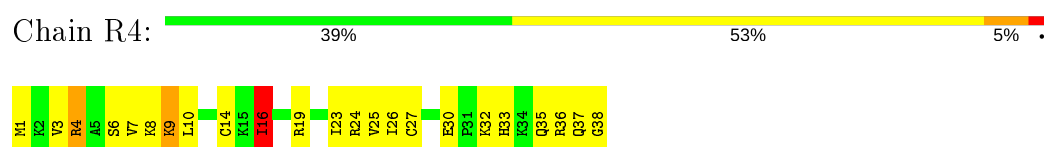
- Molecule 30: 50S ribosomal protein L35



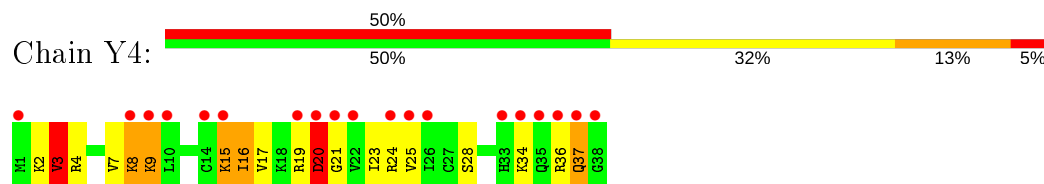
- Molecule 30: 50S ribosomal protein L35



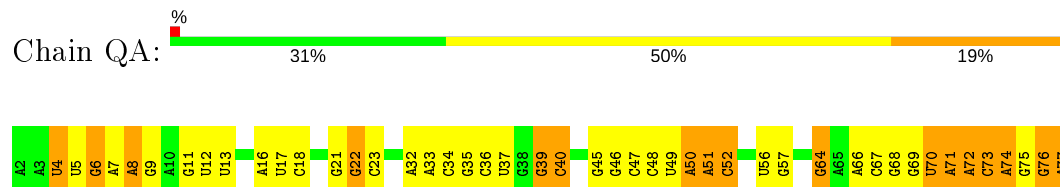
- Molecule 31: 50S ribosomal protein L36

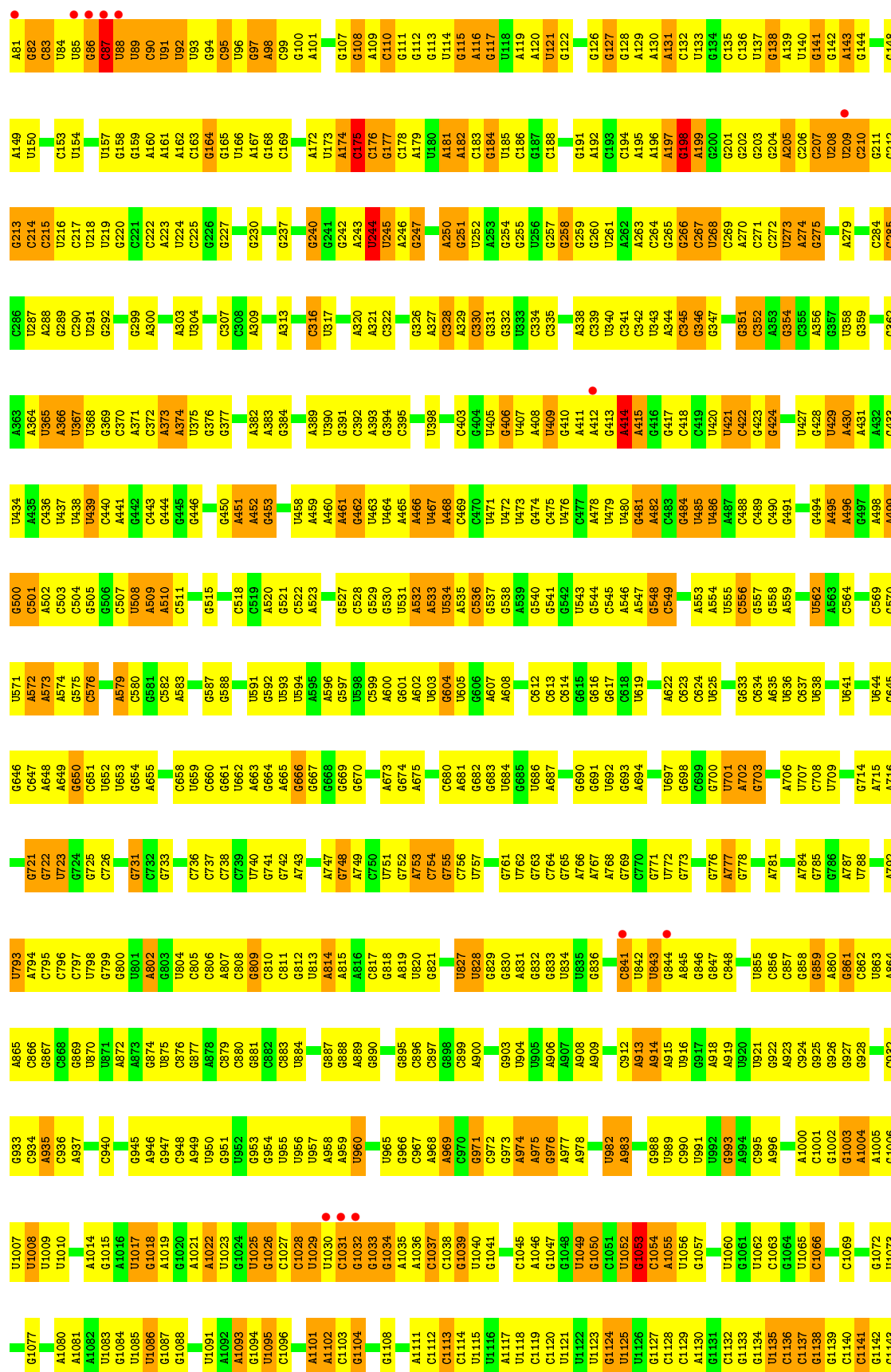


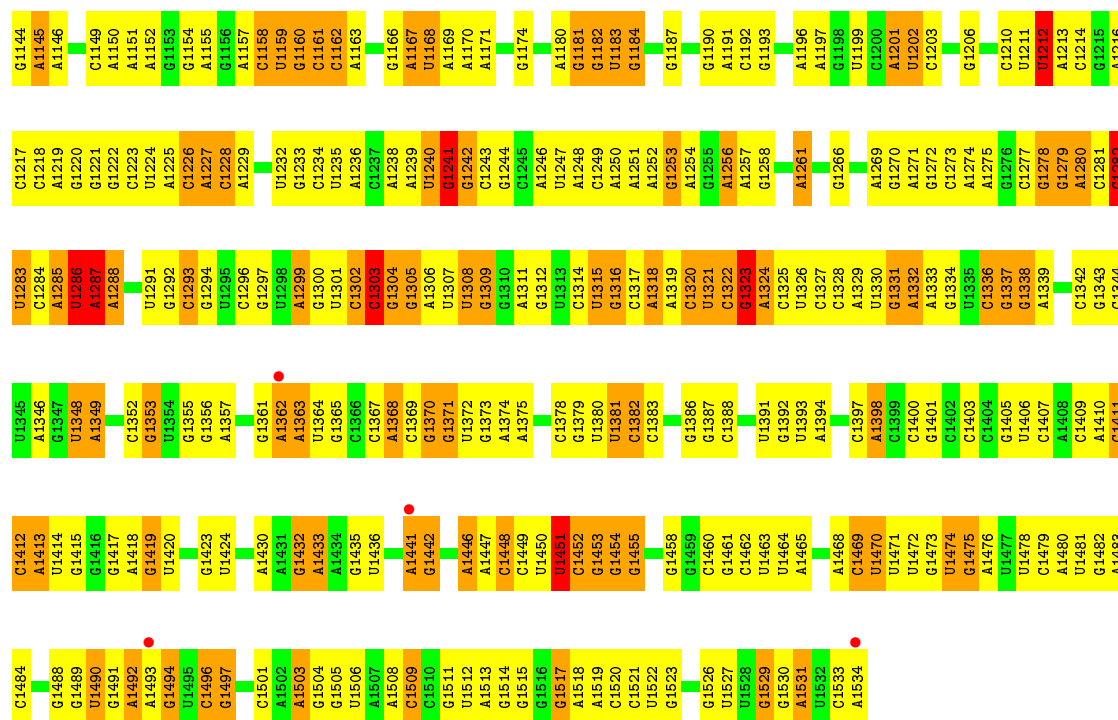
- Molecule 31: 50S ribosomal protein L36



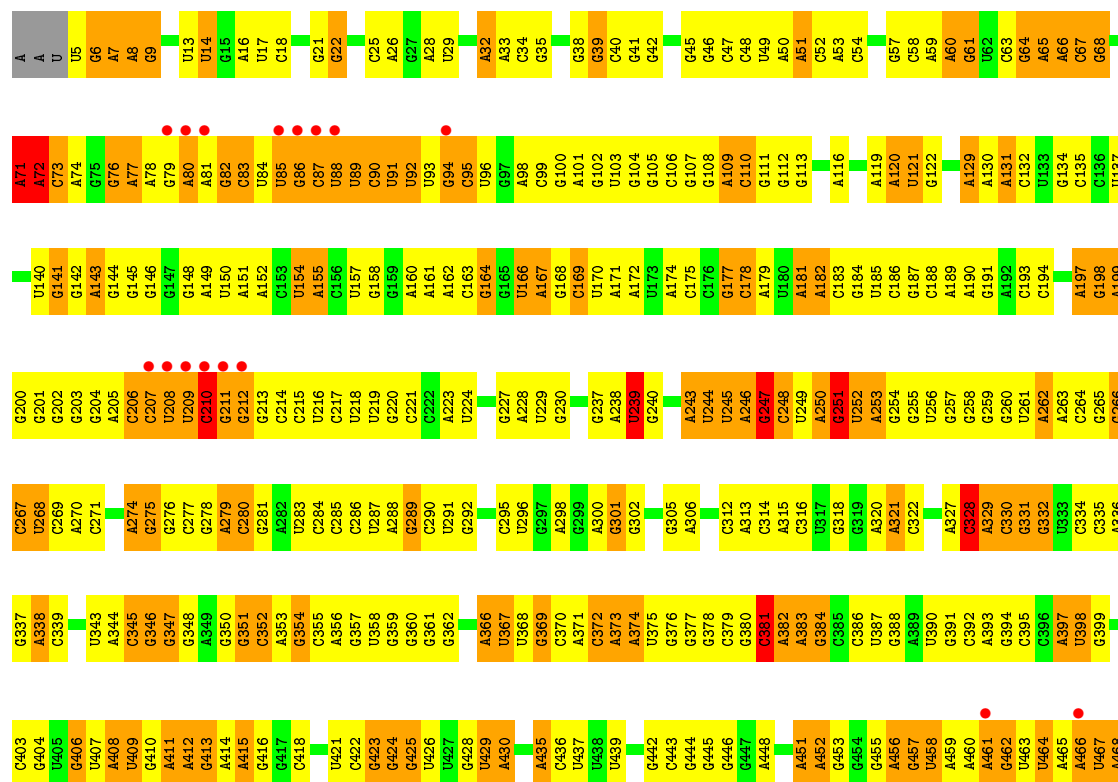
- Molecule 32: 16S rRNA







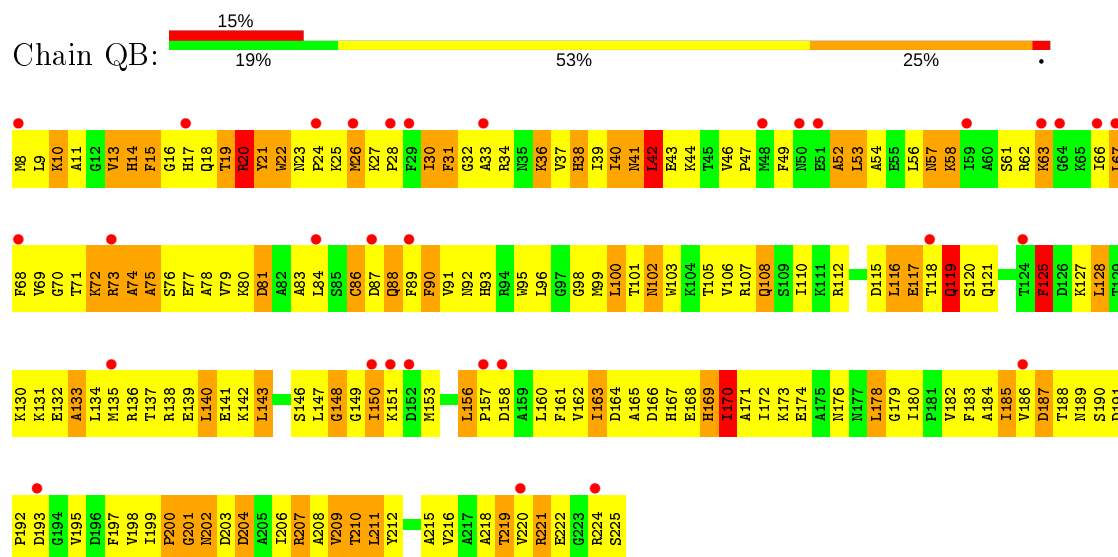
• Molecule 32: 16S rRNA



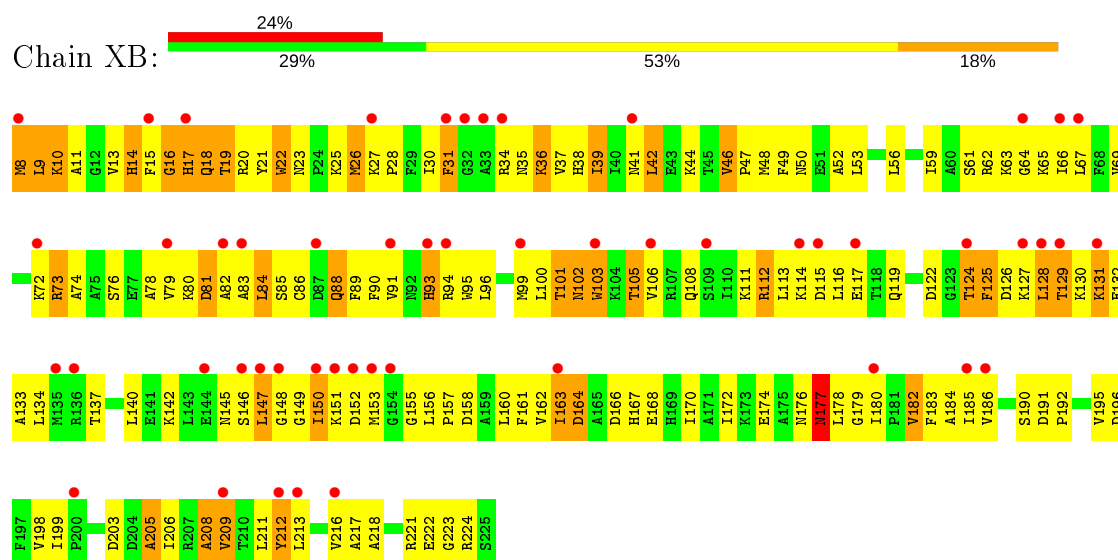
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C1409	U1345	U1283	C1214	C1147	A1081	G1020	U960	C882	A815	G752	C680	U610	A533	C470
C1410	A1347	C1284	A1215	U1148	U1082	A1021	U961	C883	A816	A753	A681	G615	U471	U471
C1411	C1346	A1285	A1216	C1149	U1083	A1022	C962	C963	C817	C754	G682	G616	A535	U472
G1415	U1348	U1286	C1217	A1150	U1084	U1023	G963	G883	G818	G755	G683	G617	C636	U473
G1416	A1349	A1287	C1218	A1151	U1085	G1024	A964	A889	A819	C756	U684	G618	U474	G474
G1417	A1350	A1288	A1219	A1152	U1086	U1025	U965	C890	U820	U757	G685	C618	C475	C475
A1418	U1351	G1292	G1220	G1153	G1089	G1026	G966	U891	G821	C758	U686	U619	U476	U476
G1422	G1352	C1293	G1221	G1154	U1090	G1027	C967	A892	U822	A759	A687	C620	U477	C477
G1423	G1356	G1294	G1222	A1157	U1091	C1028	A968	C893	C823	G760	G688	A621	A478	U479
U1429	A1357	U1295	C1223	C1158	U1092	U1029	A969	C894	C824	A762	G689	G622	U479	U479
U1358	U1358	C1296	U1224	A1159	A1092	U1030	C970	G898	C825	U762	G690	C623	U480	U480
G1359	G1359	G1297	C1225	G1160	A1093	C1031	G871	C899	C826	U763	G691	C624	G481	G481
A1360	A1360	U1298	C1226	C1161	G1094	G1032	C972	A900	U827	C764	U692	U625	G482	G482
A1361	C1361	A1299	A1227	C1162	U1095	G1033	G973	A901	U828	G765	G693	G626	U484	U484
A1362	A1362	C1300	C1228	G1163	C1096	G1034	A974	A906	G829	A766	G694	G627	C556	U486
A1363	A1363	G1301	A1229	U1167	C1097	A1035	A975	A907	G830	G775	U695	G628	C557	U487
U1364	U1364	U1302	U1232	U1168	C1098	A1036	G976	A908	G831	G776	G705	A630	C558	U488
G1365	G1365	C1303	G1233	A1169	G1099	C1037	A977	A909	U834	C770	A706	C631	C559	U489
C1366	C1366	G1304	G1234	A1170	C1100	C1038	A978	C910	U835	G771	G700	U632	C560	U490
A1367	A1367	C1305	A1238	A1171	A1101	G1039	C979	C911	U836	U772	A702	U633	U561	G491
C1368	C1368	A1306	A1239	C1172	A1102	U1040	C980	A913	G836	G773	G703	G633	C492	C492
C1369	C1369	U1307	U1240	U1173	C1103	G1041	C981	A914	U837	G774	A704	G636	A563	G493
G1370	G1370	G1308	G1241	G1174	G1104	A1042	U982	A914	C841	G775	G705	U637	C564	G494
G1371	G1371	C1309	G1242	A1176	A1105	G1043	A983	G917	U842	G776	A706	U638	A495	A495
U1372	U1372	G1310	C1243	G1177	C1106	A1046	C984	A918	U843	A777	A707	U639	A496	A496
G1373	G1373	A1311	G1244	G1178	C1107	U1047	U985	A919	U844	G778	G708	A640	C497	C497
A1374	A1374	C1312	C1245	A1179	G1108	G1048	C986	A920	G845	C779	C709	U641	A498	A498
A1375	A1375	G1313	C1246	A1180	A1111	U1049	G987	U921	U846	A780	G710	A642	G570	G570
U1376	U1376	C1314	A1246	G1181	C1112	G1050	G988	U922	G847	A781	G711	C643	G500	G500
A1377	A1377	U1315	C1249	G1182	C1113	C1051	C990	G926	C848	G783	A712	U644	C501	C501
C1378	C1378	G1316	A1250	U1183	C1114	U1052	U991	G927	G849	A784	G713	G645	A502	A502
A1379	A1379	C1317	A1251	G1184	C1115	G1053	U992	C932	G785	G786	A573	G650	C503	C503
U1380	U1380	A1318	G1252	G1185	C1116	C1054	G993	C933	C853	G787	A717	A649	C504	C504
U1381	U1381	C1319	A1254	G1186	U1056	U1055	A994	G934	U854	A788	C718	G651	G505	G505
C1382	C1382	U1320	G1255	G1187	C1117	G1056	C995	A935	U855	C789	A719	U853	A509	A509
C1383	C1383	U1321	A1256	A1188	U1123	G1057	A996	A936	C856	U790	C720	G654	C510	C510
C1384	C1384	C1322	A1257	U1189	G1124	G1058	U997	C936	C857	A791	G721	U859	C511	C511
G1385	G1385	G1323	C1258	G1190	U1125	C1059	C998	U937	G858	U792	G722	C660	U512	U512
A1386	A1386	A1324	C1259	A1191	U1126	U1060	C999	G939	G859	U793	G723	U659	C513	C513
G1387	G1387	C1325	G1260	G1192	G1127	G1061	A1000	C940	G861	A794	G724	C661	C514	C514
C1388	C1388	U1326	G1264	G1193	C1128	U1062	G1001	G941	C862	C795	A728	U662	G515	G515
C1389	C1389	C1327	C1265	U1194	C1129	G1063	G1002	G942	A865	C796	A729	A663	U516	U516
U1390	U1390	C1328	C1266	C1195	A1130	G1064	G1003	U943	C866	C797	A730	G664	G517	G517
U1391	U1391	A1329	G1267	A1196	C1131	U1065	A1004	G944	C867	U798	G731	A665	C518	C518
G1392	G1392	U1330	C1268	A1197	C1132	C1066	A1005	G945	G868	G799	C732	G666	C519	C519
U1393	U1393	G1331	G1269	G1198	G1133	A1067	G1006	A946	C869	G800	C733	G667	A520	A520
A1394	A1394	A1332	A1269	U1199	G1134	G1068	U1007	G947	U870	U801	C736	G668	G521	G521
C1395	C1395	C1333	G1270	C1200	U1135	C1069	U1008	C948	U871	A802	C737	G669	C522	C522
G1398	G1398	G1334	A1271	A1201	C1136	U1070	U1009	A949	U872	G803	C738	G670	A523	A523
U1471	U1471	U1335	G1272	C1202	C1137	C1071	U1010	U950	A873	U804	C739	G671	G524	G524
C1399	C1399	C1336	C1273	C1203	G1138	U1072	C1011	G951	A874	C805	C740	U672	C525	C525
C1400	C1400	G1337	G1274	G1204	G1139	U1073	A1012	U952	G875	C806	G741	A602	C526	C526
G1475	G1475	A1338	C1275	G1206	C1140	G1074	G1013	G953	U876	A807	G741	A603	G527	G527
A1476	A1476	A1339	G1276	G1207	C1141	U1075	A1014	G954	C877	C808	G741	A604	C528	C528
U1477	U1477	A1340	G1278	G1208	G1142	U1076	G1015	U955	G877	C811	A747	A675	G529	G529
U1478	U1478	U1341	G1279	C1209	G1143	U1077	U1016	U956	A878	G812	G748	A676	G530	G530
C1479	C1479	A1342	A1280	G1209	G1144	U1078	A1017	U957	A879	U813	C750	U677	A608	A608
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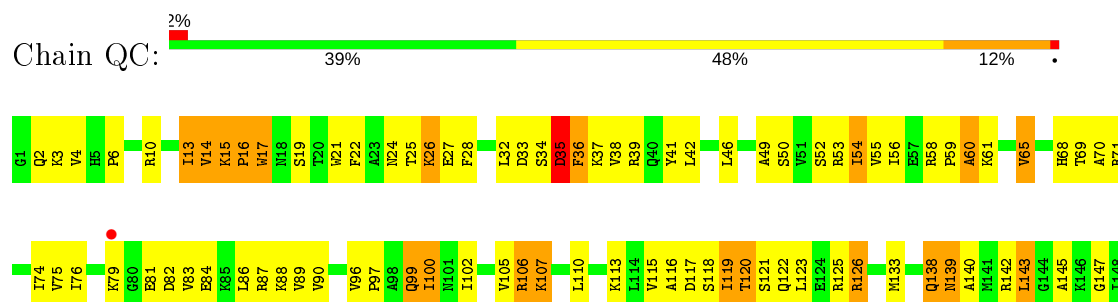
• Molecule 33: 30S ribosomal protein S2



• Molecule 33: 30S ribosomal protein S2



• Molecule 34: 30S ribosomal protein S3



K205

- Molecule 36: 30S ribosomal protein S5



E9 L10 L11 E12 K13 K14 L15 I16 A17 V17 V18 R19 R20 S21 K22 K23 K25 R28 I29 F30 L35 L36 T37 V38 R44 R45 K51 V55 P56 I59 A62 R67 R68 R69 W70 I71 I72 V73 A74 L75 N76 N77 G78 T79 L80 Q81 H82 P83 V87 H88 T89

G90 V93 F94 M95 Q96 P97 A98 S99 G101 G102 G103 I104 I105 A106 G107 G108 A109 A110 V113 L114 L115 E116 V116 A117 G118 V119 H120 H121 V122 L123 A124 K125 A126 N131 P132 I133 N134 V135 V136 R137 A138 T139 I140 D141 E144 M145 M146 N147 S148 P149 E150 M151 V152 A153 K155

R156
G157
K158

- Molecule 36: 30S ribosomal protein S5



E9 L10 L11 E12 K13 K14 L15 I16 A17 V17 V18 S21 T102 K22 K23 V24 K25 G26 T29 F30 S31 F32 T33 A34 L35 T36 V37 V38 G39 H40 D41 G41 G42 G43 R44 V45 G48 K51 E54 V55 P56 A57 A58 I59 A62 K65 A66 R67 R68 N69 W70 I71 I72 V73 A74 L75

M76 M77 G78 T79 Q81 H82 P83 V87 H88 T89 G90 S91 N95 Q96 P97 A98 S99 G101 G102 G103 I104 G107 M110 R111 A112 V113 L114 E115 V116 V119 H120 N121 V122 L123 A124 K125 A126 Y127 G128 S129 T130 N131 P132 T133 M134 V136 R137 A138 T139 L143 E144

M145 M146 N147 S148 P149 E150 M151 V152 A153 K155
G157
K158

- Molecule 37: 30S ribosomal protein S6



M1 R2 H3 Y4 I6 I7 F8 M9 H10 H11 P12 D13 Q14 S15 E16 Q17 V18 P19 T22 E23 R24 Y25 A28 I29 K35 R38 L39 E40 D41 W42 G43 Q46 L47 I51 N52 K53 L54 H55 K56 A57 H58 Y59 V60 M61 M62 M63 V64 E65 A66 P67 Q68 E69 V70

I71 D72 T77 F78 E79 F80 M81 D82 A83 V84 V85 I86 R86 S87 M88 V89 M90 R91 T92 K93 H94 T97 E98 A99 S100

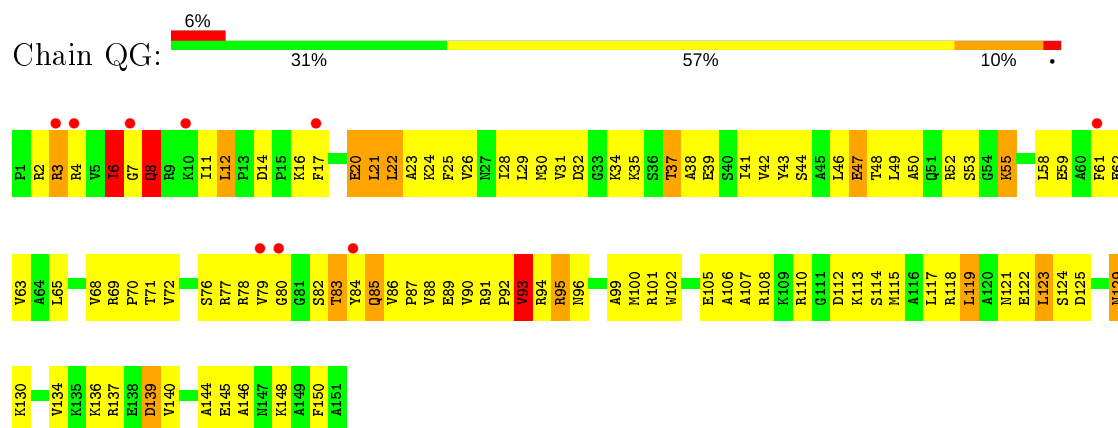
- Molecule 37: 30S ribosomal protein S6



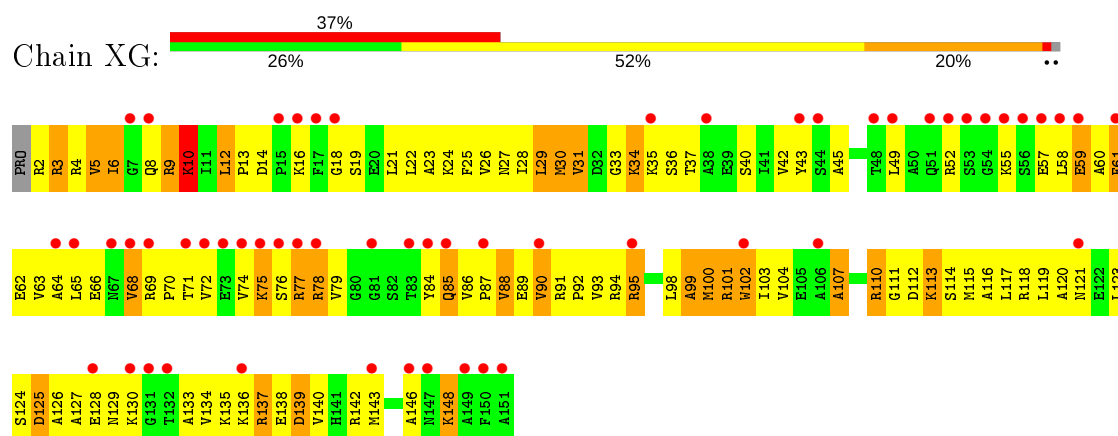
H1 R2 H3 Y4 I6 I7 F8 M9 H10 H11 P12 D13 Q14 Q17 V18 P19 T21 T22 E23 R24 Y25 A26 A27 A28 T29 T30 G31 A32 E33 G34 R38 L39 E40 D41 W42 G43 Q46 I51 N52 K53 L54 H55 K56 A57 H58 Y59 V60 M61 M62 M63 V64 E65 A66 P67 Q68 E69 V70

P67 Q68 E69 V70 I71 D72 T77 F78 E79 F80 M81 D82 A83 V84 V85 I86 R86 S87 M88 V89 M90 R91 T92 K93 H94 T97 E98 A99 S100

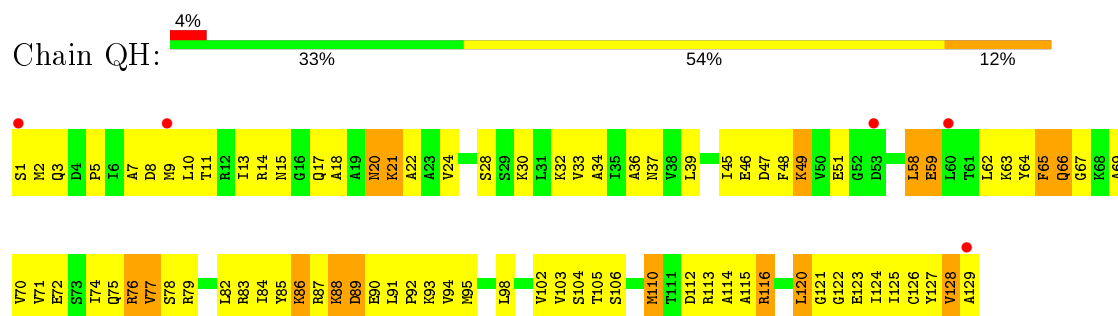
• Molecule 38: 30S ribosomal protein S7



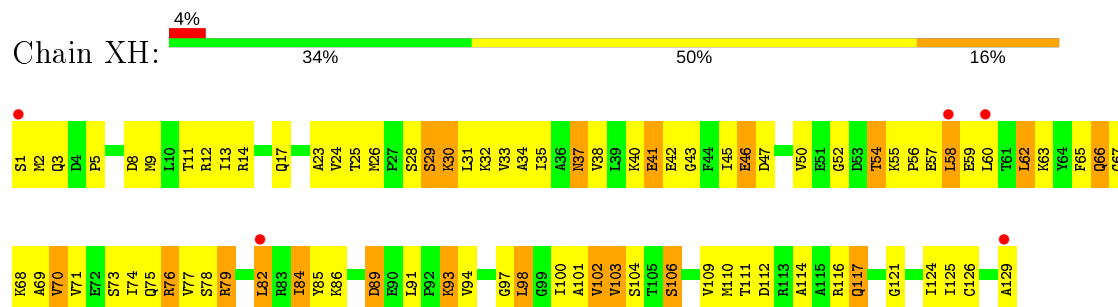
• Molecule 38: 30S ribosomal protein S7



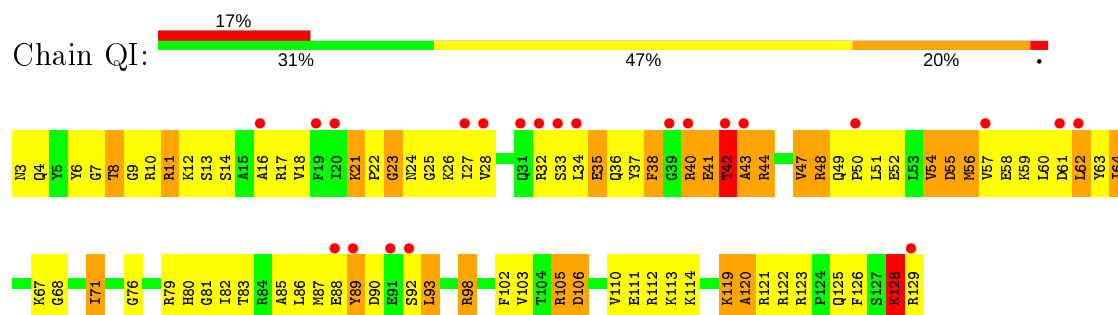
• Molecule 39: 30S ribosomal protein S8



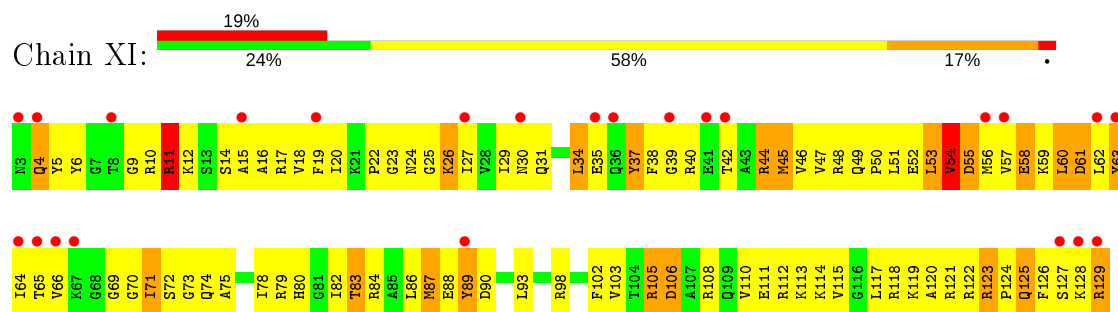
• Molecule 39: 30S ribosomal protein S8



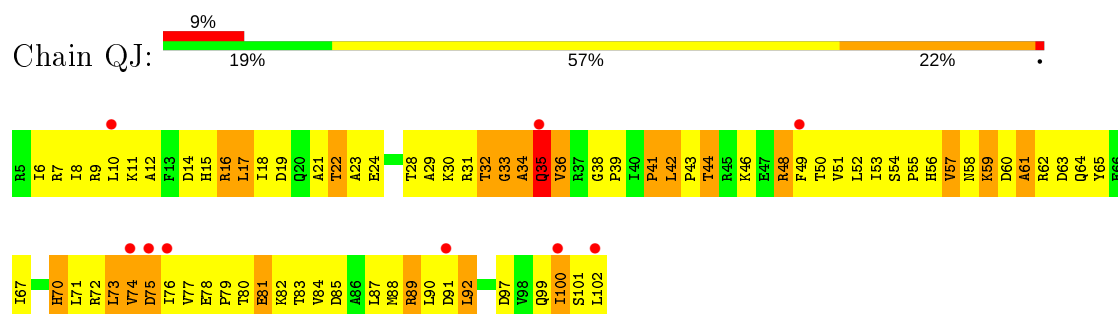
- Molecule 40: 30S ribosomal protein S9



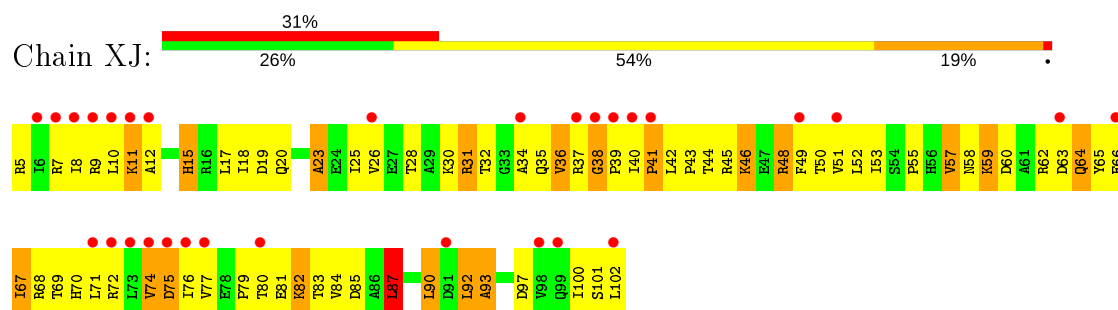
- Molecule 40: 30S ribosomal protein S9



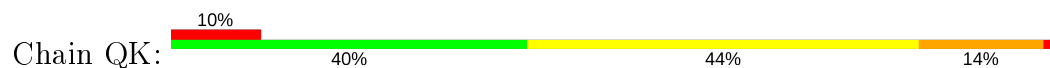
- Molecule 41: 30S ribosomal protein S10

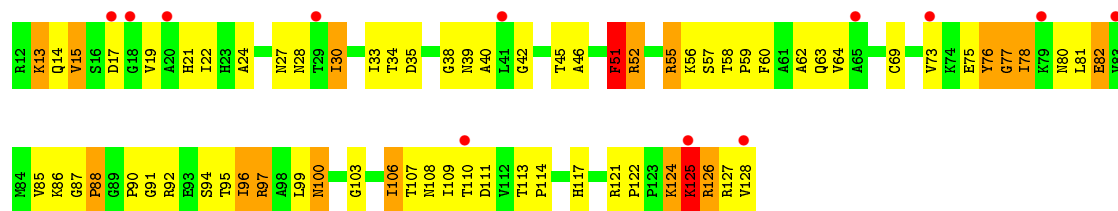


- Molecule 41: 30S ribosomal protein S10

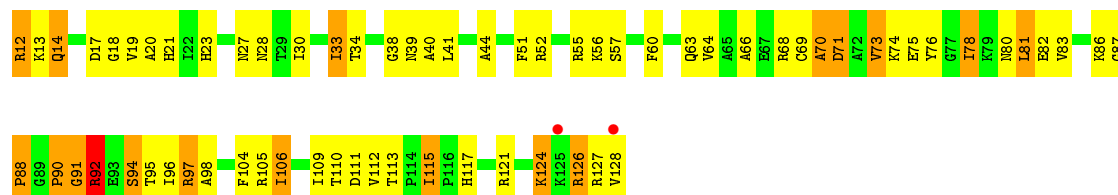
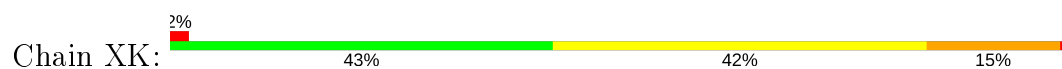


- Molecule 42: 30S ribosomal protein S11

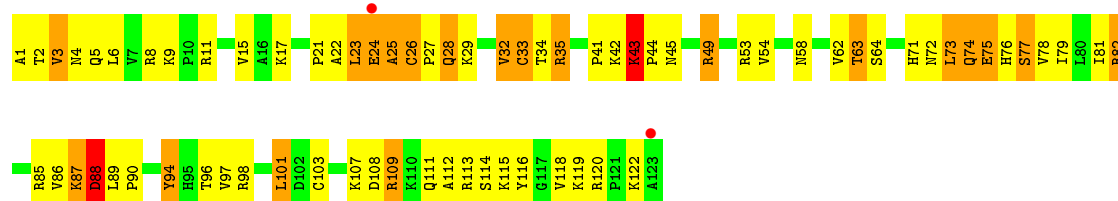




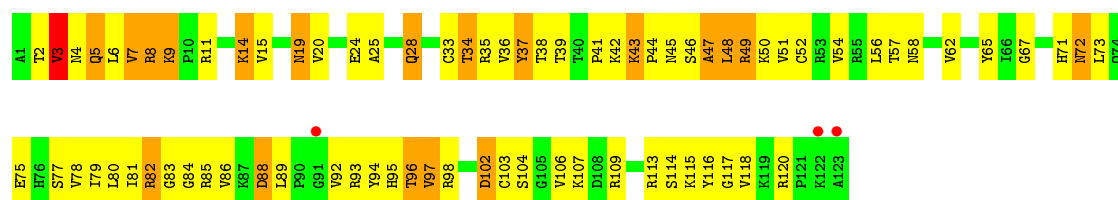
• Molecule 42: 30S ribosomal protein S11



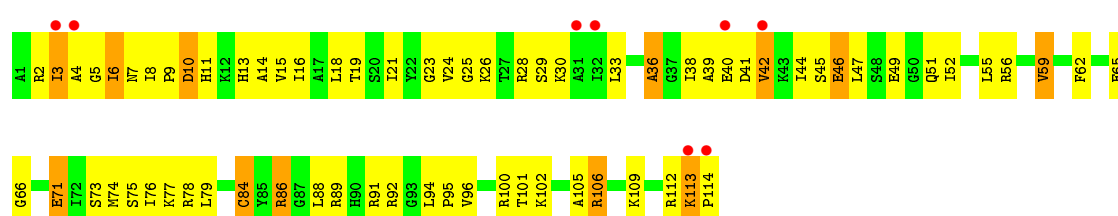
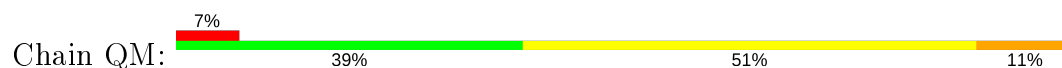
• Molecule 43: 30S ribosomal protein S12



• Molecule 43: 30S ribosomal protein S12

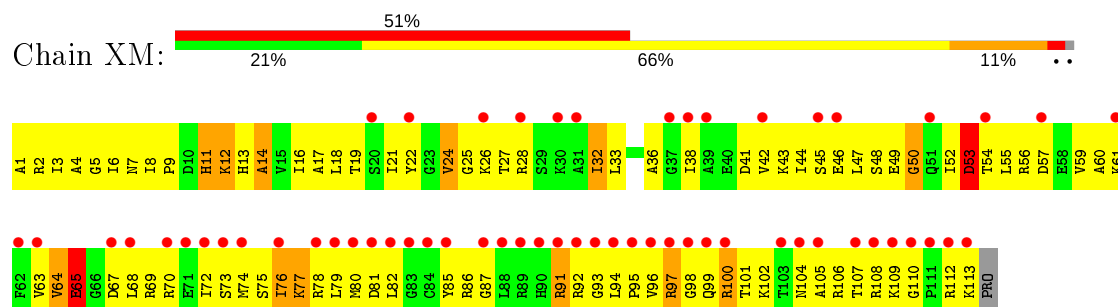


• Molecule 44: 30S ribosomal protein S13



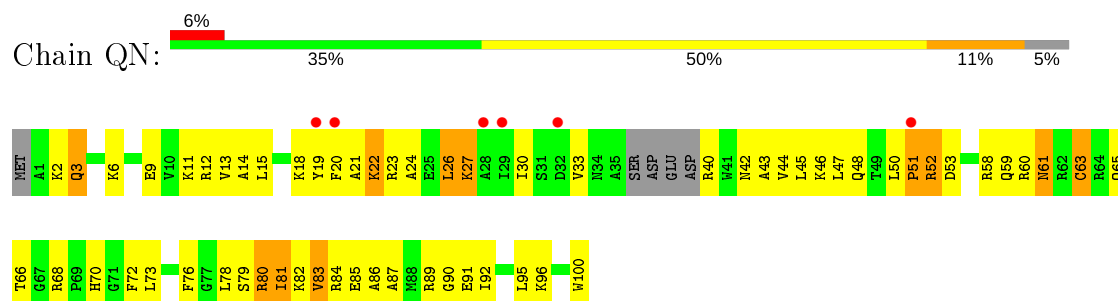
- Molecule 44: 30S ribosomal protein S13

Chain XM:



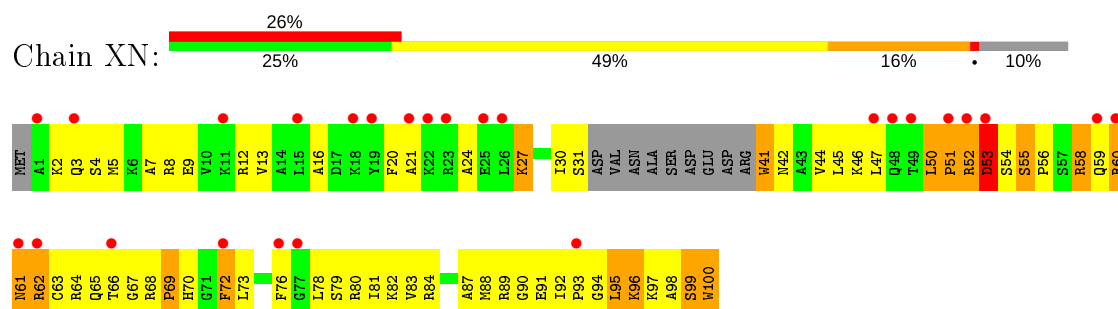
- Molecule 45: 30S ribosomal protein S14

Chain QN:



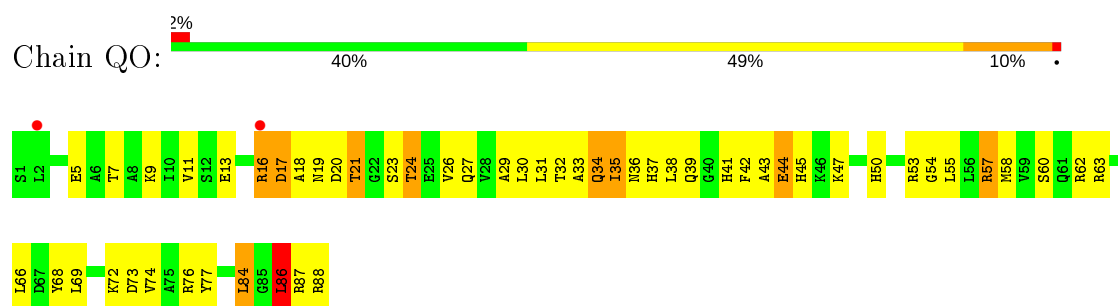
- Molecule 45: 30S ribosomal protein S14

Chain XN:



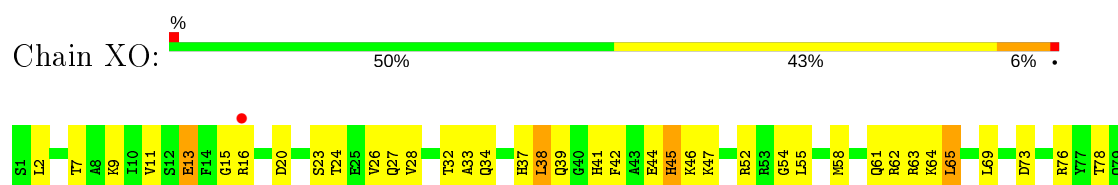
- Molecule 46: 30S ribosomal protein S15

Chain QO:



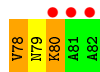
- Molecule 46: 30S ribosomal protein S15

Chain XO:

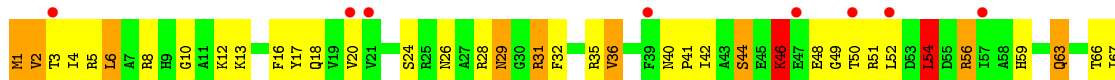




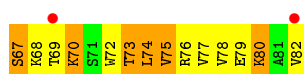
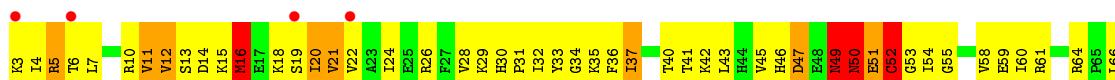
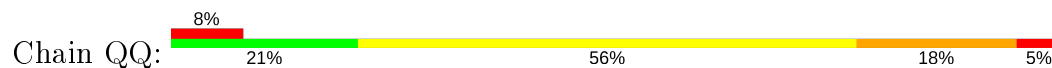
- Molecule 47: 30S ribosomal protein S16



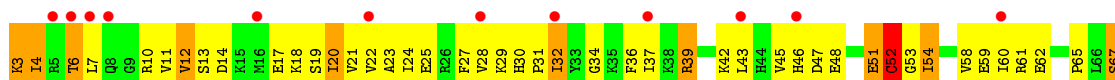
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

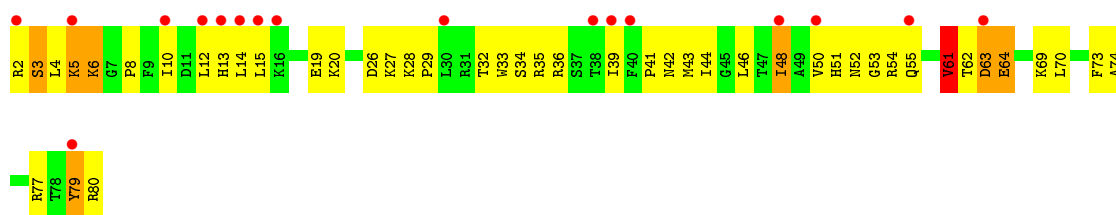




- Molecule 49: 30S ribosomal protein S18



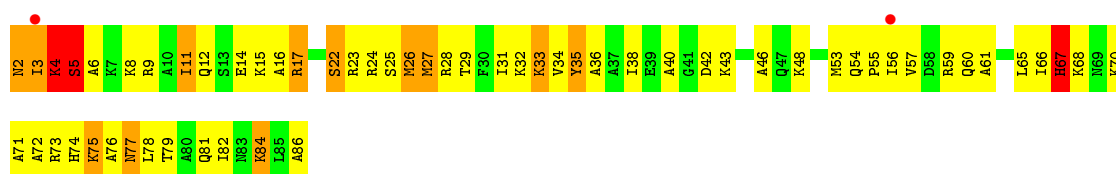
- Molecule 50: 30S ribosomal protein S19



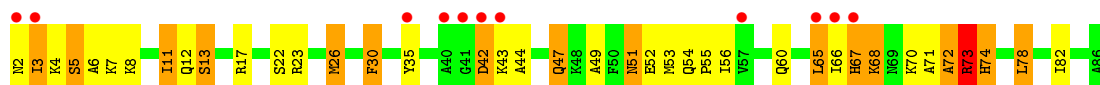
- Molecule 50: 30S ribosomal protein S19



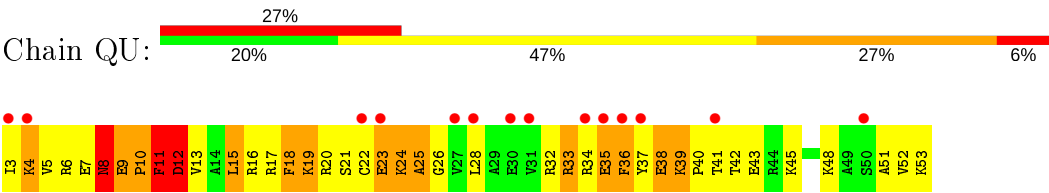
- Molecule 51: 30S ribosomal protein S20



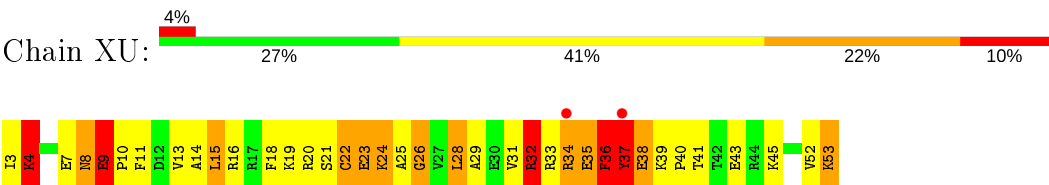
- Molecule 51: 30S ribosomal protein S20



● 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 0.210 , 0.259	Depositor DCC
R_{free} test set	19579 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 91.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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%)	0	3
3	YC	269/271 (99%)	180 (67%)	60 (22%)	29 (11%)	0	2
4	RD	207/209 (99%)	147 (71%)	31 (15%)	29 (14%)	0	1
4	YD	207/209 (99%)	128 (62%)	45 (22%)	34 (16%)	0	0
5	RE	199/201 (99%)	146 (73%)	32 (16%)	21 (11%)	0	3
5	YE	199/201 (99%)	117 (59%)	55 (28%)	27 (14%)	0	1
6	RF	175/178 (98%)	138 (79%)	22 (13%)	15 (9%)	1	4
6	YF	176/178 (99%)	102 (58%)	42 (24%)	32 (18%)	0	0
7	RG	174/176 (99%)	121 (70%)	26 (15%)	27 (16%)	0	0
7	YG	174/176 (99%)	104 (60%)	36 (21%)	34 (20%)	0	0
8	RH	147/149 (99%)	64 (44%)	49 (33%)	34 (23%)	0	0
8	YH	147/149 (99%)	73 (50%)	59 (40%)	15 (10%)	0	3
9	RI	139/141 (99%)	84 (60%)	42 (30%)	13 (9%)	0	3
9	YI	139/141 (99%)	85 (61%)	37 (27%)	17 (12%)	0	1
10	RJ	140/142 (99%)	107 (76%)	19 (14%)	14 (10%)	0	3
10	YJ	140/142 (99%)	98 (70%)	28 (20%)	14 (10%)	0	3
11	RK	120/122 (98%)	87 (72%)	16 (13%)	17 (14%)	0	1
11	YK	120/122 (98%)	83 (69%)	20 (17%)	17 (14%)	0	1
12	RL	141/143 (99%)	98 (70%)	27 (19%)	16 (11%)	0	2
12	YL	141/143 (99%)	77 (55%)	45 (32%)	19 (14%)	0	1
13	RM	134/136 (98%)	97 (72%)	22 (16%)	15 (11%)	0	2
13	YM	134/136 (98%)	92 (69%)	28 (21%)	14 (10%)	0	3
14	RN	118/120 (98%)	96 (81%)	14 (12%)	8 (7%)	1	7
14	YN	118/120 (98%)	72 (61%)	30 (25%)	16 (14%)	0	1
15	RO	114/116 (98%)	89 (78%)	17 (15%)	8 (7%)	1	7
15	YO	114/116 (98%)	74 (65%)	29 (25%)	11 (10%)	0	3
16	RP	112/114 (98%)	78 (70%)	18 (16%)	16 (14%)	0	1
16	YP	112/114 (98%)	70 (62%)	25 (22%)	17 (15%)	0	0
17	RQ	115/117 (98%)	93 (81%)	17 (15%)	5 (4%)	2	16
17	YQ	115/117 (98%)	77 (67%)	27 (24%)	11 (10%)	0	3

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

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

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

5 of 1292 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

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

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

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

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

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

Mol	Chain	Res	Type
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	-	59,64,64	2.03	14 (23%)	75,97,97	2.82	24 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	EM1	RA	3135	-	-	10/75/112/112	0/4/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	RA	3135	EM1	C76-C78	-7.12	1.37	1.48
54	RA	3135	EM1	C21-C15	-5.52	1.49	1.53
54	RA	3135	EM1	C77-C72	-4.54	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	N82-N81	-4.48	1.26	1.34

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	RA	3135	EM1	C8-C4-C2	-11.37	99.56	115.23
54	RA	3135	EM1	N82-N81-N80	9.48	114.46	107.31
54	RA	3135	EM1	C76-C77-C72	-5.96	115.50	120.66
54	RA	3135	EM1	O20-C15-C21	-5.88	117.22	123.51
54	RA	3135	EM1	C2-O5-C10	-4.91	105.41	109.29

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

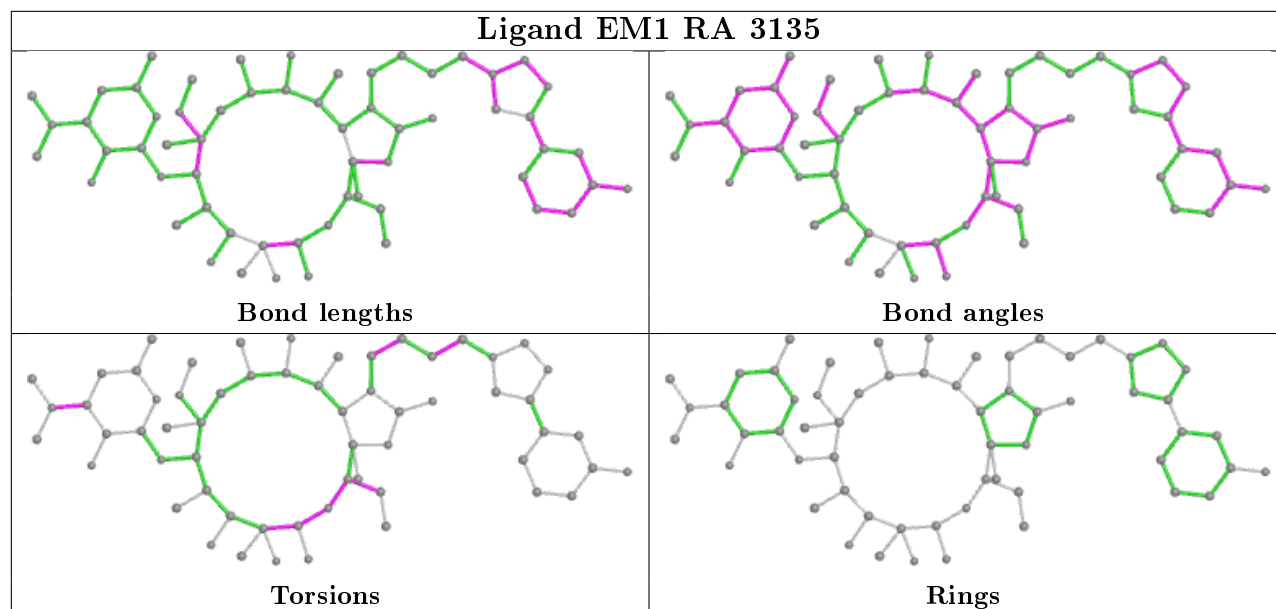
Mol	Chain	Res	Type	Atoms
54	RA	3135	EM1	O9-C4-C8-C14
54	RA	3135	EM1	C21-C15-O9-C4
54	RA	3135	EM1	O9-C15-C21-C26
54	RA	3135	EM1	O20-C15-C21-C26
54	RA	3135	EM1	O20-C15-O9-C4

There are no ring outliers.

1 monomer is involved in 4 short contacts:

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

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	RA	2854/2904 (98%)	-0.43	41 (1%) 75 56	19, 47, 175, 400	0
1	YA	2841/2904 (97%)	0.15	90 (3%) 47 25	64, 141, 260, 408	0
2	RB	118/118 (100%)	-0.63	0 100 100	32, 61, 95, 115	0
2	YB	117/118 (99%)	-0.18	0 100 100	111, 185, 242, 277	0
3	RC	271/271 (100%)	-0.25	10 (3%) 41 21	25, 57, 97, 202	0
3	YC	271/271 (100%)	0.43	19 (7%) 16 7	64, 107, 154, 181	0
4	RD	209/209 (100%)	-0.36	0 100 100	19, 41, 90, 149	0
4	YD	209/209 (100%)	0.83	26 (12%) 4 1	71, 122, 174, 236	0
5	RE	201/201 (100%)	-0.24	0 100 100	23, 58, 116, 177	0
5	YE	201/201 (100%)	1.85	76 (37%) 0 0	91, 214, 335, 378	0
6	RF	177/178 (99%)	0.22	13 (7%) 15 6	52, 93, 166, 225	0
6	YF	178/178 (100%)	2.02	80 (44%) 0 0	154, 229, 270, 299	0
7	RG	176/176 (100%)	-0.05	0 100 100	41, 75, 129, 161	0
7	YG	176/176 (100%)	1.88	64 (36%) 0 0	129, 198, 270, 312	0
8	RH	149/149 (100%)	2.56	60 (40%) 0 0	59, 178, 260, 278	0
8	YH	149/149 (100%)	2.43	63 (42%) 0 0	100, 197, 252, 272	0
9	RI	141/141 (100%)	3.30	84 (59%) 0 0	149, 241, 292, 339	0
9	YI	141/141 (100%)	4.31	102 (72%) 0 0	231, 317, 353, 360	0
10	RJ	142/142 (100%)	-0.48	1 (0%) 87 75	21, 40, 76, 139	0
10	YJ	142/142 (100%)	0.47	14 (9%) 7 2	75, 127, 168, 193	0
11	RK	122/122 (100%)	-0.36	1 (0%) 86 72	23, 45, 94, 191	0
11	YK	122/122 (100%)	0.55	12 (9%) 7 2	66, 107, 155, 228	0
12	RL	143/143 (100%)	-0.42	0 100 100	18, 55, 93, 123	0
12	YL	143/143 (100%)	1.37	40 (27%) 0 0	86, 169, 242, 284	0

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

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

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

The worst 5 of 1894 RSRZ outliers are listed below:

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

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

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

6.3 Carbohydrates ⓘ

There are no 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	YA	3062	1/1	0.69	0.55	190,190,190,190	0
53	MG	RA	3047	1/1	0.70	0.13	122,122,122,122	0
53	MG	YA	3085	1/1	0.71	0.23	158,158,158,158	0
53	MG	YA	3033	1/1	0.71	0.30	151,151,151,151	0
53	MG	RA	3129	1/1	0.71	1.07	285,285,285,285	0
53	MG	YA	3074	1/1	0.71	0.56	260,260,260,260	0
53	MG	YA	3064	1/1	0.72	0.88	256,256,256,256	0
53	MG	YA	3045	1/1	0.72	0.22	206,206,206,206	0
53	MG	YA	3097	1/1	0.72	0.21	159,159,159,159	0
53	MG	YA	3122	1/1	0.73	0.15	104,104,104,104	0
53	MG	YA	3059	1/1	0.74	0.18	232,232,232,232	0
53	MG	RA	3134	1/1	0.74	0.27	210,210,210,210	0
53	MG	XA	1619	1/1	0.74	0.12	212,212,212,212	0
53	MG	QA	1602	1/1	0.74	0.12	177,177,177,177	0
53	MG	XA	1614	1/1	0.74	0.64	236,236,236,236	0
53	MG	RA	3054	1/1	0.76	0.36	198,198,198,198	0
53	MG	YA	3008	1/1	0.77	0.24	147,147,147,147	0
53	MG	XA	1602	1/1	0.77	0.13	139,139,139,139	0
53	MG	YA	3031	1/1	0.77	0.21	80,80,80,80	0
53	MG	YA	3110	1/1	0.77	0.07	120,120,120,120	0
53	MG	XA	1634	1/1	0.78	0.13	165,165,165,165	0
53	MG	RA	3068	1/1	0.78	0.12	175,175,175,175	0
53	MG	YA	3039	1/1	0.79	0.19	105,105,105,105	0
53	MG	YA	3088	1/1	0.79	0.35	222,222,222,222	0
53	MG	YA	3083	1/1	0.79	0.10	214,214,214,214	0
53	MG	YA	3017	1/1	0.79	0.13	185,185,185,185	0
53	MG	YA	3036	1/1	0.79	0.16	205,205,205,205	0
53	MG	RA	3089	1/1	0.80	0.16	127,127,127,127	0
53	MG	XA	1610	1/1	0.80	0.13	168,168,168,168	0
53	MG	YA	3123	1/1	0.80	0.36	217,217,217,217	0
53	MG	XA	1616	1/1	0.80	0.62	195,195,195,195	0
53	MG	XA	1629	1/1	0.80	0.15	190,190,190,190	0
53	MG	RB	202	1/1	0.80	0.11	82,82,82,82	0
53	MG	YA	3050	1/1	0.80	0.16	154,154,154,154	0
53	MG	YA	3101	1/1	0.80	0.20	96,96,96,96	0
53	MG	YA	3010	1/1	0.80	1.07	272,272,272,272	0
53	MG	RA	3096	1/1	0.81	0.18	169,169,169,169	0
53	MG	RA	3069	1/1	0.81	0.24	197,197,197,197	0
53	MG	RA	3024	1/1	0.81	0.47	210,210,210,210	0
53	MG	YA	3082	1/1	0.82	0.19	164,164,164,164	0
53	MG	YA	3084	1/1	0.82	0.16	168,168,168,168	0
53	MG	XA	1620	1/1	0.82	0.19	182,182,182,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	RA	3060	1/1	0.82	0.47	236,236,236,236	0
53	MG	RA	3011	1/1	0.82	0.18	129,129,129,129	0
53	MG	RA	3086	1/1	0.82	0.09	151,151,151,151	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	XA	1635	1/1	0.83	0.11	76,76,76,76	0
53	MG	YA	3079	1/1	0.83	0.79	225,225,225,225	0
53	MG	YA	3038	1/1	0.83	0.07	234,234,234,234	0
53	MG	YA	3047	1/1	0.83	0.18	174,174,174,174	0
53	MG	YA	3007	1/1	0.83	0.45	232,232,232,232	0
53	MG	RA	3085	1/1	0.83	0.17	133,133,133,133	0
53	MG	YA	3128	1/1	0.84	0.81	163,163,163,163	0
53	MG	QA	1610	1/1	0.84	0.11	197,197,197,197	0
53	MG	RA	3090	1/1	0.84	0.17	135,135,135,135	0
53	MG	XA	1632	1/1	0.84	0.10	122,122,122,122	0
53	MG	YE	301	1/1	0.84	0.29	199,199,199,199	0
53	MG	YA	3071	1/1	0.84	0.20	102,102,102,102	0
53	MG	YA	3106	1/1	0.84	0.17	218,218,218,218	0
53	MG	RA	3020	1/1	0.85	0.37	200,200,200,200	0
53	MG	QA	1632	1/1	0.85	0.15	85,85,85,85	0
53	MG	YA	3060	1/1	0.85	0.76	235,235,235,235	0
53	MG	YA	3020	1/1	0.85	0.21	53,53,53,53	0
53	MG	YA	3098	1/1	0.85	0.21	183,183,183,183	0
53	MG	YA	3043	1/1	0.85	0.23	155,155,155,155	0
53	MG	YA	3072	1/1	0.86	0.12	183,183,183,183	0
53	MG	RA	3056	1/1	0.86	0.12	148,148,148,148	0
53	MG	YA	3004	1/1	0.86	0.17	134,134,134,134	0
53	MG	YA	3026	1/1	0.86	0.77	242,242,242,242	0
53	MG	XA	1601	1/1	0.86	0.08	106,106,106,106	0
53	MG	RA	3004	1/1	0.86	0.19	184,184,184,184	0
53	MG	QA	1630	1/1	0.86	0.14	196,196,196,196	0
53	MG	YA	3025	1/1	0.87	0.15	162,162,162,162	0
53	MG	YA	3093	1/1	0.87	0.36	188,188,188,188	0
53	MG	YA	3022	1/1	0.87	0.23	149,149,149,149	0
53	MG	QA	1641	1/1	0.87	0.16	171,171,171,171	0
53	MG	QA	1638	1/1	0.88	0.13	67,67,67,67	0
53	MG	YA	3132	1/1	0.88	0.49	240,240,240,240	0
53	MG	YA	3100	1/1	0.88	0.13	124,124,124,124	0
53	MG	RA	3070	1/1	0.89	0.34	137,137,137,137	0
53	MG	RA	3091	1/1	0.89	0.10	84,84,84,84	0
53	MG	YA	3092	1/1	0.89	0.16	169,169,169,169	0
53	MG	XA	1606	1/1	0.89	0.13	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	XA	1611	1/1	0.89	0.11	110,110,110,110	0
53	MG	YA	3001	1/1	0.89	0.15	141,141,141,141	0
53	MG	YA	3077	1/1	0.89	0.07	109,109,109,109	0
53	MG	YA	3070	1/1	0.89	0.13	91,91,91,91	0
53	MG	RA	3103	1/1	0.89	0.15	30,30,30,30	0
53	MG	YA	3027	1/1	0.89	0.23	194,194,194,194	0
53	MG	RA	3131	1/1	0.89	0.60	187,187,187,187	0
53	MG	RA	3035	1/1	0.89	0.33	189,189,189,189	0
53	MG	YA	3015	1/1	0.89	0.19	219,219,219,219	0
53	MG	XA	1638	1/1	0.89	0.15	204,204,204,204	0
53	MG	QA	1624	1/1	0.89	0.14	143,143,143,143	0
53	MG	YA	3058	1/1	0.90	0.39	249,249,249,249	0
53	MG	XA	1618	1/1	0.90	0.11	136,136,136,136	0
53	MG	RA	3130	1/1	0.90	0.24	118,118,118,118	0
53	MG	QA	1605	1/1	0.90	0.18	72,72,72,72	0
53	MG	YA	3054	1/1	0.90	0.12	86,86,86,86	0
53	MG	QA	1625	1/1	0.90	0.14	101,101,101,101	0
53	MG	RA	3055	1/1	0.90	0.33	252,252,252,252	0
53	MG	YA	3114	1/1	0.90	0.12	182,182,182,182	0
53	MG	YA	3080	1/1	0.90	0.18	154,154,154,154	0
53	MG	XA	1623	1/1	0.90	0.11	108,108,108,108	0
53	MG	RA	3003	1/1	0.90	0.14	77,77,77,77	0
53	MG	YA	3042	1/1	0.90	0.17	81,81,81,81	0
53	MG	YA	3030	1/1	0.91	0.13	130,130,130,130	0
53	MG	RA	3014	1/1	0.91	0.18	38,38,38,38	0
53	MG	YA	3069	1/1	0.91	0.23	267,267,267,267	0
53	MG	RA	3051	1/1	0.91	0.16	70,70,70,70	0
53	MG	YA	3094	1/1	0.91	0.14	145,145,145,145	0
53	MG	YA	3029	1/1	0.91	0.21	178,178,178,178	0
53	MG	QA	1643	1/1	0.91	0.11	67,67,67,67	0
53	MG	XA	1628	1/1	0.91	0.44	224,224,224,224	0
53	MG	XA	1615	1/1	0.91	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	3089	1/1	0.91	0.21	101,101,101,101	0
53	MG	YA	3104	1/1	0.91	0.22	52,52,52,52	0
53	MG	YA	3011	1/1	0.91	0.21	150,150,150,150	0
53	MG	YA	3111	1/1	0.91	0.14	202,202,202,202	0
53	MG	YA	3096	1/1	0.91	0.14	127,127,127,127	0
53	MG	YA	3126	1/1	0.91	0.19	120,120,120,120	0
53	MG	YA	3034	1/1	0.91	0.09	88,88,88,88	0
53	MG	YA	3115	1/1	0.92	0.26	176,176,176,176	0
53	MG	XA	1627	1/1	0.92	0.23	197,197,197,197	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	YA	3116	1/1	0.92	0.12	84,84,84,84	0
53	MG	YA	3021	1/1	0.92	0.28	183,183,183,183	0
53	MG	RA	3119	1/1	0.92	0.08	56,56,56,56	0
53	MG	XA	1640	1/1	0.92	0.17	137,137,137,137	0
53	MG	RA	3110	1/1	0.92	0.15	84,84,84,84	0
53	MG	QA	1640	1/1	0.92	0.05	79,79,79,79	0
53	MG	YA	3013	1/1	0.92	0.39	241,241,241,241	0
53	MG	QA	1609	1/1	0.92	0.08	77,77,77,77	0
53	MG	YA	3044	1/1	0.92	0.15	87,87,87,87	0
53	MG	RA	3100	1/1	0.92	0.27	119,119,119,119	0
53	MG	YA	3124	1/1	0.92	0.16	82,82,82,82	0
53	MG	YA	3081	1/1	0.92	0.10	83,83,83,83	0
53	MG	XA	1625	1/1	0.92	0.23	111,111,111,111	0
53	MG	YA	3016	1/1	0.92	0.10	60,60,60,60	0
53	MG	QA	1616	1/1	0.92	0.18	98,98,98,98	0
53	MG	QA	1606	1/1	0.92	0.13	80,80,80,80	0
53	MG	YA	3051	1/1	0.92	0.14	88,88,88,88	0
53	MG	YA	3103	1/1	0.92	0.13	86,86,86,86	0
53	MG	RA	3031	1/1	0.93	0.14	37,37,37,37	0
53	MG	QA	1621	1/1	0.93	0.13	131,131,131,131	0
54	EM1	RA	3135	60/60	0.93	0.26	0,23,85,88	0
53	MG	XA	1604	1/1	0.93	0.10	96,96,96,96	0
53	MG	RA	3117	1/1	0.93	0.16	162,162,162,162	0
53	MG	RA	3050	1/1	0.93	0.18	39,39,39,39	0
53	MG	RA	3046	1/1	0.93	0.08	176,176,176,176	0
53	MG	YA	3067	1/1	0.93	0.11	72,72,72,72	0
53	MG	YA	3035	1/1	0.93	0.09	90,90,90,90	0
53	MG	XA	1612	1/1	0.93	0.19	125,125,125,125	0
53	MG	RA	3113	1/1	0.93	0.14	190,190,190,190	0
53	MG	XA	1642	1/1	0.93	0.10	139,139,139,139	0
53	MG	RA	3083	1/1	0.93	0.16	53,53,53,53	0
53	MG	RB	203	1/1	0.93	0.12	58,58,58,58	0
53	MG	QA	1636	1/1	0.93	0.37	218,218,218,218	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
53	MG	RA	3018	1/1	0.94	0.34	32,32,32,32	0
53	MG	YA	3118	1/1	0.94	0.17	100,100,100,100	0
53	MG	RA	3072	1/1	0.94	0.05	61,61,61,61	0
53	MG	RA	3118	1/1	0.94	0.15	48,48,48,48	0
53	MG	QA	1607	1/1	0.94	0.13	136,136,136,136	0
53	MG	RA	3133	1/1	0.94	0.28	116,116,116,116	0
53	MG	XA	1637	1/1	0.94	0.13	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	YA	3040	1/1	0.94	0.17	72,72,72,72	0
53	MG	RA	3061	1/1	0.94	0.12	18,18,18,18	0
53	MG	RA	3017	1/1	0.94	0.09	57,57,57,57	0
53	MG	YA	3113	1/1	0.94	0.07	128,128,128,128	0
53	MG	RA	3122	1/1	0.94	0.70	164,164,164,164	0
53	MG	RA	3045	1/1	0.94	0.14	25,25,25,25	0
53	MG	QA	1618	1/1	0.94	0.12	78,78,78,78	0
53	MG	RA	3057	1/1	0.94	0.08	71,71,71,71	0
53	MG	RA	3001	1/1	0.94	0.09	98,98,98,98	0
53	MG	QA	1634	1/1	0.94	0.15	94,94,94,94	0
53	MG	YA	3119	1/1	0.94	0.12	60,60,60,60	0
53	MG	XA	1613	1/1	0.94	0.17	147,147,147,147	0
53	MG	XA	1639	1/1	0.94	0.05	159,159,159,159	0
53	MG	QA	1635	1/1	0.95	0.10	87,87,87,87	0
53	MG	RA	3121	1/1	0.95	0.17	45,45,45,45	0
53	MG	RA	3041	1/1	0.95	0.14	38,38,38,38	0
53	MG	QA	1613	1/1	0.95	0.07	76,76,76,76	0
53	MG	RA	3088	1/1	0.95	0.08	59,59,59,59	0
53	MG	YA	3066	1/1	0.95	0.17	105,105,105,105	0
53	MG	RA	3030	1/1	0.95	0.11	56,56,56,56	0
53	MG	YA	3112	1/1	0.95	0.09	79,79,79,79	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	YA	3107	1/1	0.95	0.20	91,91,91,91	0
53	MG	YA	3037	1/1	0.95	0.13	81,81,81,81	0
53	MG	YA	3086	1/1	0.95	0.13	109,109,109,109	0
53	MG	YA	3048	1/1	0.95	0.10	103,103,103,103	0
53	MG	QA	1629	1/1	0.95	0.06	97,97,97,97	0
53	MG	RA	3084	1/1	0.95	0.15	26,26,26,26	0
53	MG	YA	3131	1/1	0.95	0.14	94,94,94,94	0
53	MG	YA	3075	1/1	0.95	0.54	209,209,209,209	0
53	MG	RA	3002	1/1	0.95	0.10	75,75,75,75	0
53	MG	YA	3065	1/1	0.95	0.13	88,88,88,88	0
53	MG	YA	3134	1/1	0.95	0.33	201,201,201,201	0
53	MG	XA	1621	1/1	0.95	0.13	57,57,57,57	0
53	MG	XA	1607	1/1	0.95	0.13	167,167,167,167	0
53	MG	XA	1631	1/1	0.95	0.23	82,82,82,82	0
53	MG	RA	3052	1/1	0.95	0.14	34,34,34,34	0
53	MG	YA	3018	1/1	0.95	0.10	185,185,185,185	0
53	MG	QA	1604	1/1	0.96	0.04	139,139,139,139	0
53	MG	YA	3056	1/1	0.96	0.07	85,85,85,85	0
53	MG	RA	3065	1/1	0.96	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	RA	3048	1/1	0.96	0.17	25,25,25,25	0
53	MG	XA	1633	1/1	0.96	0.10	79,79,79,79	0
53	MG	YA	3095	1/1	0.96	0.15	138,138,138,138	0
53	MG	RB	204	1/1	0.96	0.14	45,45,45,45	0
53	MG	QA	1628	1/1	0.96	0.24	142,142,142,142	0
53	MG	RA	3099	1/1	0.96	0.19	34,34,34,34	0
53	MG	RA	3105	1/1	0.96	0.21	66,66,66,66	0
53	MG	YA	3053	1/1	0.96	0.18	127,127,127,127	0
53	MG	RA	3028	1/1	0.96	0.14	92,92,92,92	0
53	MG	YA	3012	1/1	0.96	0.09	72,72,72,72	0
53	MG	RA	3049	1/1	0.96	0.14	76,76,76,76	0
53	MG	YA	3099	1/1	0.96	0.17	188,188,188,188	0
53	MG	RA	3095	1/1	0.96	0.16	139,139,139,139	0
53	MG	QA	1622	1/1	0.96	0.17	54,54,54,54	0
55	ZN	Y4	101	1/1	0.96	0.07	169,169,169,169	0
53	MG	RA	3120	1/1	0.96	0.31	45,45,45,45	0
53	MG	QA	1608	1/1	0.96	0.26	61,61,61,61	0
53	MG	RA	3008	1/1	0.96	0.14	45,45,45,45	0
53	MG	YA	3102	1/1	0.96	0.10	118,118,118,118	0
53	MG	XA	1630	1/1	0.96	0.16	160,160,160,160	0
53	MG	QA	1623	1/1	0.96	0.11	77,77,77,77	0
53	MG	RA	3116	1/1	0.96	0.10	72,72,72,72	0
53	MG	RA	3005	1/1	0.96	0.12	74,74,74,74	0
53	MG	RA	3029	1/1	0.96	0.19	14,14,14,14	0
53	MG	RA	3059	1/1	0.96	0.43	207,207,207,207	0
53	MG	QA	1631	1/1	0.96	0.19	228,228,228,228	0
53	MG	RA	3074	1/1	0.96	0.10	93,93,93,93	0
53	MG	RA	3112	1/1	0.96	0.10	49,49,49,49	0
53	MG	RA	3075	1/1	0.96	0.05	43,43,43,43	0
53	MG	RA	3124	1/1	0.97	0.20	63,63,63,63	0
53	MG	QA	1642	1/1	0.97	0.13	79,79,79,79	0
53	MG	RA	3132	1/1	0.97	0.12	20,20,20,20	0
53	MG	QA	1611	1/1	0.97	0.14	57,57,57,57	0
53	MG	YB	201	1/1	0.97	0.09	111,111,111,111	0
53	MG	RA	3037	1/1	0.97	0.14	30,30,30,30	0
53	MG	RA	3036	1/1	0.97	0.18	23,23,23,23	0
53	MG	YA	3105	1/1	0.97	0.19	97,97,97,97	0
53	MG	RA	3080	1/1	0.97	0.07	60,60,60,60	0
53	MG	RA	3063	1/1	0.97	0.13	26,26,26,26	0
53	MG	RA	3010	1/1	0.97	0.12	31,31,31,31	0
53	MG	RA	3109	1/1	0.97	0.16	46,46,46,46	0
53	MG	YA	3046	1/1	0.97	0.22	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	RA	3108	1/1	0.97	0.13	95,95,95,95	0
53	MG	QA	1639	1/1	0.97	0.18	118,118,118,118	0
53	MG	RA	3077	1/1	0.97	0.10	63,63,63,63	0
53	MG	RA	3114	1/1	0.97	0.19	28,28,28,28	0
53	MG	RA	3067	1/1	0.97	0.14	28,28,28,28	0
53	MG	XA	1609	1/1	0.97	0.15	98,98,98,98	0
53	MG	QA	1620	1/1	0.97	0.08	116,116,116,116	0
53	MG	QA	1612	1/1	0.97	0.18	113,113,113,113	0
53	MG	XA	1603	1/1	0.97	0.09	136,136,136,136	0
53	MG	RA	3097	1/1	0.97	0.13	54,54,54,54	0
53	MG	XA	1605	1/1	0.97	0.19	54,54,54,54	0
53	MG	RA	3012	1/1	0.97	0.12	20,20,20,20	0
53	MG	YA	3061	1/1	0.97	0.14	110,110,110,110	0
53	MG	RA	3016	1/1	0.97	0.11	22,22,22,22	0
53	MG	RA	3064	1/1	0.97	0.14	28,28,28,28	0
53	MG	RA	3127	1/1	0.97	0.09	8,8,8,8	0
53	MG	YA	3024	1/1	0.97	0.15	102,102,102,102	0
53	MG	RA	3019	1/1	0.97	0.06	34,34,34,34	0
53	MG	YA	3117	1/1	0.97	0.17	73,73,73,73	0
53	MG	RA	3007	1/1	0.97	0.13	112,112,112,112	0
53	MG	RA	3073	1/1	0.97	0.24	43,43,43,43	0
53	MG	RA	3079	1/1	0.97	0.15	32,32,32,32	0
53	MG	RA	3098	1/1	0.97	0.07	49,49,49,49	0
53	MG	YA	3121	1/1	0.97	0.17	168,168,168,168	0
53	MG	RA	3025	1/1	0.97	0.06	40,40,40,40	0
53	MG	RA	3053	1/1	0.97	0.17	55,55,55,55	0
53	MG	RA	3101	1/1	0.97	0.11	48,48,48,48	0
53	MG	RA	3126	1/1	0.97	0.14	40,40,40,40	0
53	MG	RA	3006	1/1	0.97	0.13	54,54,54,54	0
53	MG	QA	1614	1/1	0.97	0.15	159,159,159,159	0
53	MG	RA	3081	1/1	0.97	0.17	99,99,99,99	0
53	MG	RA	3107	1/1	0.98	0.22	17,17,17,17	0
53	MG	RA	3027	1/1	0.98	0.12	33,33,33,33	0
53	MG	QA	1601	1/1	0.98	0.07	94,94,94,94	0
53	MG	RA	3111	1/1	0.98	0.15	31,31,31,31	0
53	MG	RA	3009	1/1	0.98	0.14	38,38,38,38	0
53	MG	QA	1633	1/1	0.98	0.12	70,70,70,70	0
53	MG	RA	3032	1/1	0.98	0.14	23,23,23,23	0
53	MG	RA	3115	1/1	0.98	0.07	22,22,22,22	0
53	MG	YA	3068	1/1	0.98	0.07	98,98,98,98	0
53	MG	XA	1626	1/1	0.98	0.24	20,20,20,20	0
53	MG	RA	3040	1/1	0.98	0.13	47,47,47,47	0

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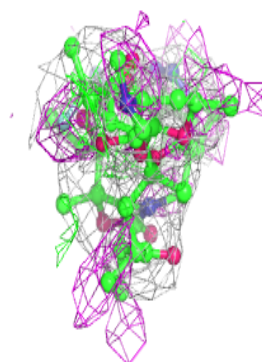
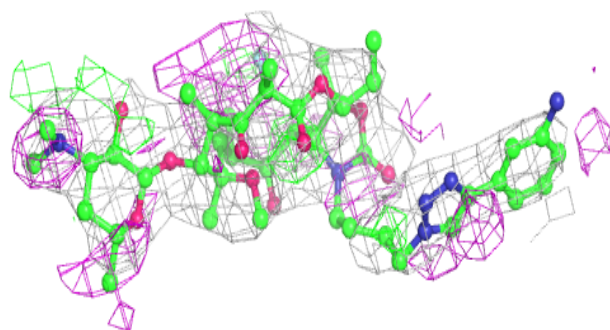
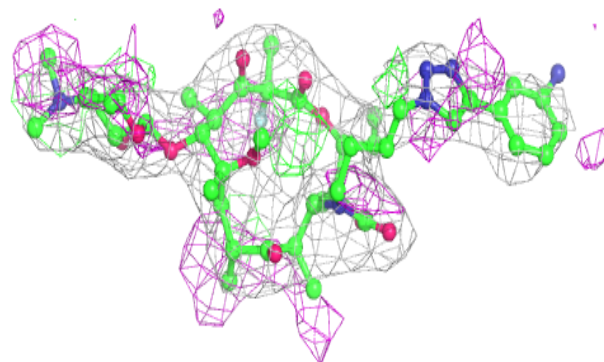
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
53	MG	RA	3136	1/1	0.98	0.07	61,61,61,61	0
53	MG	RA	3106	1/1	0.98	0.19	13,13,13,13	0
53	MG	YA	3014	1/1	0.98	0.20	113,113,113,113	0
53	MG	RA	3087	1/1	0.98	0.08	47,47,47,47	0
53	MG	QA	1603	1/1	0.98	0.09	65,65,65,65	0
53	MG	QA	1617	1/1	0.98	0.17	129,129,129,129	0
53	MG	RA	3104	1/1	0.98	0.17	23,23,23,23	0
53	MG	RA	3033	1/1	0.98	0.15	159,159,159,159	0
53	MG	XA	1641	1/1	0.98	0.15	116,116,116,116	0
53	MG	RA	3039	1/1	0.98	0.24	7,7,7,7	0
53	MG	RA	3094	1/1	0.98	0.10	32,32,32,32	0
53	MG	RA	3125	1/1	0.98	0.14	40,40,40,40	0
53	MG	RA	3015	1/1	0.98	0.06	65,65,65,65	0
53	MG	RA	3066	1/1	0.98	0.16	32,32,32,32	0
53	MG	RA	3102	1/1	0.98	0.17	24,24,24,24	0
53	MG	RA	3078	1/1	0.98	0.13	58,58,58,58	0
53	MG	RA	3042	1/1	0.98	0.07	60,60,60,60	0
53	MG	RA	3038	1/1	0.98	0.17	19,19,19,19	0
53	MG	RA	3026	1/1	0.98	0.17	143,143,143,143	0
53	MG	YA	3090	1/1	0.98	0.10	112,112,112,112	0
53	MG	YA	3052	1/1	0.98	0.07	72,72,72,72	0
53	MG	YA	3055	1/1	0.98	0.16	103,103,103,103	0
53	MG	XA	1608	1/1	0.98	0.27	46,46,46,46	0
53	MG	RA	3022	1/1	0.98	0.12	27,27,27,27	0
53	MG	RA	3123	1/1	0.98	0.11	24,24,24,24	0
53	MG	QA	1615	1/1	0.98	0.11	152,152,152,152	0
53	MG	RA	3093	1/1	0.98	0.08	45,45,45,45	0
53	MG	RA	3044	1/1	0.98	0.14	34,34,34,34	0
53	MG	RA	3128	1/1	0.99	0.16	33,33,33,33	0
53	MG	RA	3021	1/1	0.99	0.12	24,24,24,24	0
53	MG	QA	1626	1/1	0.99	0.20	29,29,29,29	0
53	MG	RA	3043	1/1	0.99	0.26	11,11,11,11	0
53	MG	RA	3023	1/1	0.99	0.12	22,22,22,22	0
53	MG	RA	3034	1/1	0.99	0.10	11,11,11,11	0
55	ZN	R4	101	1/1	0.99	0.10	108,108,108,108	0
53	MG	RA	3013	1/1	0.99	0.16	18,18,18,18	0
53	MG	RA	3076	1/1	0.99	0.07	107,107,107,107	0
53	MG	RA	3092	1/1	0.99	0.09	68,68,68,68	0
53	MG	RA	3062	1/1	1.00	0.15	19,19,19,19	0

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

orientation to approximate a three-dimensional view.

Electron density around EM1 RA 3135:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.