



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 04:20 pm BST

PDB ID : 4V4G  
Title : Crystal structure of five 70s ribosomes from Escherichia Coli in complex with protein Y.  
Authors : Vila-Sanjurjo, A.; Schuwirth, B.S.; Hau, C.W.; Cate, J.H.  
Deposited on : 2004-10-06  
Resolution : 11.50 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](mailto: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.

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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
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

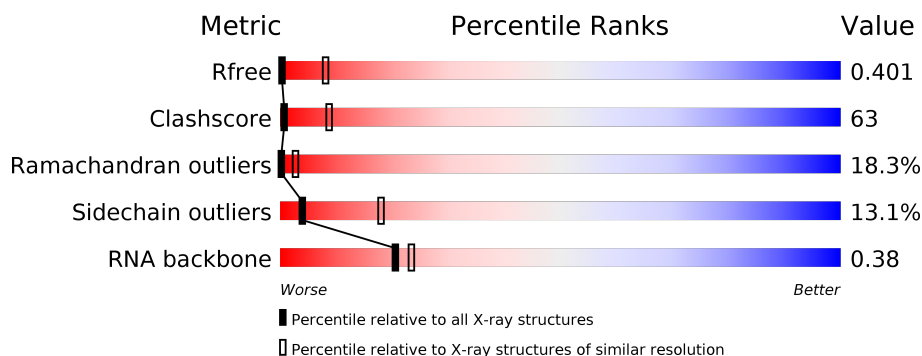
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 11.50 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.






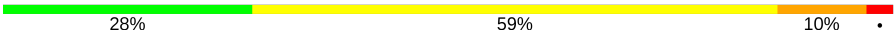
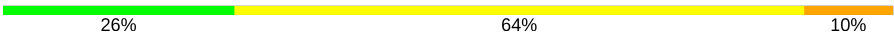
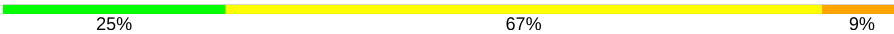
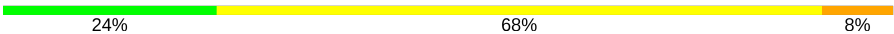
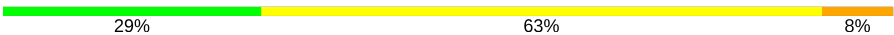
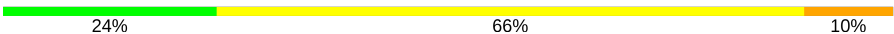
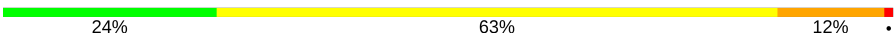
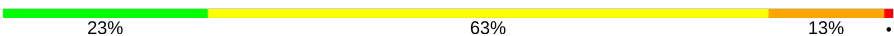
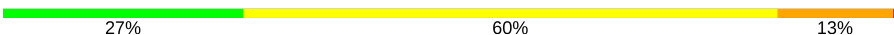
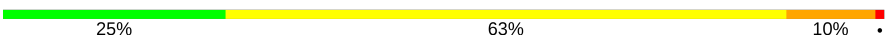












Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1005 (11.50-3.90)
Clashscore	141614	1071 (15.00-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RNA backbone	3102	1079 (11.50-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	AA	1526	20% 61% 19% .
1	CA	1526	20% 60% 19%
1	EA	1526	20% 60% 19%
1	GA	1526	20% 61% 19% .
1	IA	1526	20% 60% 19%
2	AB	234	29% 59% 10% .



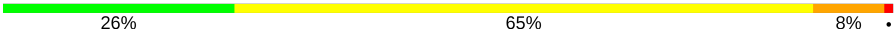
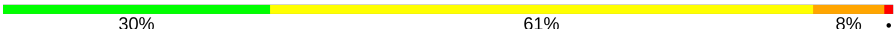
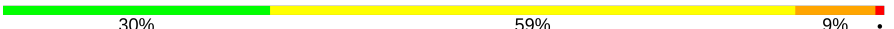
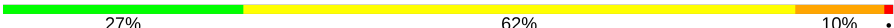
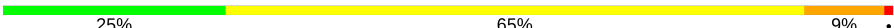


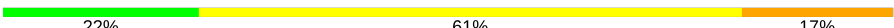
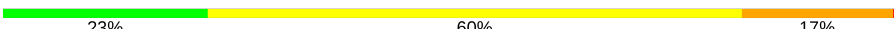
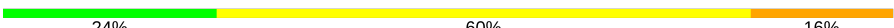

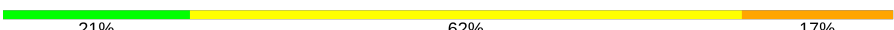

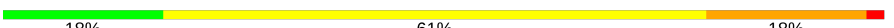
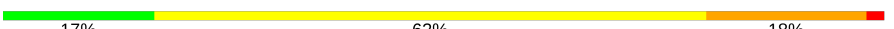
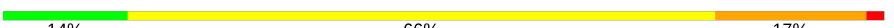
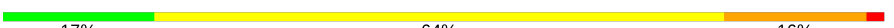
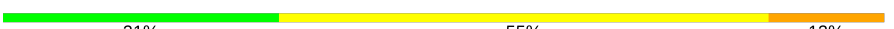
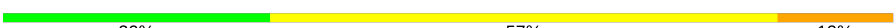

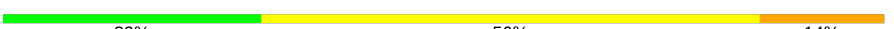


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Mol	Chain	Length	Quality of chain
2	CB	234	
2	EB	234	
2	GB	234	
2	IB	234	
3	AC	206	
3	CC	206	
3	EC	206	
3	GC	206	
3	IC	206	
4	AD	208	
4	CD	208	
4	ED	208	
4	GD	208	
4	ID	208	
5	AE	150	
5	CE	150	
5	EE	150	
5	GE	150	
5	IE	150	
6	AF	101	
6	CF	101	
6	EF	101	
6	GF	101	
6	IF	101	
7	AG	155	

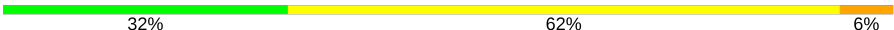

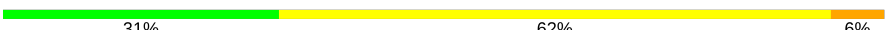
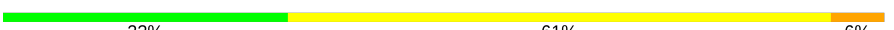
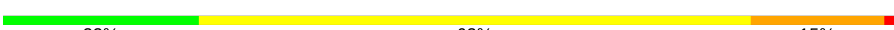
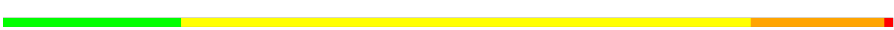


















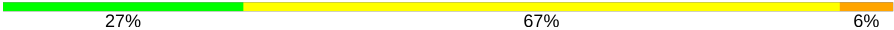
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Mol	Chain	Length	Quality of chain
7	CG	155	
7	EG	155	
7	GG	155	
7	IG	155	
8	AH	138	
8	CH	138	
8	EH	138	
8	GH	138	
8	IH	138	
9	AI	127	
9	CI	127	
9	EI	127	
9	GI	127	
9	II	127	
10	AJ	98	
10	CJ	98	
10	EJ	98	
10	GJ	98	
10	IJ	98	
11	AK	119	
11	CK	119	
11	EK	119	
11	GK	119	
11	IK	119	
12	AL	124	

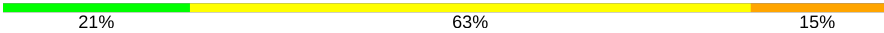
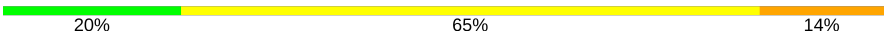
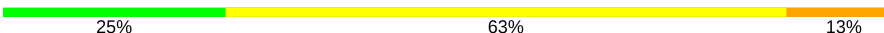


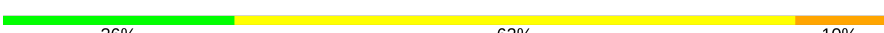
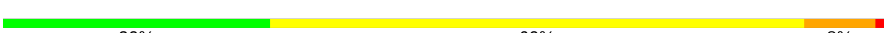




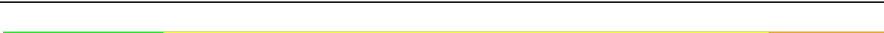


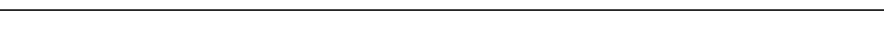




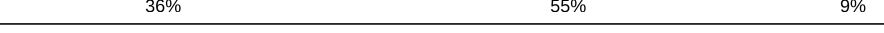





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Mol	Chain	Length	Quality of chain
12	CL	124	
12	EL	124	
12	GL	124	
12	IL	124	
13	AM	125	
13	CM	125	
13	EM	125	
13	GM	125	
13	IM	125	
14	AN	60	
14	CN	60	
14	EN	60	
14	GN	60	
14	IN	60	
15	AO	88	
15	CO	88	
15	EO	88	
15	GO	88	
15	IO	88	
16	AP	83	
16	CP	83	
16	EP	83	
16	GP	83	
16	IP	83	
17	AQ	104	

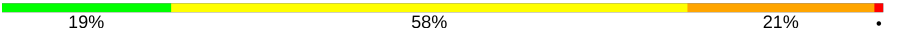
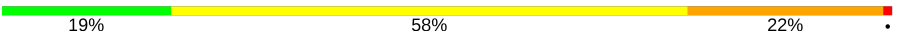
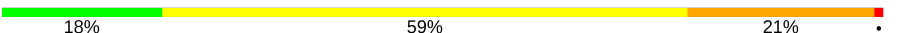
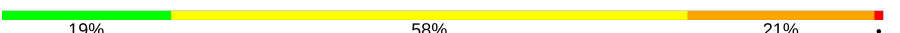
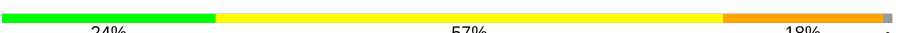
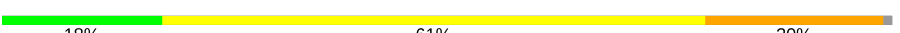
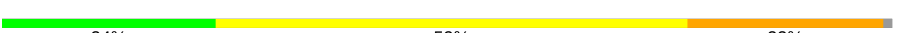




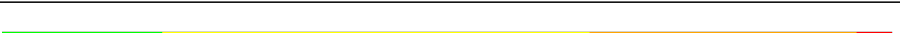


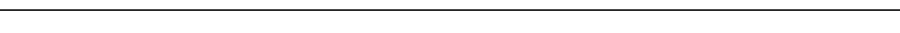
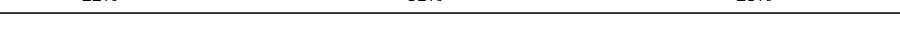
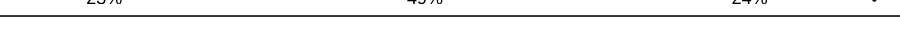
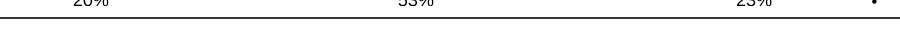
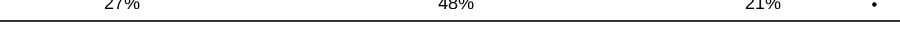
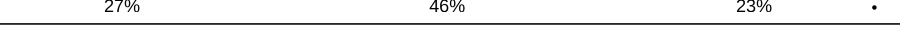

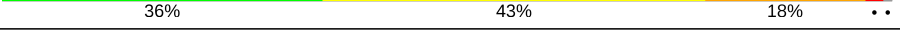


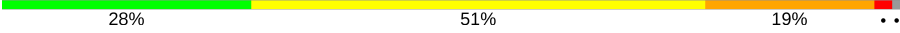
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Mol	Chain	Length	Quality of chain
17	CQ	104	
17	EQ	104	
17	GQ	104	
17	IQ	104	
18	AR	73	
18	CR	73	
18	ER	73	
18	GR	73	
18	IR	73	
19	AS	80	
19	CS	80	
19	ES	80	
19	GS	80	
19	IS	80	
20	AT	99	
20	CT	99	
20	ET	99	
20	GT	99	
20	IT	99	
21	Aa	90	
21	Ca	90	
21	Ea	90	
21	Ga	90	
21	Ia	90	
22	BB	2825	

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Mol	Chain	Length	Quality of chain
22	DB	2825	 19% 58% 21% .
22	FB	2825	 19% 58% 22% .
22	HB	2825	 18% 59% 21% .
22	JB	2825	 19% 58% 21% .
23	BA	119	 24% 57% 18% .
23	DA	119	 18% 61% 20% .
23	FA	119	 24% 53% 22% .
23	HA	119	 24% 56% 18% .
23	JA	119	 27% 50% 22% .
24	BD	270	 20% 46% 30% .
24	DD	270	 18% 50% 28% .
24	FD	270	 18% 48% 30% .
24	HD	270	 20% 47% 28% .
24	JD	270	 19% 47% 30% .
25	BE	205	 22% 51% 23% .
25	DE	205	 23% 49% 24% .
25	FE	205	 20% 53% 23% .
25	HE	205	 27% 48% 21% .
25	JE	205	 27% 46% 23% .
26	BF	198	 36% 43% 19% ..
26	DF	198	 36% 43% 18% ..
26	FF	198	 30% 49% 19% ..
26	HF	198	 34% 46% 18% ..
26	JF	198	 28% 51% 19% ..
27	BG	178	 20% 46% 29% 6%

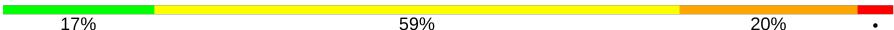
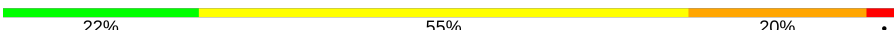
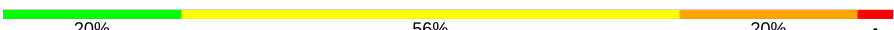
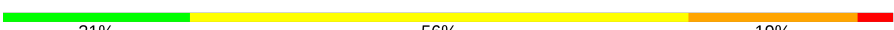

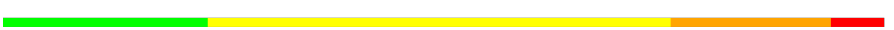









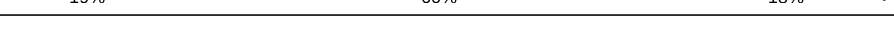
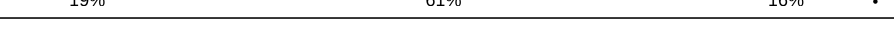
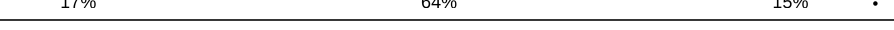
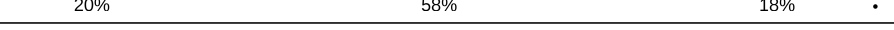
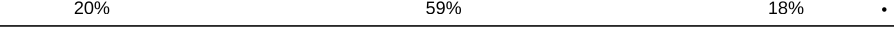




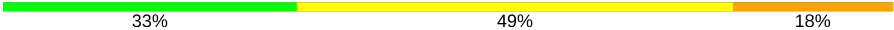
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Mol	Chain	Length	Quality of chain
27	DG	178	
27	FG	178	
27	HG	178	
27	JG	178	
28	BH	177	
28	DH	177	
28	FH	177	
28	HH	177	
28	JH	177	
29	BI	52	
29	DI	52	
29	FI	52	
29	HI	52	
29	JI	52	
30	BJ	143	
30	DJ	143	
30	FJ	143	
30	HJ	143	
30	JJ	143	
31	BK	143	
31	DK	143	
31	FK	143	
31	HK	143	
31	JK	143	
32	BL	132	

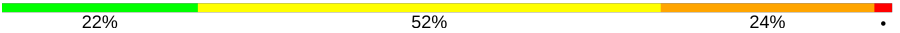
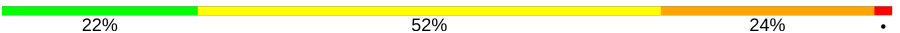
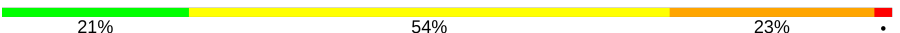



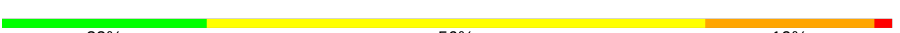




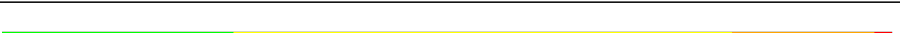


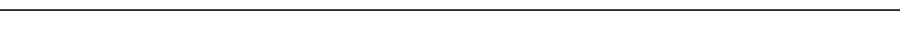


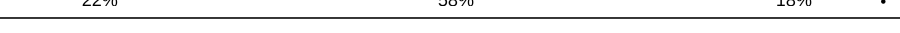
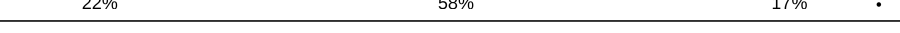
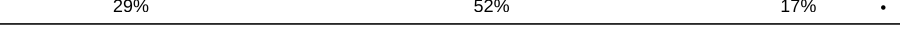
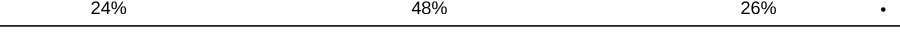
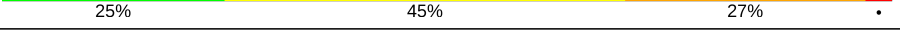
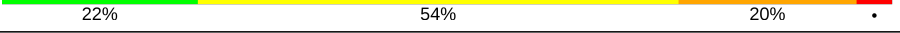
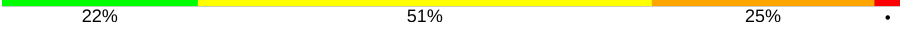

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Mol	Chain	Length	Quality of chain
32	DL	132	
32	FL	132	
32	HL	132	
32	JL	132	
33	BM	141	
33	DM	141	
33	FM	141	
33	HM	141	
33	JM	141	
34	BN	124	
34	DN	124	
34	FN	124	
34	HN	124	
34	JN	124	
35	BO	114	
35	DO	114	
35	FO	114	
35	HO	114	
35	JO	114	
36	BP	111	
36	DP	111	
36	FP	111	
36	HP	111	
36	JP	111	
37	BQ	125	

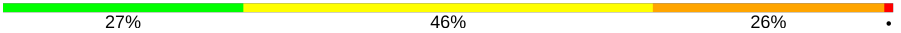
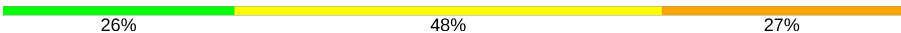
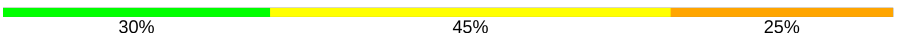


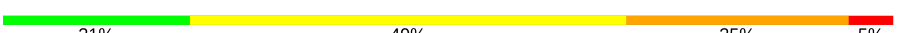
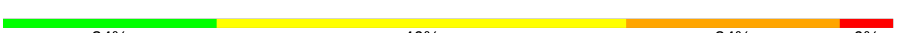




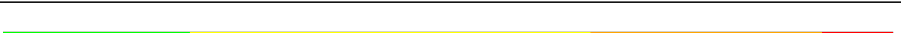


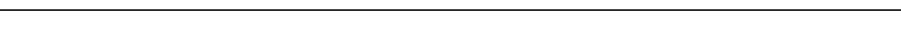
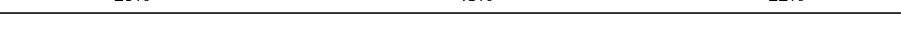
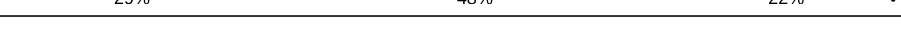
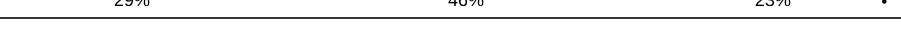
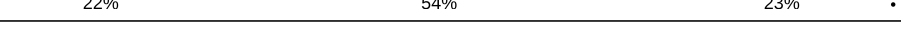
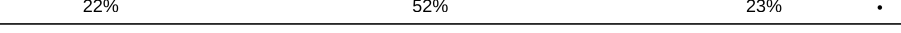

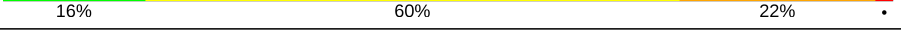



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Mol	Chain	Length	Quality of chain
37	DQ	125	
37	FQ	125	
37	HQ	125	
37	JQ	125	
38	BR	117	
38	DR	117	
38	FR	117	
38	HR	117	
38	JR	117	
39	BS	100	
39	DS	100	
39	FS	100	
39	HS	100	
39	JS	100	
40	BT	130	
40	DT	130	
40	FT	130	
40	HT	130	
40	JT	130	
41	BU	93	
41	DU	93	
41	FU	93	
41	HU	93	
41	JU	93	
42	BV	113	

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Mol	Chain	Length	Quality of chain
42	DV	113	
42	FV	113	
42	HV	113	
42	JV	113	
43	BW	173	
43	DW	173	
43	FW	173	
43	HW	173	
43	JW	173	
44	BX	86	
44	DX	86	
44	FX	86	
44	HX	86	
44	JX	86	
45	BY	65	
45	DY	65	
45	FY	65	
45	HY	65	
45	JY	65	
46	BZ	55	
46	DZ	55	
46	FZ	55	
46	HZ	55	
46	JZ	55	
47	B1	73	


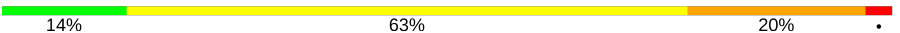
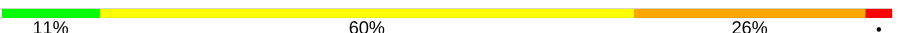


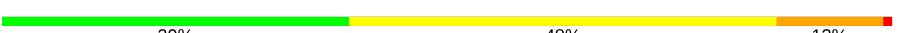
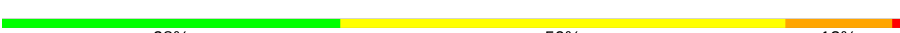


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Mol	Chain	Length	Quality of chain
47	D1	73	
47	F1	73	
47	H1	73	
47	J1	73	
48	B2	58	
48	D2	58	
48	F2	58	
48	H2	58	
48	J2	58	
49	B3	53	
49	D3	53	
49	F3	53	
49	H3	53	
49	J3	53	
50	B4	46	
50	D4	46	
50	F4	46	
50	H4	46	
50	J4	46	
51	B5	63	
51	D5	63	
51	F5	63	
51	H5	63	
51	J5	63	
52	B6	35	

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Mol	Chain	Length	Quality of chain
52	D6	35	 9% 66% 23% .
52	F6	35	 14% 63% 20% .
52	H6	35	 11% 60% 26% .
52	J6	35	 11% 63% 23% .
53	B7	217	 38% 49% 12% .
53	D7	217	 39% 48% 12% .
53	F7	217	 38% 50% 12% .
53	H7	217	 36% 51% 12% .
53	J7	217	 34% 54% 12% .

## 2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 717805 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1526	Total	C	N	O	P	0	0	0
			32799	14601	6082	10590	1526			
1	CA	1526	Total	C	N	O	P	0	0	0
			32799	14601	6082	10590	1526			
1	EA	1526	Total	C	N	O	P	0	0	0
			32799	14601	6082	10590	1526			
1	GA	1526	Total	C	N	O	P	0	0	0
			32799	14601	6082	10590	1526			
1	IA	1526	Total	C	N	O	P	0	0	0
			32799	14601	6082	10590	1526			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
2	CB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
2	EB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
2	GB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
2	IB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	EC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
3	GC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
3	IC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	ED	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	GD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	ID	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	4			
5	CE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	4			
5	EE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	4			
5	GE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	4			
5	IE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	4			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	EG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	GG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	IG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	EH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	GH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	IH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
9	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	EI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
9	GI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
9	II	127	Total	C	N	O	0	0	0
			1011	639	198	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			
10	CJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			
10	EJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			
10	GJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			
10	IJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	EK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	GK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	IK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	CL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	EL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	GL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	IL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			
13	CM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			
13	EM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			
13	GM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			
13	IM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	EN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	GN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	IN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	CP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	EP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	GP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	IP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			
17	CQ	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			
17	EQ	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			
17	GQ	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			
17	IQ	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	73	Total	C	N	O	0	0	0
			597	380	118	99			
18	CR	73	Total	C	N	O	0	0	0
			597	380	118	99			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	ER	73	Total	C	N	O	0	0	0
			597	380	118	99			
18	GR	73	Total	C	N	O	0	0	0
			597	380	118	99			
18	IR	73	Total	C	N	O	0	0	0
			597	380	118	99			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	80	Total	C	N	O	S	0	0	0
			648	414	119	113	2			
19	CS	80	Total	C	N	O	S	0	0	0
			648	414	119	113	2			
19	ES	80	Total	C	N	O	S	0	0	0
			648	414	119	113	2			
19	GS	80	Total	C	N	O	S	0	0	0
			648	414	119	113	2			
19	IS	80	Total	C	N	O	S	0	0	0
			648	414	119	113	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
20	ET	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
20	GT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
20	IT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 21 is a protein called protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Aa	90	Total	C	N	O	S	0	0	0
			719	452	131	133	3			
21	Ca	90	Total	C	N	O	S	0	0	0
			719	452	131	133	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Ea	90	Total	C	N	O	S	0	0	0
			719	452	131	133	3			
21	Ga	90	Total	C	N	O	S	0	0	0
			719	452	131	133	3			
21	Ia	90	Total	C	N	O	S	0	0	0
			719	452	131	133	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BB	2825	Total	C	N	O	P	0	0	0
			60635	27047	11190	19573	2825			
22	DB	2825	Total	C	N	O	P	0	0	0
			60635	27047	11190	19573	2825			
22	FB	2825	Total	C	N	O	P	0	0	0
			60635	27047	11190	19573	2825			
22	HB	2825	Total	C	N	O	P	0	0	0
			60635	27047	11190	19573	2825			
22	JB	2825	Total	C	N	O	P	0	0	0
			60635	27047	11190	19573	2825			

- Molecule 23 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	118	Total	C	N	O	P	0	0	0
			2519	1124	464	813	118			
23	DA	118	Total	C	N	O	P	0	0	0
			2519	1124	464	813	118			
23	FA	118	Total	C	N	O	P	0	0	0
			2519	1124	464	813	118			
23	HA	118	Total	C	N	O	P	0	0	0
			2519	1124	464	813	118			
23	JA	118	Total	C	N	O	P	0	0	0
			2519	1124	464	813	118			

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BD	270	Total	C	N	O	S	0	0	0
			2079	1294	417	365	3			
24	DD	270	Total	C	N	O	S	0	0	0
			2079	1294	417	365	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	FD	270	Total	C	N	O	S	0	0	0
			2079	1294	417	365	3			
24	HD	270	Total	C	N	O	S	0	0	0
			2079	1294	417	365	3			
24	JD	270	Total	C	N	O	S	0	0	0
			2079	1294	417	365	3			

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BE	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			
25	DE	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			
25	FE	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			
25	HE	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			
25	JE	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BF	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			
26	DF	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			
26	FF	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			
26	HF	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			
26	JF	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BG	178	Total	C	N	O	S	0	0	0
			1410	897	249	257	7			
27	DG	178	Total	C	N	O	S	0	0	0
			1410	897	249	257	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	FG	178	Total	C	N	O	S	0	0	0
			1410	897	249	257	7			
27	HG	178	Total	C	N	O	S	0	0	0
			1410	897	249	257	7			
27	JG	178	Total	C	N	O	S	0	0	0
			1410	897	249	257	7			

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BH	177	Total	C	N	O	S	0	0	0
			1316	828	243	244	1			
28	DH	177	Total	C	N	O	S	0	0	0
			1316	828	243	244	1			
28	FH	177	Total	C	N	O	S	0	0	0
			1316	828	243	244	1			
28	HH	177	Total	C	N	O	S	0	0	0
			1316	828	243	244	1			
28	JH	177	Total	C	N	O	S	0	0	0
			1316	828	243	244	1			

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BI	52	Total	C	N	O	S	0	0	0
			401	251	73	75	2			
29	DI	52	Total	C	N	O	S	0	0	0
			401	251	73	75	2			
29	FI	52	Total	C	N	O	S	0	0	0
			401	251	73	75	2			
29	HI	52	Total	C	N	O	S	0	0	0
			401	251	73	75	2			
29	JI	52	Total	C	N	O	S	0	0	0
			401	251	73	75	2			

- Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BJ	143	Total	C	N	O	S	0	0	0
			1039	660	178	196	5			
30	DJ	143	Total	C	N	O	S	0	0	0
			1039	660	178	196	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	FJ	143	Total	C	N	O	S	0	0	0
			1039	660	178	196	5			
30	HJ	143	Total	C	N	O	S	0	0	0
			1039	660	178	196	5			
30	JJ	143	Total	C	N	O	S	0	0	0
			1039	660	178	196	5			

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BK	143	Total	C	N	O	S	0	0	0
			1122	709	210	200	3			
31	DK	143	Total	C	N	O	S	0	0	0
			1122	709	210	200	3			
31	FK	143	Total	C	N	O	S	0	0	0
			1122	709	210	200	3			
31	HK	143	Total	C	N	O	S	0	0	0
			1122	709	210	200	3			
31	JK	143	Total	C	N	O	S	0	0	0
			1122	709	210	200	3			

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BL	132	Total	C	N	O	S	0	0	0
			981	603	196	178	4			
32	DL	132	Total	C	N	O	S	0	0	0
			981	603	196	178	4			
32	FL	132	Total	C	N	O	S	0	0	0
			981	603	196	178	4			
32	HL	132	Total	C	N	O	S	0	0	0
			981	603	196	178	4			
32	JL	132	Total	C	N	O	S	0	0	0
			981	603	196	178	4			

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	BM	141	Total	C	N	O	0	0	0
			1068	655	216	197			
33	DM	141	Total	C	N	O	0	0	0
			1068	655	216	197			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	FM	141	Total	C	N	O	0	0	0
			1068	655	216	197			
33	HM	141	Total	C	N	O	0	0	0
			1068	655	216	197			
33	JM	141	Total	C	N	O	0	0	0
			1068	655	216	197			

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	124	Total	C	N	O	S	0	0	0
			986	631	182	167	6			
34	DN	124	Total	C	N	O	S	0	0	0
			986	631	182	167	6			
34	FN	124	Total	C	N	O	S	0	0	0
			986	631	182	167	6			
34	HN	124	Total	C	N	O	S	0	0	0
			986	631	182	167	6			
34	JN	124	Total	C	N	O	S	0	0	0
			986	631	182	167	6			

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	114	Total	C	N	O	S	0	0	0
			886	546	179	159	2			
35	DO	114	Total	C	N	O	S	0	0	0
			886	546	179	159	2			
35	FO	114	Total	C	N	O	S	0	0	0
			886	546	179	159	2			
35	HO	114	Total	C	N	O	S	0	0	0
			886	546	179	159	2			
35	JO	114	Total	C	N	O	S	0	0	0
			886	546	179	159	2			

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BP	111	Total	C	N	O	8	0	0
			834	512	168	154			
36	DP	111	Total	C	N	O	8	0	0
			834	512	168	154			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	FP	111	Total	C	N	O	8	0	0
			834	512	168	154			
36	HP	111	Total	C	N	O	8	0	0
			834	512	168	154			
36	JP	111	Total	C	N	O	8	0	0
			834	512	168	154			

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	125	Total	C	N	O	S	0	0	0
			1008	625	204	178	1			
37	DQ	125	Total	C	N	O	S	0	0	0
			1008	625	204	178	1			
37	FQ	125	Total	C	N	O	S	0	0	0
			1008	625	204	178	1			
37	HQ	125	Total	C	N	O	S	0	0	0
			1008	625	204	178	1			
37	JQ	125	Total	C	N	O	S	0	0	0
			1008	625	204	178	1			

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	117	Total	C	N	O	S	16	0	0
			978	608	210	159	1			
38	DR	117	Total	C	N	O	S	16	0	0
			978	608	210	159	1			
38	FR	117	Total	C	N	O	S	16	0	0
			978	608	210	159	1			
38	HR	117	Total	C	N	O	S	16	0	0
			978	608	210	159	1			
38	JR	117	Total	C	N	O	S	16	0	0
			978	608	210	159	1			

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BS	100	Total	C	N	O	S	0	0	0
			787	495	146	145	1			
39	DS	100	Total	C	N	O	S	0	0	0
			787	495	146	145	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	FS	100	Total	C	N	O	S	0	0	0
			787	495	146	145	1			
39	HS	100	Total	C	N	O	S	0	0	0
			787	495	146	145	1			
39	JS	100	Total	C	N	O	S	0	0	0
			787	495	146	145	1			

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	130	Total	C	N	O	S	0	0	0
			1039	653	203	181	2			
40	DT	130	Total	C	N	O	S	0	0	0
			1039	653	203	181	2			
40	FT	130	Total	C	N	O	S	0	0	0
			1039	653	203	181	2			
40	HT	130	Total	C	N	O	S	0	0	0
			1039	653	203	181	2			
40	JT	130	Total	C	N	O	S	0	0	0
			1039	653	203	181	2			

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	93	Total	C	N	O	S	0	0	0
			727	458	136	131	2			
41	DU	93	Total	C	N	O	S	0	0	0
			727	458	136	131	2			
41	FU	93	Total	C	N	O	S	0	0	0
			727	458	136	131	2			
41	HU	93	Total	C	N	O	S	0	0	0
			727	458	136	131	2			
41	JU	93	Total	C	N	O	S	0	0	0
			727	458	136	131	2			

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BV	113	Total	C	N	O	S	0	0	0
			852	530	166	155	1			
42	DV	113	Total	C	N	O	S	0	0	0
			852	530	166	155	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	FV	113	Total	C	N	O	S	0	0	0
			852	530	166	155	1			
42	HV	113	Total	C	N	O	S	0	0	0
			852	530	166	155	1			
42	JV	113	Total	C	N	O	S	0	0	0
			852	530	166	155	1			

- Molecule 43 is a protein called general stress protein Ctc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	173	Total	C	N	O	S	0	0	0
			1328	838	231	253	6			
43	DW	173	Total	C	N	O	S	0	0	0
			1328	838	231	253	6			
43	FW	173	Total	C	N	O	S	0	0	0
			1328	838	231	253	6			
43	HW	173	Total	C	N	O	S	0	0	0
			1328	838	231	253	6			
43	JW	173	Total	C	N	O	S	0	0	0
			1328	838	231	253	6			

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BX	86	Total	C	N	O	S	0	0	0
			642	402	124	115	1			
44	DX	86	Total	C	N	O	S	0	0	0
			642	402	124	115	1			
44	FX	86	Total	C	N	O	S	0	0	0
			642	402	124	115	1			
44	HX	86	Total	C	N	O	S	0	0	0
			642	402	124	115	1			
44	JX	86	Total	C	N	O	S	0	0	0
			642	402	124	115	1			

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	65	Total	C	N	O	S	0	0	0
			526	322	106	96	2			
45	DY	65	Total	C	N	O	S	0	0	0
			526	322	106	96	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	FY	65	Total	C	N	O	S	0	0	0
			526	322	106	96	2			
45	HY	65	Total	C	N	O	S	0	0	0
			526	322	106	96	2			
45	JY	65	Total	C	N	O	S	0	0	0
			526	322	106	96	2			

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	55	Total	C	N	O	S	4	0	0
			424	264	82	76	2			
46	DZ	55	Total	C	N	O	S	4	0	0
			424	264	82	76	2			
46	FZ	55	Total	C	N	O	S	4	0	0
			424	264	82	76	2			
46	HZ	55	Total	C	N	O	S	4	0	0
			424	264	82	76	2			
46	JZ	55	Total	C	N	O	S	4	0	0
			424	264	82	76	2			

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B1	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			
47	D1	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			
47	F1	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			
47	H1	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			
47	J1	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B2	58	Total	C	N	O	S	0	0	0
			458	281	94	78	5			
48	D2	58	Total	C	N	O	S	0	0	0
			458	281	94	78	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	F2	58	Total	C	N	O	S	0	0	0
			458	281	94	78	5			
48	H2	58	Total	C	N	O	S	0	0	0
			458	281	94	78	5			
48	J2	58	Total	C	N	O	S	0	0	0
			458	281	94	78	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B3	53	Total	C	N	O	S	0	0	0
			432	274	80	77	1			
49	D3	53	Total	C	N	O	S	0	0	0
			432	274	80	77	1			
49	F3	53	Total	C	N	O	S	0	0	0
			432	274	80	77	1			
49	H3	53	Total	C	N	O	S	0	0	0
			432	274	80	77	1			
49	J3	53	Total	C	N	O	S	0	0	0
			432	274	80	77	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	46	Total	C	N	O	S	0	0	0
			384	230	91	61	2			
50	D4	46	Total	C	N	O	S	0	0	0
			384	230	91	61	2			
50	F4	46	Total	C	N	O	S	0	0	0
			384	230	91	61	2			
50	H4	46	Total	C	N	O	S	0	0	0
			384	230	91	61	2			
50	J4	46	Total	C	N	O	S	0	0	0
			384	230	91	61	2			

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			
51	D5	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	F5	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			
51	H5	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			
51	J5	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			
52	D6	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			
52	F6	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			
52	H6	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			
52	J6	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			

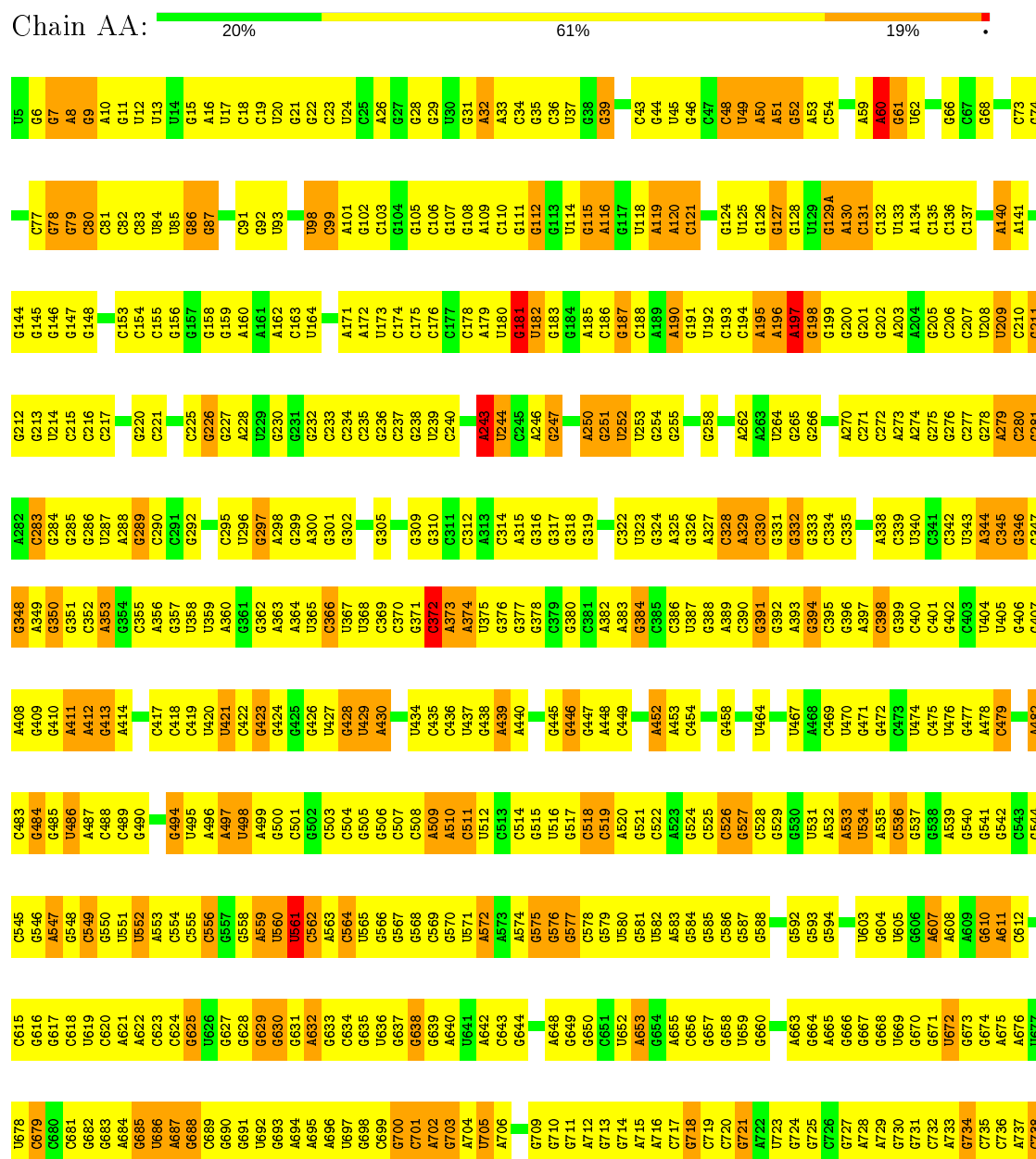
- Molecule 53 is a protein called 50S ribosomal protein L1P.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
53	B7	217	Total	C	N	O	S	Se	0	0	0
			1720	1098	304	313	1	4			
53	D7	217	Total	C	N	O	S	Se	0	0	0
			1720	1098	304	313	1	4			
53	F7	217	Total	C	N	O	S	Se	0	0	0
			1720	1098	304	313	1	4			
53	H7	217	Total	C	N	O	S	Se	0	0	0
			1720	1098	304	313	1	4			
53	J7	217	Total	C	N	O	S	Se	0	0	0
			1720	1098	304	313	1	4			

### 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 16S ribosomal RNA

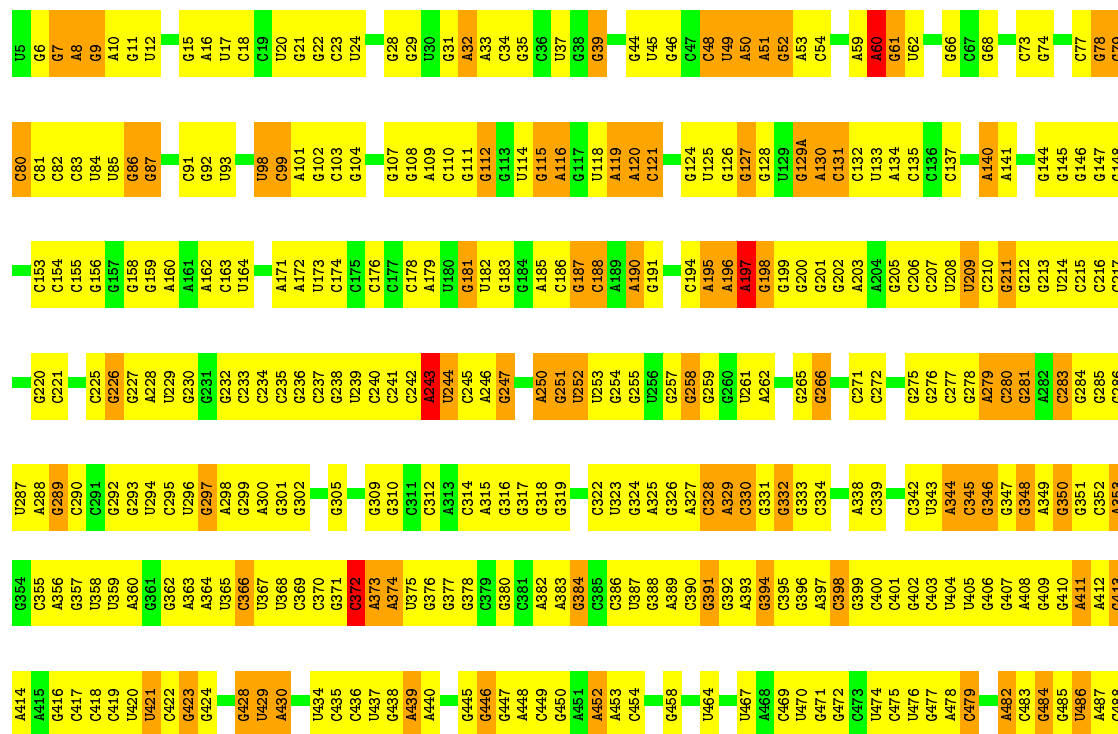




Response	Percentage
Yes	20%
No	60%
Don't know	19%



U1073	U1012	A946	G881	A814	G742	C681	G617	A553	G490	C417	C355	A288	G220	G147	G79
G1074	G1013	G947	G888	A815	C748	G682	C618	C554	G494	C418	A356	G289	C221	G146	C80
C1075	A1014	C948	A816	C817	C749	G683	U619	C555	G495	C419	U358	C290	C225	C153	C81
G1077	A1015	U950	G890	G818	G752	G685	A621	G557	U495	U420	U359	G291	G226	C154	C82
U1078	A1016	G951	G891	A819	A622	U686	A622	G558	A497	U421	A360	G292	G227	G158	C83
U1079	C1017	U952	A892	U820	A753	A687	C623	U559	U498	C422	A228	G297	U229	U85	U84
A1080	C1018	G953	C893	G821	C754	G688	G625	U560	A499	G423	U230	C230	A160	G86	U85
G1081	C1019	G954	G894	G822	G755	C689	G626	U561	G500	G424	A362	C231	G230	A161	G87
U1082	U1020	U955	G895	G825	C756	G690	U626	A562	C501	G425	A364	A298	G232	A162	C91
U1083	G1021	U956	C896	G826	U757	G691	G627	A563	G502	G426	U365	G299	G233	A163	G92
G1084	G1022	U957	C897	U827	G758	U692	G628	A564	C503	U427	C366	A300	C234	U164	U93
U1085	G1023	A958	G898	A828	A759	G693	G629	U565	C504	G428	U367	G301	C235	G168	
U1086	G1024	A959	C899	G829	G760	A694	G630	G566	G505	U429	U368	G302	C236		
	U1025	U960	A900	U833	G761	A695	A631	G567	G506	A430	C369	G305	G236	A171	U98
	G1026	U961	A901	U834	G762	A696	A632	G568	C507	U434	C370	G371	C237	A172	C99
	C1027	G962	G902	C834	G765	G697	G633	C569	C508	C435	G372	G372	G238	U173	A101
	C1028	G963	G903	G835	A766	G698	C634	U571	A509	C436	A373	G310	U239	U174	G102
	U1029	A964	C904	G837	A767	C699	G635	A572	A510	U437	A374	G311	C240	C175	C103
	U1030	A965	U905	C838	A768	G700	U636	A573	C511	G438	U375	C241	C242	G177	G104
	G1094	G966	G906	G839	A769	G701	G637	A574	U512	A439	G376	A313	C243	G178	G105
	U1095	C967	A907	G840	G770	A702	G638	G575	C514	A440	G377	C314	U244	A179	C106
	C1096	A968	A908	C841	C771	G703	G639	G576	G515	G445	C378	A315	C245	U180	G107
	G1097	A969	A909	U842	G772	A704	A640	G577	U516	G446	G380	G317	C246	U181	G108
	A1035	C970	C910	U843	G773	U705	A641	G578	G517	G447	G381	G318	G247	U182	A109
	G1036	G971	U811	A844	G774	A706	A642	C579	C518	G448	A382	G319	C250	G183	C110
	C1037	C972	C912	A845	G775	G709	C643	U580	C519	C449	A383	G320	A251	G184	G111
	A1101	G973	A913	C846	G776	G710	G644	U581	A520	C452	C385	G321	U252	C185	G112
	C1038	A974	A914	G847	C779	G711	A648	U582	G521	A453	C386	G322	U253	C186	U114
	U1039	A975	A915	G848	A781	A712	G649	U583	C522	A454	U387	G323	U254	C187	G115
	C1040	U976	G916	G849	A782	A713	G650	U584	C523	C455	U388	G324	G255	C188	G116
	U1041	A977	G917	G851	A783	G714	C651	G585	C526	C456	U389	A325	G256	A189	G117
	C1045	A978	A918	G852	A784	A715	C652	G586	C527	G458	A390	A327	G258	A190	U118
	A1046	C979	A919	G853	C784	A716	A653	G587	G528	U464	C391	A329	A262	A195	A120
	G1047	C980	U920	G854	G785	C717	G654	G588	G529	C472	C392	A330	A263	A196	C121
	U1048	U981	G921	C857	G786	G718	A655	C589	G530	U467	G393	G331	U264	A197	G124
	A1110	U982	G922	G858	A787	C719	C656	C590	U531	A468	G394	G332	G265	G198	U125
	U1050	A983	A923	G859	C792	C720	G657	G592	A532	U469	G395	G333	G266	G199	G126
	C1051	C984	C924	A860	A792	G721	G658	G593	A533	U470	G396	G334	A270	G201	G127
	U1052	A986	G925	G861	U793	A722	U659	G594	U534	G471	A397	G335	C271	G202	U128
	G1053	C987	G926	C862	A794	U723	A663	G597	A535	G472	C398	A338	C272	G203	U129
	C1054	U987	G927	C863	C795	A724	G664	U598	C536	C473	G399	G339	A273	A204	G129A
	A1055	G988	G928	U863	C796	G725	G665	C599	G537	U474	C400	C339	A274	G205	A130
	C1116	C989	G929	A864	C797	G726	G666	U603	A538	U475	C401	G342	G275	G206	C132
	G1117	C990	C930	A865	G798	C727	G667	U604	A539	U476	G402	G343	G276	G207	U133
	C1118	U991	C931	G866	G799	A728	G668	U605	G541	G477	G403	U344	C277	U208	A134
	G1119	U992	G932	C867	G800	A729	G669	G542	G542	A478	U404	C345	G278	U209	C135
	C1120	G993	G933	C868	G801	A730	U669	A607	C543	C479	U405	G346	A279	G210	G136
	U1121	A994	C934	G869	U801	G730	G670	U608	G544	A482	G407	G347	C280	G211	C137
		C995	A835	U870	A802	G731	G671	A609	C545	C483	A408	G348	G281	G212	A140
	U1124	A996	C936	U871	G803	C732	U672	A611	A547	G484	G409	A349	A282	G213	A141
	U1126		A937	U872	U804	A733	G673	A612	G548	G485	G410	G350	C283	U214	
	G1126		A938	A873	A807	C734	G674	A613	C549	U486	A411	G351	G284	C215	
	C1127		A939	G874	C735	G735	G675	A614	G550	A487	A412	C352	G285	C216	G144
	G1128		G940	C875	C736	G736	A675	A615	U551	C488	G413	A353	G286	C217	G145
	U1129		G941	G876	A737	G737	A676	C612	C549	U487	G414	G354	U287		G146
	A1130		G942	C877	C738	C738	U677	C613							
	G1131		U943	G878	C739	C739	U678	C614							
	C1132		U944	C879	U740	C740	C679	C615							
	G1133		G945	C880	G741	C741	C680	G616							



A1374	U1313	G1253	G1190	G1127	C1066	G874	C806	A737	U677	U551	C489
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C1377	G1316	A1256	G1193	C1130	C1069	C877	G809	U740	C680	C654	U495
C1378	C1317	U1257	U1194	G1131	C1070	C878	C810	G741	C681	C655	A496
G1379	A1318	G1258	C1195	C1132	C1071	C879	C811	G742	C682	C656	A497
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U1381	C1320	C1260	G1197	G1134	U1073	C881	U813	C748	A684	C658	U499
C1382	C1321	A1261	U1198	U1135	G1074		A814	C749	C685	A622	U498
C1383	C1322	C1262	U1199	G1136	C1075	G888	A815	G750	U686	U600	C501
C1384	C1323	C1263	C1200	C1137	A1076	A889	A816	U751	A687	U601	C502
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G1386	C1325	G1265	G1202	G1139	U1078	U891	C818	A753	C689	U625	C504
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C1389	C1328	A1268	U1205	G1142	U1081	G894	U821	C755	U692	G629	G507
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G1392	G1331	C1272	C1208	C1145	G1084	C897	C826	A759	A695	A632	A509
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C1395	G1334	G1275	U1211	U1148	G1087	A900	G829	C762	C698	U635	U512
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C1397	G1336	G1277	A1213	U1150	U1089	G902	U834	G765	G700	G637	C514
A1398	C1337	C1278	C1214	A1151	U1090	G903	C835	A766	C701	G638	G515
C1399	G1338	U1278	G1215	A1152	A1092	C904		A767	A702	G639	U516
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C1409	G1347	C1287	A1225		A1101	A913	C846	A777	G711	G585	C525
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		U1292		A1167	G1051	A923	G858	A781	G721	A535	A535
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G1421	A1357	G1295	U1235	G1171	G1109	U921	C862	G785	G718	U591	A532
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G1423	C1359	C1297	C1237	G1173	A1111	C923	C857	A787	C720	G594	U534
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U1425	G1361	A1299	A1239	A1176	C1112	C925	A864		A722	G597	C536
C1426	C2361	G1300	U1240	G1177	C1113	C926	A865	A792	U723	U598	G537
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A1428	A1363	U1302	C1242	A1179	C1115	G928	U863	A794	G725	A539	A539
C1429	U1364	C1303	C1243	A1180	G1117	C929	A864	C795	G726	G666	G540
C1430	G1365	G1304	C1244	G1181	C1118	C930	A865	G796	G727	G667	G541
C1431	C1366	G1305	A1245	G1182	C1119	C931	A866	C797	A728	G668	G542
G1432	C1367	A1306	C1246	A1183	G1120	C932	C866	G798	A729	U669	C543
A1433	U1368	U1307	U1247	G1184	C1059	C933	C867	G799	G730	G670	G544
C1369	C1369	U1308	A1248	G1185	C1060	G934	C868	G800	G731	G671	A608
G1370	G1370	C1249	A1248	G1186	C1061	C935	C869	U801	G732	U672	C545
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C1437	U1372	A1251	G1250	G1188	C1063	C936	U871	G803	G734	G674	G548
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											G550



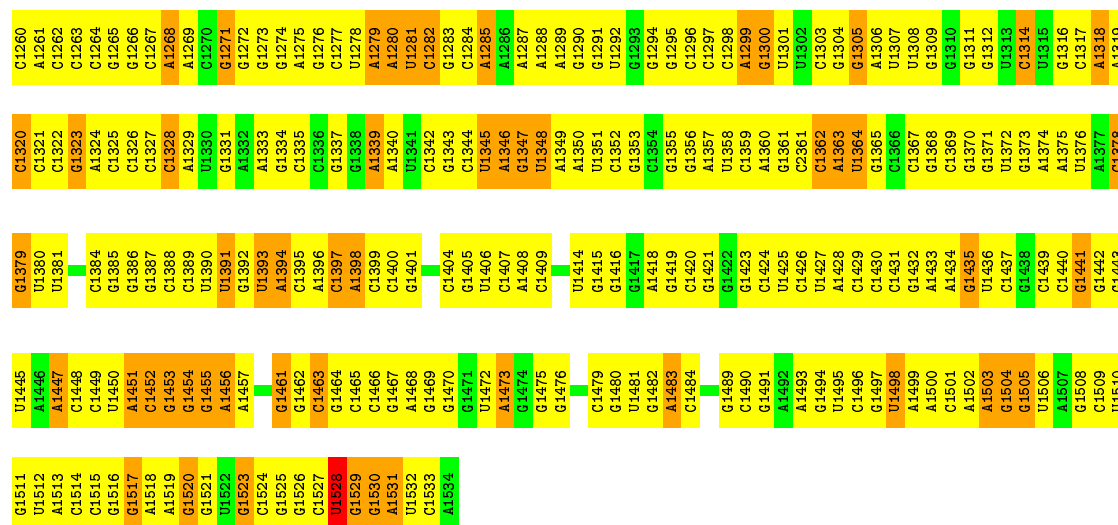
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U1510	G1443	C1378	G1317	G1256	C1192	C1129	C1066	G2003	G941	G379
G1511	U1445	G1379	A1318	U1257	G1196	A1130	A1067	A1004	G942	G380
U1512	U1446	U1380	A1319	G1258	C1195	G1131	G1068	A1005	U943	G381
A1513	A1447	U1381	C1320	C1259	U1196	C1132	C1069	C1006	G944	G382
G1514	G1448	C1382	G1321	G1260	G1197	G1133	U1070	C1007	G945	G385
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G1516	U1450	G1385	G1323	C1262	U1199	U1135	U1073	G1013	G948	G388
G1517	A1451	G1386	A1324	G1263	C1200	U1136	G1074	A1014	U949	A889
A1518	G1452	G1387	G1325	C1264	A1201	C1137	G1075	A1015	U950	G890
A1519	G1453	C1388	C1326	G1265	G1202	G1138	G1076	A1016	G951	G892
G1520	G1454	C1389	G1327	G1266	G1203	G1139	U1078	G1017	U952	A893
U1521	G1455	U1390	C1328	A1267	U1205	C1141	G1079	C1018	G953	G894
U1522	A1456	U1391	A1329	G1268	G1206	C1142	A1080	C1019	G954	G895
G1523	A1457	U1392	U1330	A1269	G1207	G1143	G1081	U1020	U955	G896
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G1525	G1462	A1394	A1332	G1271	G1209	G1145	U1078	G1022	U957	G898
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G1529	G1466	A1398	G1336	A1275	C1213	C1149	G1087	G1026	U961	G902
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G1533	G1469	U1470	U1340	A1279	C1217	C1153	A1092	U1030	A965	G906
A1534	G1471	C1404	G1342	U1281	G1222	G1155	G1094	G1032	G966	G907
U1472	U1473	U1406	G1343	C1282	C1223	G1156	U1095	G1033	C967	A908
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G1476	G1476	C1409	A1346	A1285	C1226	U1159	G1098	U1036	G971	U911
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G1505	G1505	G1438	G1373	G1311	A1251	G1187	G1124	G1061	A996	C936
U1506	U1506	C1439	A1374	G1312	A1252	C1188	U1125	C1062	A997	A937
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## • Molecule 1: 16S ribosomal RNA

Chain IA:

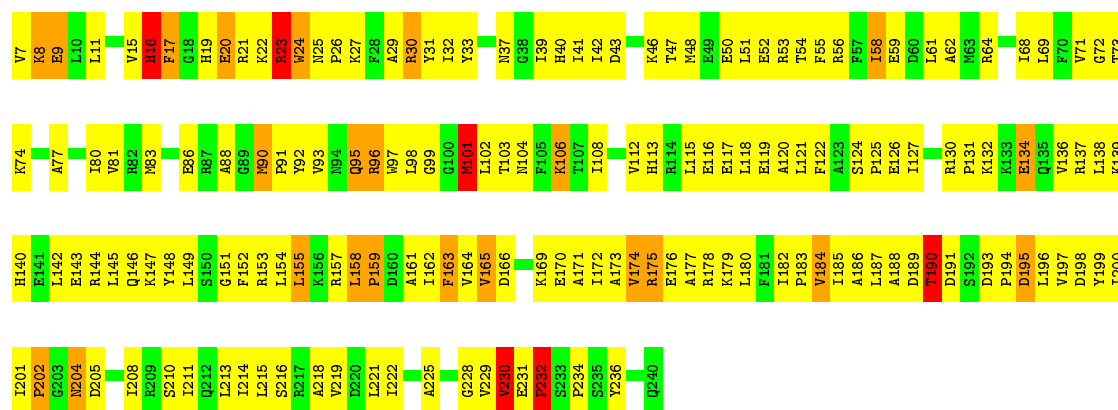


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G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768
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A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641
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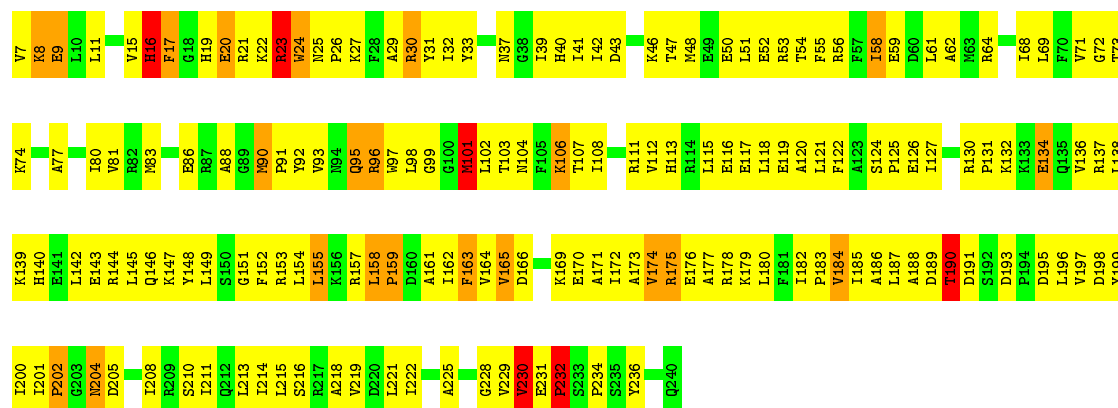
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Chain AB: 29% 59% 10% .

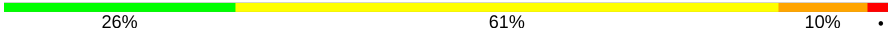


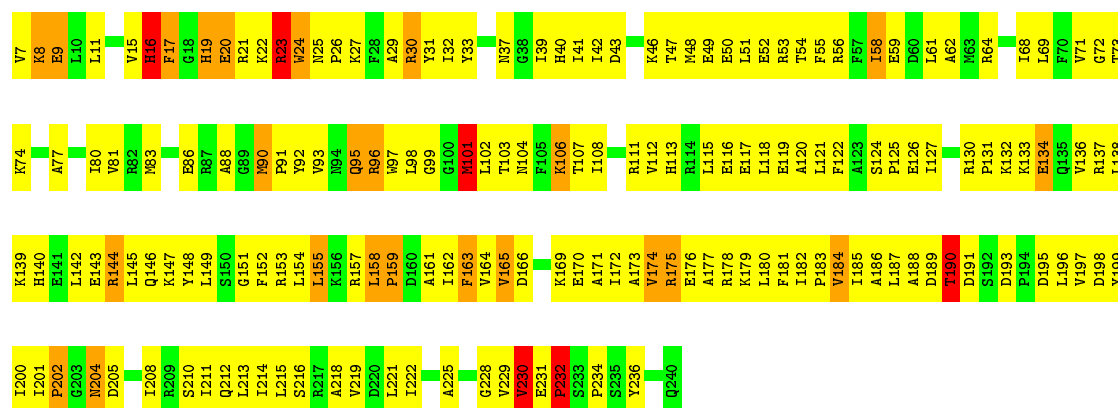
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Chain CB: 28% 60% 9% .



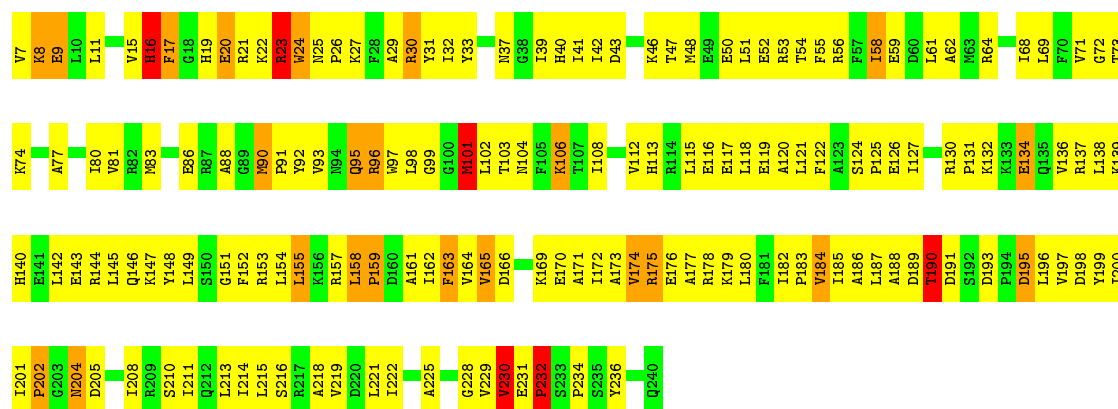
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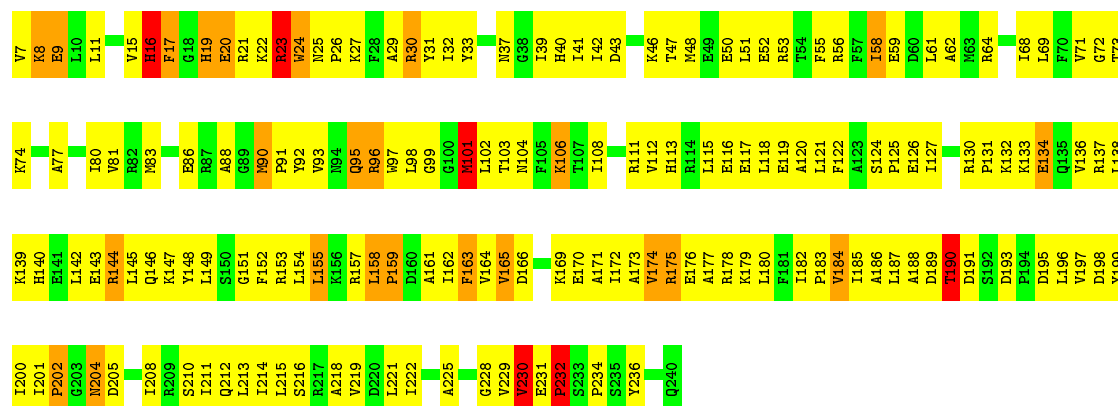
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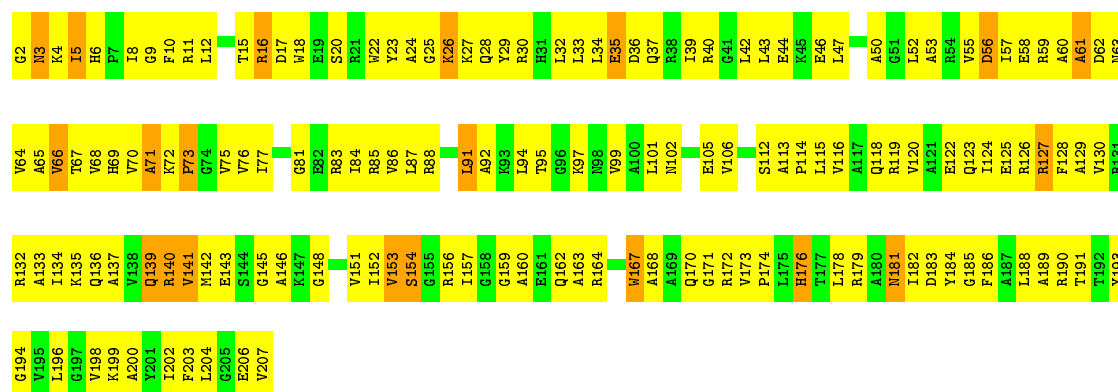
• Molecule 2: 30S ribosomal protein S2

Chain IB: 



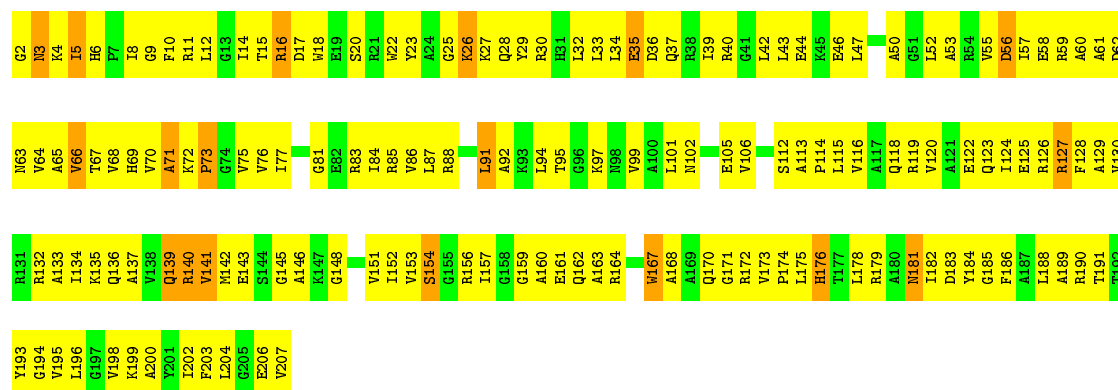
• Molecule 3: 30S ribosomal protein S3

Chain AC: 



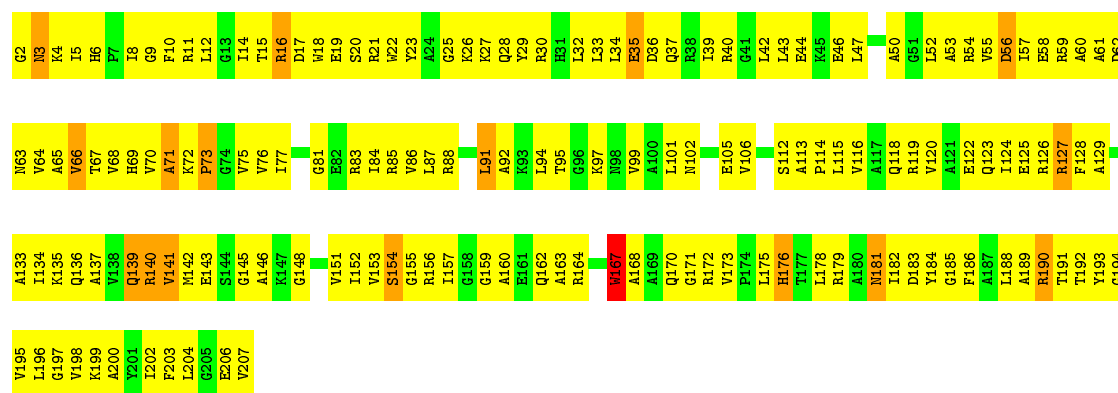
• Molecule 3: 30S ribosomal protein S3

Chain CC: 



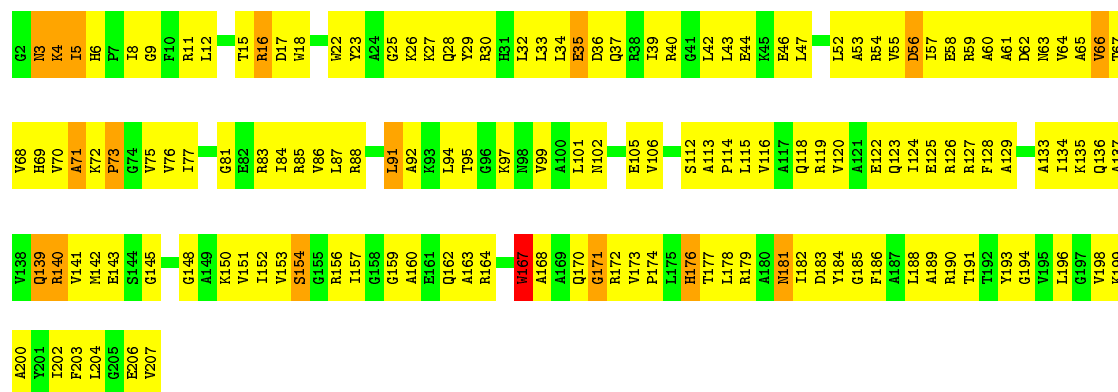
• Molecule 3: 30S ribosomal protein S3

Chain EC: 

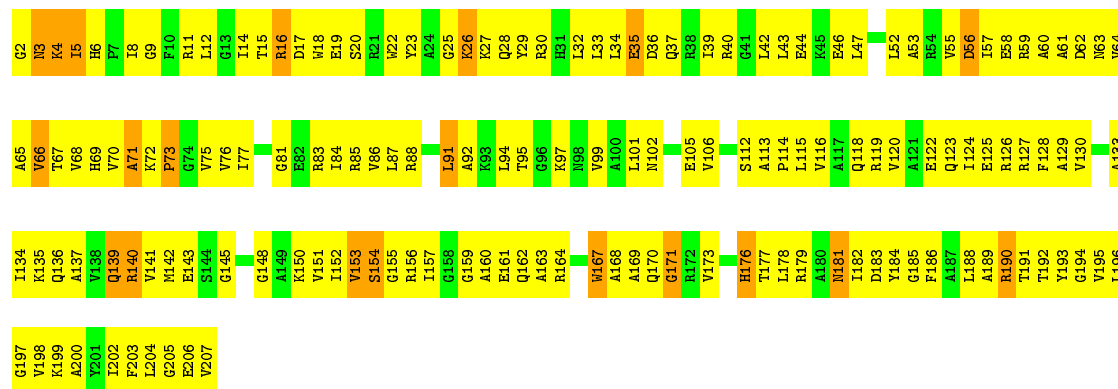


• Molecule 3: 30S ribosomal protein S3

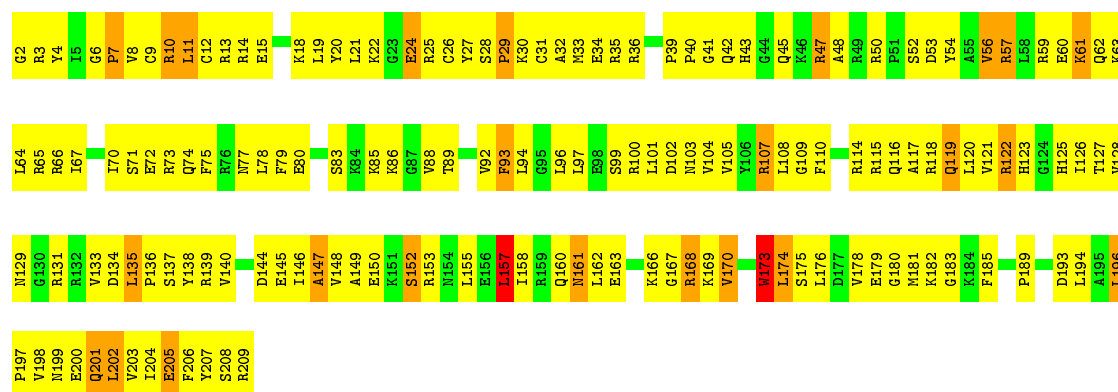
Chain GC: 



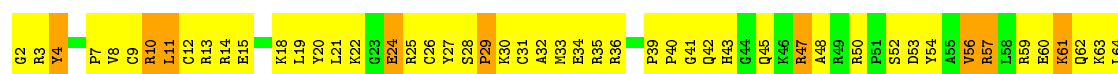
• Molecule 3: 30S ribosomal protein S3

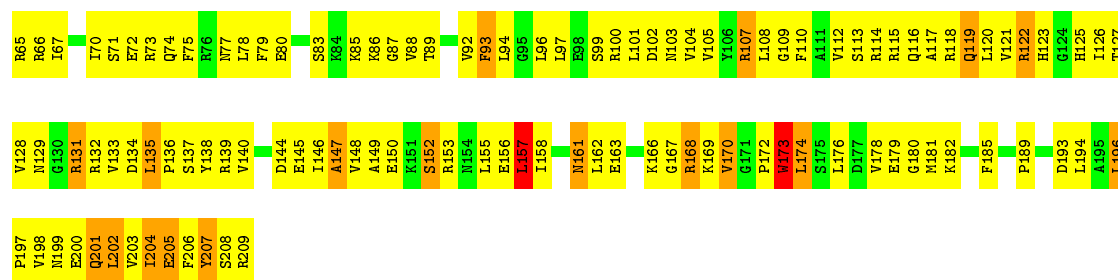


• Molecule 4: 30S ribosomal protein S4



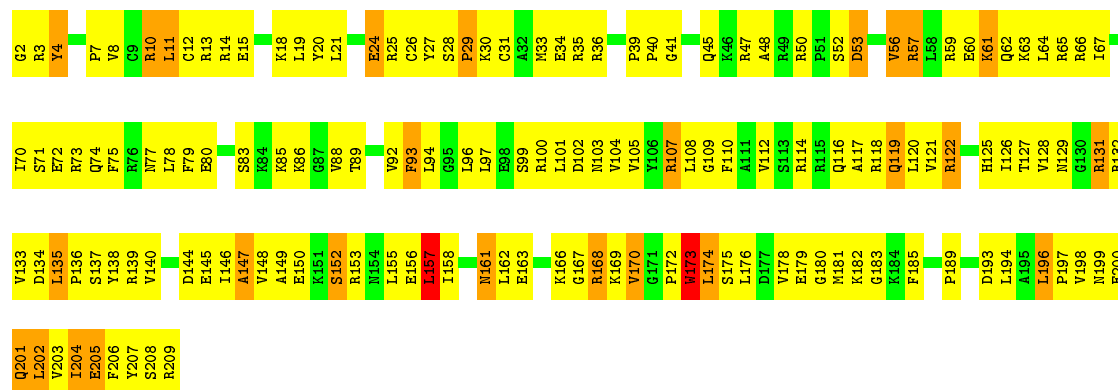
• Molecule 4: 30S ribosomal protein S4





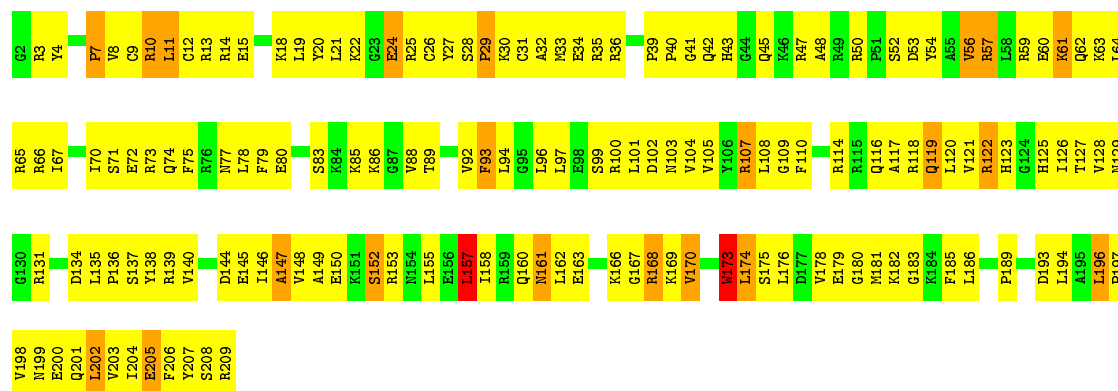
• Molecule 4: 30S ribosomal protein S4

Chain ED: 27% 60% 13%



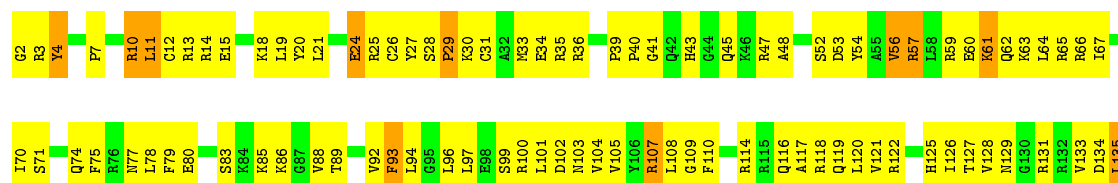
• Molecule 4: 30S ribosomal protein S4

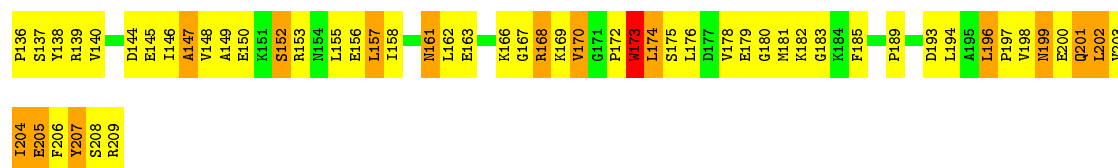
Chain GD: 25% 63% 10%



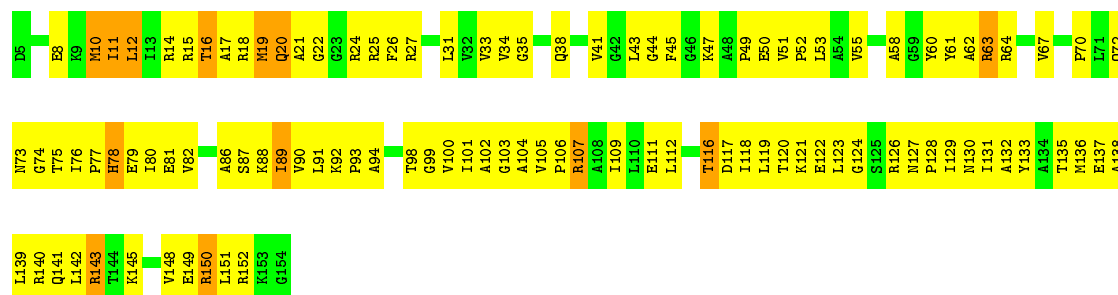
• Molecule 4: 30S ribosomal protein S4

Chain ID: 29% 59% 12%

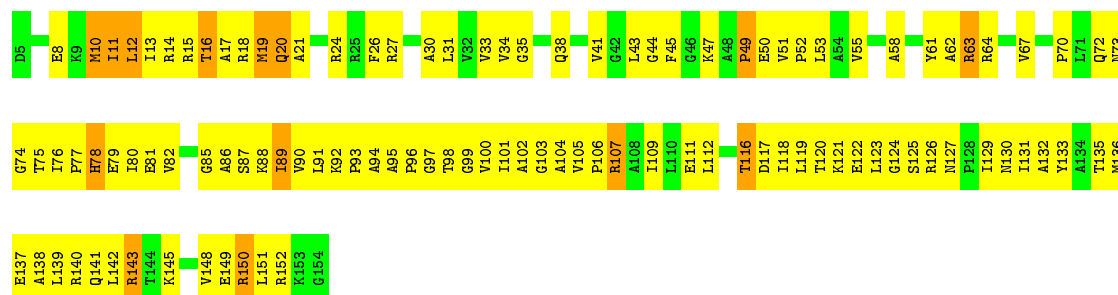
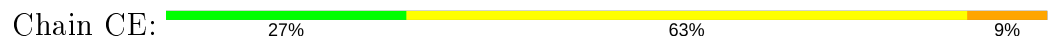




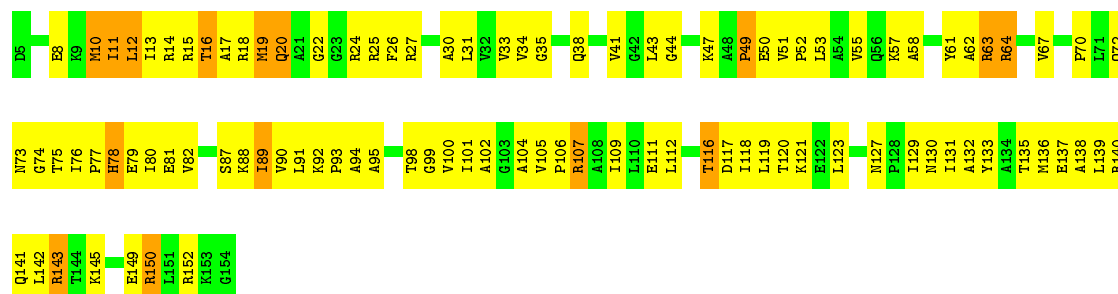
• Molecule 5: 30S ribosomal protein S5



• Molecule 5: 30S ribosomal protein S5

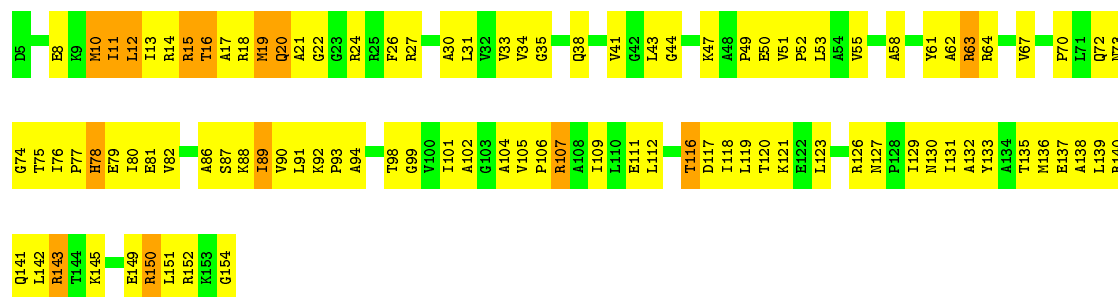


• Molecule 5: 30S ribosomal protein S5



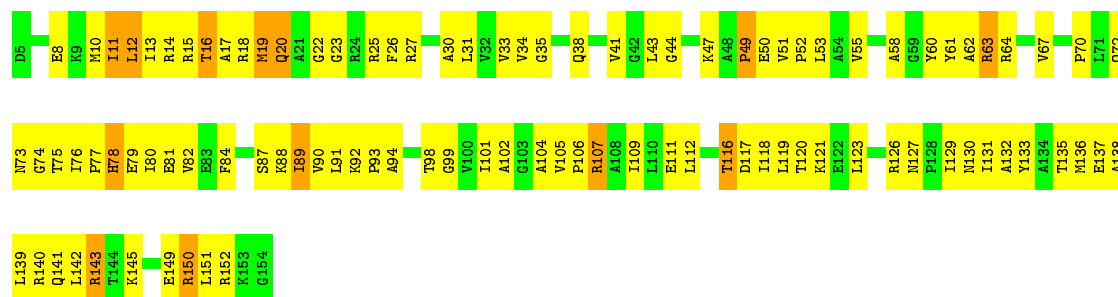
• Molecule 5: 30S ribosomal protein S5





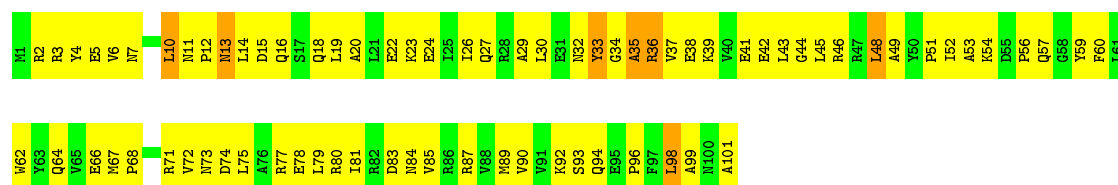
- Molecule 5: 30S ribosomal protein S5

Chain IE: 33% 58% 9%



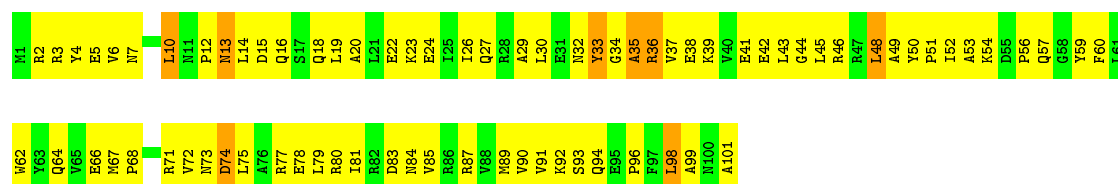
- Molecule 6: 30S ribosomal protein S6

Chain AF: 26% 67% 7%



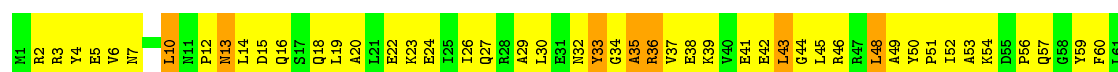
- Molecule 6: 30S ribosomal protein S6

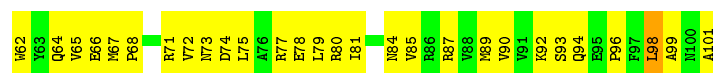
Chain CF: 25% 67% 8%



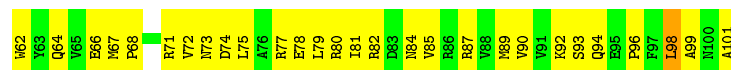
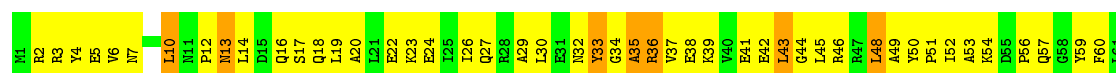
- Molecule 6: 30S ribosomal protein S6

Chain EF: 26% 66% 8%

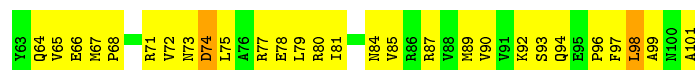
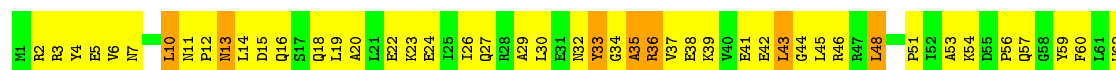




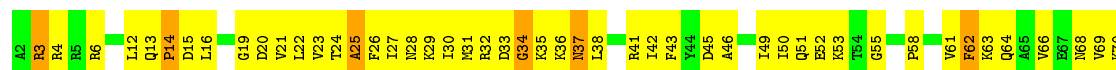
- Molecule 6: 30S ribosomal protein S6



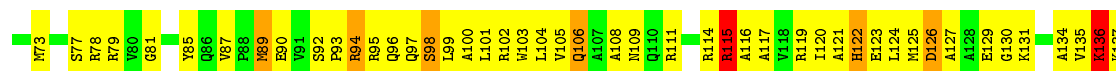
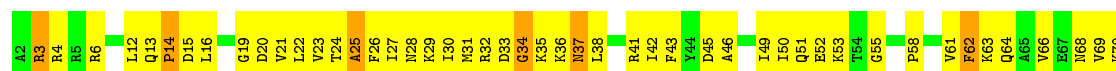
- Molecule 6: 30S ribosomal protein S6



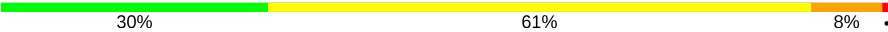
- Molecule 7: 30S ribosomal protein S7

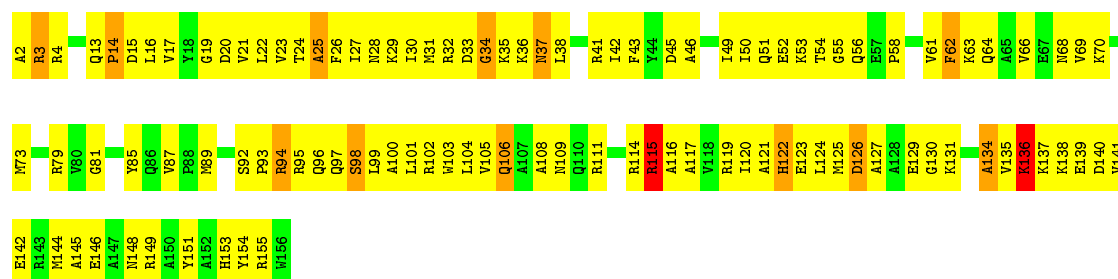


- Molecule 7: 30S ribosomal protein S7



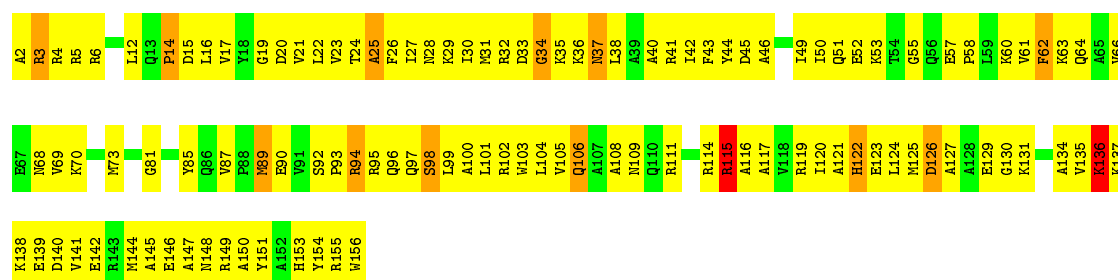
- Molecule 7: 30S ribosomal protein S7

Chain EG: 



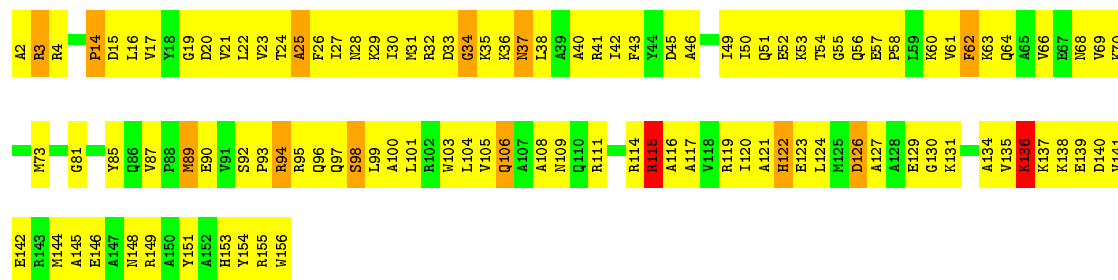
• Molecule 7: 30S ribosomal protein S7

Chain GG: 

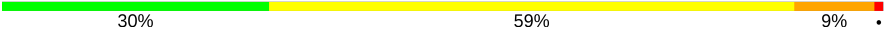


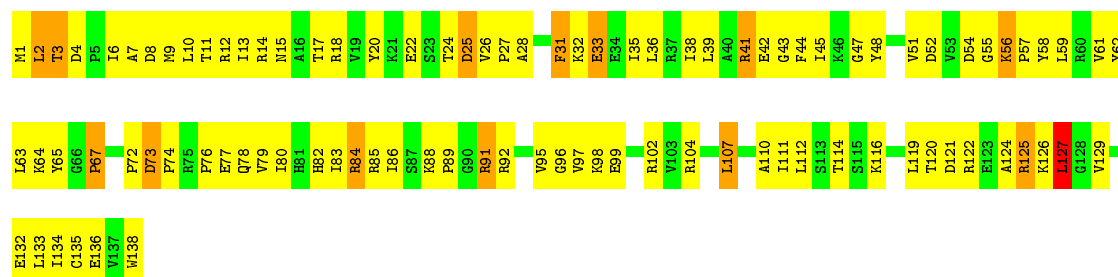
• Molecule 7: 30S ribosomal protein S7

Chain IG: 

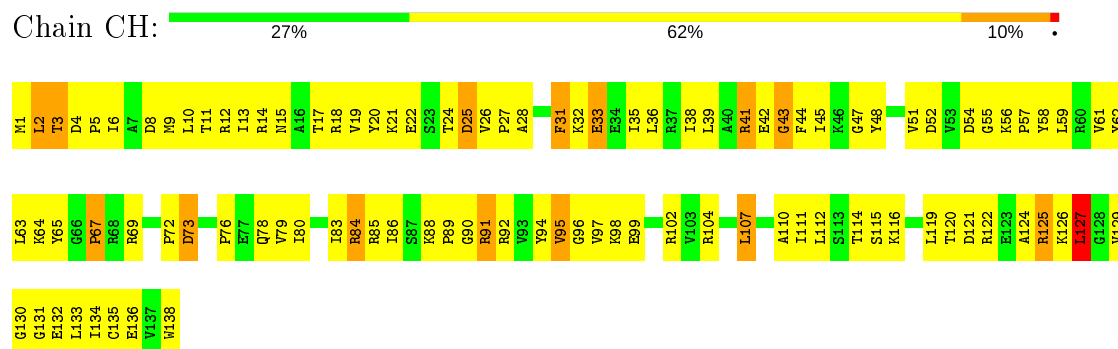


• Molecule 8: 30S ribosomal protein S8

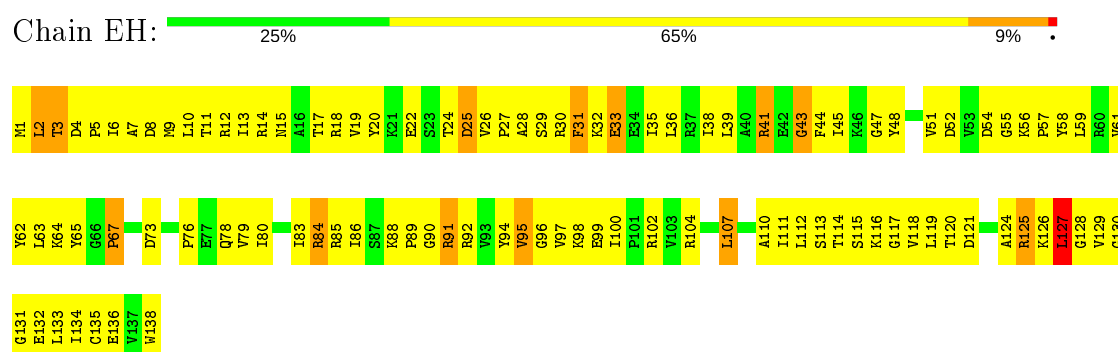
Chain AH: 



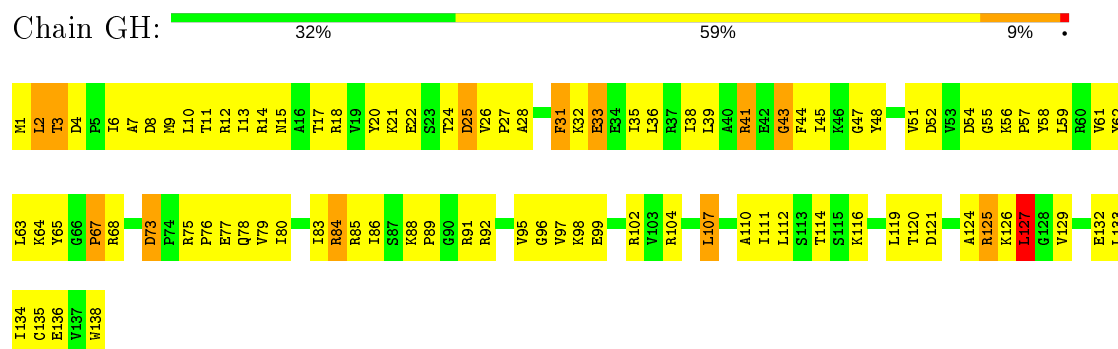
- Molecule 8: 30S ribosomal protein S8



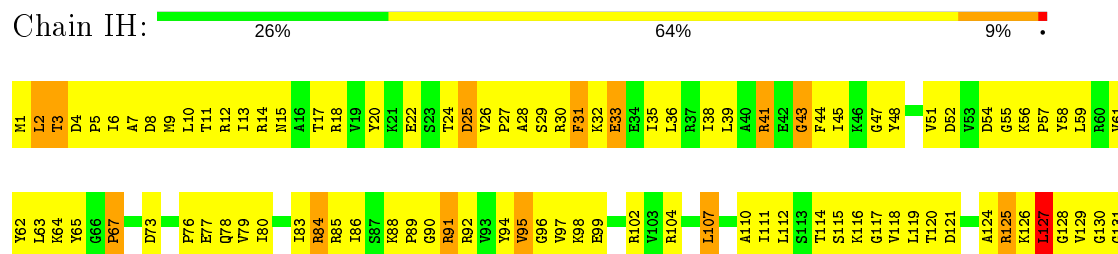
- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8



E132  
L133  
I134  
C135  
E136  
V137  
W138

• Molecule 9: 30S ribosomal protein S9

Chain AI: 22% 61% 17%

E2 Q3 Y4 Y5 G6 T7 G8 R9 R10 K11 K12 E12 A13 A14 V14 A15 A16 R16 V17 I77 F18 F19 L19 R20 R21 P21 G22 N23 G24 G25 R25 V26 V27 T27 V28 N29 N30 G30 Q31 Q32 D32 F33 F34 N34 E35 Y36 Y37 F37 Q38 Q39 G39 L40 V41 R42 A43 A44 V44 A45 A46 L47 E48 E49 P49 L50 R51 R52 V53 D54 A55 A56 P123 L56 G57 A58 F59 D60 A61

Y62 I63 T64 V65 R66 G67 G68 G69 K70 S71 G72 G73 Q73 I74 I75 D75 A76 A77 I77 F78 K78 L79 R80 R81 I81 A82 R83 N83 G84 A84 L85 L86 V86 N89 Y92 R93 R94 A94 K95 L96 R97 P98 L102 L103 T103 R104 D105 A106 R107 A108 V109 E110 R111 K116 H117 K118 A119 R120 A121 A122 P123 Q124 Y125 R128

• Molecule 9: 30S ribosomal protein S9

Chain CI: 23% 60% 17%

E2 Q3 Y4 Y5 G6 T7 G8 R9 R10 K11 K12 E12 A13 A14 V14 A15 A16 R16 V17 I77 F18 F19 L19 R20 R21 P21 G22 N23 G24 G25 R25 V26 V27 T27 V28 N29 N30 G30 Q31 Q32 D32 F33 F34 N34 E35 Y36 Y37 F37 Q38 Q39 G39 L40 V41 R42 A43 A44 V44 A45 A46 L47 E48 E49 P49 L50 R51 R52 V53 D54 A55 A56 P123 L56 G57 A58 F59 D60 A61

Y62 I63 T64 V65 R66 G67 G68 G69 K70 S71 G72 G73 Q73 I74 I75 D75 A76 A77 I77 F78 K78 L79 R80 R81 I81 A82 R83 N83 G84 A84 L85 L86 V86 N89 Y92 R93 R94 A94 K95 L96 R97 P98 L102 L103 T103 R104 D105 A106 R107 A108 V109 E110 R111 K112 K113 K116 H117 K118 A119 R120 A121 A122 P123 Q124 Y125 S126

K127 R128

• Molecule 9: 30S ribosomal protein S9

Chain EI: 24% 60% 16%

E2 Q3 Y4 Y5 G6 T7 G8 R9 R10 K11 K12 E12 A13 A14 V14 A15 A16 R16 V17 I77 F18 F19 L19 R20 R21 P21 G22 N23 G24 G25 R25 V26 V27 T27 V28 N29 N30 G30 Q31 Q32 D32 F33 F34 N34 E35 Y36 Y37 F37 Q38 Q39 G39 L40 V41 R42 A43 A44 V44 A45 A46 L47 E48 E49 P49 L50 R51 R52 V53 D54 A55 A56 P123 L56 G57 A58 F59 D60 A61

I63 T64 V65 R66 G67 G68 G69 K70 S71 G72 G73 Q73 I74 I75 D75 A76 A77 I77 F78 K78 L79 R80 R81 I81 A82 R83 N83 G84 A84 L85 L86 V86 N89 Y92 R93 R94 A94 K95 L96 R97 P98 L102 L103 T103 R104 D105 A106 R107 A108 V109 E110 R111 K112 K113 K116 H117 K118 A119 R120 A121 A122 P123 Q124 Y125 S126

K127 R128

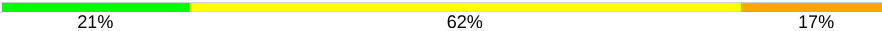
• Molecule 9: 30S ribosomal protein S9

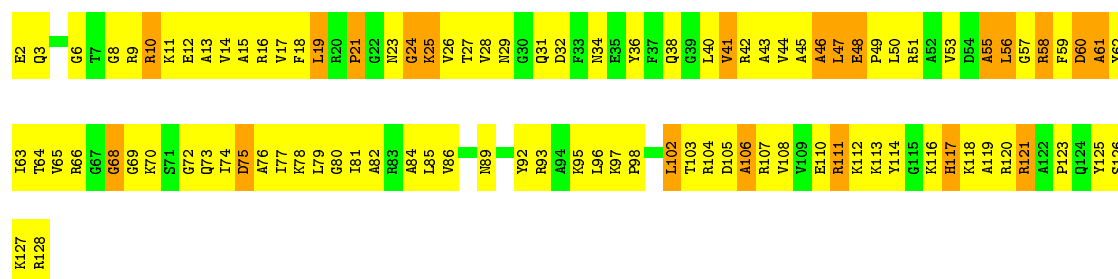
Chain GI: 23% 61% 16%

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Y62 I63 T64 V65 R66 G67 G68 G69 K70 S71 G72 G73 Q73 I74 I75 D75 A76 A77 I77 F78 K78 L79 R80 R81 I81 A82 R83 N83 G84 A84 L85 L86 V86 N89 Y92 R93 R94 A94 K95 L96 R97 P98 L102 L103 T103 R104 D105 A106 R107 A108 V109 E110 R111 K112 K113 K114 G115 K116 H117 K118 A119 R120 A121 A122 P123 Q124 R128

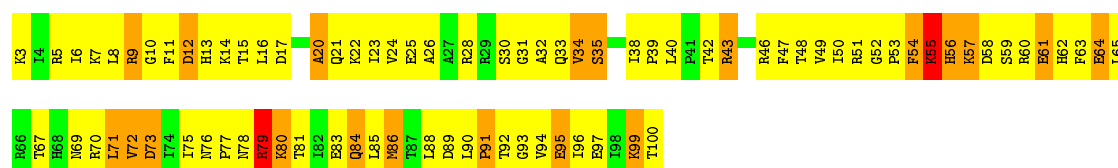
• Molecule 9: 30S ribosomal protein S9

Chain II: 



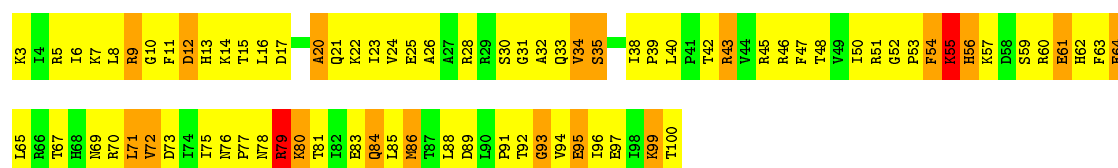
- Molecule 10: 30S ribosomal protein S10

Chain AJ: 



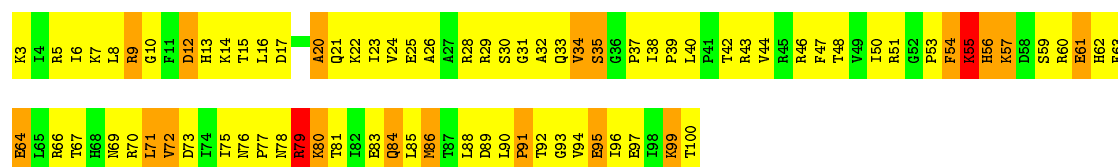
- Molecule 10: 30S ribosomal protein S10

Chain CJ: 




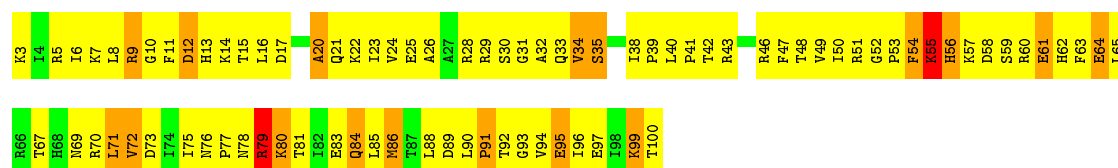
- Molecule 10: 30S ribosomal protein S10

Chain EJ: 

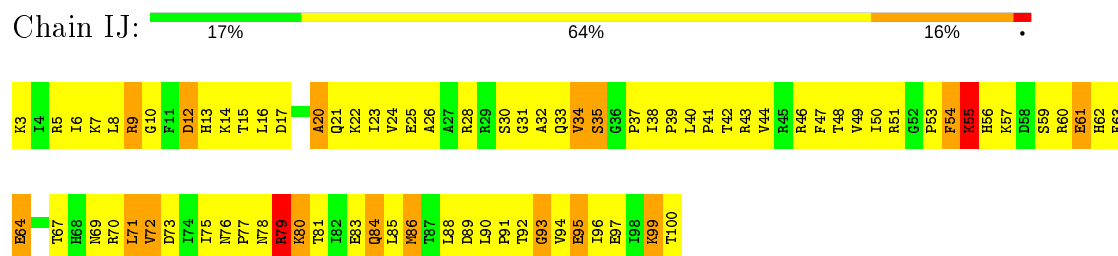


- Molecule 10: 30S ribosomal protein S10

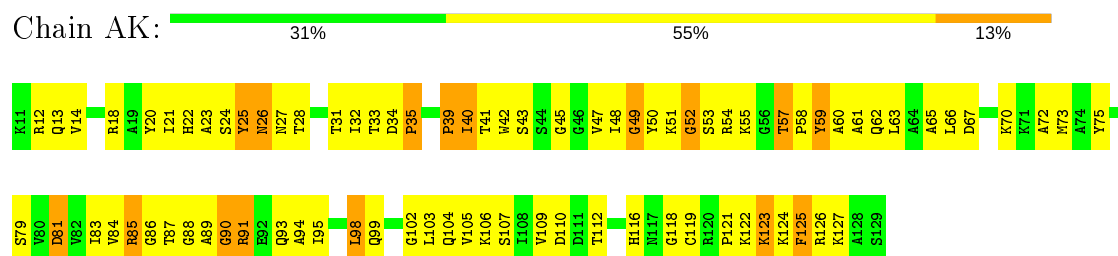
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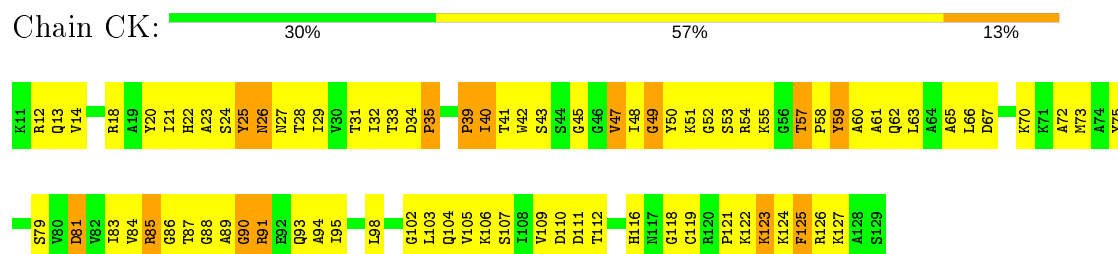
- Molecule 10: 30S ribosomal protein S10



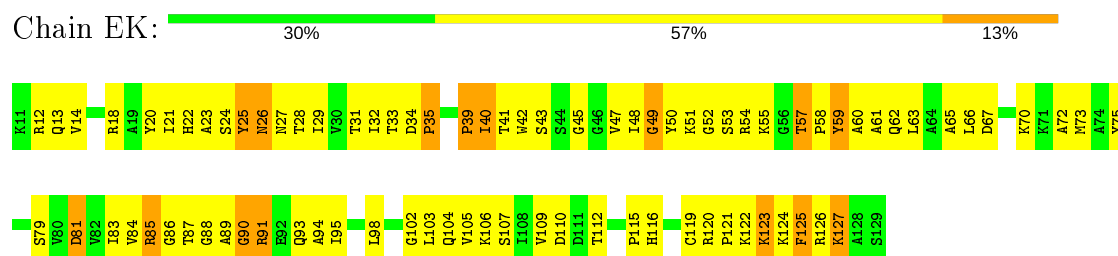
- Molecule 11: 30S ribosomal protein S11



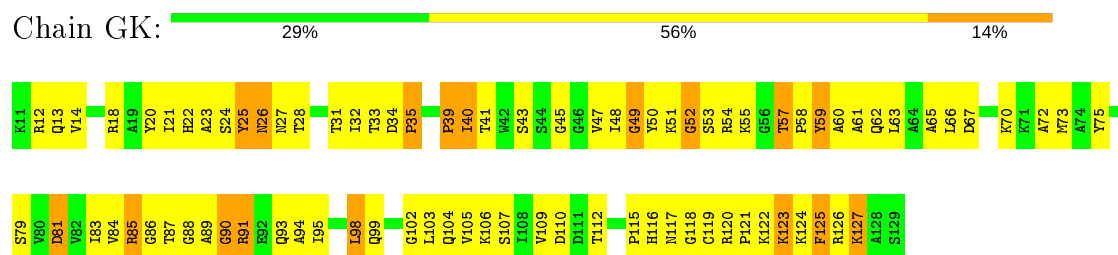
- Molecule 11: 30S ribosomal protein S11



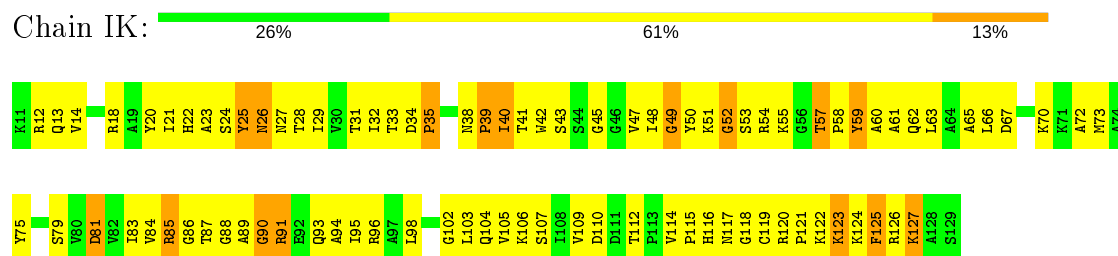
- Molecule 11: 30S ribosomal protein S11



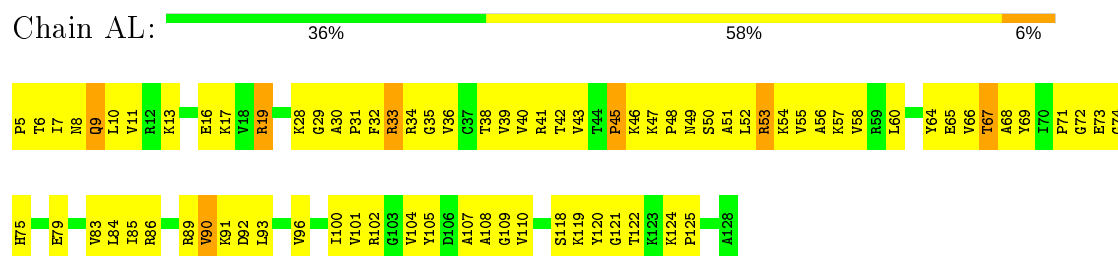
- Molecule 11: 30S ribosomal protein S11



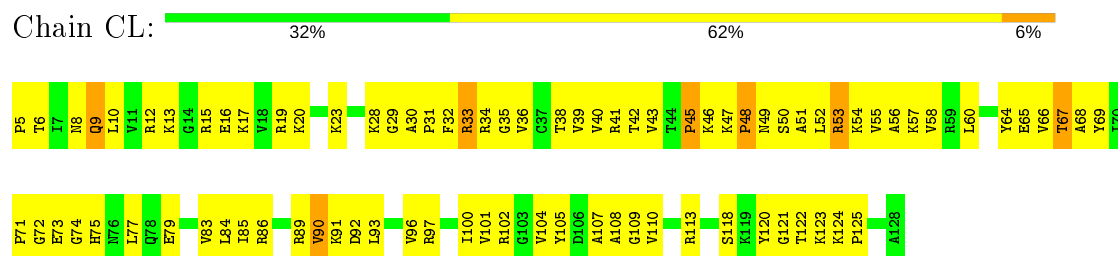
- Molecule 11: 30S ribosomal protein S11



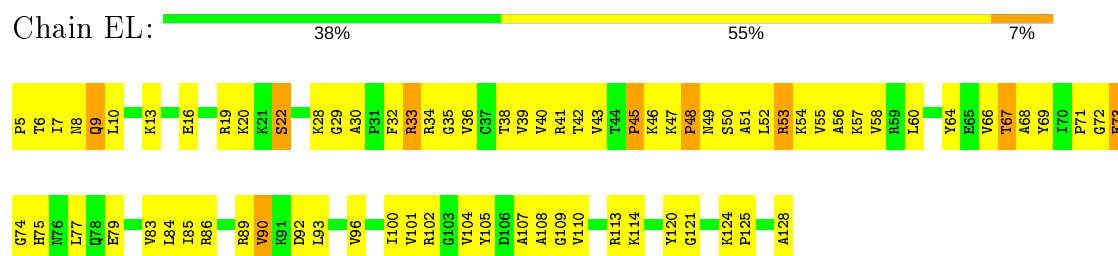
- Molecule 12: 30S ribosomal protein S12



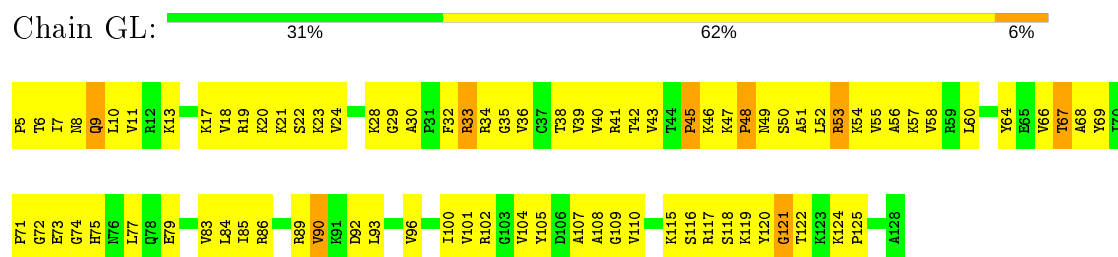
- Molecule 12: 30S ribosomal protein S12



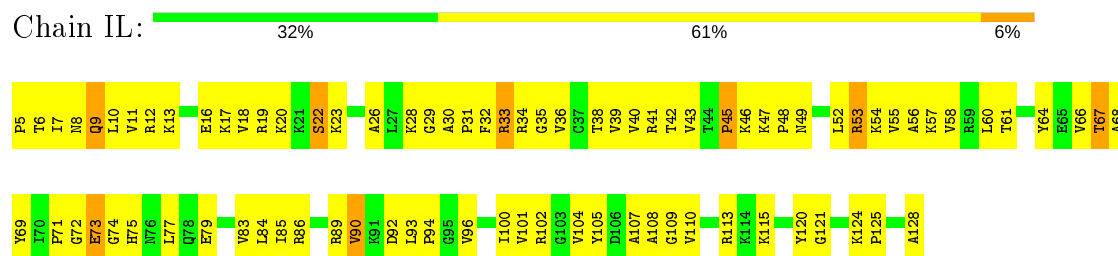
- Molecule 12: 30S ribosomal protein S12



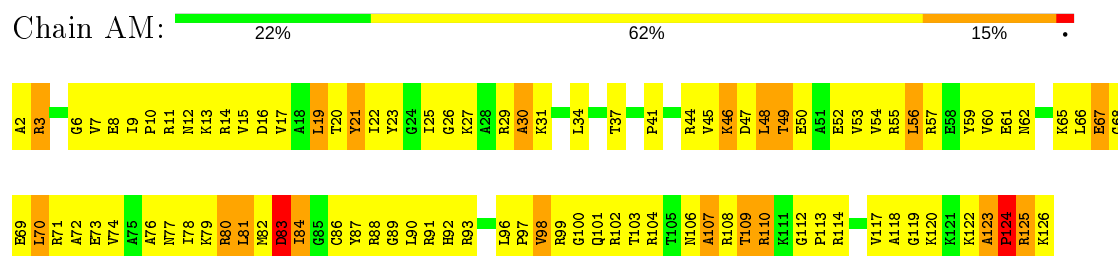
- Molecule 12: 30S ribosomal protein S12



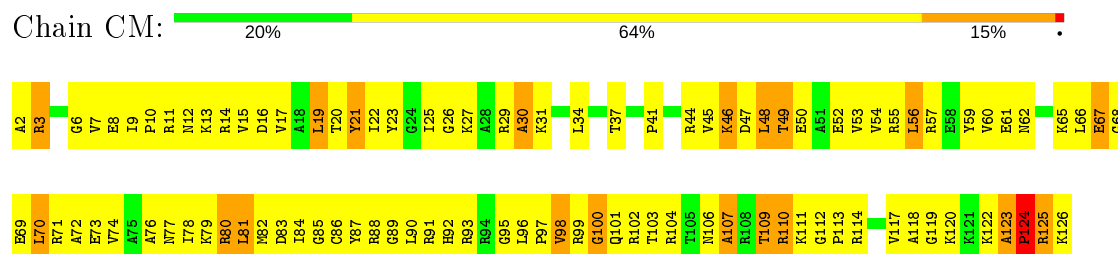
- Molecule 12: 30S ribosomal protein S12



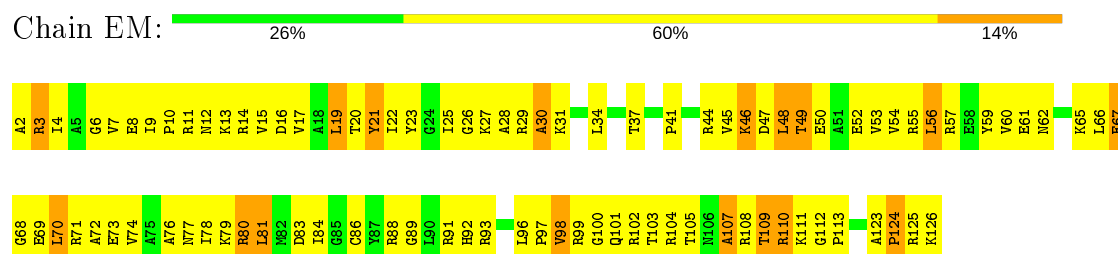
- Molecule 13: 30S ribosomal protein S13



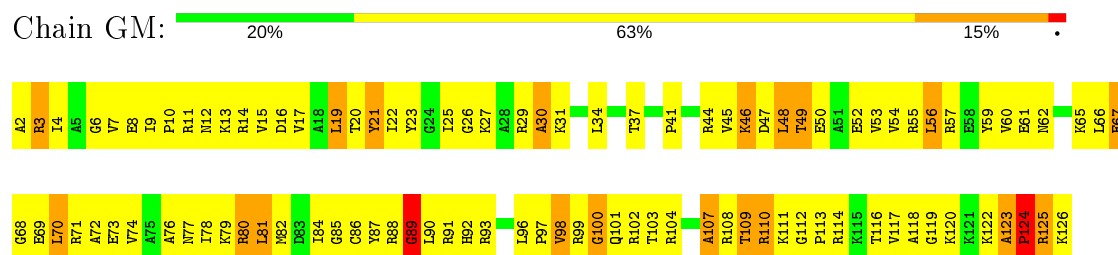
- Molecule 13: 30S ribosomal protein S13



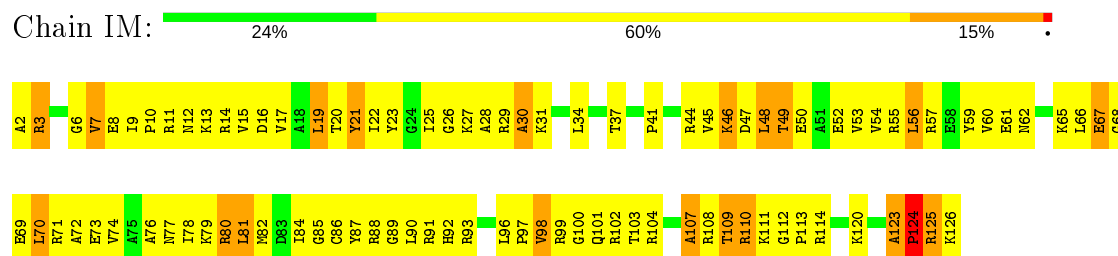
- Molecule 13: 30S ribosomal protein S13



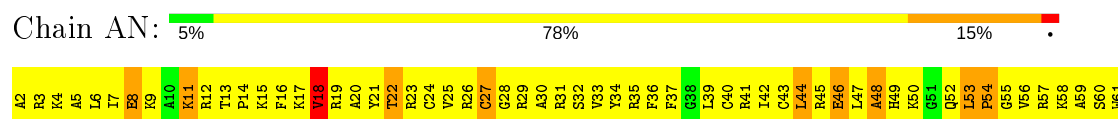
- Molecule 13: 30S ribosomal protein S13



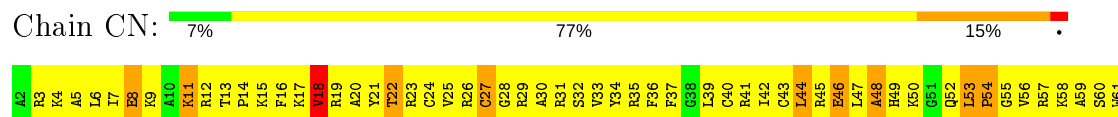
- Molecule 13: 30S ribosomal protein S13



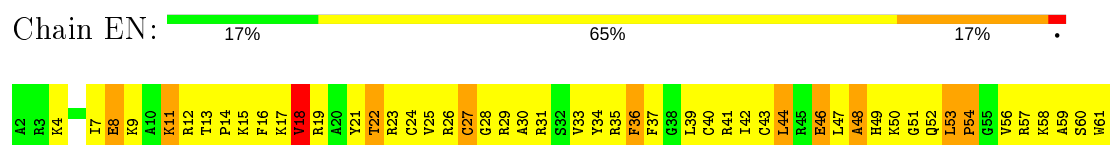
- Molecule 14: 30S ribosomal protein S14



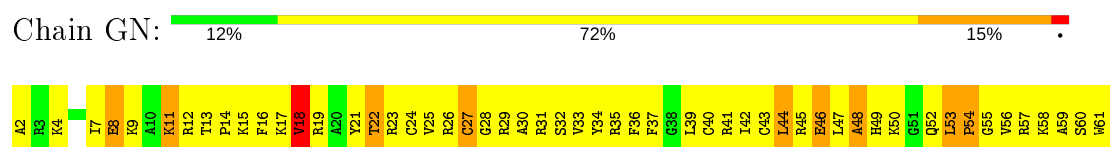
- Molecule 14: 30S ribosomal protein S14



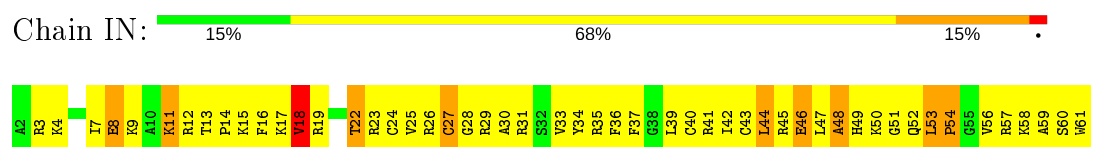
- Molecule 14: 30S ribosomal protein S14



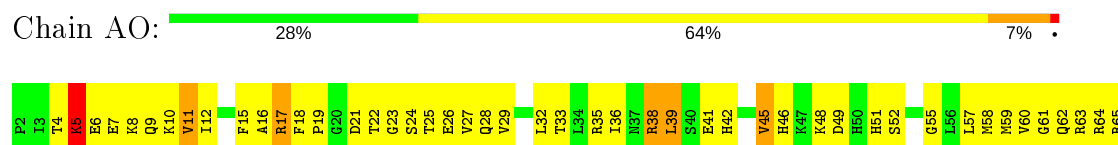
- Molecule 14: 30S ribosomal protein S14

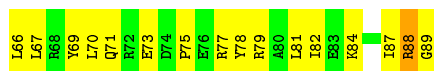


- Molecule 14: 30S ribosomal protein S14



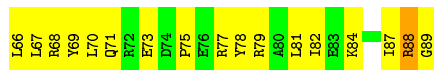
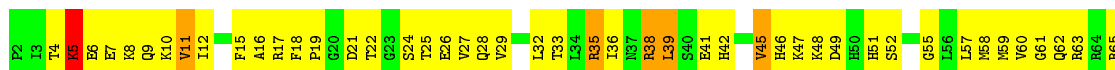
- Molecule 15: 30S ribosomal protein S15





- Molecule 15: 30S ribosomal protein S15

Chain CO: 28% 64% 7%



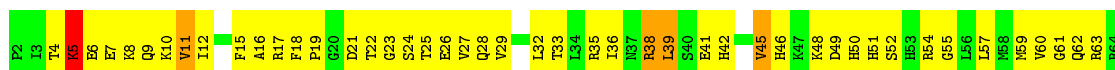
- Molecule 15: 30S ribosomal protein S15

Chain EO: 28% 63% 9%



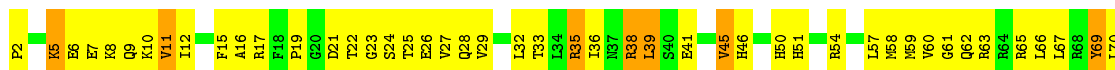
- Molecule 15: 30S ribosomal protein S15

Chain GO: 28% 64% 7%



- Molecule 15: 30S ribosomal protein S15

Chain IO: 34% 57% 9%



- Molecule 16: 30S ribosomal protein S16

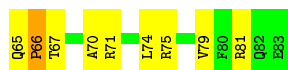
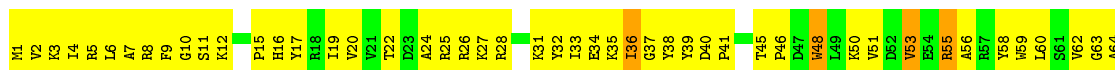
Chain AP: 31% 61% 7%





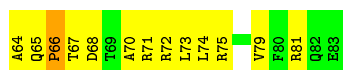
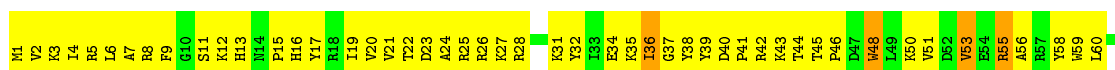
- Molecule 16: 30S ribosomal protein S16

Chain CP: 31% 63% 6%



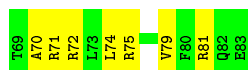
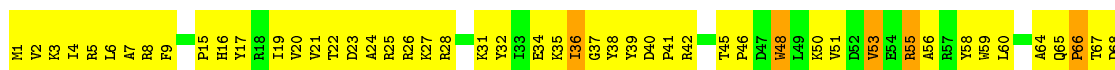
- Molecule 16: 30S ribosomal protein S16

Chain EP: 25% 69% 6%



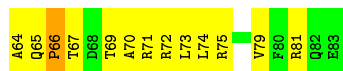
- Molecule 16: 30S ribosomal protein S16

Chain GP: 33% 61% 6%



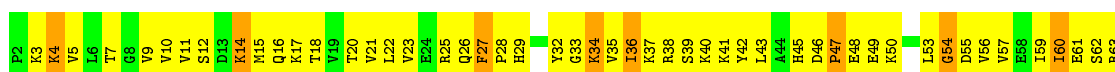
- Molecule 16: 30S ribosomal protein S16

Chain IP: 27% 67% 6%



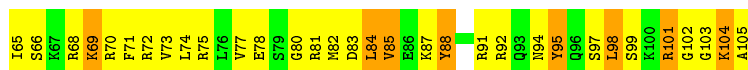
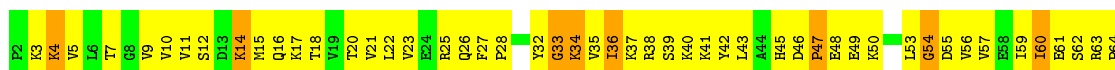
- Molecule 17: 30S ribosomal protein S17

Chain AQ: 21% 63% 15%

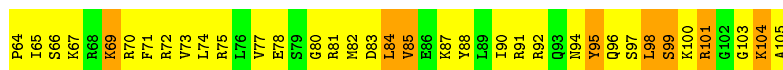
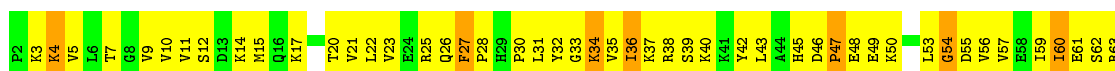




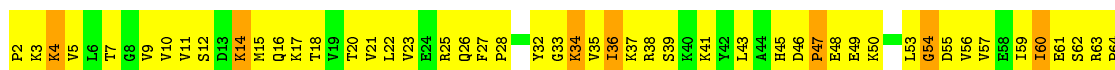
- Molecule 17: 30S ribosomal protein S17



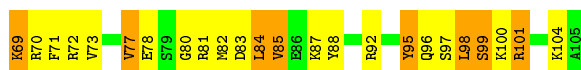
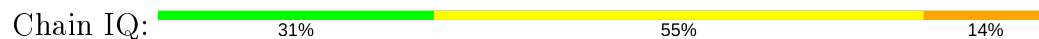
- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17

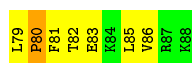


- Molecule 17: 30S ribosomal protein S17



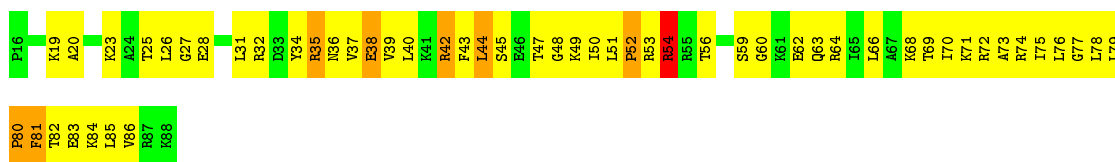
- Molecule 18: 30S ribosomal protein S18





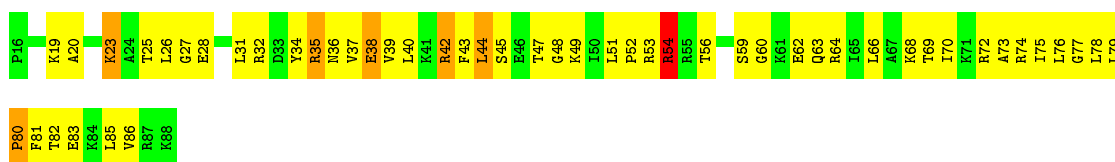
- Molecule 18: 30S ribosomal protein S18

Chain CR: 26% 63% 10% .



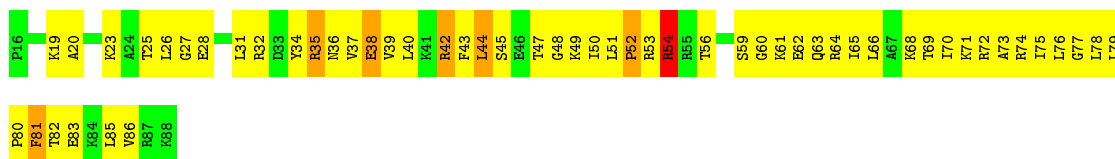
- Molecule 18: 30S ribosomal protein S18

Chain ER: 30% 60% 8% .



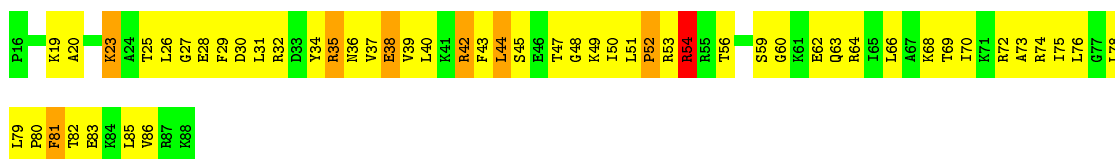
- Molecule 18: 30S ribosomal protein S18

Chain GR: 25% 66% 8% .



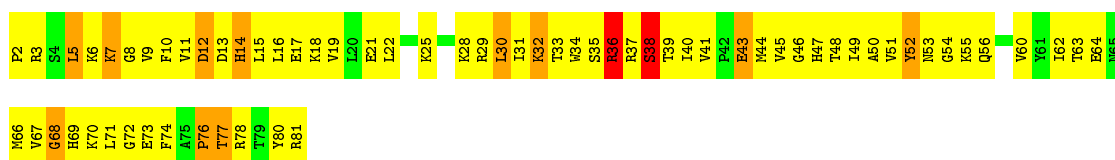
- Molecule 18: 30S ribosomal protein S18

Chain IR: 27% 62% 10% .

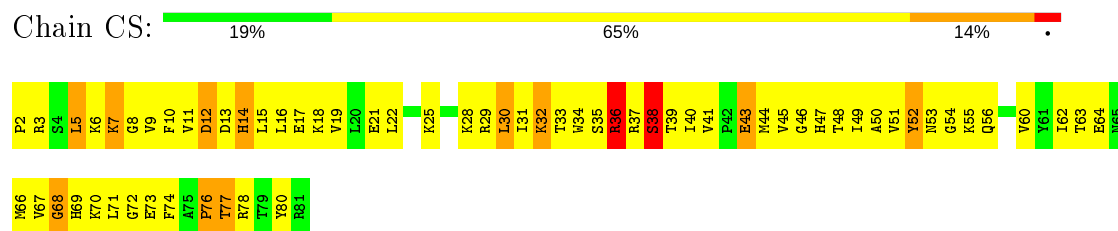


- Molecule 19: 30S ribosomal protein S19

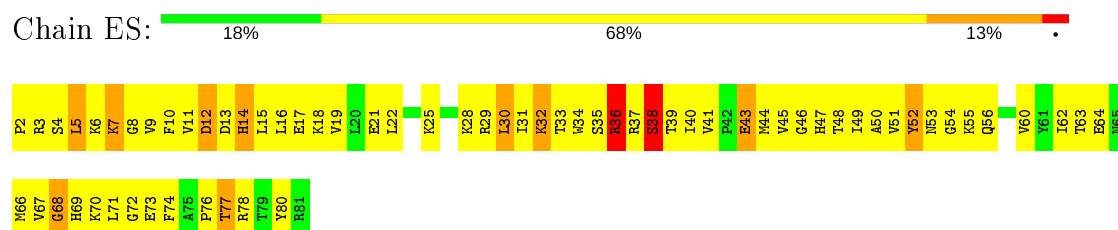
Chain AS: 18% 66% 14% .



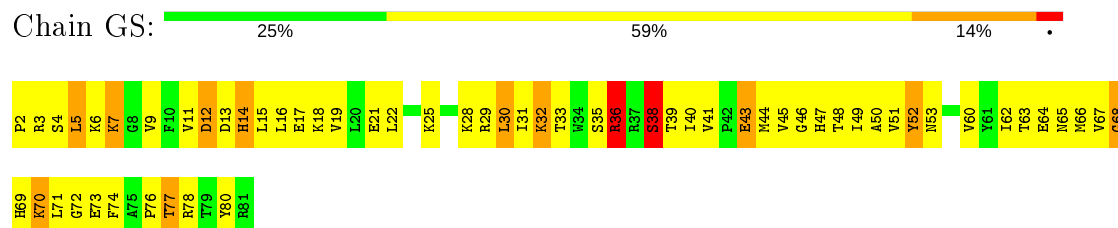
## • Molecule 19: 30S ribosomal protein S19



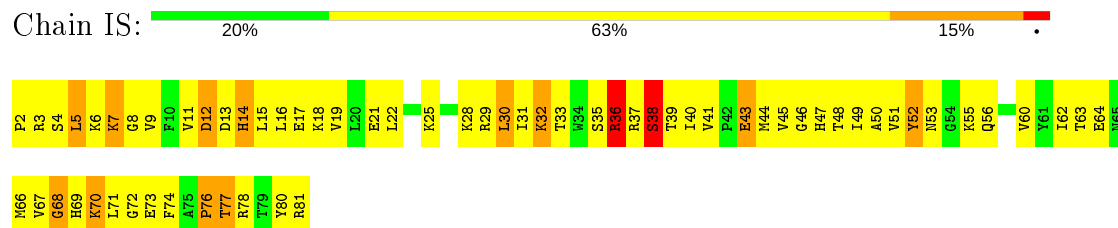
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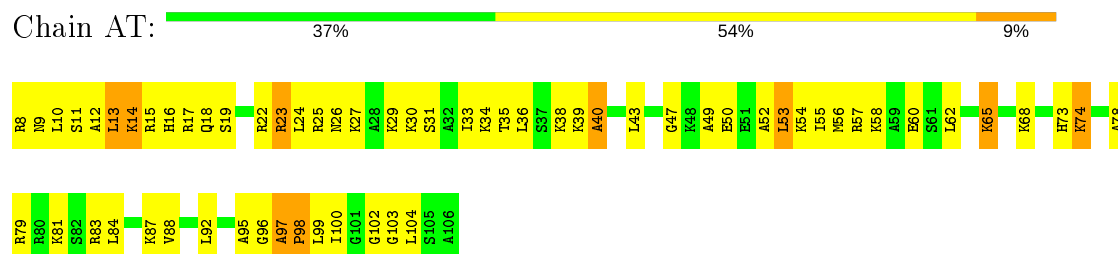
## • Molecule 19: 30S ribosomal protein S19



## • Molecule 19: 30S ribosomal protein S19

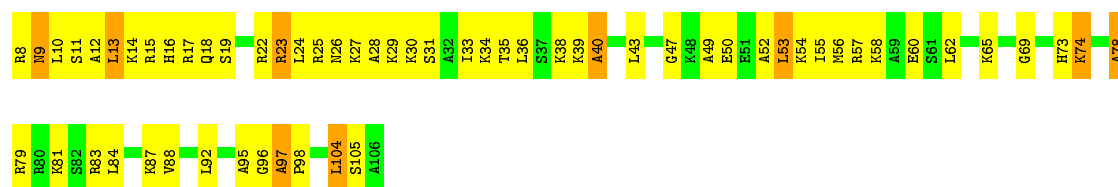


## • Molecule 20: 30S ribosomal protein S20




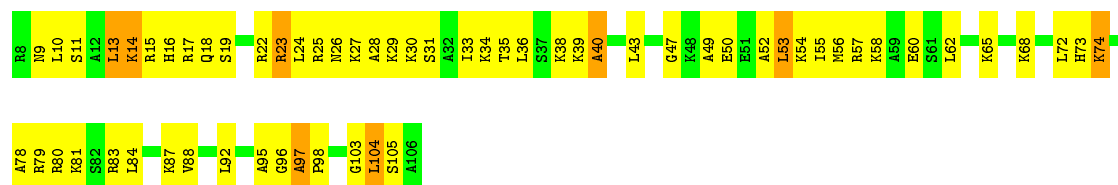
## • Molecule 20: 30S ribosomal protein S20

Chain CT:  39% 52% 9%



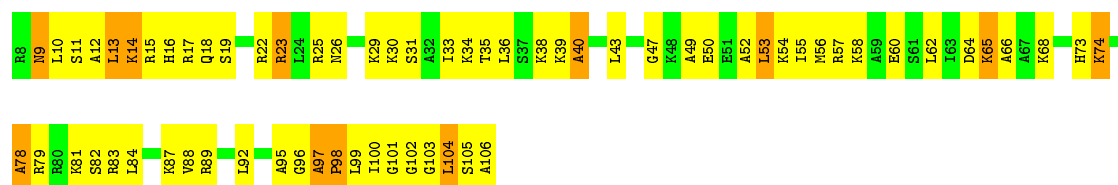
- Molecule 20: 30S ribosomal protein S20

Chain ET:  38% 54% 8%



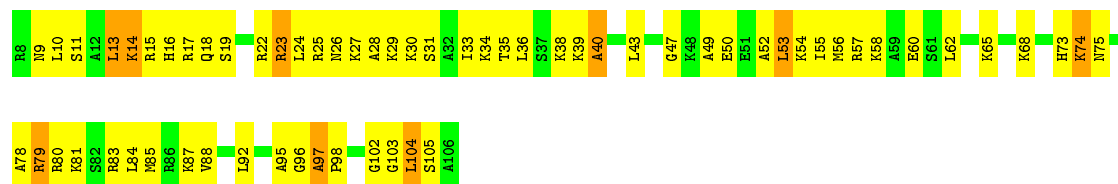
- Molecule 20: 30S ribosomal protein S20

Chain GT:  33% 55% 12%




- Molecule 20: 30S ribosomal protein S20

Chain IT:  36% 55% 9%




- Molecule 21: protein Y

Chain Aa:  79% 21%

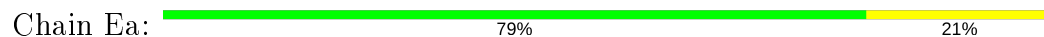


- Molecule 21: protein Y

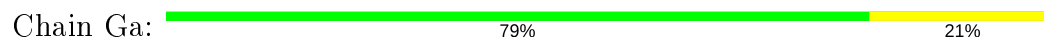
Chain Ca:  79% 21%



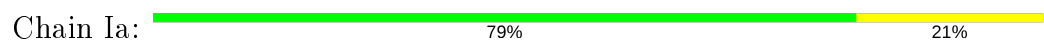
- Molecule 21: protein Y



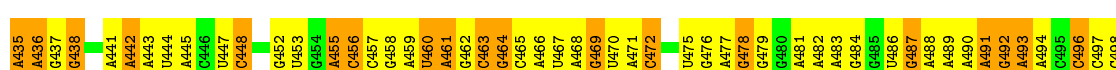
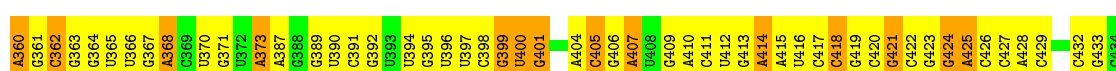
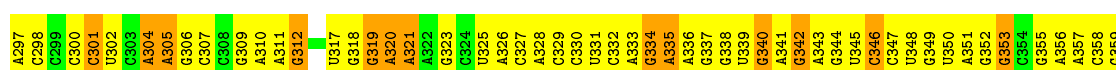
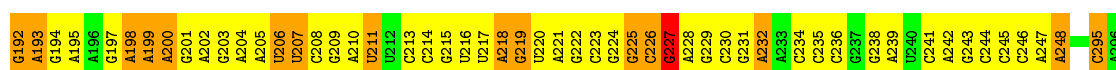
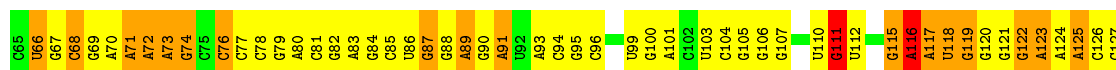
- Molecule 21: protein Y



- Molecule 21: protein Y

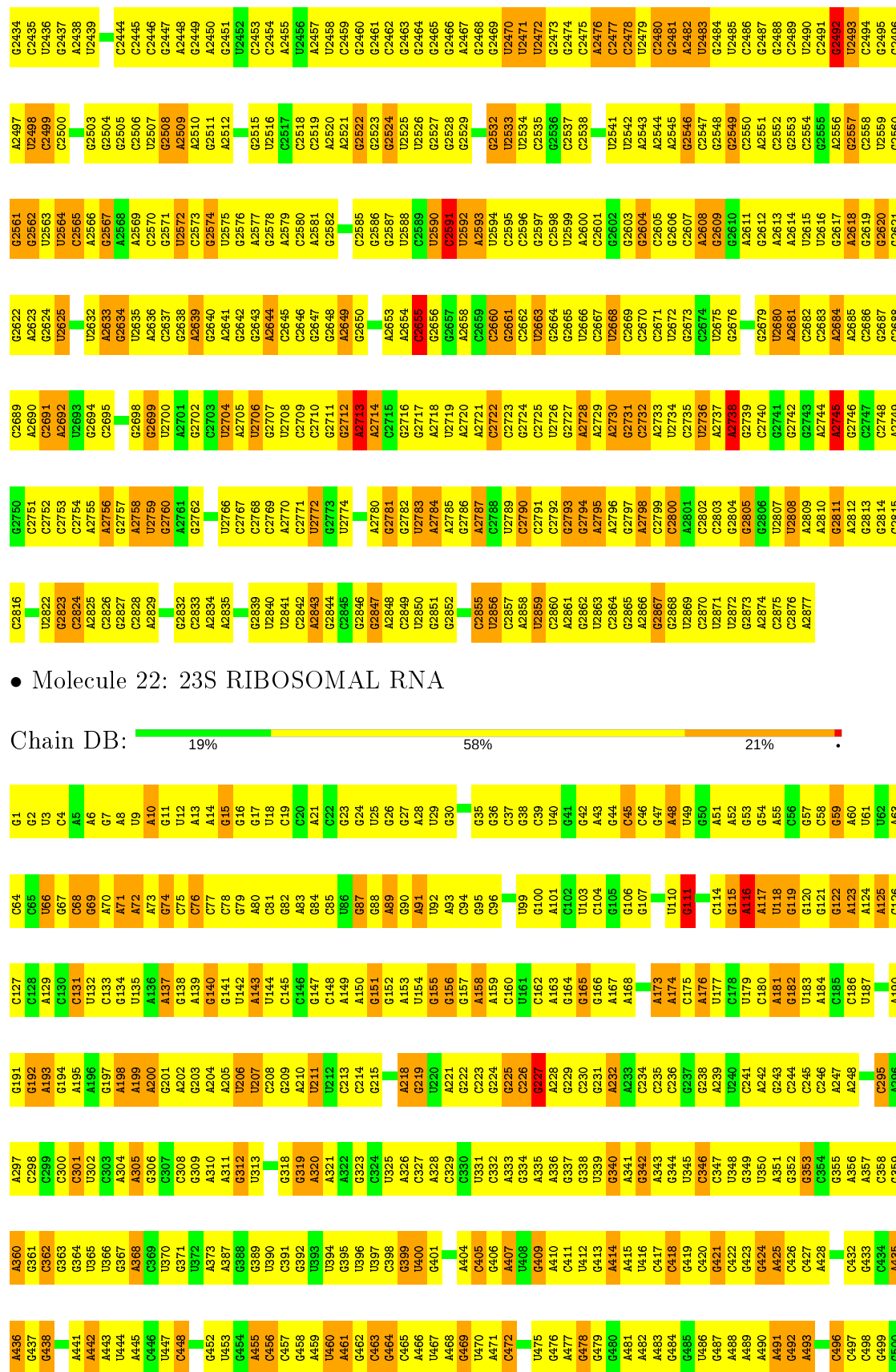


- Molecule 22: 23S RIBOSOMAL RNA



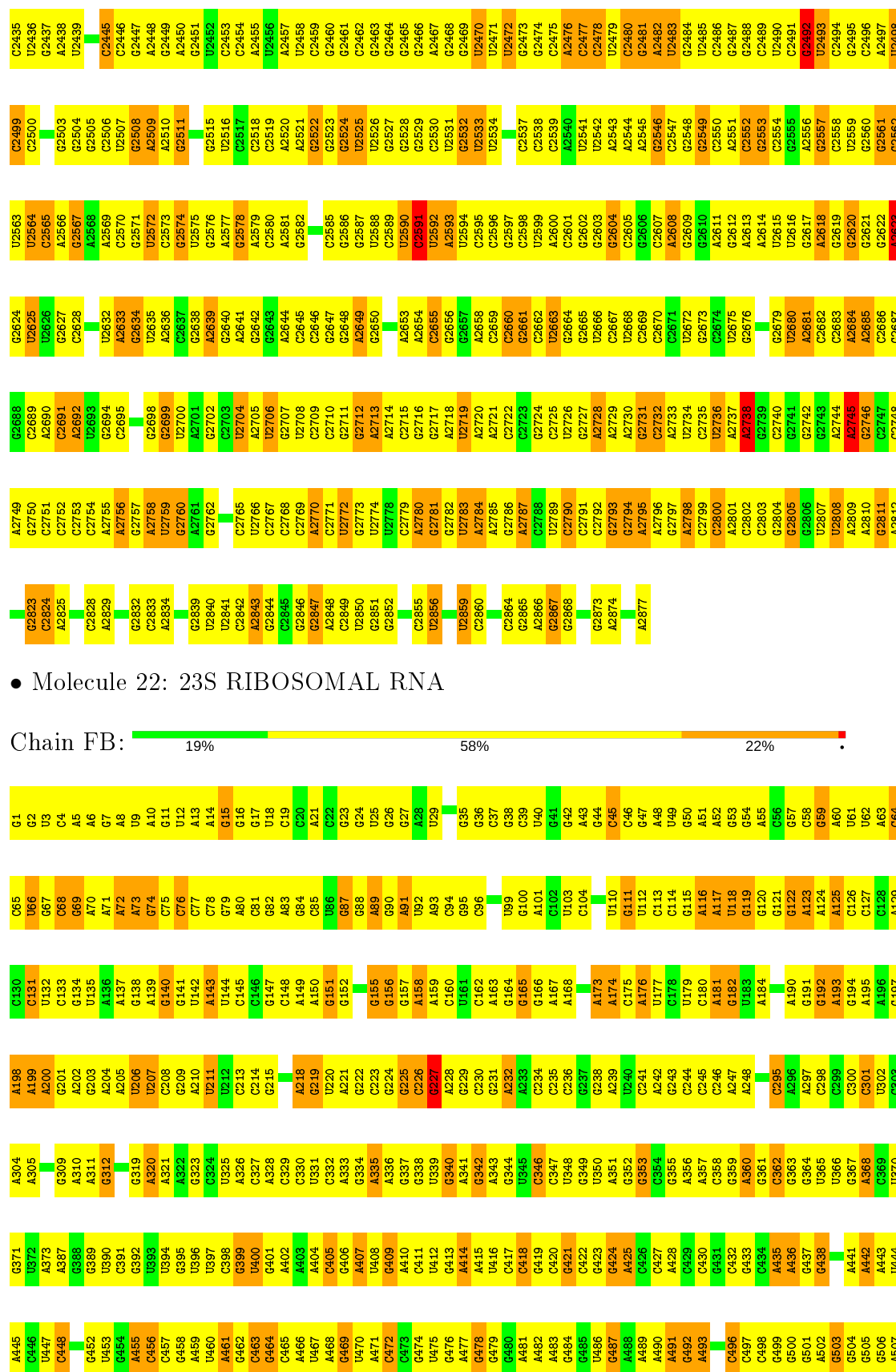
WORLDWIDE  
**PDB**  
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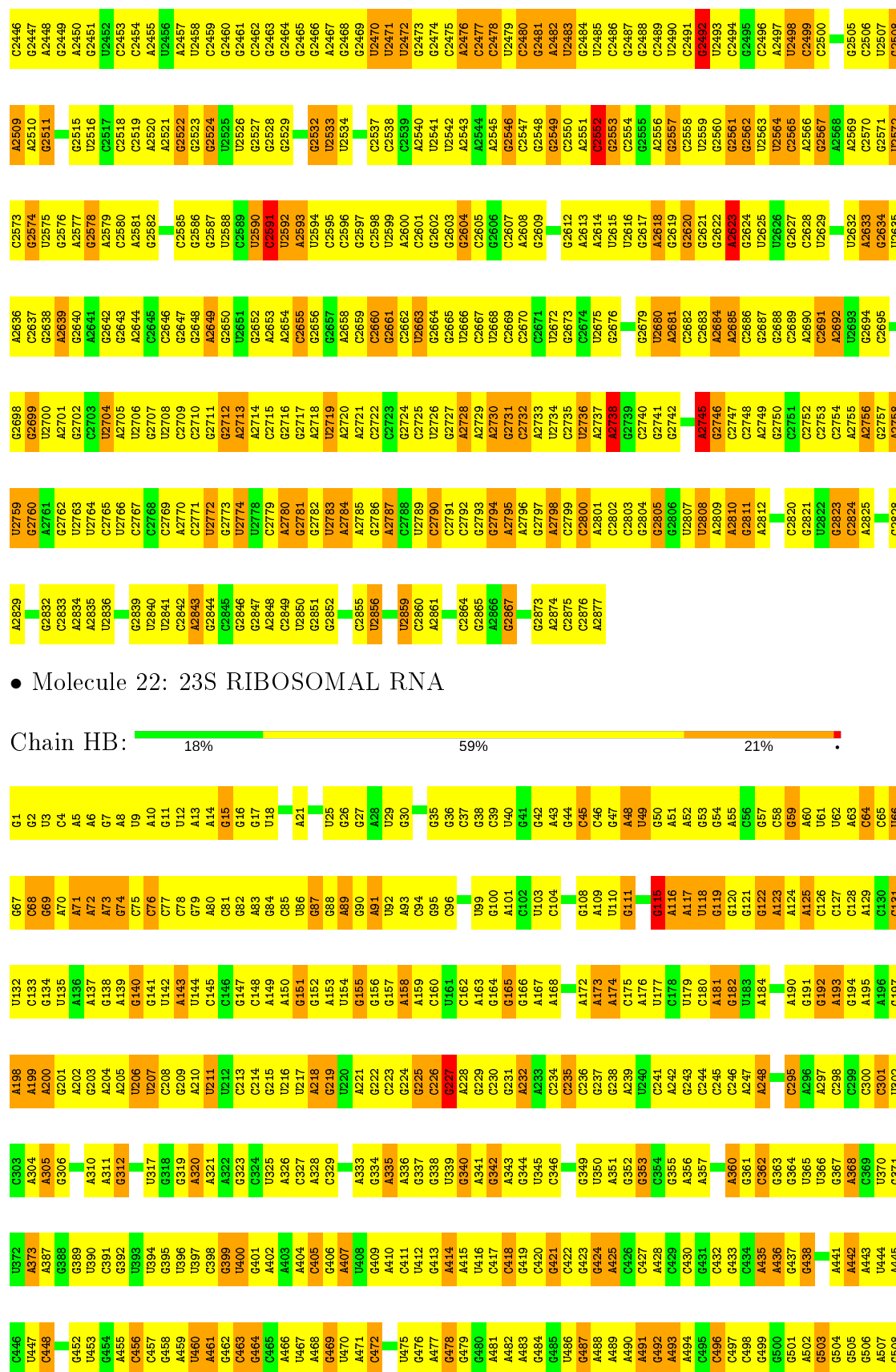
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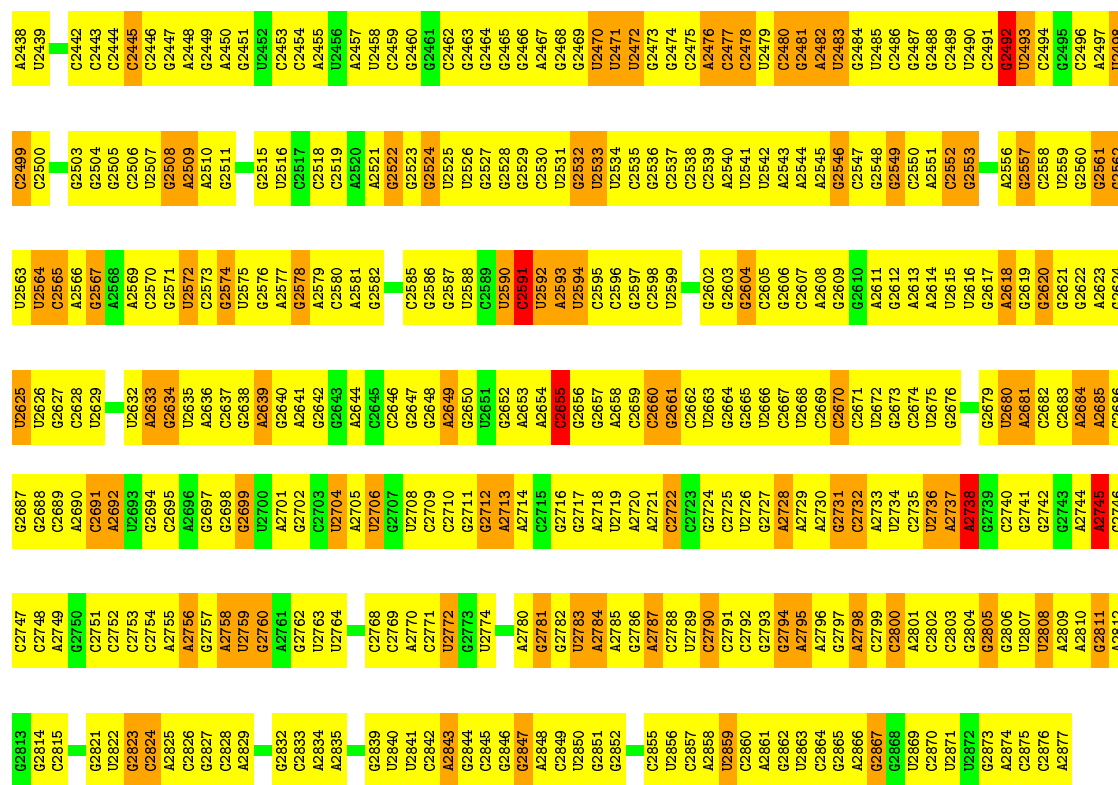




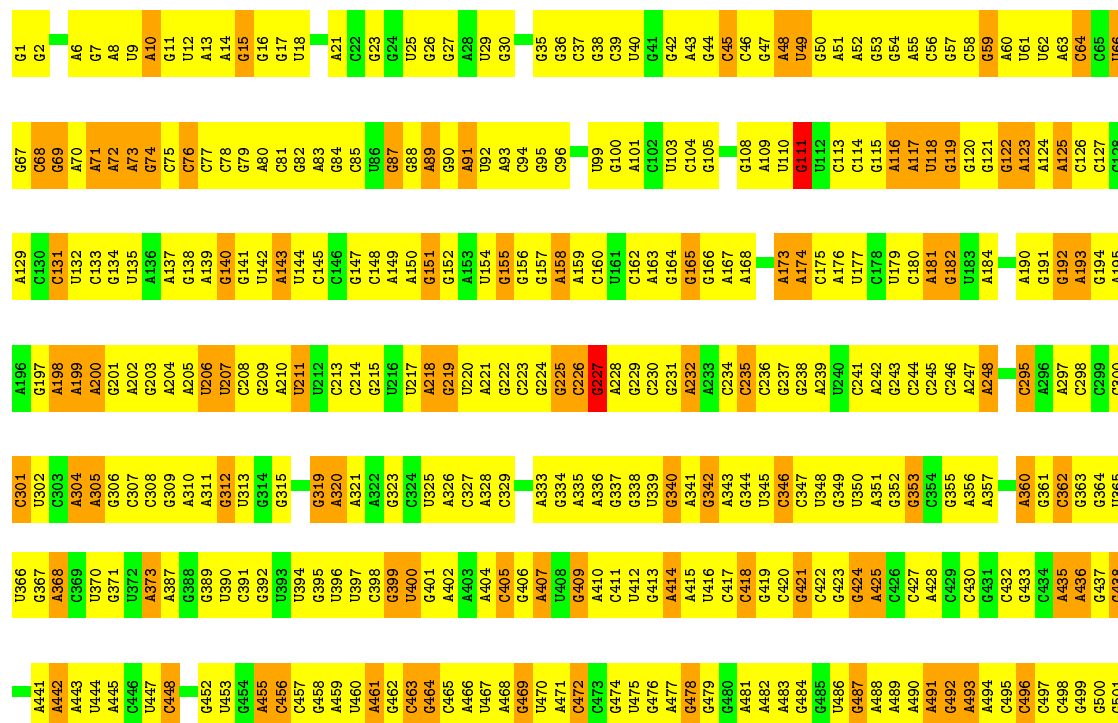


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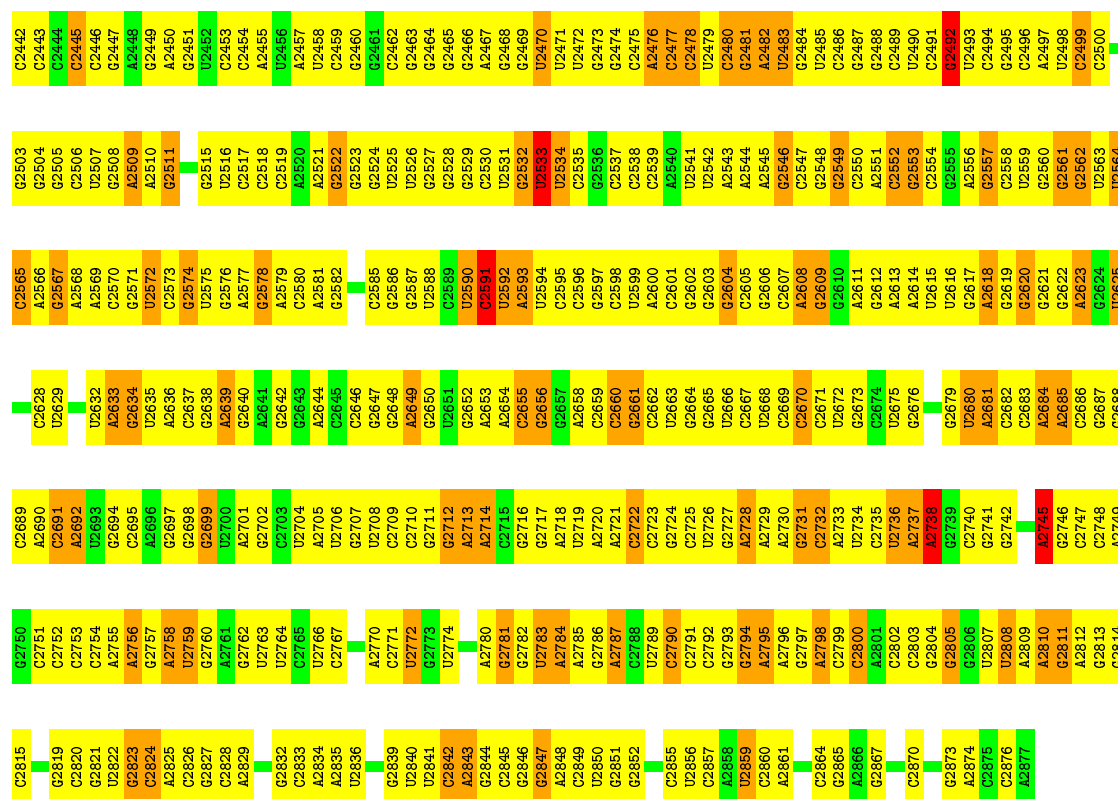


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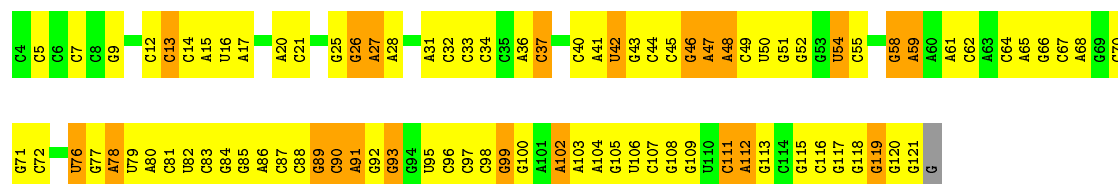


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	G1356	A1292	A1227		A1084	U1015	G953	C889	A821	C759	G696	G634	U570	U509
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A2412	A2352	A2288	A2226	A3176	G3110	U2024	U1959	A1898	A1845	A1780	A1714	G1652	C1581	A1511
A2413	G2353	C3177	C2227	C3178	C3111	A2025	A1960	U1900	A1846	C1781	A1715	C1653	A1582	
G2414	G2354	C3179	U2228	C3179	G3112	C2026	A1961	A1901	G1847	A1782	A1717	C1655	A1583	C1514
	A2355	U3180	G2229	U3180	U3113	C2027	A1964	A1902	U1848	G1783	A1718	U1656	A1584	
G2419	A2356	C2292	G2230	U3185	G3116	U2030	U1967	G1905	G1850	C1786	G1721	A1658	A1588	A1525
C2420	A2357	G2293	G2231	U3186	G3116	A2035	G1968	G1906	G1852	U1787	G1722	G1660	G1589	U1526
C2421	C2358	U2294	G2232	C3187	A3117	U2031	G1969	C1907	G1854	U1788	U1723	C1661	G1527	G1527
C2422	G2359	C2295	C2233	U3188	U3118	A2034	G1970	C1908	G1855	U1789	C1725	G1662	C1528	C1528
G2423	G2360	U2296	G2234	U3189	A3119	G2036	C1971	U1909	G1856	C1791	U1726	G1663	A1595	U1529
G2424	C2361	G2297	G2235	U3190	G3120	A2037	C1972	A1910	U1857	C1791	C1727	G1665	A1596	C1531
C2425	G2362	U2298	G2236	G3190	G3121	G2038	U1971	A1911	G1858	C1792	C1727	C1666	A1597	A1532
G2426	C2363	A2299	G2237	A3191	G3122	A2040	U1976	G1912	G1859	A1793	C1731	A1667	U1600	C1535
A2427	G2364	G2300	C2239	A3191	G3123	A2041	C1977	A1915	G1860	A1796	U1732	G1668	U1601	G1536
U2428	U2365	A2301	C2240	G3191	G3124	A2042	U1978	G1916	C3870	A1800	C1734	G1670	U1537	A1523
A2429	U2366	G2302	U2241	G3196	G3125	A2043	U1979	C1917	A3871	C1801	U1738	A1671	U1608	A1538
A2430	A2367	C2303	C2242	U3197	G3126	A2044	A1980	A1918	A3872	C1802	U1739	A1672	G1609	U1539
C2431	G2368	C2304	C2243	A2181	A3126	A2045	A1981	A1919	G3873	A1803	G1740	C1673	G1540	G1541
A2432	U2369	C2305	C2244	U3198	G3127	C2046	C1982	A1920	C3874	G1804	G1741	C1675	C1614	G1542
G2433	G2370	A2306	A2245	C2183	G3128	C2047	G1983	U1921	A3875	U1805	G1742	G1676	G1543	G1544
G2434	G2371	A2307	A2246	C2184	G3129	C2048	A1984	U1922	A3876	G1806	C1743	G1678		
C2435	A2372	A2308	A2247	U2185	C3129	A2049	A1985	U1923	A3877					
A2436	G2373	G2309	A2248	G2186	G3130	C2046								
G2437	C2374	G2310	U2249	A2187	G3131	C2047								
A2438	G2375	U2311	G2250	A2188	A3134	C2048								
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U2440	G2377	G2313	A2252	A2191	C3136									

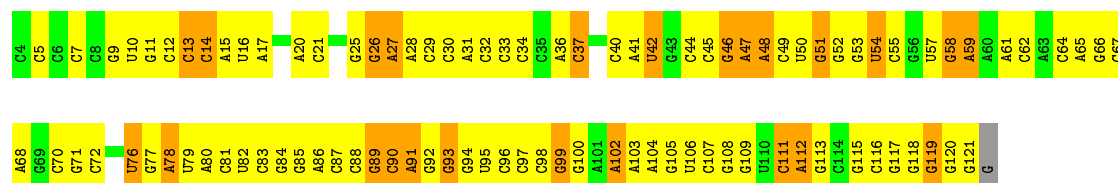


Chain BA: 24% 57% 18%



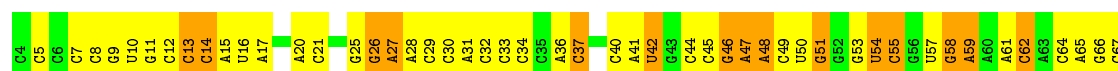
• Molecule 23: 5S RIBOSOMAL RNA

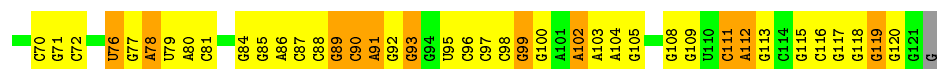
Chain DA: 18% 61% 20%



• Molecule 23: 5S RIBOSOMAL RNA

Chain FA: 24% 53% 22%





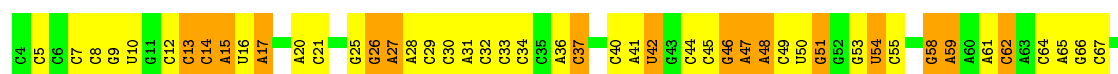
• Molecule 23: 5S RIBOSOMAL RNA

Chain HA: 24% 56% 18%



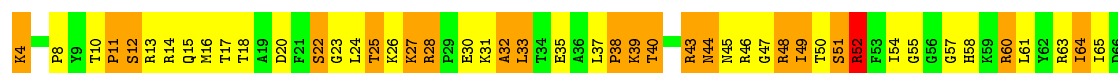
• Molecule 23: 5S RIBOSOMAL RNA

Chain JA: 27% 50% 22%



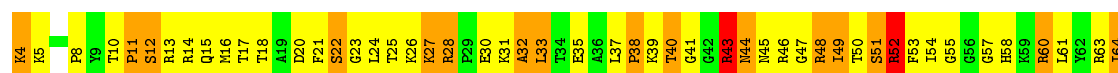
• Molecule 24: 50S ribosomal protein L2

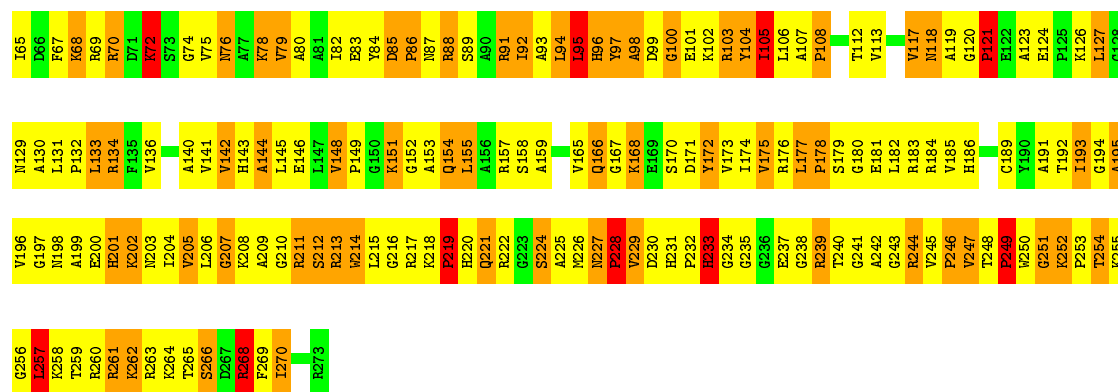
Chain BD: 20% 46% 30%



• Molecule 24: 50S ribosomal protein L2

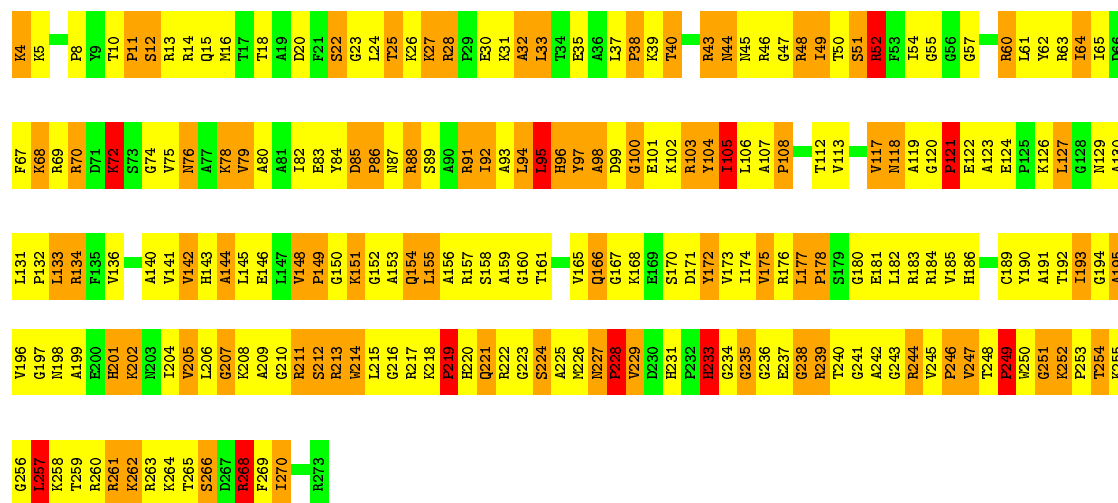
Chain DD: 18% 50% 28%





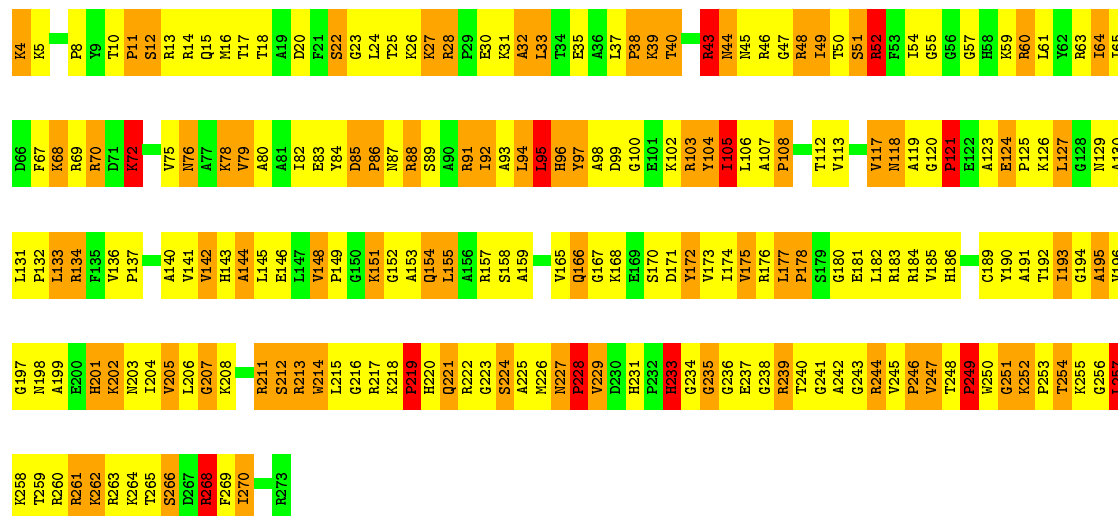
• Molecule 24: 50S ribosomal protein L2

Chain FD: 18% 48% 30%

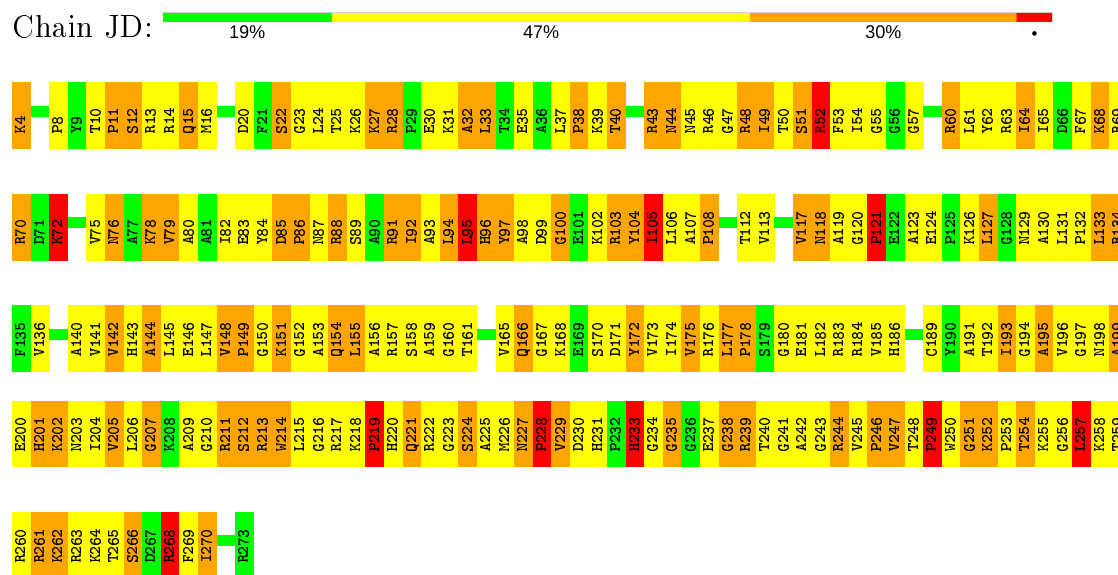


• Molecule 24: 50S ribosomal protein L2

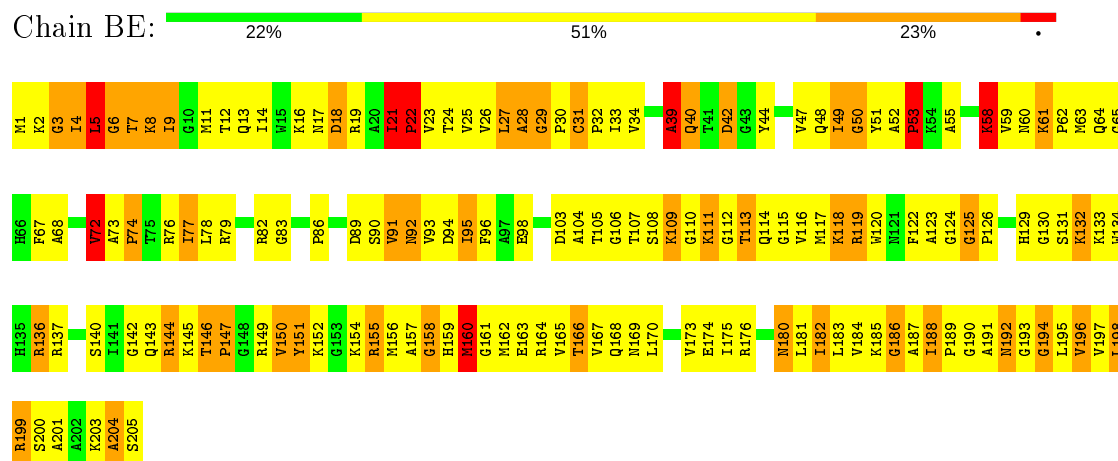
Chain HD: 20% 47% 28%



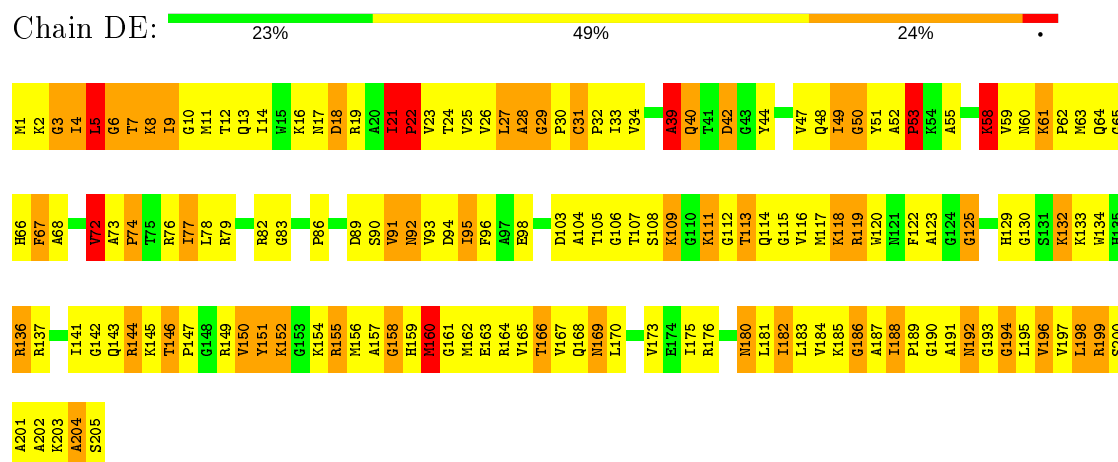
- Molecule 24: 50S ribosomal protein L2



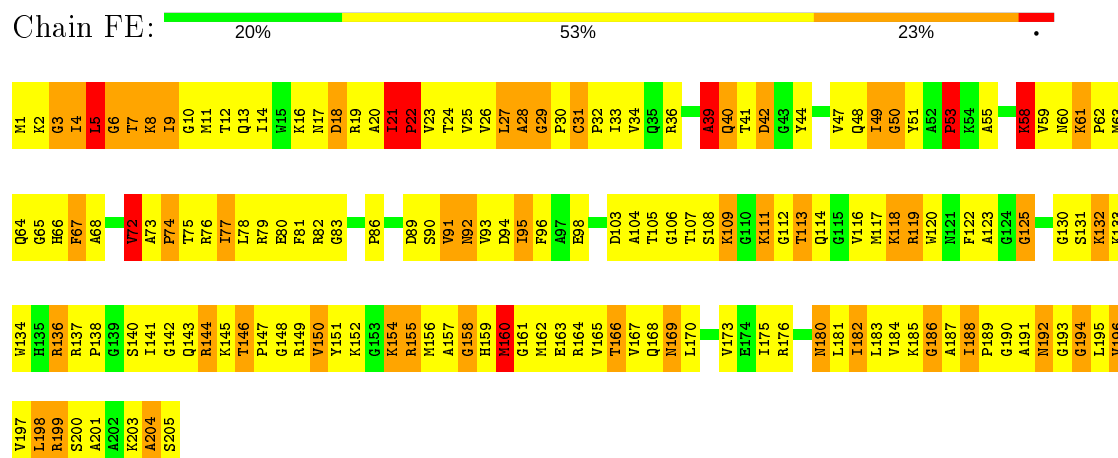
- Molecule 25: 50S ribosomal protein L3



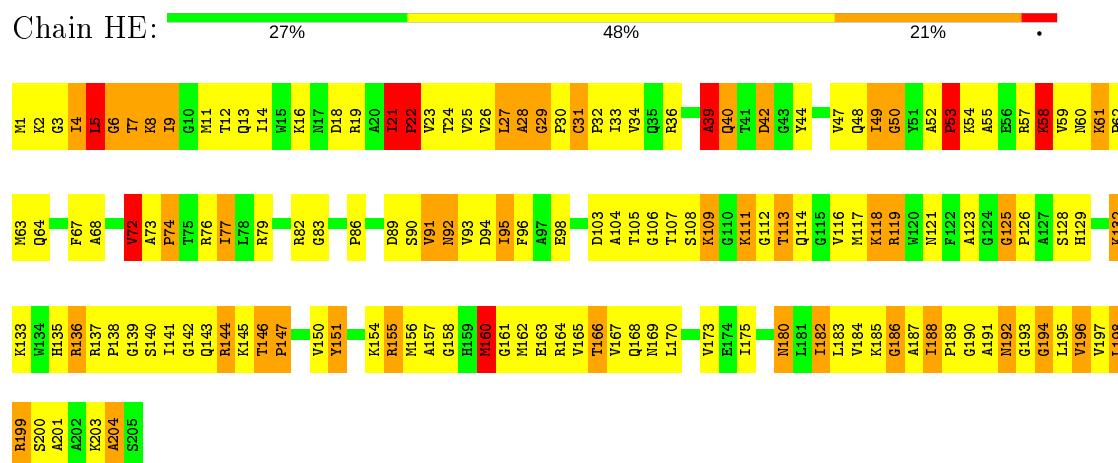
- Molecule 25: 50S ribosomal protein L3



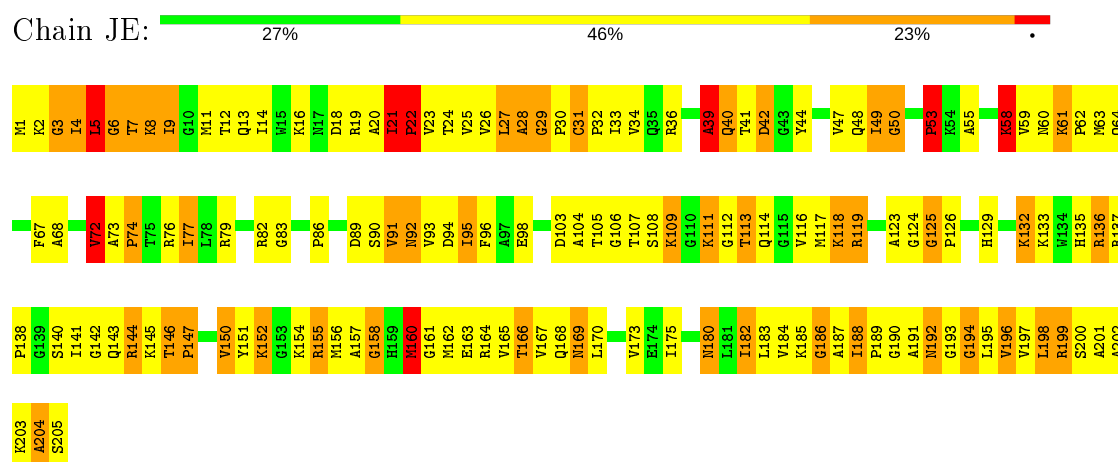
- Molecule 25: 50S ribosomal protein L3



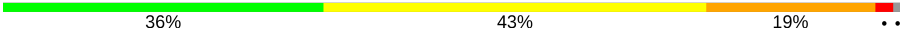
- Molecule 25: 50S ribosomal protein L3

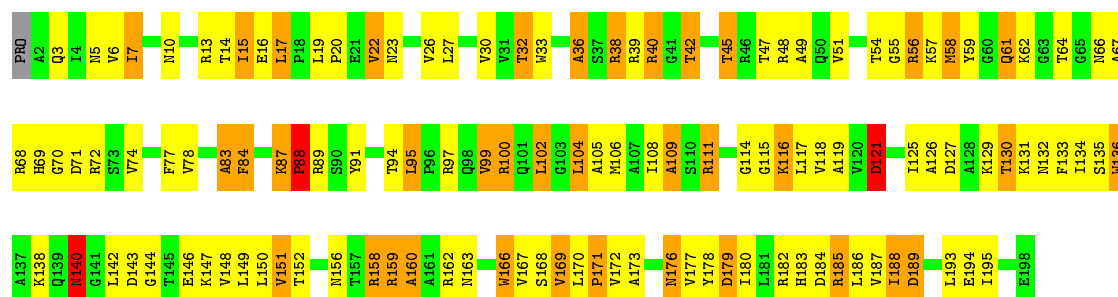


- Molecule 25: 50S ribosomal protein L3



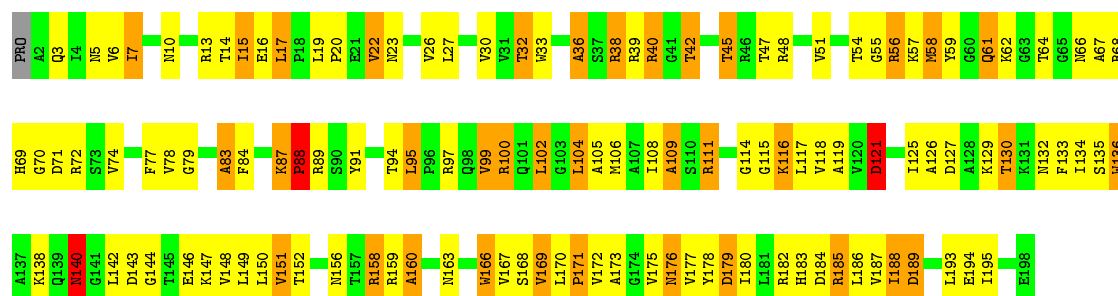
- Molecule 26: 50S ribosomal protein L4

Chain BF: 



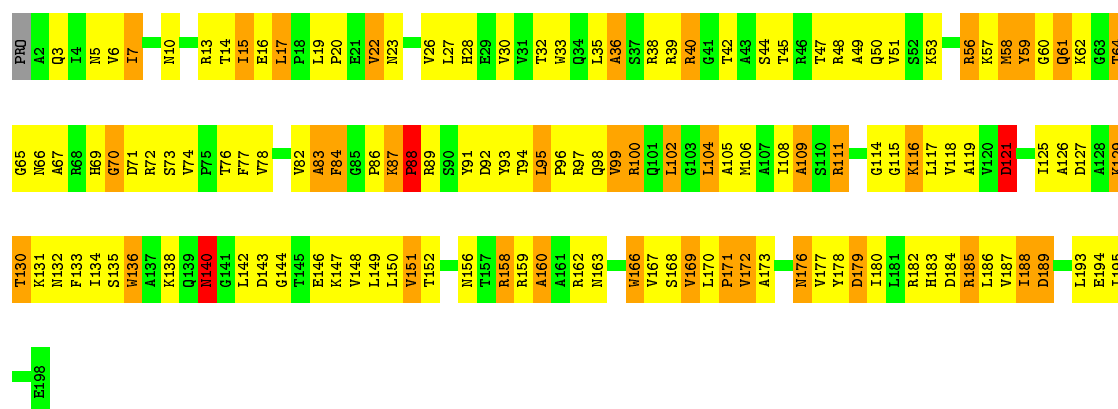
• Molecule 26: 50S ribosomal protein L4

Chain DF: 

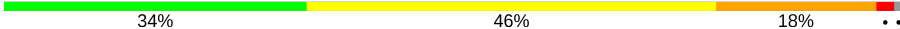


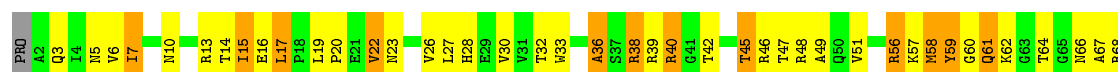
• Molecule 26: 50S ribosomal protein L4

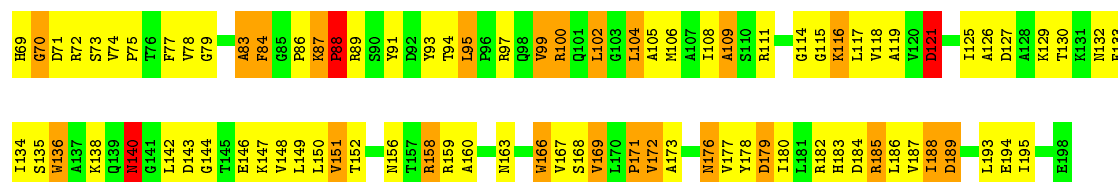
Chain FF: 



• Molecule 26: 50S ribosomal protein L4

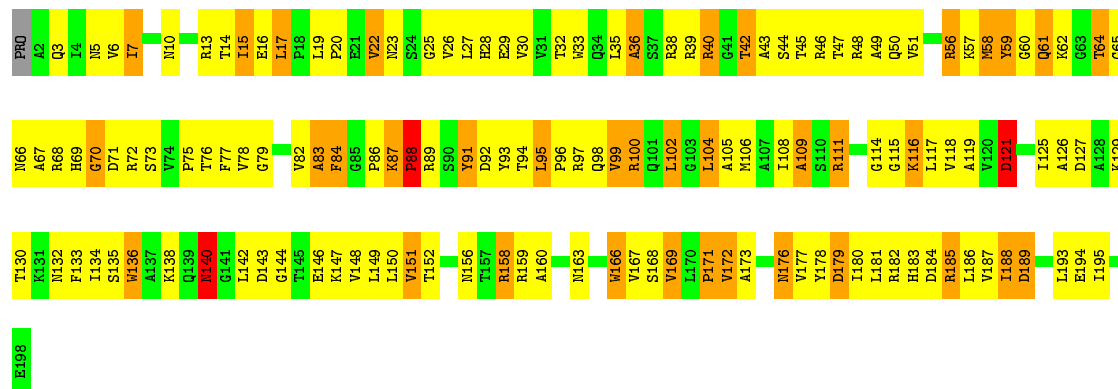
Chain HF: 





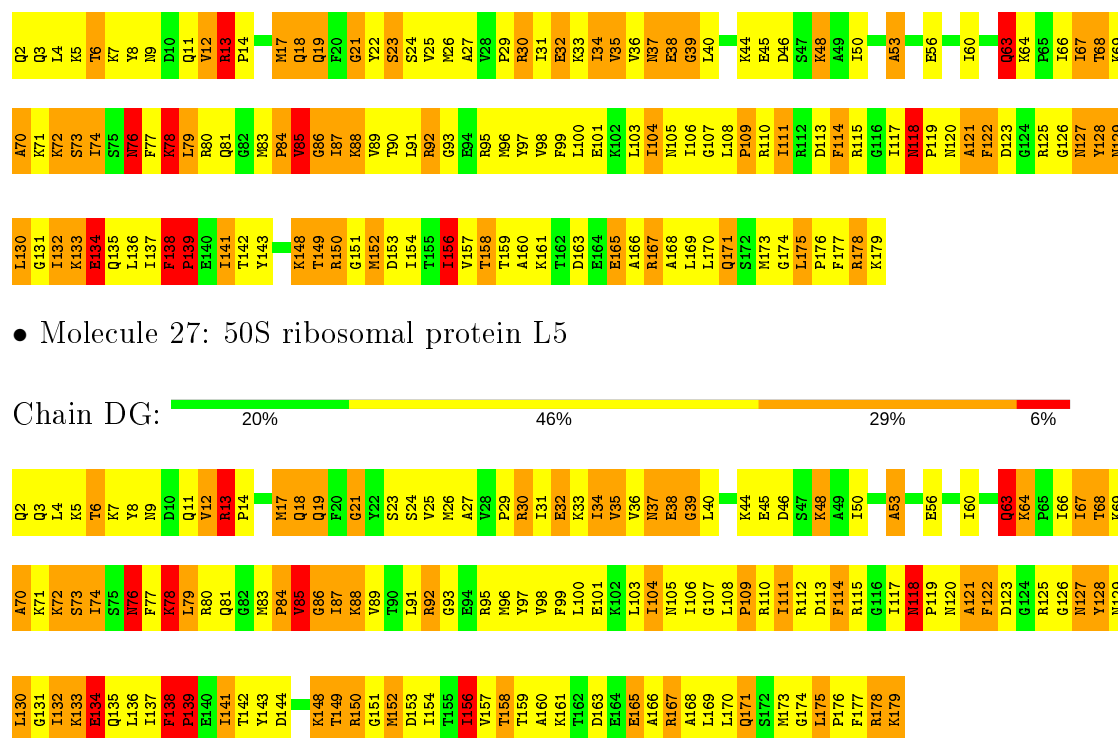
• Molecule 26: 50S ribosomal protein L4

Chain JF: 28% 51% 19% ..



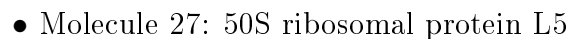
• Molecule 27: 50S ribosomal protein L5

Chain BG: 20% 46% 29% 6%

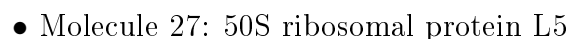


• Molecule 27: 50S ribosomal protein L5

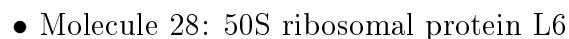
Frequency	Percentage
Daily	21%
Often	44%
Sometimes	29%
Never	6%



Frequency	Percentage
Daily	21%
Often	46%
Sometimes	28%
Never	6%



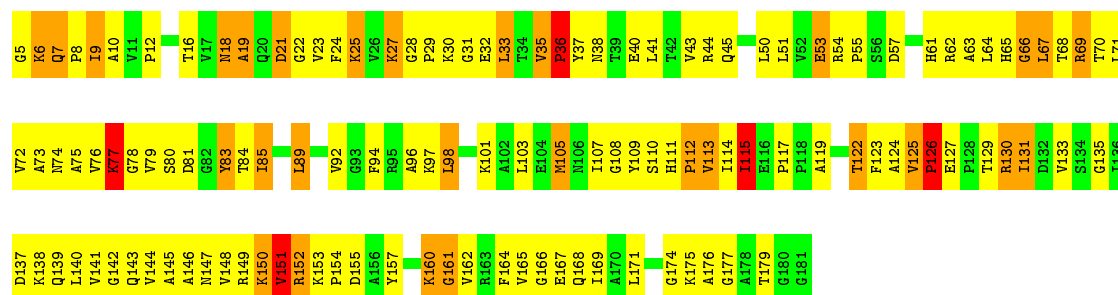
Frequency	Percentage
Daily	21%
Weekly	44%
Monthly	29%
Never	6%



Response	Percentage
Yes	30%
No	51%
Don't know	16%

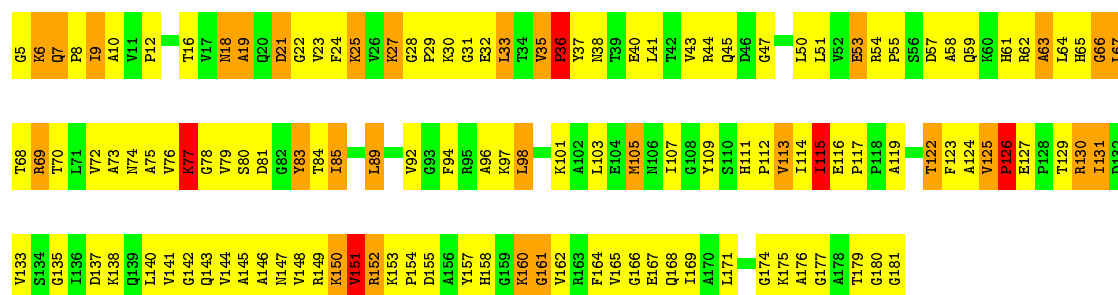
- Molecule 28: 50S ribosomal protein L6

Chain DH:  28% 53% 16% •

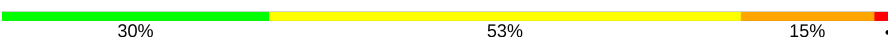


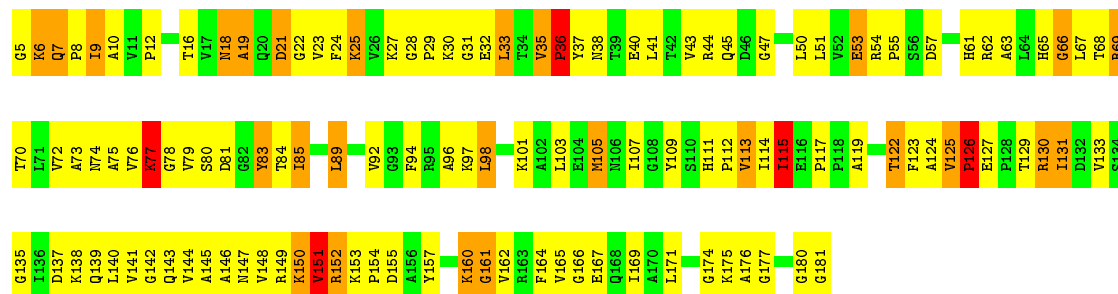
- Molecule 28: 50S ribosomal protein L6

Chain FH:  27% 54% 16% •



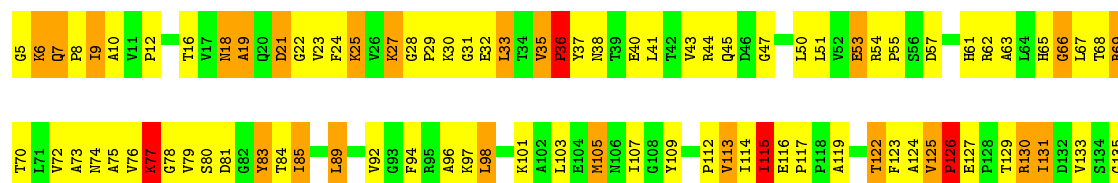
- Molecule 28: 50S ribosomal protein L6

Chain HH:  30% 53% 15% •



- Molecule 28: 50S ribosomal protein L6

Chain JH:  29% 53% 15% •

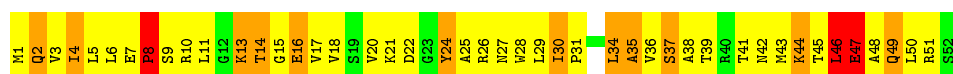
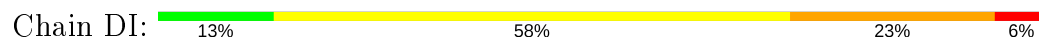




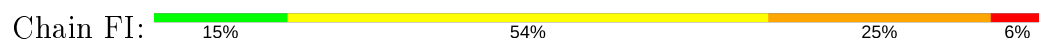
- Molecule 29: 50S ribosomal protein L9



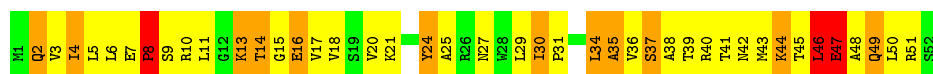
- Molecule 29: 50S ribosomal protein L9



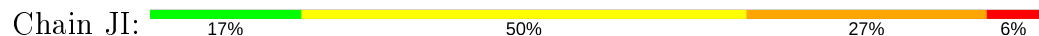
- Molecule 29: 50S ribosomal protein L9



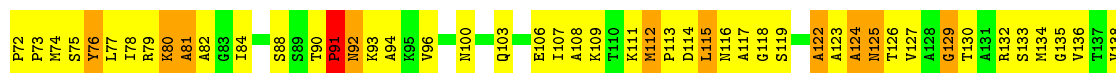
- Molecule 29: 50S ribosomal protein L9



- Molecule 29: 50S ribosomal protein L9



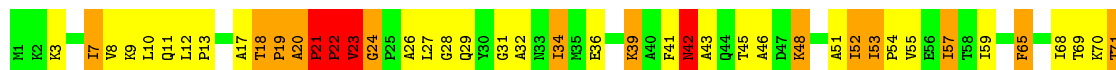
- Molecule 30: 50S ribosomal protein L11





- Molecule 30: 50S ribosomal protein L11

Chain DJ: 39% 40% 17%



- Molecule 30: 50S ribosomal protein L11

Chain FJ: 39% 41% 17%



- Molecule 30: 50S ribosomal protein L11

Chain HJ: 38% 41% 18%



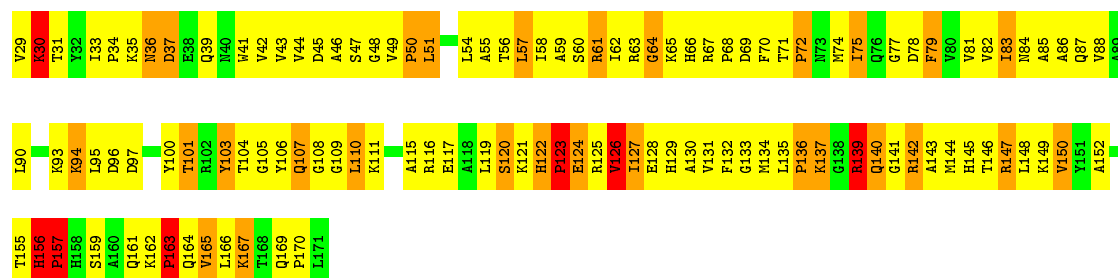
- Molecule 30: 50S ribosomal protein L11

Chain JJ: 36% 44% 17%



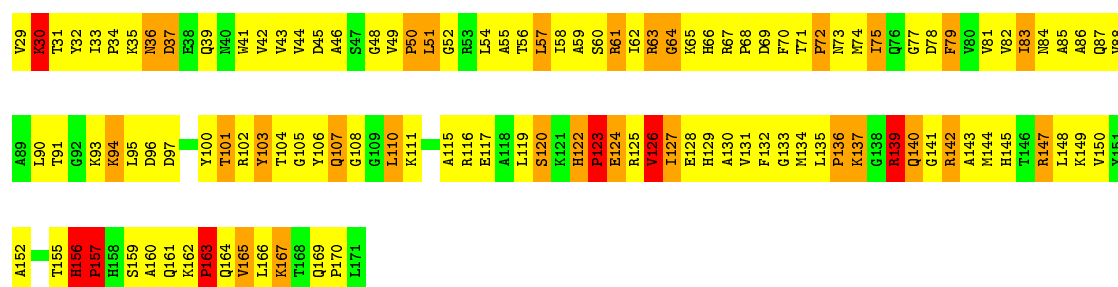
- Molecule 31: 50S ribosomal protein L13

Chain BK: 



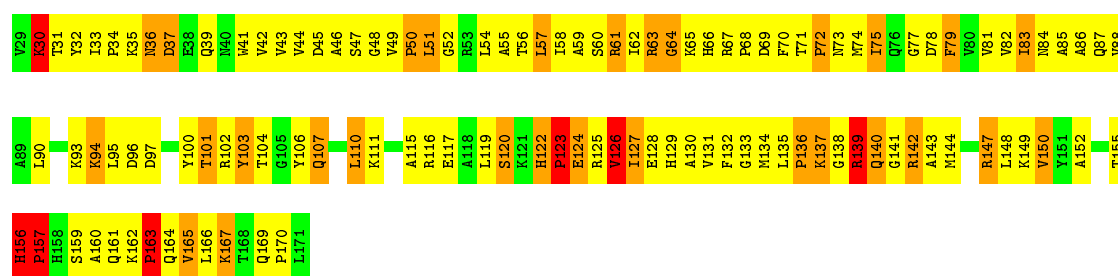
- Molecule 31: 50S ribosomal protein L13

Chain DK: 



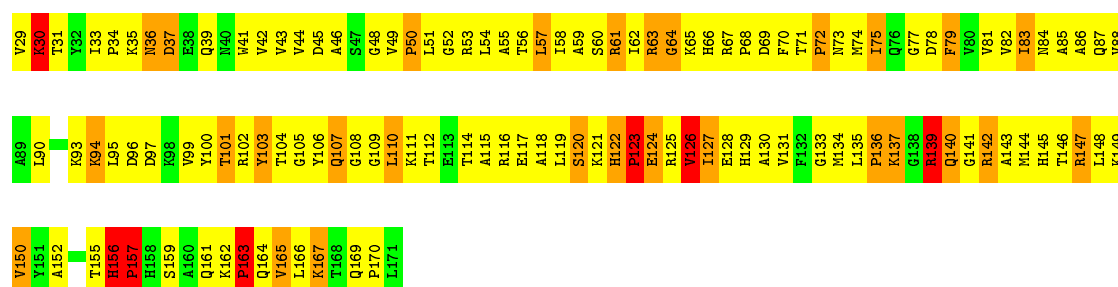
- Molecule 31: 50S ribosomal protein L13

Chain FK: 

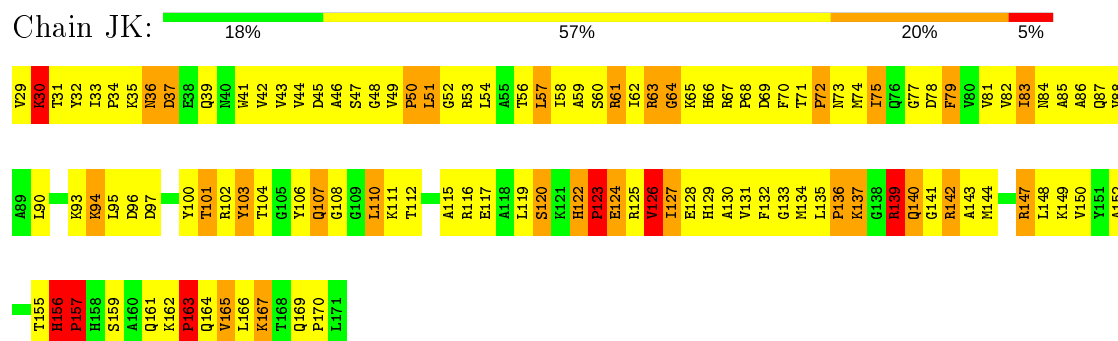


- Molecule 31: 50S ribosomal protein L13

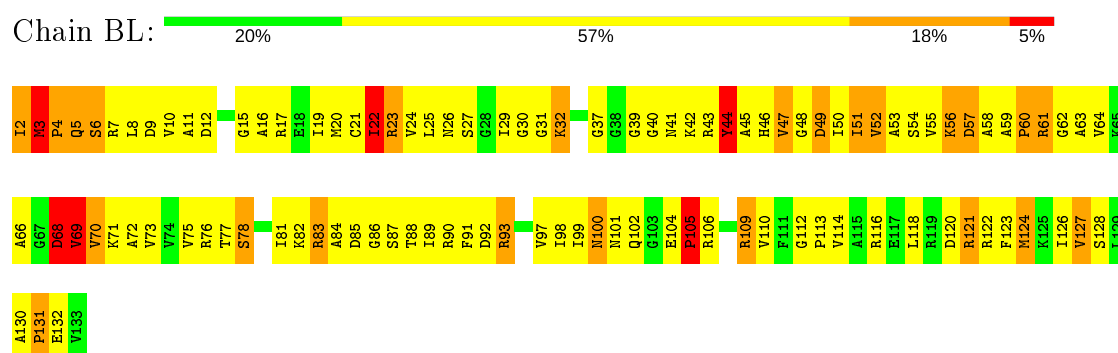
Chain HK: 



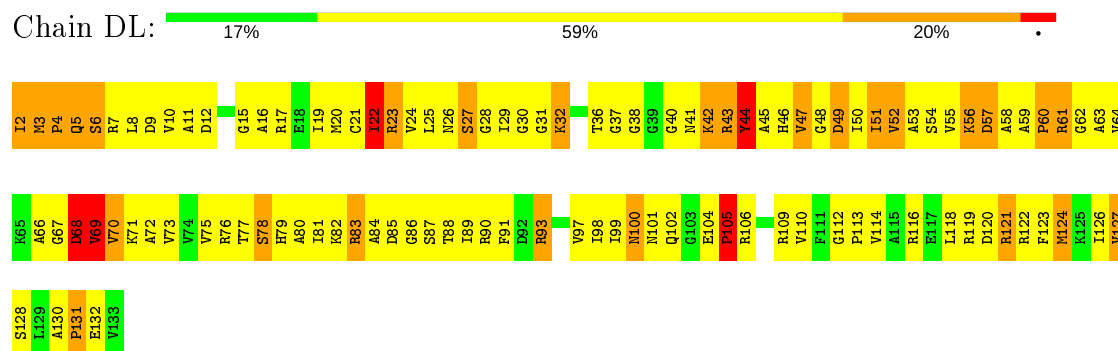
- Molecule 31: 50S ribosomal protein L13



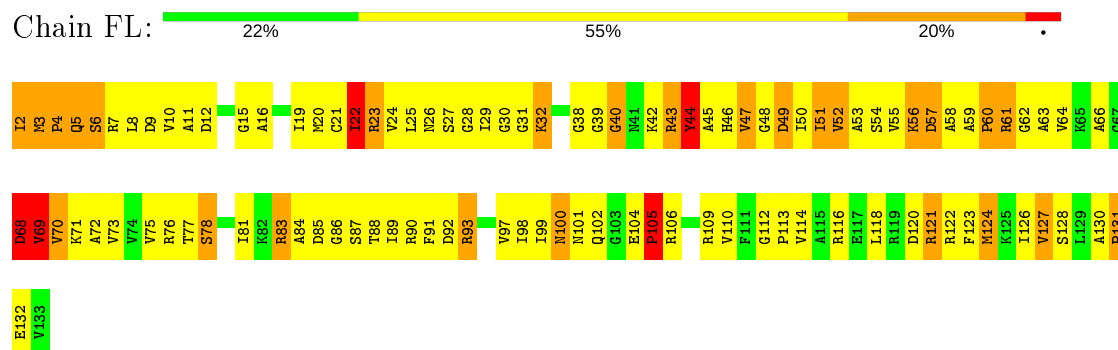
- Molecule 32: 50S ribosomal protein L14



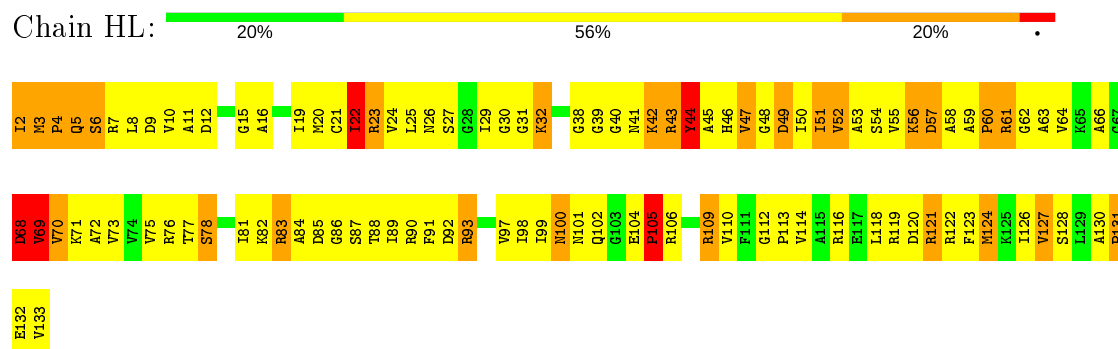
- Molecule 32: 50S ribosomal protein L14



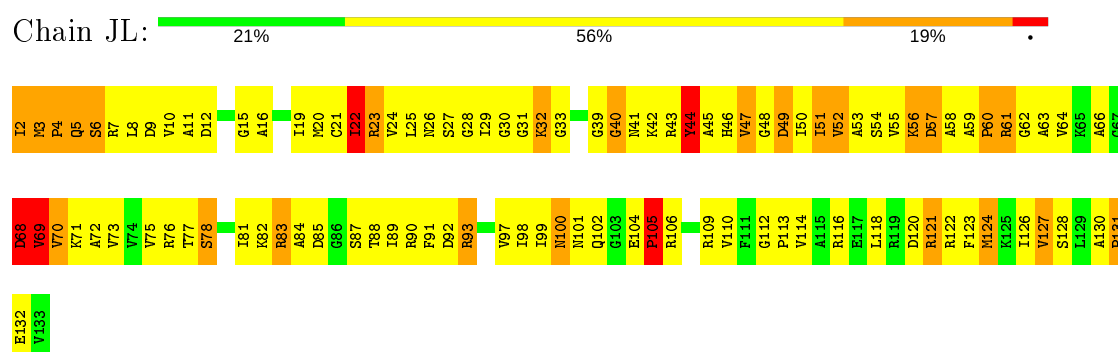
- Molecule 32: 50S ribosomal protein L14



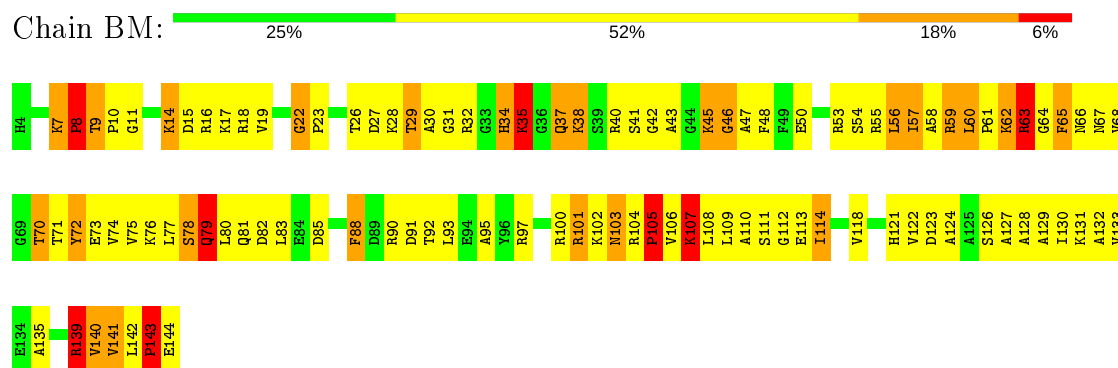
- Molecule 32: 50S ribosomal protein L14



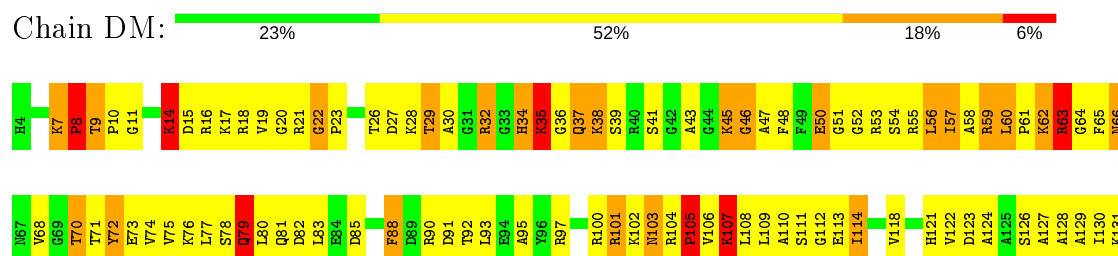
- Molecule 32: 50S ribosomal protein L14

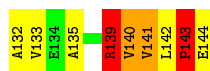


- Molecule 33: 50S ribosomal protein L15

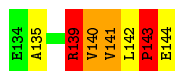
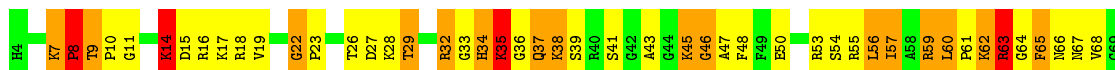


- Molecule 33: 50S ribosomal protein L15

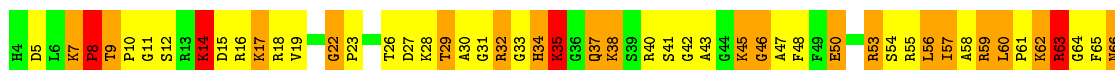
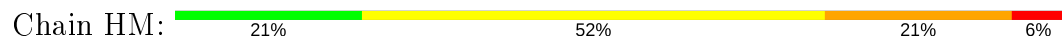




- Molecule 33: 50S ribosomal protein L15



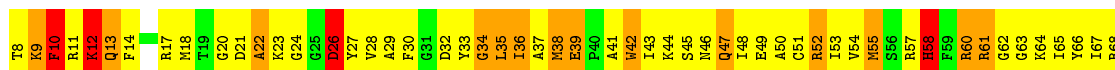
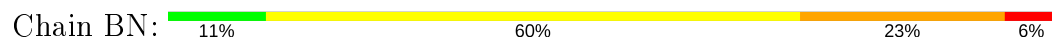
- Molecule 33: 50S ribosomal protein L15

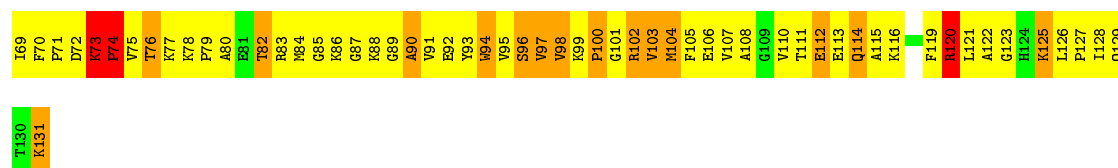


- Molecule 33: 50S ribosomal protein L15



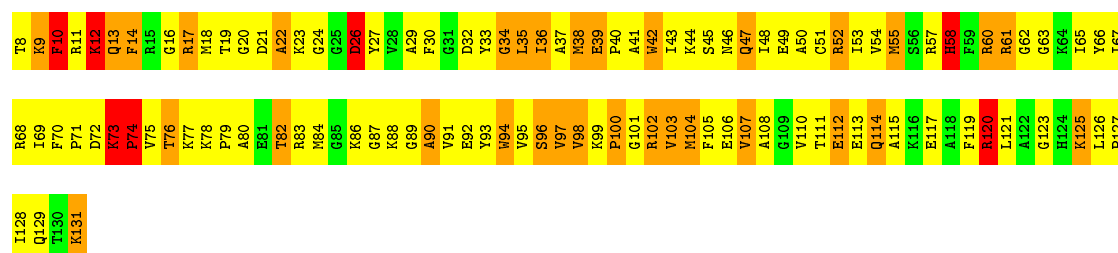
- Molecule 34: 50S ribosomal protein L16





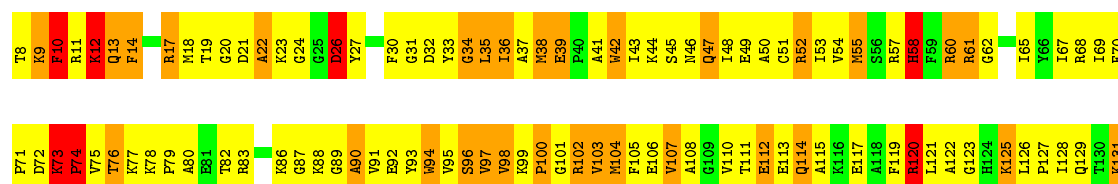
• Molecule 34: 50S ribosomal protein L16

Chain DN: 12% 56% 26% 6%



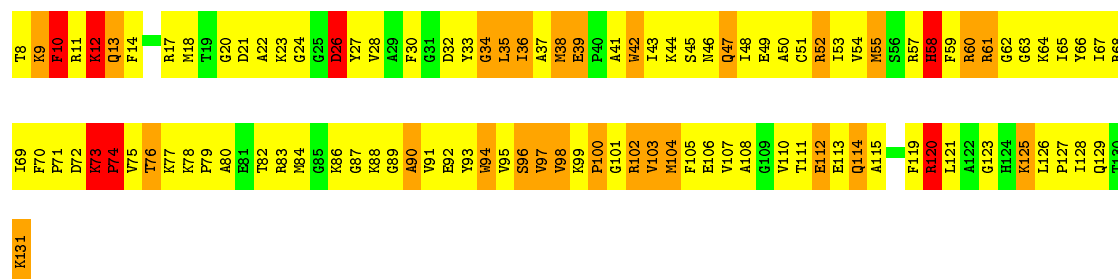
• Molecule 34: 50S ribosomal protein L16

Chain FN: 15% 54% 25% 6%



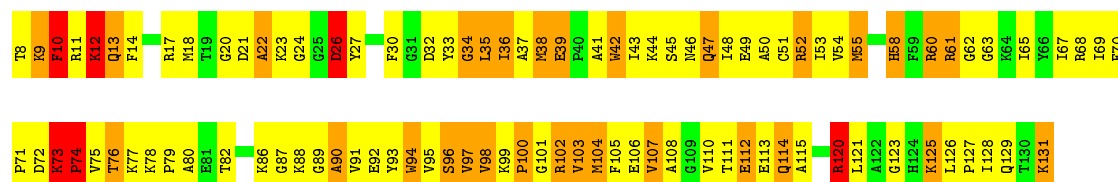
• Molecule 34: 50S ribosomal protein L16

Chain HN: 14% 59% 22% 6%



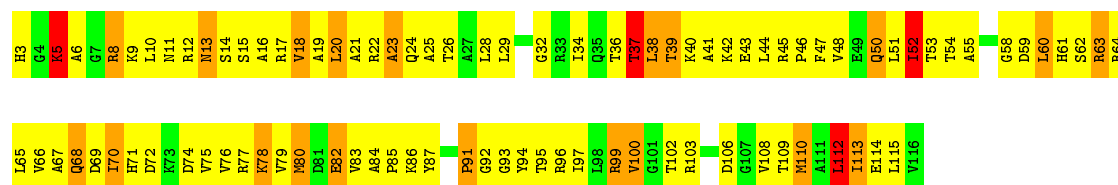
• Molecule 34: 50S ribosomal protein L16

Chain JN: 20% 51% 24% 5%

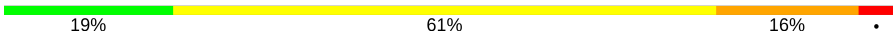


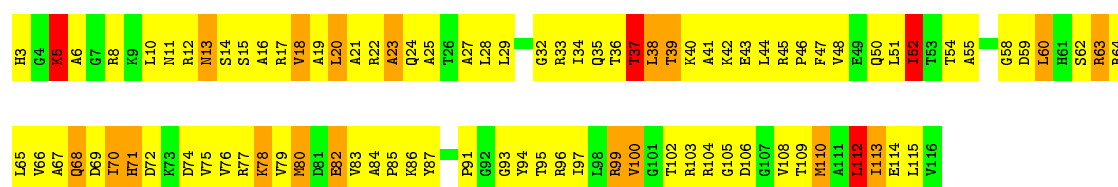
- Molecule 35: 50S ribosomal protein L17

Chain BO: 



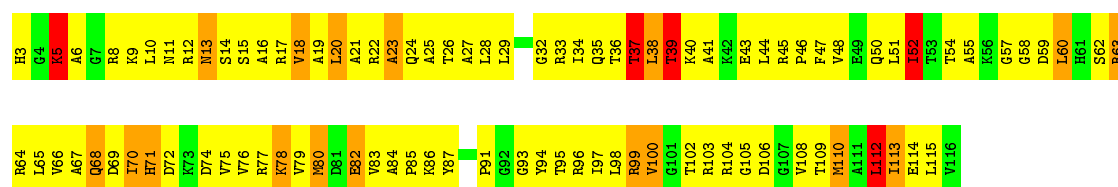
- Molecule 35: 50S ribosomal protein L17

Chain DO: 



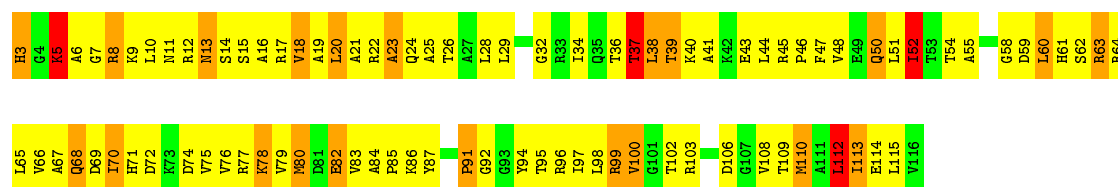
- Molecule 35: 50S ribosomal protein L17

Chain FO: 



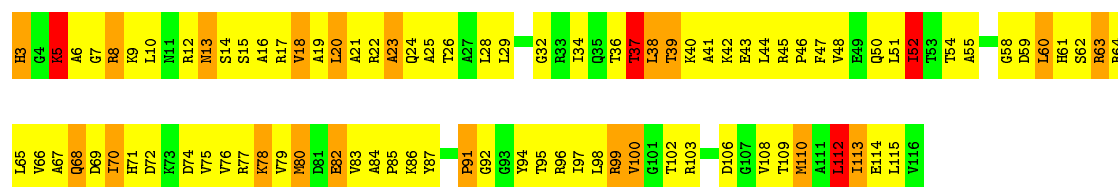
- Molecule 35: 50S ribosomal protein L17

Chain HO: 

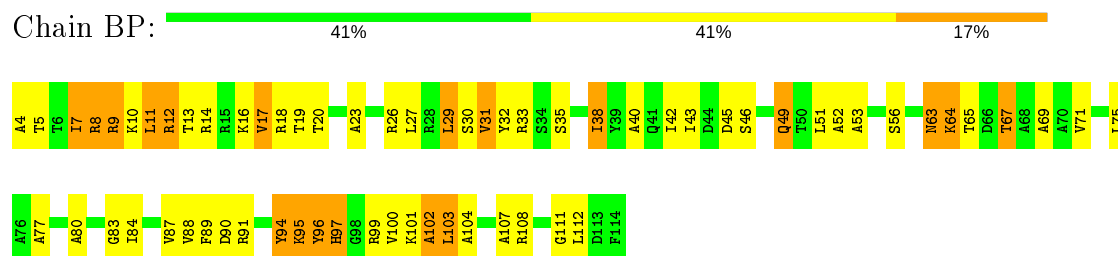


- Molecule 35: 50S ribosomal protein L17

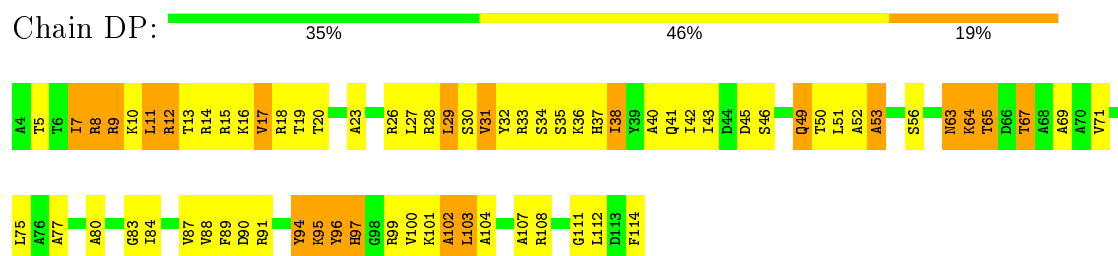
Chain JO: 



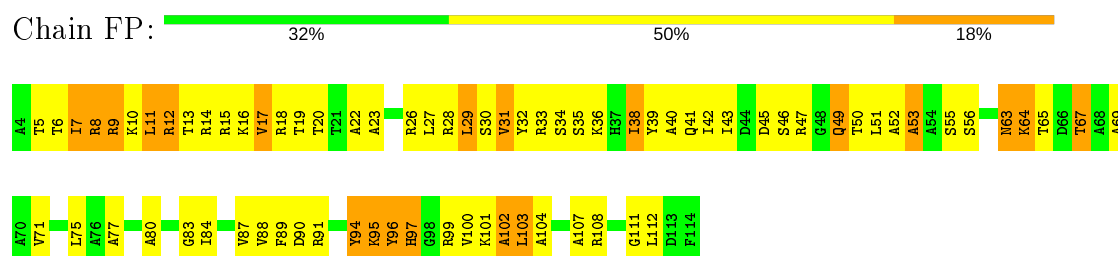
- Molecule 36: 50S ribosomal protein L18



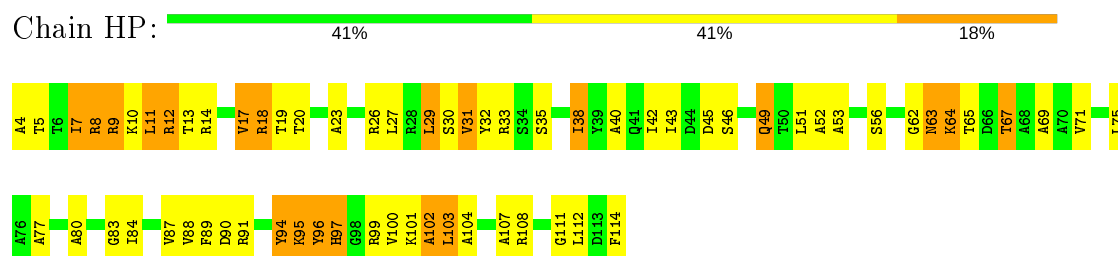
- Molecule 36: 50S ribosomal protein L18



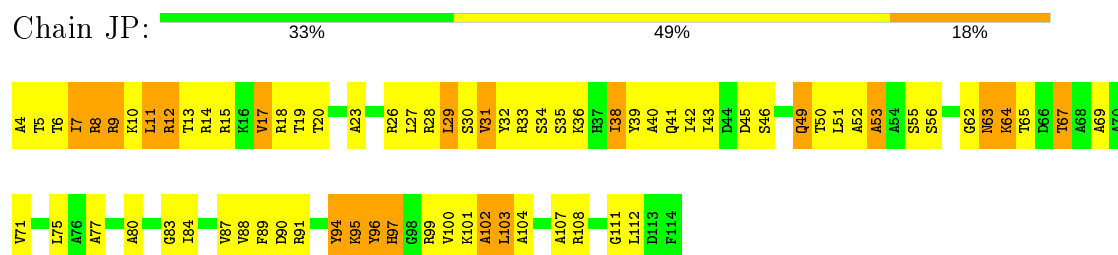
- Molecule 36: 50S ribosomal protein L18



- Molecule 36: 50S ribosomal protein L18



- Molecule 36: 50S ribosomal protein L18




- Chain BQ:**

19% 55% 24%

Category	Value
Q2	1
T3	1
H4	1
J5	1
K6	1
L7	1
M8	1
N9	1
O10	1
P11	1
Q12	1
R13	1
S14	1
T15	1
U16	1
V17	1
W18	1
X19	1
Y20	1
Z21	1
AA22	1
AB23	1
AC24	1
AD25	1
AE26	1
AF27	1
AG28	1
AH29	1
AI30	1
AJ31	1
AK32	1
AL33	1
AM34	1
AN35	1
AO36	1
AP37	1
AP38	1
AP39	1
AP40	1
AP41	1
AP42	1
AP43	1
AP44	1
AP45	1
AP46	1
AP47	1
AP48	1
AP49	1
AP50	1
AP51	1
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AP114	1
AP115	1
AP116	1
AP117	1
AP118	1
AP119	1
AP120	1
AP121	1
AP122	1
AP123	1
AP124	1
AP125	1
AP126	1

- Chain DQ:  22%  52%  24%

Item	Category
K2	Yellow
T3	Yellow
H4	Yellow
K6	Yellow
I7	Yellow
R8	Yellow
R9	Yellow
G10	Yellow
E11	Yellow
L12	Yellow
L13	Yellow
R14	Yellow
I16	Yellow
E17	Yellow
Q18	Yellow
D19	Yellow
H20	Yellow
T21	Yellow
R22	Yellow
Q23	Yellow
L24	Yellow
P25	Yellow
D26	Yellow
F27	Yellow
R28	Yellow
P29	Yellow
G30	Yellow
D31	Yellow
T32	Yellow
V33	Yellow
R34	Yellow
V35	Yellow
D36	Yellow
T37	Yellow
K38	Yellow
V39	Yellow
R40	Yellow
E41	Yellow
G42	Yellow
R43	Red
R44	Red
T45	Yellow
R46	Yellow
S47	Yellow
Q48	Yellow
A49	Yellow
P50	Yellow
V53	Yellow
V54	Yellow
A56	Yellow
I57	Yellow
N58	Yellow
G59	Yellow
S60	Yellow
G61	Yellow
S62	Yellow
K63	Red
K64	Yellow
S65	Yellow
F66	Yellow
T67	Yellow
V68	Yellow
R69	Yellow
K70	Yellow
S71	Yellow
F72	Yellow
F73	Yellow
G74	Yellow
E75	Yellow
G76	Yellow
V77	Yellow
E78	Yellow
R79	Yellow
V80	Yellow
F81	Yellow
P82	Yellow
F83	Yellow
A84	Yellow
S85	Yellow
P86	Yellow
L87	Yellow
V88	Yellow
N89	Yellow
Q90	Yellow
V91	Yellow
T92	Yellow
I93	Yellow
V94	Yellow
E95	Yellow
R96	Yellow
V99	Yellow
R100	Yellow
R101	Yellow
A102	Yellow
K103	Yellow
K104	Yellow
L104	Yellow
K105	Yellow
K106	Yellow
L107	Yellow
R108	Yellow
E109	Yellow
L110	Yellow
R111	Yellow
G112	Yellow
K113	Yellow
A114	Yellow
A115	Yellow
R116	Yellow
D120	Yellow
R121	Yellow
R122	Yellow
G123	Yellow
R124	Yellow
V124	Yellow
A125	Yellow

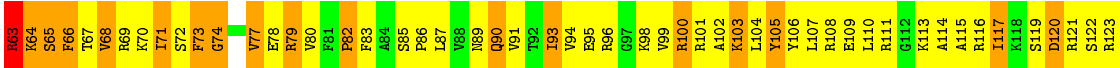
- Chain FQ: 
- |      |      |     |
|------|------|-----|
| M125 | R63  | Q2  |
| K126 | K64  | T3  |
|      | S65  | R4  |
|      | F66  | R5  |
|      | T67  | K6  |
|      | V68  | I7  |
|      | R69  | R8  |
|      | K70  | R9  |
|      | I71  | G10 |
|      | S72  | E11 |
|      | F73  | L12 |
|      | G74  | L13 |
|      | E75  | R14 |
|      | G76  | G15 |
|      | V77  | I16 |
|      | E78  | E17 |
|      | R79  | Q18 |
|      | V80  | D19 |
|      | F81  | E20 |
|      | R82  | T21 |
|      | F83  | R22 |
|      | A84  | Q23 |
|      | S85  | L24 |
|      | P86  | P25 |
|      | L87  | D26 |
|      | V88  | F27 |
|      | R89  | R28 |
|      | Q90  | P29 |
|      | V91  | G30 |
|      | T92  | D31 |
|      | I93  | T32 |
|      | V94  | V33 |
|      | E95  | R34 |
|      | R96  | V35 |
|      |      | D36 |
|      |      | T37 |
|      | V99  | R38 |
|      | R100 | V39 |
|      | R101 | R40 |
|      | A102 | E41 |
|      | K103 | G42 |
|      | L104 | R43 |
|      | I105 | R44 |
|      | Y106 | T45 |
|      | L107 | R46 |
|      | R108 | S47 |
|      | E109 | Q48 |
|      | L110 | A49 |
|      | R111 | F50 |
|      | G112 |     |
|      | K113 | V53 |
|      | A114 | E54 |
|      | A115 | V55 |
|      | R116 | I56 |
|      | I117 | A56 |
|      |      | I57 |
|      |      | N58 |
|      | D120 | G59 |
|      | R121 | S60 |
|      | S122 | G61 |
|      | R123 | R62 |
|      | V124 | S63 |

- Chain HQ:

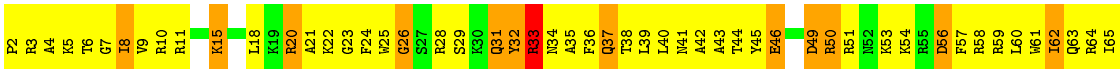
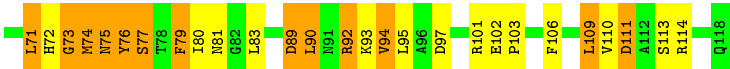
K126

- Molecule 37: 50S ribosomal protein L19

Chain JQ:  18% 56% 25%


V124  
M125  
K126

- Molecule 38: 50S ribosomal protein L20

Chain BR:  32% 45% 21%



- Molecule 38: 50S ribosomal protein L20

Chain DR:  26% 53% 20%



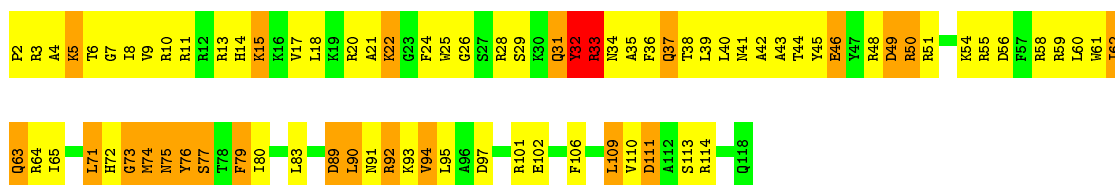
- Molecule 38: 50S ribosomal protein L20

Chain FR:  23% 56% 19%



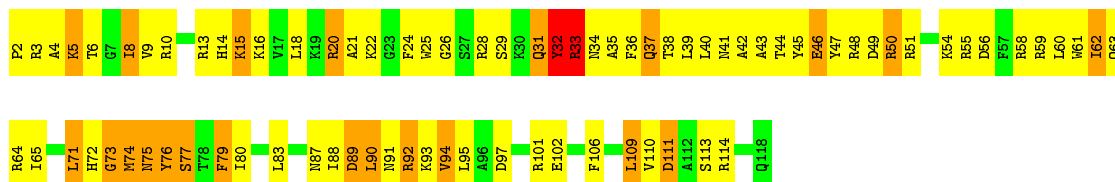
- Molecule 38: 50S ribosomal protein L20

Chain HR:  32% 47% 20%



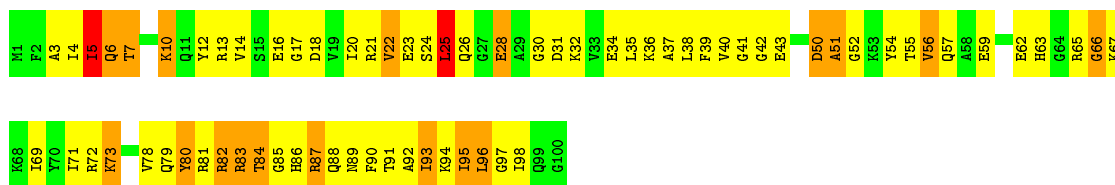
- Molecule 38: 50S ribosomal protein L20

Chain JR: 31% 49% 19%



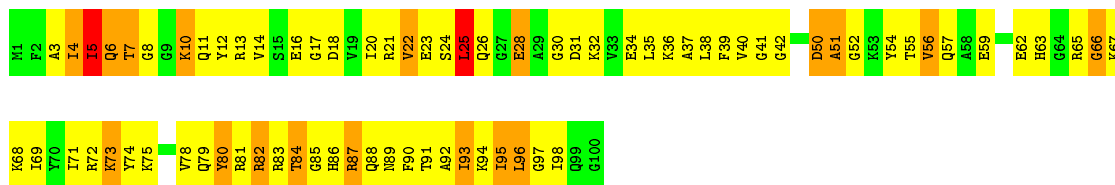
- Molecule 39: 50S ribosomal protein L21

Chain BS: 29% 51% 18%



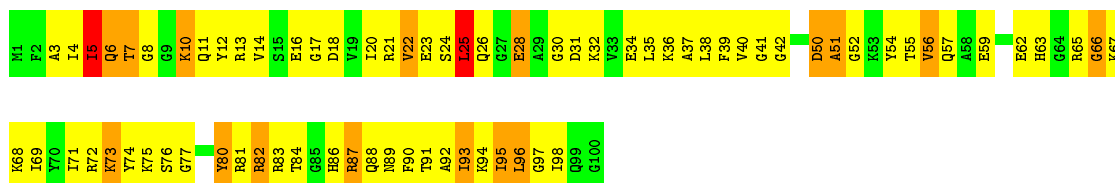
- Molecule 39: 50S ribosomal protein L21

Chain DS: 25% 55% 18%



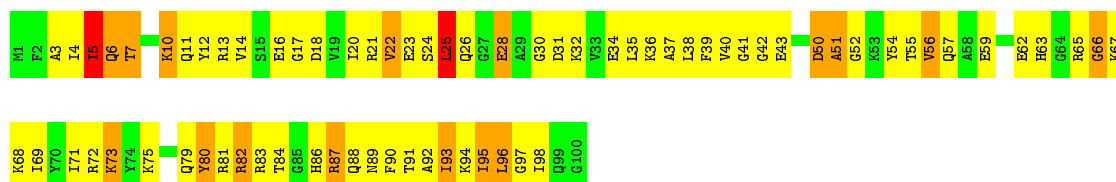
- Molecule 39: 50S ribosomal protein L21

Chain FS: 26% 56% 16%

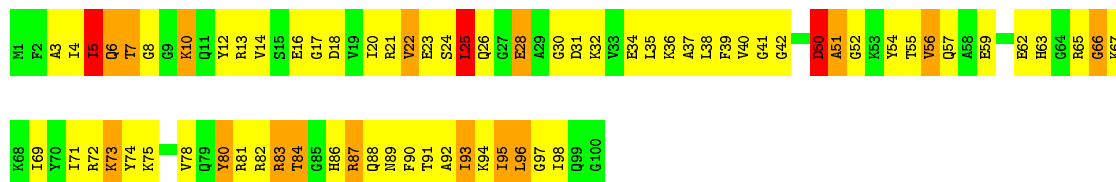


- Molecule 39: 50S ribosomal protein L21

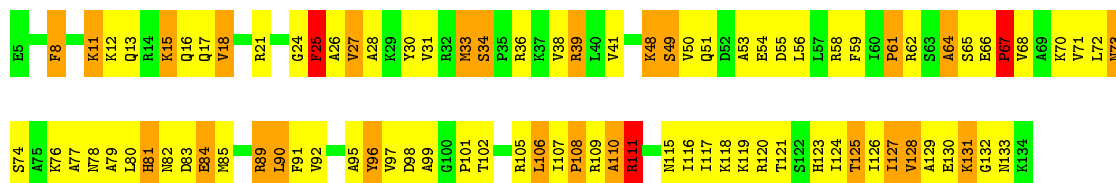
Chain HS: 28% 54% 16%



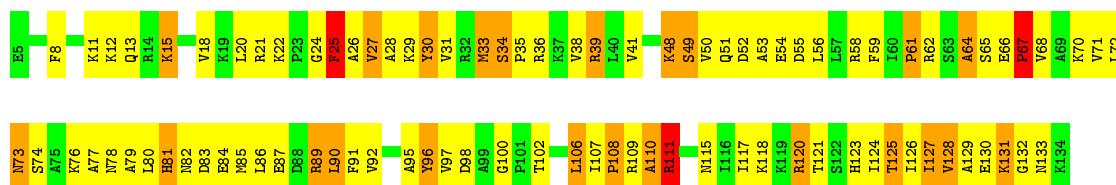
- Molecule 39: 50S ribosomal protein L21



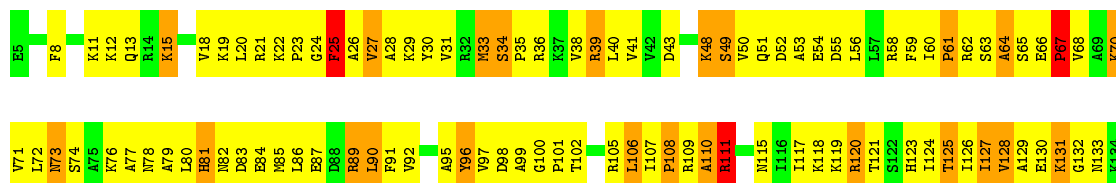
- Molecule 40: 50S ribosomal protein L22



- Molecule 40: 50S ribosomal protein L22

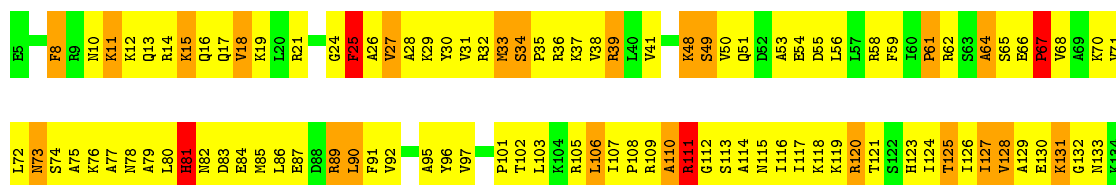


- Molecule 40: 50S ribosomal protein L22

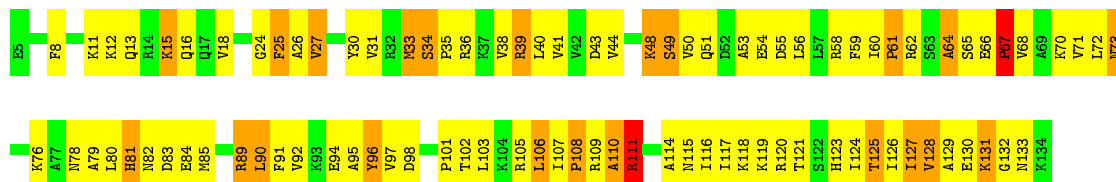


- Molecule 40: 50S ribosomal protein L22

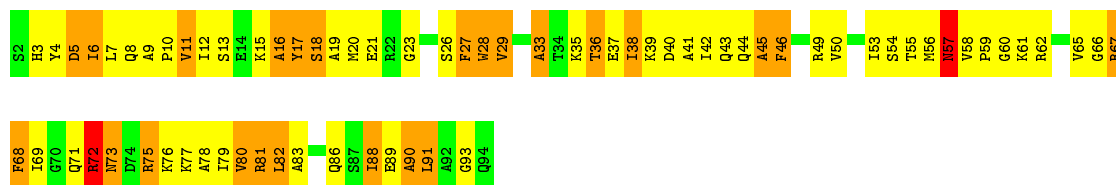




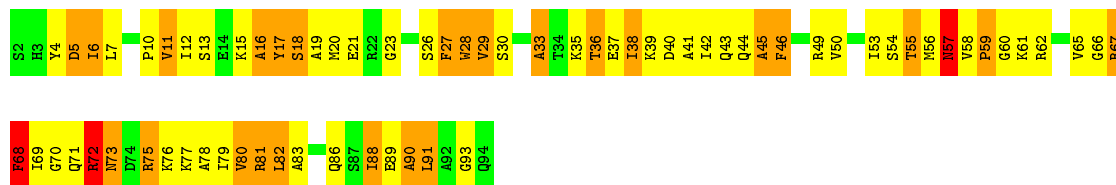
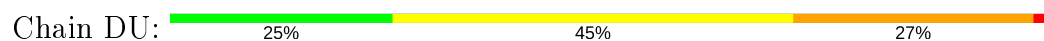
- Molecule 40: 50S ribosomal protein L22



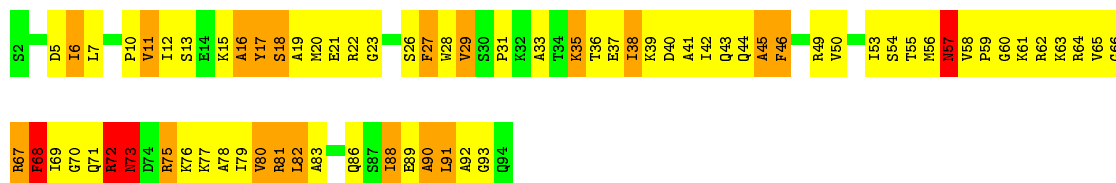
- Molecule 41: 50S ribosomal protein L23



- Molecule 41: 50S ribosomal protein L23

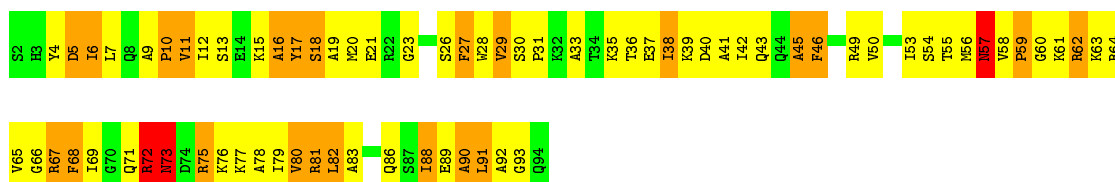


- Molecule 41: 50S ribosomal protein L23

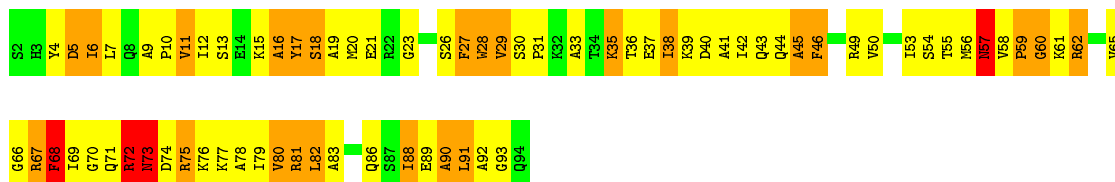


- Molecule 41: 50S ribosomal protein L23

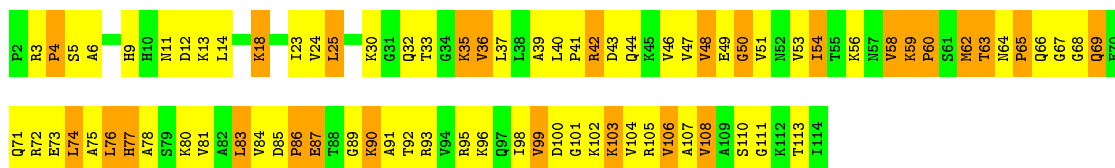




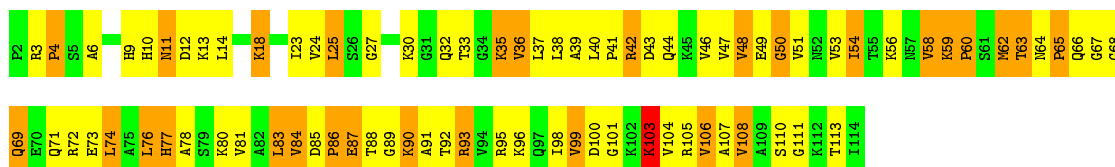
- Molecule 41: 50S ribosomal protein L23



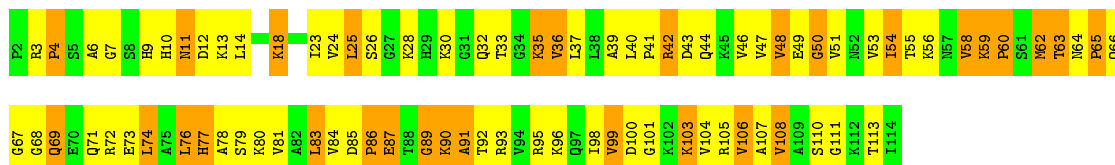
- Molecule 42: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L24

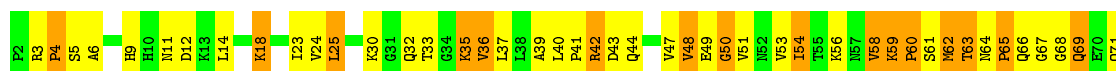


- Molecule 42: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L24

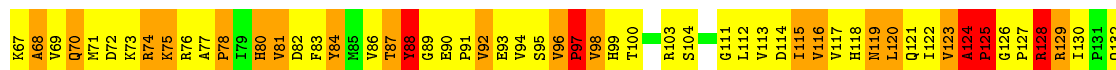




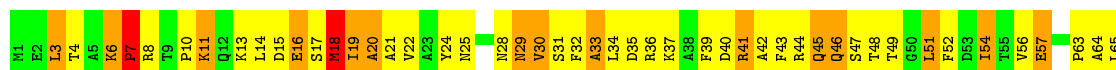
- Molecule 42: 50S ribosomal protein L24



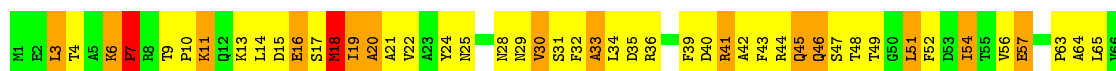
- Molecule 43: general stress protein Ctc

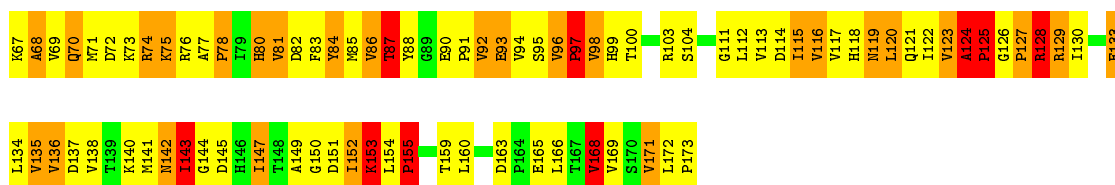


- Molecule 43: general stress protein Ctc



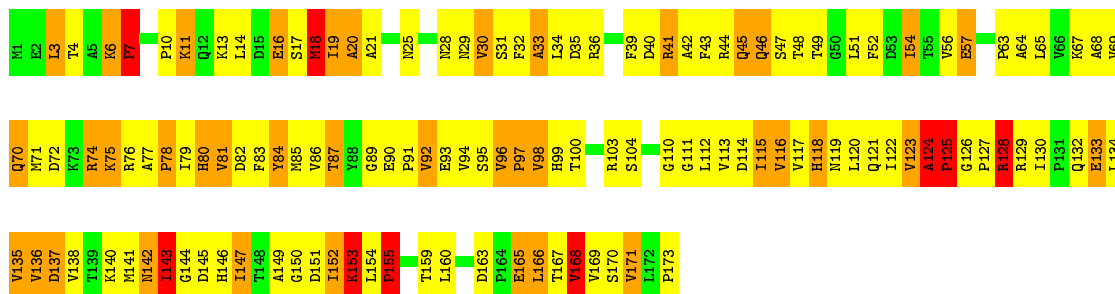
- Molecule 43: general stress protein Ctc





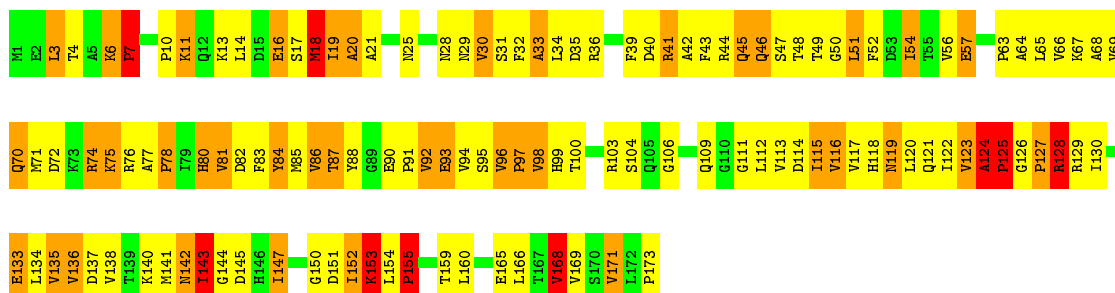
- Molecule 43: general stress protein Ctc

Chain HW: 24% 48% 23% 5%



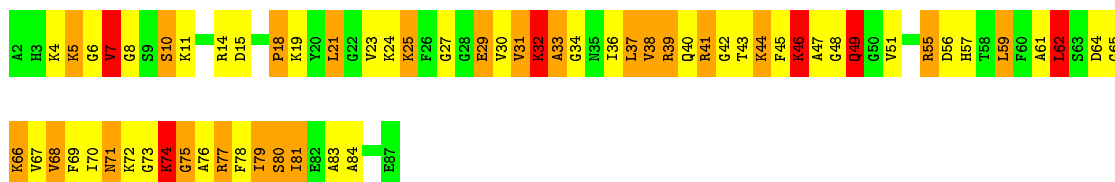
- Molecule 43: general stress protein Ctc

Chain JW: 27% 45% 23% 5%



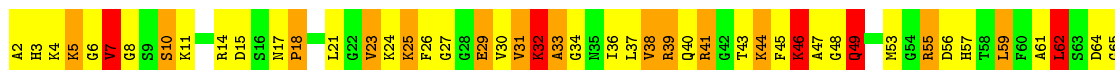
- Molecule 44: 50S ribosomal protein L27

Chain BX: 27% 40% 27% 7%



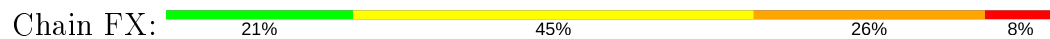
- Molecule 44: 50S ribosomal protein L27

Chain DX: 26% 43% 24% 7%

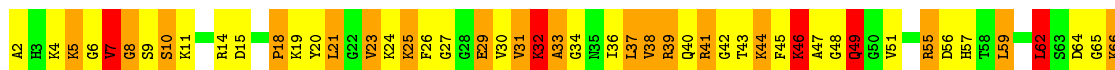
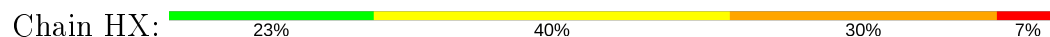




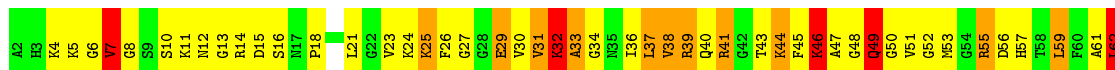
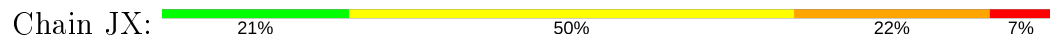
- Molecule 44: 50S ribosomal protein L27



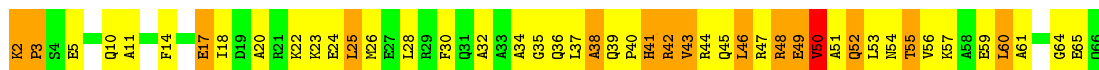
- Molecule 44: 50S ribosomal protein L27



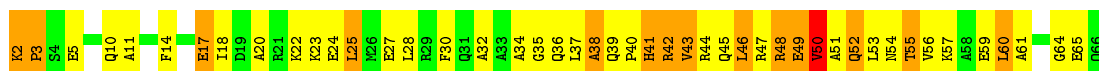
- Molecule 44: 50S ribosomal protein L27



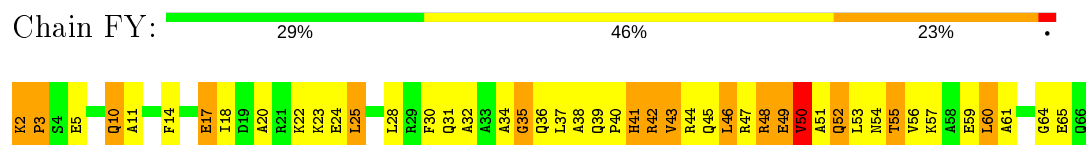
- Molecule 45: 50S ribosomal protein L29



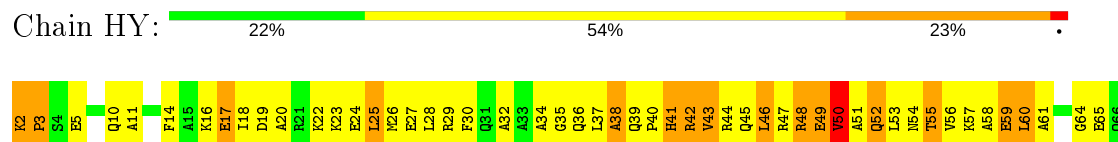
- Molecule 45: 50S ribosomal protein L29



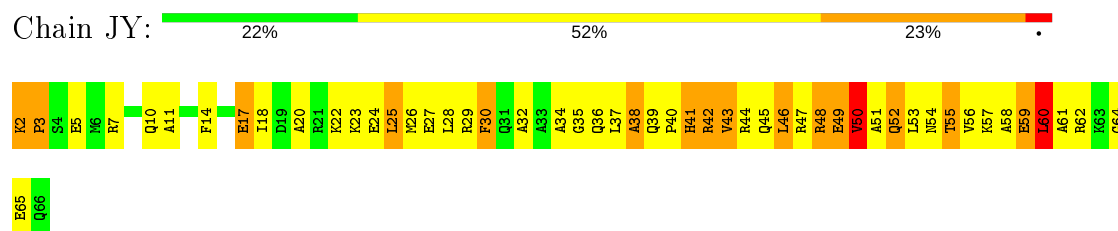
- Molecule 45: 50S ribosomal protein L29



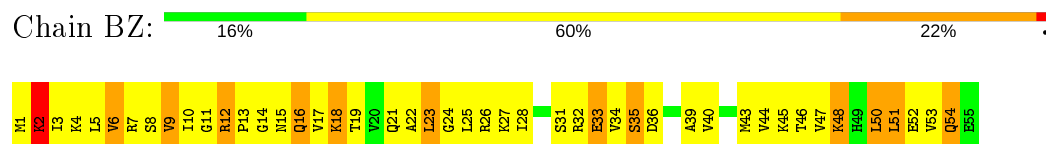
- Molecule 45: 50S ribosomal protein L29



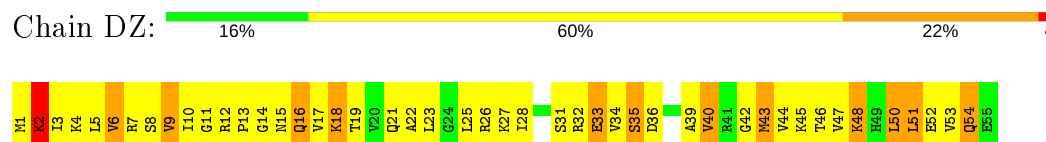
- Molecule 45: 50S ribosomal protein L29



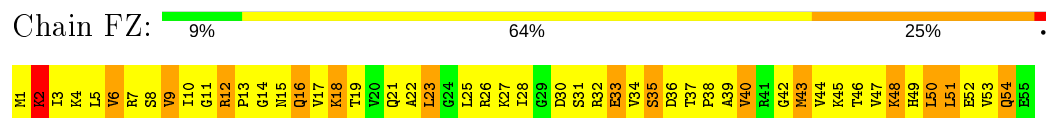
- Molecule 46: 50S ribosomal protein L30



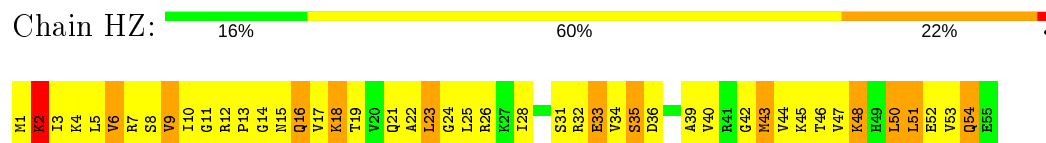
- Molecule 46: 50S ribosomal protein L30



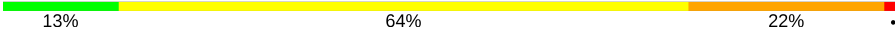
- Molecule 46: 50S ribosomal protein L30

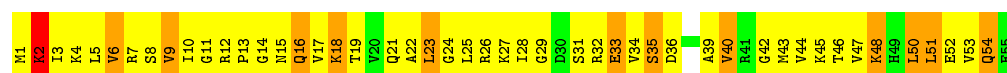


- Molecule 46: 50S ribosomal protein L30



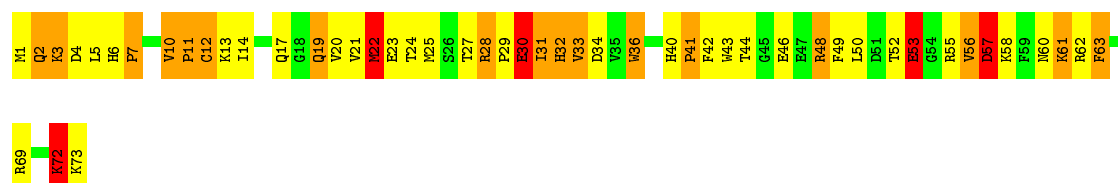
- Molecule 46: 50S ribosomal protein L30

Chain JZ: 



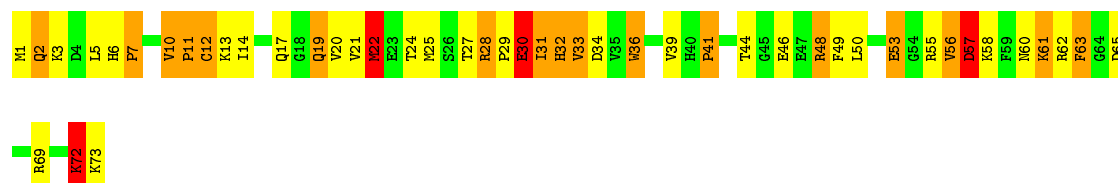
• Molecule 47: 50S ribosomal protein L31

Chain B1: 

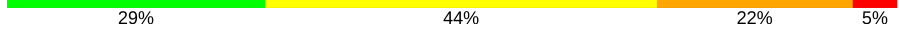


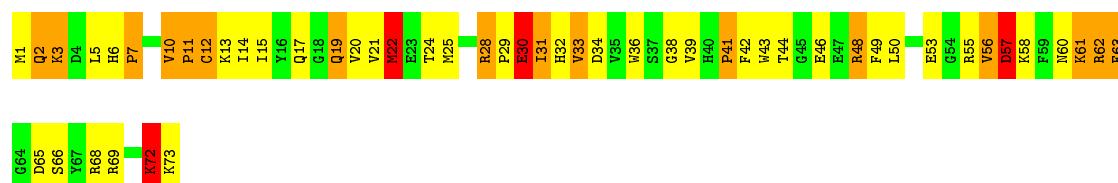
• Molecule 47: 50S ribosomal protein L31

Chain D1: 

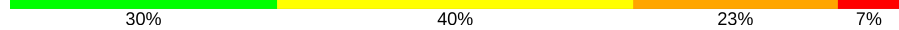


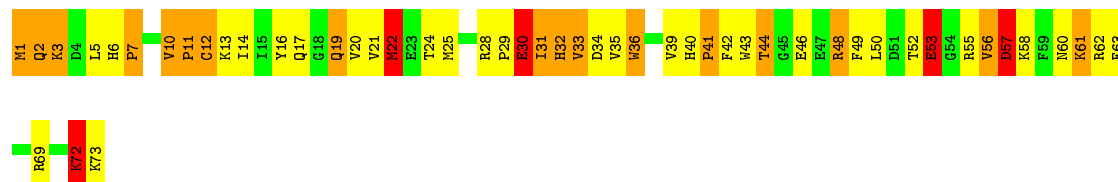
• Molecule 47: 50S ribosomal protein L31

Chain F1: 

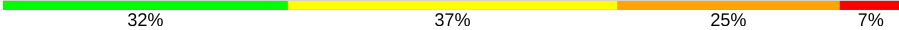


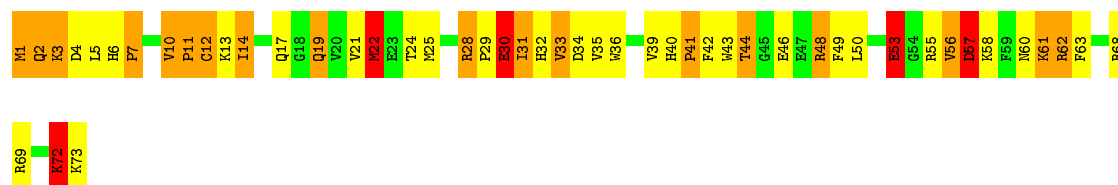
• Molecule 47: 50S ribosomal protein L31

Chain H1: 



• Molecule 47: 50S ribosomal protein L31

Chain J1: 



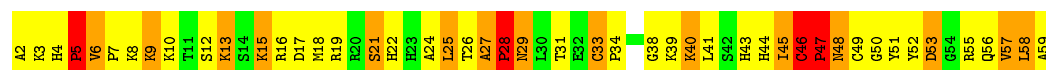
- Molecule 48: 50S ribosomal protein L32

Chain B2: 16% 53% 26% 5%



- Molecule 48: 50S ribosomal protein L32

Chain D2: 19% 48% 26% 7%



- Molecule 48: 50S ribosomal protein L32

Chain F2: 24% 48% 21% 7%



- Molecule 48: 50S ribosomal protein L32

Chain H2: 12% 57% 26% 5%



- Molecule 48: 50S ribosomal protein L32

Chain J2: 16% 50% 28% 7%



- Molecule 49: 50S ribosomal protein L33

Chain B3: 21% 38% 32% 9%



- Molecule 49: 50S ribosomal protein L33

Chain D3: 13% 47% 30% 9%



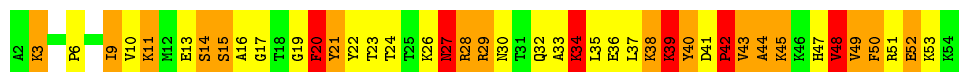
- Molecule 49: 50S ribosomal protein L33

Chain F3: 11% 45% 32% 11%



- Molecule 49: 50S ribosomal protein L33

Chain H3: 21% 38% 30% 11%



- Molecule 49: 50S ribosomal protein L33

Chain J3: 11% 47% 30% 11%



- Molecule 50: 50S ribosomal protein L34

Chain B4: 17% 54% 22% 7%



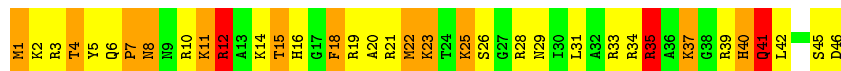
- Molecule 50: 50S ribosomal protein L34

Chain D4: 24% 43% 26% 7%



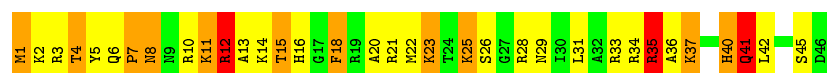
- Molecule 50: 50S ribosomal protein L34

Chain F4: 24% 43% 26% 7%

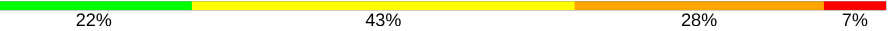


- Molecule 50: 50S ribosomal protein L34

Chain H4: 

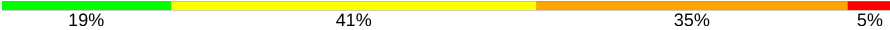


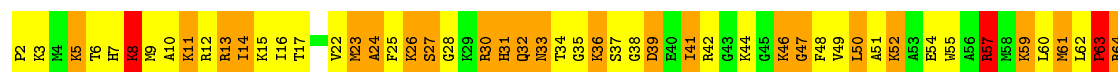
- Molecule 50: 50S ribosomal protein L34

Chain J4: 




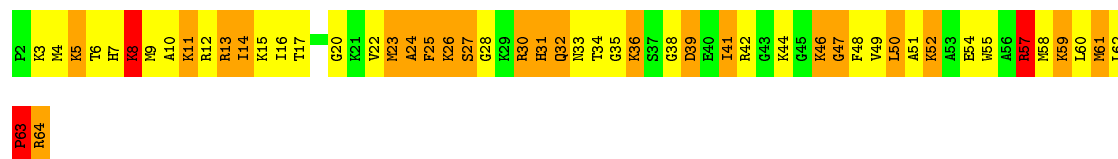
- Molecule 51: 50S ribosomal protein L35

Chain B5: 



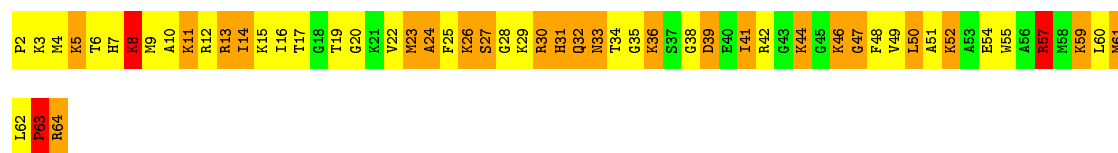
- Molecule 51: 50S ribosomal protein L35

Chain D5: 

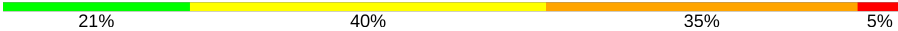


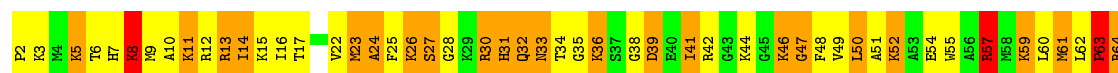
- Molecule 51: 50S ribosomal protein L35

Chain F5: 




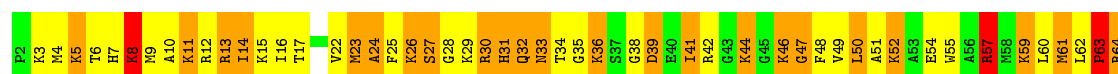
- Molecule 51: 50S ribosomal protein L35

Chain H5: 

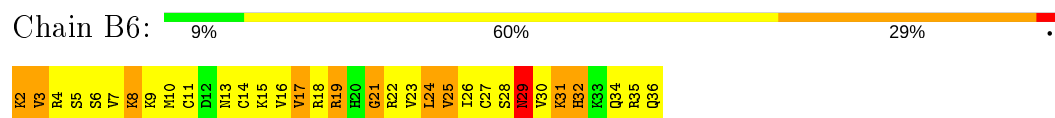


- Molecule 51: 50S ribosomal protein L35

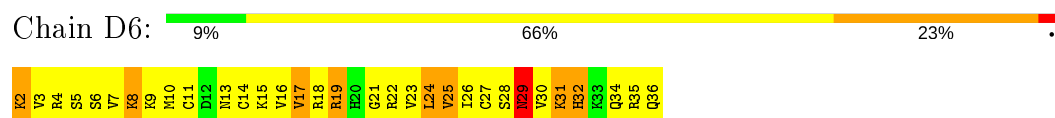
Chain J5: 



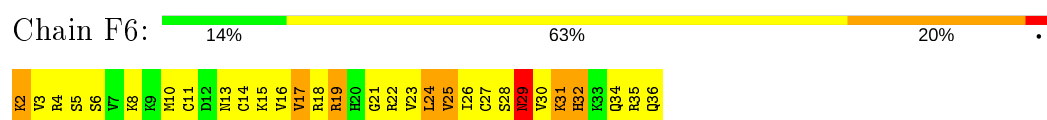
- Molecule 52: 50S ribosomal protein L36



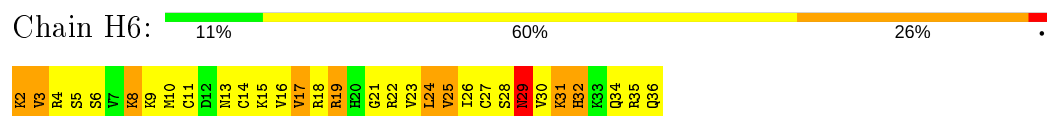
- Molecule 52: 50S ribosomal protein L36



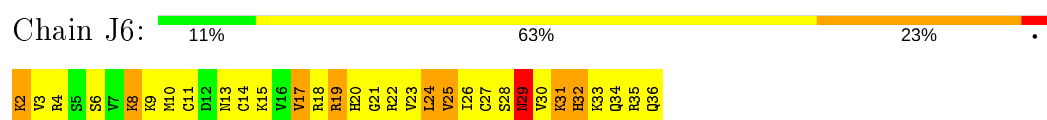
- Molecule 52: 50S ribosomal protein L36



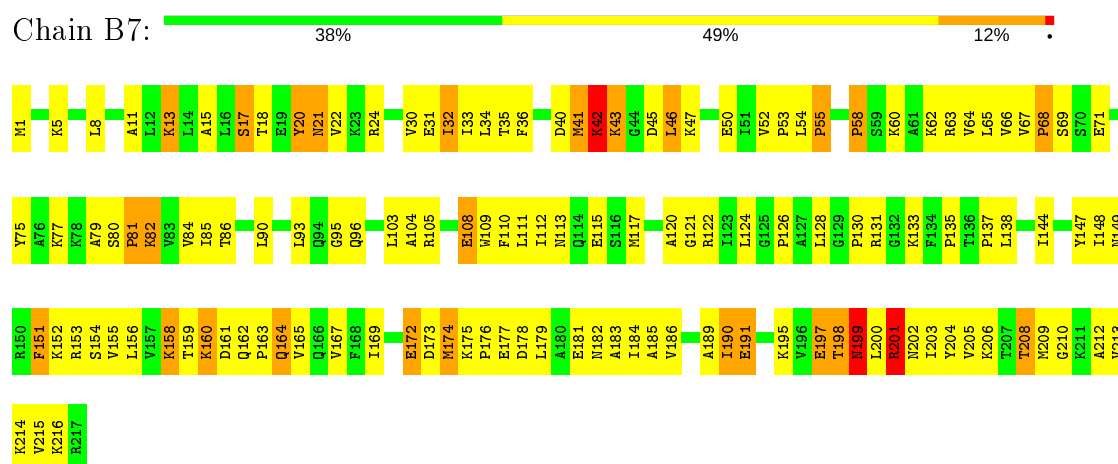
- Molecule 52: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L36

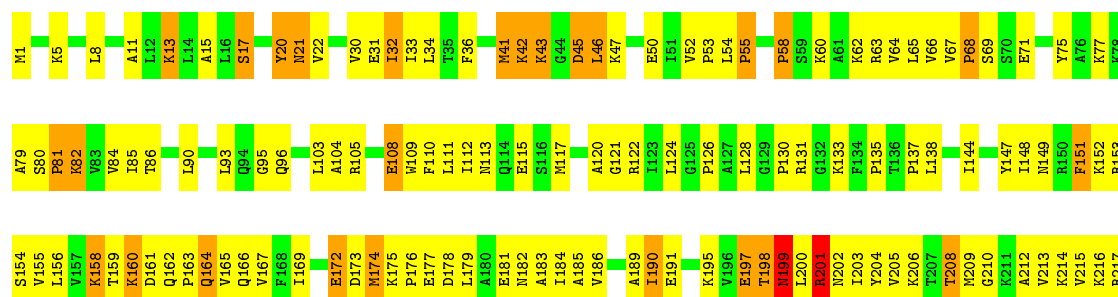


- Molecule 53: 50S ribosomal protein L1P



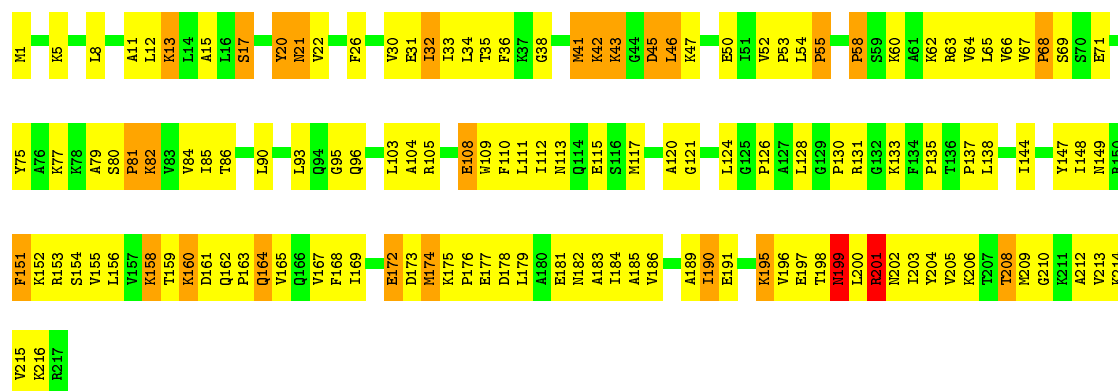
- Molecule 53: 50S ribosomal protein L1P

Chain D7: 



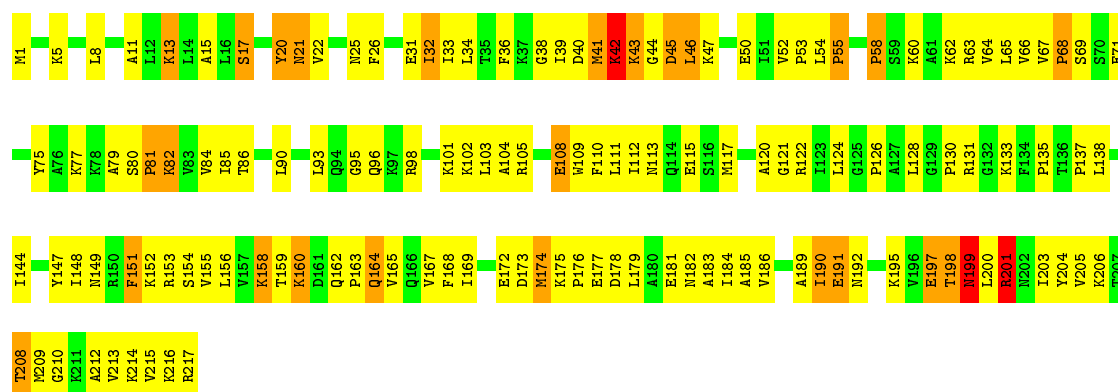
• Molecule 53: 50S ribosomal protein L1P

Chain F7: 

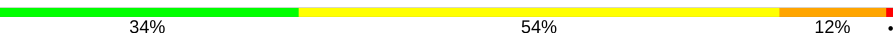


• Molecule 53: 50S ribosomal protein L1P

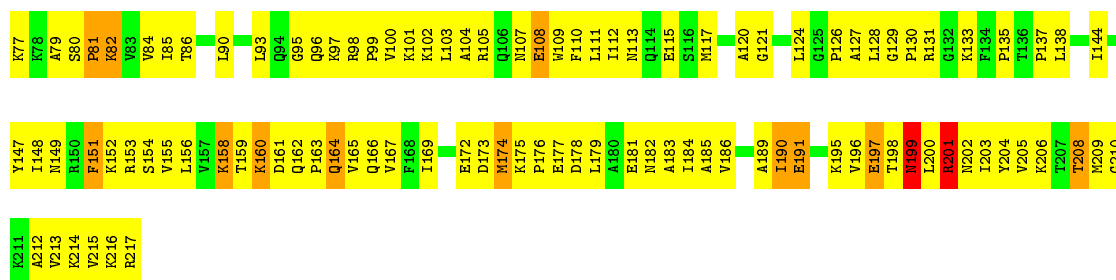
Chain H7: 



• Molecule 53: 50S ribosomal protein L1P

Chain J7: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	687.90Å 687.90Å 1933.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 11.50 486.42 – 11.53	Depositor EDS
% Data completeness (in resolution range)	93.9 (500.00-11.50) 76.3 (486.42-11.53)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.395 , 0.401 0.386 , 0.401	Depositor DCC
$R_{free}$ test set	7421 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.93 , -10.0	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	717805	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	803.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

<sup>1</sup>Theoretical 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 ⓘ

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	AA	0.30	1/36713 (0.0%)	0.74	16/57289 (0.0%)
1	CA	0.30	1/36713 (0.0%)	0.74	15/57289 (0.0%)
1	EA	0.39	2/36714 (0.0%)	0.77	21/57293 (0.0%)
1	GA	0.39	2/36714 (0.0%)	0.75	19/57293 (0.0%)
1	IA	0.36	1/36714 (0.0%)	0.78	20/57293 (0.0%)
2	AB	0.26	0/1936	0.55	0/2609
2	CB	0.26	0/1936	0.55	0/2609
2	EB	0.26	0/1936	0.55	0/2609
2	GB	0.26	0/1936	0.55	0/2609
2	IB	0.26	0/1936	0.55	0/2609
3	AC	0.24	0/1637	0.53	0/2205
3	CC	0.24	0/1637	0.53	0/2205
3	EC	0.24	0/1637	0.53	0/2205
3	GC	0.24	0/1637	0.53	0/2205
3	IC	0.25	0/1637	0.53	0/2205
4	AD	0.24	0/1733	0.49	0/2318
4	CD	0.25	0/1733	0.49	0/2318
4	ED	0.25	0/1733	0.49	0/2318
4	GD	0.25	0/1733	0.49	0/2318
4	ID	0.25	0/1733	0.49	0/2318
5	AE	0.28	0/1163	0.59	0/1564
5	CE	0.28	0/1163	0.59	0/1564
5	EE	0.28	0/1163	0.59	0/1564
5	GE	0.28	0/1163	0.59	0/1564
5	IE	0.27	0/1163	0.59	0/1564
6	AF	0.24	0/856	0.52	0/1154
6	CF	0.24	0/856	0.52	0/1154
6	EF	0.24	0/856	0.52	0/1154
6	GF	0.24	0/856	0.52	0/1154
6	IF	0.24	0/856	0.52	0/1154
7	AG	0.24	0/1276	0.50	0/1709
7	CG	0.24	0/1276	0.50	0/1709
7	EG	0.25	0/1276	0.50	0/1709
7	GG	0.25	0/1276	0.50	0/1709

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
7	IG	0.25	0/1276	0.50	0/1709
8	AH	0.25	0/1136	0.56	0/1527
8	CH	0.25	0/1136	0.56	0/1527
8	EH	0.25	0/1136	0.56	0/1527
8	GH	0.25	0/1136	0.56	0/1527
8	IH	0.25	0/1136	0.56	0/1527
9	AI	0.26	0/1029	0.51	0/1378
9	CI	0.26	0/1029	0.51	0/1378
9	EI	0.25	0/1029	0.51	0/1378
9	GI	0.25	0/1029	0.51	0/1378
9	II	0.25	0/1029	0.51	0/1378
10	AJ	0.25	0/808	0.59	0/1085
10	CJ	0.25	0/808	0.59	0/1085
10	EJ	0.25	0/808	0.59	0/1085
10	GJ	0.25	0/808	0.58	0/1085
10	IJ	0.25	0/808	0.59	0/1085
11	AK	0.24	0/900	0.56	0/1213
11	CK	0.24	0/900	0.56	0/1213
11	EK	0.24	0/900	0.56	0/1213
11	GK	0.24	0/900	0.56	0/1213
11	IK	0.24	0/900	0.56	0/1213
12	AL	0.49	1/985 (0.1%)	0.68	1/1314 (0.1%)
12	CL	0.25	0/984	0.58	0/1311
12	EL	0.35	1/985 (0.1%)	0.83	3/1314 (0.2%)
12	GL	0.25	0/984	0.58	0/1311
12	IL	0.86	1/985 (0.1%)	0.70	2/1314 (0.2%)
13	AM	0.27	0/1007	0.87	3/1344 (0.2%)
13	CM	0.26	0/1006	0.59	1/1341 (0.1%)
13	EM	0.26	0/1006	0.58	1/1341 (0.1%)
13	GM	0.52	1/1007 (0.1%)	1.07	3/1344 (0.2%)
13	IM	0.27	0/1006	0.58	1/1341 (0.1%)
14	AN	0.27	0/501	0.59	0/664
14	CN	0.27	0/501	0.59	0/664
14	EN	0.27	0/501	0.59	0/664
14	GN	0.27	0/501	0.59	0/664
14	IN	0.28	0/501	0.59	0/664
15	AO	0.24	0/745	0.51	0/992
15	CO	0.24	0/745	0.51	0/992
15	EO	0.24	0/745	0.51	0/992
15	GO	0.24	0/745	0.51	0/992
15	IO	0.24	0/745	0.51	0/992
16	AP	0.26	0/717	0.58	0/963
16	CP	0.26	0/717	0.58	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	EP	0.26	0/717	0.58	0/963
16	GP	0.26	0/717	0.58	0/963
16	IP	0.26	0/717	0.59	0/963
17	AQ	0.26	0/870	0.59	0/1159
17	CQ	0.26	0/870	0.59	0/1159
17	EQ	0.26	0/870	0.59	0/1159
17	GQ	0.26	0/870	0.59	0/1159
17	IQ	0.26	0/870	0.59	0/1159
18	AR	0.26	0/603	0.52	0/799
18	CR	0.26	0/603	0.52	0/799
18	ER	0.26	0/603	0.52	0/799
18	GR	0.26	0/603	0.52	0/799
18	IR	0.26	0/603	0.52	0/799
19	AS	0.25	0/662	0.60	0/890
19	CS	0.25	0/662	0.60	0/890
19	ES	0.25	0/662	0.60	0/890
19	GS	0.25	0/662	0.60	0/890
19	IS	0.25	0/662	0.60	0/890
20	AT	0.30	0/764	0.68	1/1006 (0.1%)
20	CT	0.29	0/764	0.68	1/1006 (0.1%)
20	ET	0.30	0/764	0.68	1/1006 (0.1%)
20	GT	0.29	0/764	0.68	1/1006 (0.1%)
20	IT	0.29	0/764	0.68	1/1006 (0.1%)
21	Aa	0.23	0/731	0.36	0/987
21	Ca	0.23	0/731	0.36	0/987
21	Ea	0.23	0/731	0.36	0/987
21	Ga	0.23	0/731	0.36	0/987
21	Ia	0.23	0/731	0.36	0/987
22	BB	0.90	55/67883 (0.1%)	0.93	143/105846 (0.1%)
22	DB	0.87	62/67886 (0.1%)	0.89	142/105858 (0.1%)
22	FB	0.85	58/67883 (0.1%)	0.92	138/105846 (0.1%)
22	HB	0.80	57/67884 (0.1%)	0.92	146/105850 (0.1%)
22	JB	0.81	56/67885 (0.1%)	0.85	130/105854 (0.1%)
23	BA	0.35	0/2816	0.75	0/4388
23	DA	0.35	0/2816	0.75	0/4388
23	FA	0.35	0/2816	0.75	0/4388
23	HA	0.35	0/2816	0.75	0/4388
23	JA	0.34	0/2816	0.75	0/4388
24	BD	0.33	0/2121	0.90	2/2854 (0.1%)
24	DD	0.33	0/2121	0.90	2/2854 (0.1%)
24	FD	0.33	0/2121	0.90	2/2854 (0.1%)
24	HD	0.32	0/2121	0.90	2/2854 (0.1%)
24	JD	0.33	0/2121	0.90	2/2854 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
25	BE	0.33	0/1568	0.92	8/2105 (0.4%)
25	DE	0.33	0/1568	0.92	8/2105 (0.4%)
25	FE	0.33	0/1568	0.92	8/2105 (0.4%)
25	HE	0.33	0/1568	0.92	8/2105 (0.4%)
25	JE	0.33	0/1568	0.92	8/2105 (0.4%)
26	BF	0.29	0/1530	0.75	0/2070
26	DF	0.29	0/1530	0.75	0/2070
26	FF	0.29	0/1530	0.75	0/2070
26	HF	0.30	0/1530	0.75	0/2070
26	JF	0.29	0/1530	0.75	0/2070
27	BG	0.32	0/1429	0.87	3/1915 (0.2%)
27	DG	0.32	0/1429	0.87	3/1915 (0.2%)
27	FG	0.32	0/1429	0.87	3/1915 (0.2%)
27	HG	0.31	0/1429	0.87	3/1915 (0.2%)
27	JG	0.32	0/1429	0.87	3/1915 (0.2%)
28	BH	0.29	0/1338	0.80	3/1810 (0.2%)
28	DH	0.29	0/1338	0.79	3/1810 (0.2%)
28	FH	0.29	0/1338	0.79	3/1810 (0.2%)
28	HH	0.29	0/1338	0.79	3/1810 (0.2%)
28	JH	0.29	0/1338	0.80	3/1810 (0.2%)
29	BI	0.36	0/405	0.96	3/545 (0.6%)
29	DI	0.35	0/405	0.97	3/545 (0.6%)
29	FI	0.35	0/405	0.97	3/545 (0.6%)
29	HI	0.35	0/405	0.97	3/545 (0.6%)
29	JI	0.36	0/405	0.97	3/545 (0.6%)
30	BJ	0.31	0/1058	0.88	2/1433 (0.1%)
30	DJ	0.31	0/1058	0.88	2/1433 (0.1%)
30	FJ	0.31	0/1058	0.88	2/1433 (0.1%)
30	HJ	0.31	0/1058	0.88	2/1433 (0.1%)
30	JJ	0.31	0/1058	0.88	2/1433 (0.1%)
31	BK	0.32	0/1146	0.87	3/1549 (0.2%)
31	DK	0.32	0/1146	0.87	3/1549 (0.2%)
31	FK	0.32	0/1146	0.87	3/1549 (0.2%)
31	HK	0.32	0/1146	0.87	3/1549 (0.2%)
31	JK	0.32	0/1146	0.87	3/1549 (0.2%)
32	BL	0.28	0/991	0.76	1/1331 (0.1%)
32	DL	0.28	0/991	0.76	1/1331 (0.1%)
32	FL	0.28	0/991	0.76	1/1331 (0.1%)
32	HL	0.28	0/991	0.76	1/1331 (0.1%)
32	JL	0.28	0/991	0.76	1/1331 (0.1%)
33	BM	0.32	0/1082	0.82	1/1448 (0.1%)
33	DM	0.32	0/1082	0.82	1/1448 (0.1%)
33	FM	0.32	0/1082	0.82	1/1448 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	HM	0.32	0/1082	0.82	1/1448 (0.1%)
33	JM	0.32	0/1082	0.82	1/1448 (0.1%)
34	BN	0.36	0/1008	1.07	4/1346 (0.3%)
34	DN	0.36	0/1008	1.07	4/1346 (0.3%)
34	FN	0.36	0/1008	1.07	4/1346 (0.3%)
34	HN	0.36	0/1008	1.07	4/1346 (0.3%)
34	JN	0.36	0/1008	1.07	4/1346 (0.3%)
35	BO	0.28	0/894	0.79	0/1198
35	DO	0.28	0/894	0.79	0/1198
35	FO	0.27	0/894	0.79	0/1198
35	HO	0.27	0/894	0.79	0/1198
35	JO	0.28	0/894	0.79	0/1198
36	BP	0.29	0/841	0.70	0/1124
36	DP	0.28	0/841	0.70	0/1124
36	FP	0.28	0/841	0.70	0/1124
36	HP	0.28	0/841	0.70	0/1124
36	JP	0.28	0/841	0.70	0/1124
37	BQ	0.32	0/1021	0.90	3/1363 (0.2%)
37	DQ	0.32	0/1021	0.90	3/1363 (0.2%)
37	FQ	0.32	0/1021	0.90	3/1363 (0.2%)
37	HQ	0.32	0/1021	0.90	3/1363 (0.2%)
37	JQ	0.33	0/1021	0.90	3/1363 (0.2%)
38	BR	0.34	0/994	0.82	0/1323
38	DR	0.33	0/994	0.82	0/1323
38	FR	0.33	0/994	0.82	0/1323
38	HR	0.33	0/994	0.82	0/1323
38	JR	0.33	0/994	0.82	0/1323
39	BS	0.36	0/797	0.96	3/1061 (0.3%)
39	DS	0.35	0/797	0.96	3/1061 (0.3%)
39	FS	0.36	0/797	0.96	3/1061 (0.3%)
39	HS	0.36	0/797	0.96	3/1061 (0.3%)
39	JS	0.35	0/797	0.96	3/1061 (0.3%)
40	BT	0.31	0/1052	0.93	4/1407 (0.3%)
40	DT	0.31	0/1052	0.93	4/1407 (0.3%)
40	FT	0.31	0/1052	0.93	4/1407 (0.3%)
40	HT	0.31	0/1052	0.93	4/1407 (0.3%)
40	JT	0.31	0/1052	0.93	4/1407 (0.3%)
41	BU	0.33	0/738	0.87	2/988 (0.2%)
41	DU	0.32	0/738	0.87	2/988 (0.2%)
41	FU	0.33	0/738	0.87	2/988 (0.2%)
41	HU	0.33	0/738	0.87	2/988 (0.2%)
41	JU	0.33	0/738	0.87	2/988 (0.2%)
42	BV	0.28	0/863	0.92	1/1158 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
42	DV	0.28	0/863	0.92	1/1158 (0.1%)
42	FV	0.29	0/863	0.92	1/1158 (0.1%)
42	HV	0.29	0/863	0.92	1/1158 (0.1%)
42	JV	0.29	0/863	0.92	1/1158 (0.1%)
43	BW	0.43	1/1351 (0.1%)	1.39	10/1833 (0.5%)
43	DW	0.32	0/1350	0.89	7/1830 (0.4%)
43	FW	0.33	0/1350	0.89	7/1830 (0.4%)
43	HW	0.32	0/1350	0.89	7/1830 (0.4%)
43	JW	0.32	0/1350	0.89	7/1830 (0.4%)
44	BX	0.35	0/650	1.09	5/860 (0.6%)
44	DX	0.36	0/650	1.09	5/860 (0.6%)
44	FX	0.36	0/650	1.09	5/860 (0.6%)
44	HX	0.36	0/650	1.08	5/860 (0.6%)
44	JX	0.36	0/650	1.09	5/860 (0.6%)
45	BY	0.32	0/530	1.08	5/704 (0.7%)
45	DY	0.32	0/530	1.08	5/704 (0.7%)
45	FY	0.32	0/530	1.08	5/704 (0.7%)
45	HY	0.32	0/530	1.08	5/704 (0.7%)
45	JY	0.32	0/530	1.08	5/704 (0.7%)
46	BZ	0.27	0/426	0.70	0/568
46	DZ	0.27	0/426	0.71	0/568
46	FZ	0.27	0/426	0.70	0/568
46	HZ	0.27	0/426	0.70	0/568
46	JZ	0.27	0/426	0.71	0/568
47	B1	0.40	0/620	0.87	2/831 (0.2%)
47	D1	0.40	0/620	0.87	2/831 (0.2%)
47	F1	0.40	0/620	0.87	1/831 (0.1%)
47	H1	0.40	0/620	0.88	2/831 (0.2%)
47	J1	0.40	0/620	0.87	1/831 (0.1%)
48	B2	0.33	0/470	1.37	5/629 (0.8%)
48	D2	0.33	0/470	1.37	6/629 (1.0%)
48	F2	0.33	0/470	1.37	5/629 (0.8%)
48	H2	0.33	0/470	1.37	5/629 (0.8%)
48	J2	0.33	0/470	1.37	6/629 (1.0%)
49	B3	0.45	0/439	0.89	0/583
49	D3	0.45	0/439	0.90	0/583
49	F3	0.45	0/439	0.89	0/583
49	H3	0.44	0/439	0.89	0/583
49	J3	0.45	0/439	0.89	0/583
50	B4	0.30	0/388	0.82	0/509
50	D4	0.30	0/388	0.82	0/509
50	F4	0.30	0/388	0.82	0/509
50	H4	0.30	0/388	0.82	0/509

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
50	J4	0.30	0/388	0.82	0/509
51	B5	0.32	0/503	0.81	2/657 (0.3%)
51	D5	0.32	0/503	0.81	2/657 (0.3%)
51	F5	0.32	0/503	0.81	2/657 (0.3%)
51	H5	0.33	0/503	0.81	2/657 (0.3%)
51	J5	0.32	0/503	0.82	2/657 (0.3%)
52	B6	0.28	0/286	0.76	0/375
52	D6	0.27	0/286	0.76	0/375
52	F6	0.27	0/286	0.76	0/375
52	H6	0.28	0/286	0.76	0/375
52	J6	0.28	0/286	0.76	0/375
53	B7	0.49	3/1740 (0.2%)	0.76	11/2333 (0.5%)
53	D7	0.49	3/1740 (0.2%)	0.76	11/2333 (0.5%)
53	F7	0.49	3/1740 (0.2%)	0.76	11/2333 (0.5%)
53	H7	0.49	3/1740 (0.2%)	0.76	11/2333 (0.5%)
53	J7	0.49	3/1740 (0.2%)	0.76	11/2333 (0.5%)
All	All	0.61	315/778750 (0.0%)	0.83	1213/1161574 (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
1	AA	0	5
1	CA	0	5
1	EA	0	5
1	GA	0	5
1	IA	0	6
12	AL	0	1
12	EL	0	1
13	AM	0	1
13	GM	0	1
22	BB	0	21
22	DB	0	21
22	FB	0	21
22	HB	0	21
22	JB	0	21
24	BD	0	1
24	DD	0	1
24	FD	0	1
24	HD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	JD	0	1
27	BG	0	1
27	DG	0	1
27	FG	0	1
27	HG	0	1
27	JG	0	1
43	BW	0	1
All	All	0	146

The worst 5 of 315 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BB	1888	C	O3'-P	-87.06	0.56	1.61
22	DB	1411	C	O3'-P	-62.45	0.86	1.61
22	FB	1047	G	O3'-P	-62.19	0.86	1.61
22	DB	1437	A	O3'-P	-58.70	0.90	1.61
22	FB	1586	A	O3'-P	-55.84	0.94	1.61

The worst 5 of 1213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	DB	1888	C	P-O3'-C3'	-81.68	21.69	119.70
22	HB	910	U	P-O3'-C3'	-72.53	32.66	119.70
22	BB	1888	C	P-O3'-C3'	-66.03	40.47	119.70
22	FB	3197	U	P-O3'-C3'	-60.64	46.93	119.70
22	FB	1411	C	O3'-P-O5'	-53.08	3.15	104.00

There are no chirality outliers.

5 of 146 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	188	C	Sidechain
1	AA	190	A	Sidechain
1	AA	197	A	Sidechain
1	AA	916	G	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32799	0	16508	3508	4
1	CA	32799	0	16515	3468	3
1	EA	32799	0	16515	3290	2
1	GA	32799	0	16500	3234	3
1	IA	32799	0	16508	3429	10
2	AB	1901	0	1950	183	0
2	CB	1901	0	1951	212	0
2	EB	1901	0	1948	269	0
2	GB	1901	0	1951	188	0
2	IB	1901	0	1951	207	0
3	AC	1613	0	1677	235	0
3	CC	1613	0	1677	271	0
3	EC	1613	0	1674	311	0
3	GC	1613	0	1676	221	0
3	IC	1613	0	1676	319	0
4	AD	1703	0	1765	340	2
4	CD	1703	0	1765	475	24
4	ED	1703	0	1762	358	12
4	GD	1703	0	1767	242	1
4	ID	1703	0	1766	225	2
5	AE	1147	0	1195	303	0
5	CE	1147	0	1198	360	0
5	EE	1147	0	1205	202	0
5	GE	1147	0	1199	236	0
5	IE	1147	0	1202	169	0
6	AF	843	0	857	106	2
6	CF	843	0	857	123	12
6	EF	843	0	857	127	11
6	GF	843	0	857	99	1
6	IF	843	0	857	140	2
7	AG	1257	0	1284	306	0
7	CG	1257	0	1292	310	0
7	EG	1257	0	1296	252	1
7	GG	1257	0	1294	306	21
7	IG	1257	0	1290	237	10
8	AH	1116	0	1175	239	0
8	CH	1116	0	1169	296	0
8	EH	1116	0	1166	369	0
8	GH	1116	0	1176	198	0
8	IH	1116	0	1168	368	0
9	AI	1011	0	1036	313	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	CI	1011	0	1039	268	0
9	EI	1011	0	1017	278	0
9	GI	1011	0	1038	262	0
9	II	1011	0	1031	331	1
10	AJ	795	0	837	303	0
10	CJ	795	0	839	192	0
10	EJ	795	0	831	188	1
10	GJ	795	0	835	260	21
10	IJ	795	0	838	211	11
11	AK	885	0	904	112	0
11	CK	885	0	903	118	12
11	EK	885	0	904	163	1
11	GK	885	0	899	174	0
11	IK	885	0	900	239	0
12	AL	971	0	1046	198	0
12	CL	971	0	1041	188	0
12	EL	971	0	1049	248	3
12	GL	971	0	1044	190	0
12	IL	971	0	1052	198	21
13	AM	997	0	1052	373	0
13	CM	997	0	1047	387	0
13	EM	997	0	1061	198	0
13	GM	997	0	1051	335	0
13	IM	997	0	1057	274	0
14	AN	492	0	531	320	0
14	CN	492	0	532	190	0
14	EN	492	0	532	207	0
14	GN	492	0	533	224	0
14	IN	492	0	532	159	0
15	AO	734	0	771	244	0
15	CO	734	0	767	148	0
15	EO	734	0	769	110	0
15	GO	734	0	770	179	0
15	IO	734	0	768	153	0
16	AP	701	0	718	117	0
16	CP	701	0	719	125	0
16	EP	701	0	712	184	0
16	GP	701	0	716	107	0
16	IP	701	0	713	178	0
17	AQ	857	0	917	348	0
17	CQ	857	0	916	300	0
17	EQ	857	0	920	289	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	GQ	857	0	916	320	0
17	IQ	857	0	923	252	0
18	AR	597	0	667	114	0
18	CR	597	0	666	123	0
18	ER	597	0	668	96	0
18	GR	597	0	666	155	0
18	IR	597	0	668	126	0
19	AS	648	0	673	215	0
19	CS	648	0	673	177	0
19	ES	648	0	671	227	0
19	GS	648	0	673	168	0
19	IS	648	0	668	233	0
20	AT	762	0	856	194	0
20	CT	762	0	854	132	0
20	ET	762	0	848	142	0
20	GT	762	0	850	336	0
20	IT	762	0	848	154	0
21	Aa	719	0	735	0	0
21	Ca	719	0	734	0	0
21	Ea	719	0	737	0	0
21	Ga	719	0	738	0	0
21	Ia	719	0	735	0	0
22	BB	60635	0	30507	6789	5
22	DB	60635	0	30501	6512	4
22	FB	60635	0	30479	6851	6
22	HB	60635	0	30492	6628	2
22	JB	60635	0	30478	7310	31
23	BA	2519	0	1281	279	6
23	DA	2519	0	1279	352	3
23	FA	2519	0	1279	281	0
23	HA	2519	0	1283	137	4
23	JA	2519	0	1284	252	9
24	BD	2079	0	2144	622	0
24	DD	2079	0	2144	593	0
24	FD	2079	0	2152	466	0
24	HD	2079	0	2149	544	0
24	JD	2079	0	2146	636	0
25	BE	1540	0	1592	596	0
25	DE	1540	0	1579	737	0
25	FE	1540	0	1582	628	0
25	HE	1540	0	1597	338	0
25	JE	1540	0	1600	367	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	BF	1507	0	1521	251	0
26	DF	1507	0	1520	196	0
26	FF	1507	0	1523	253	0
26	HF	1507	0	1525	180	0
26	JF	1507	0	1518	322	0
27	BG	1410	0	1489	221	0
27	DG	1410	0	1485	267	0
27	FG	1410	0	1488	320	0
27	HG	1410	0	1487	187	0
27	JG	1410	0	1486	229	0
28	BH	1316	0	1362	246	0
28	DH	1316	0	1360	253	0
28	FH	1316	0	1361	210	0
28	HH	1316	0	1361	164	0
28	JH	1316	0	1361	212	0
29	BI	401	0	426	36	0
29	DI	401	0	424	78	0
29	FI	401	0	425	99	0
29	HI	401	0	426	48	1
29	JI	401	0	426	102	0
30	BJ	1039	0	1083	201	0
30	DJ	1039	0	1083	105	0
30	FJ	1039	0	1083	103	0
30	HJ	1039	0	1083	151	0
30	JJ	1039	0	1080	160	0
31	BK	1122	0	1141	432	0
31	DK	1122	0	1132	390	0
31	FK	1122	0	1146	312	0
31	HK	1122	0	1143	329	0
31	JK	1122	0	1153	200	0
32	BL	981	0	1020	247	0
32	DL	981	0	1020	313	0
32	FL	981	0	1017	246	0
32	HL	981	0	1018	276	0
32	JL	981	0	1019	179	0
33	BM	1068	0	1098	308	0
33	DM	1068	0	1099	305	0
33	FM	1068	0	1100	290	0
33	HM	1068	0	1103	358	0
33	JM	1068	0	1091	414	0
34	BN	986	0	1010	489	0
34	DN	986	0	1006	542	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	FN	986	0	1006	381	0
34	HN	986	0	1011	371	0
34	JN	986	0	1012	300	0
35	BO	886	0	939	236	0
35	DO	886	0	939	252	0
35	FO	886	0	934	286	0
35	HO	886	0	936	259	0
35	JO	886	0	936	247	0
36	BP	834	0	874	71	0
36	DP	834	0	874	147	0
36	FP	834	0	863	177	0
36	HP	834	0	872	114	0
36	JP	834	0	868	170	0
37	BQ	1008	0	1048	323	0
37	DQ	1008	0	1050	269	0
37	FQ	1008	0	1048	212	0
37	HQ	1008	0	1050	276	0
37	JQ	1008	0	1045	336	0
38	BR	978	0	1018	183	0
38	DR	978	0	1015	377	0
38	FR	978	0	1011	513	0
38	HR	978	0	1009	306	0
38	JR	978	0	999	354	0
39	BS	787	0	803	206	0
39	DS	787	0	804	257	0
39	FS	787	0	800	291	0
39	HS	787	0	804	152	0
39	JS	787	0	798	247	0
40	BT	1039	0	1111	284	0
40	DT	1039	0	1105	328	0
40	FT	1039	0	1107	323	0
40	HT	1039	0	1107	453	0
40	JT	1039	0	1110	312	0
41	BU	727	0	752	108	0
41	DU	727	0	749	117	0
41	FU	727	0	736	211	0
41	HU	727	0	751	157	0
41	JU	727	0	747	183	0
42	BV	852	0	909	121	0
42	DV	852	0	911	104	0
42	FV	852	0	908	201	0
42	HV	852	0	908	132	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	JV	852	0	905	292	0
43	BW	1328	0	1343	486	0
43	DW	1328	0	1338	594	0
43	FW	1328	0	1341	325	0
43	HW	1328	0	1350	306	0
43	JW	1328	0	1342	254	0
44	BX	642	0	664	280	0
44	DX	642	0	665	210	0
44	FX	642	0	658	257	0
44	HX	642	0	663	295	0
44	JX	642	0	661	246	0
45	BY	526	0	546	72	0
45	DY	526	0	543	49	0
45	FY	526	0	538	102	0
45	HY	526	0	535	211	0
45	JY	526	0	535	196	0
46	BZ	424	0	468	76	0
46	DZ	424	0	468	109	0
46	FZ	424	0	467	204	0
46	HZ	424	0	466	82	0
46	JZ	424	0	468	135	0
47	B1	604	0	594	201	0
47	D1	604	0	593	193	0
47	F1	604	0	592	177	0
47	H1	604	0	582	203	0
47	J1	604	0	592	232	0
48	B2	458	0	457	218	0
48	D2	458	0	461	188	0
48	F2	458	0	459	178	0
48	H2	458	0	456	286	0
48	J2	458	0	460	221	0
49	B3	432	0	456	53	0
49	D3	432	0	456	87	0
49	F3	432	0	453	181	0
49	H3	432	0	455	74	0
49	J3	432	0	452	154	0
50	B4	384	0	406	139	0
50	D4	384	0	403	166	0
50	F4	384	0	408	198	0
50	H4	384	0	409	115	0
50	J4	384	0	401	167	0
51	B5	496	0	547	162	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	D5	496	0	542	191	0
51	F5	496	0	542	251	0
51	H5	496	0	545	230	0
51	J5	496	0	536	298	0
52	B6	285	0	305	210	0
52	D6	285	0	313	119	0
52	F6	285	0	309	72	0
52	H6	285	0	310	88	0
52	J6	285	0	311	114	0
53	B7	1720	0	1842	221	6
53	D7	1720	0	1842	167	4
53	F7	1720	0	1847	223	9
53	H7	1720	0	1843	360	3
53	J7	1720	0	1826	472	0
All	All	717805	0	489246	75816	144

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 63.

The worst 5 of 75816 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)
34:DN:66:TYR:CE2	43:DW:118:HIS:CE1	1.77	1.72
22:HB:2733:A:C2	52:H6:15:LYS:HE2	1.22	1.72
22:BB:1437:A:H2'	22:BB:1438:G:C8	1.25	1.70
22:BB:1805:G:C2	24:BD:52:ARG:HD3	1.26	1.69
34:BN:66:TYR:CD1	43:BW:115:ILE:HG21	1.25	1.69

The worst 5 of 144 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:435:C:OP1	22:BB:3096:C:OP1[3_465]	0.46	1.74
12:IL:128:ALA:C	22:JB:3157:G:C4'[4_445]	0.52	1.68
7:GG:60:LYS:CD	10:GJ:90:LEU:CD1[3_465]	0.58	1.62
7:GG:60:LYS:CE	10:GJ:90:LEU:CG[3_465]	0.60	1.60
4:CD:173:TRP:N	6:CF:15:ASP:OD2[3_465]	0.63	1.57

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	232/234 (99%)	129 (56%)	74 (32%)	29 (12%)	0	5
2	CB	232/234 (99%)	128 (55%)	75 (32%)	29 (12%)	0	5
2	EB	232/234 (99%)	127 (55%)	76 (33%)	29 (12%)	0	5
2	GB	232/234 (99%)	129 (56%)	74 (32%)	29 (12%)	0	5
2	IB	232/234 (99%)	128 (55%)	75 (32%)	29 (12%)	0	5
3	AC	204/206 (99%)	125 (61%)	60 (29%)	19 (9%)	0	11
3	CC	204/206 (99%)	124 (61%)	61 (30%)	19 (9%)	0	11
3	EC	204/206 (99%)	125 (61%)	60 (29%)	19 (9%)	0	11
3	GC	204/206 (99%)	124 (61%)	61 (30%)	19 (9%)	0	11
3	IC	204/206 (99%)	124 (61%)	61 (30%)	19 (9%)	0	11
4	AD	206/208 (99%)	130 (63%)	56 (27%)	20 (10%)	0	10
4	CD	206/208 (99%)	129 (63%)	57 (28%)	20 (10%)	0	10
4	ED	206/208 (99%)	130 (63%)	56 (27%)	20 (10%)	0	10
4	GD	206/208 (99%)	128 (62%)	58 (28%)	20 (10%)	0	10
4	ID	206/208 (99%)	129 (63%)	57 (28%)	20 (10%)	0	10
5	AE	148/150 (99%)	93 (63%)	43 (29%)	12 (8%)	1	12
5	CE	148/150 (99%)	91 (62%)	45 (30%)	12 (8%)	1	12
5	EE	148/150 (99%)	92 (62%)	44 (30%)	12 (8%)	1	12
5	GE	148/150 (99%)	92 (62%)	44 (30%)	12 (8%)	1	12
5	IE	148/150 (99%)	92 (62%)	44 (30%)	12 (8%)	1	12
6	AF	99/101 (98%)	67 (68%)	25 (25%)	7 (7%)	1	14
6	CF	99/101 (98%)	67 (68%)	25 (25%)	7 (7%)	1	14
6	EF	99/101 (98%)	67 (68%)	25 (25%)	7 (7%)	1	14
6	GF	99/101 (98%)	67 (68%)	25 (25%)	7 (7%)	1	14
6	IF	99/101 (98%)	67 (68%)	25 (25%)	7 (7%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	153/155 (99%)	94 (61%)	47 (31%)	12 (8%)	1	13
7	CG	153/155 (99%)	94 (61%)	47 (31%)	12 (8%)	1	13
7	EG	153/155 (99%)	93 (61%)	48 (31%)	12 (8%)	1	13
7	GG	153/155 (99%)	94 (61%)	47 (31%)	12 (8%)	1	13
7	IG	153/155 (99%)	94 (61%)	47 (31%)	12 (8%)	1	13
8	AH	136/138 (99%)	83 (61%)	38 (28%)	15 (11%)	0	7
8	CH	136/138 (99%)	83 (61%)	37 (27%)	16 (12%)	0	6
8	EH	136/138 (99%)	83 (61%)	37 (27%)	16 (12%)	0	6
8	GH	136/138 (99%)	83 (61%)	37 (27%)	16 (12%)	0	6
8	IH	136/138 (99%)	83 (61%)	37 (27%)	16 (12%)	0	6
9	AI	125/127 (98%)	68 (54%)	43 (34%)	14 (11%)	0	7
9	CI	125/127 (98%)	68 (54%)	43 (34%)	14 (11%)	0	7
9	EI	125/127 (98%)	68 (54%)	43 (34%)	14 (11%)	0	7
9	GI	125/127 (98%)	68 (54%)	43 (34%)	14 (11%)	0	7
9	II	125/127 (98%)	68 (54%)	43 (34%)	14 (11%)	0	7
10	AJ	96/98 (98%)	52 (54%)	22 (23%)	22 (23%)	0	1
10	CJ	96/98 (98%)	53 (55%)	21 (22%)	22 (23%)	0	1
10	EJ	96/98 (98%)	52 (54%)	22 (23%)	22 (23%)	0	1
10	GJ	96/98 (98%)	52 (54%)	22 (23%)	22 (23%)	0	1
10	IJ	96/98 (98%)	52 (54%)	22 (23%)	22 (23%)	0	1
11	AK	117/119 (98%)	72 (62%)	32 (27%)	13 (11%)	0	7
11	CK	117/119 (98%)	74 (63%)	30 (26%)	13 (11%)	0	7
11	EK	117/119 (98%)	73 (62%)	31 (26%)	13 (11%)	0	7
11	GK	117/119 (98%)	73 (62%)	31 (26%)	13 (11%)	0	7
11	IK	117/119 (98%)	73 (62%)	31 (26%)	13 (11%)	0	7
12	AL	118/124 (95%)	77 (65%)	34 (29%)	7 (6%)	1	17
12	CL	116/124 (94%)	76 (66%)	32 (28%)	8 (7%)	1	15
12	EL	118/124 (95%)	76 (64%)	34 (29%)	8 (7%)	1	15
12	GL	116/124 (94%)	77 (66%)	31 (27%)	8 (7%)	1	15
12	IL	118/124 (95%)	78 (66%)	33 (28%)	7 (6%)	1	17
13	AM	121/125 (97%)	77 (64%)	32 (26%)	12 (10%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	CM	119/125 (95%)	77 (65%)	32 (27%)	10 (8%)	1	12
13	EM	119/125 (95%)	77 (65%)	32 (27%)	10 (8%)	1	12
13	GM	121/125 (97%)	77 (64%)	32 (26%)	12 (10%)	0	9
13	IM	119/125 (95%)	78 (66%)	30 (25%)	11 (9%)	1	11
14	AN	58/60 (97%)	22 (38%)	27 (47%)	9 (16%)	0	3
14	CN	58/60 (97%)	23 (40%)	26 (45%)	9 (16%)	0	3
14	EN	58/60 (97%)	22 (38%)	27 (47%)	9 (16%)	0	3
14	GN	58/60 (97%)	22 (38%)	27 (47%)	9 (16%)	0	3
14	IN	58/60 (97%)	22 (38%)	27 (47%)	9 (16%)	0	3
15	AO	86/88 (98%)	59 (69%)	19 (22%)	8 (9%)	0	11
15	CO	86/88 (98%)	59 (69%)	20 (23%)	7 (8%)	1	12
15	EO	86/88 (98%)	59 (69%)	19 (22%)	8 (9%)	0	11
15	GO	86/88 (98%)	59 (69%)	20 (23%)	7 (8%)	1	12
15	IO	86/88 (98%)	59 (69%)	19 (22%)	8 (9%)	0	11
16	AP	81/83 (98%)	48 (59%)	29 (36%)	4 (5%)	2	20
16	CP	81/83 (98%)	48 (59%)	29 (36%)	4 (5%)	2	20
16	EP	81/83 (98%)	48 (59%)	29 (36%)	4 (5%)	2	20
16	GP	81/83 (98%)	48 (59%)	29 (36%)	4 (5%)	2	20
16	IP	81/83 (98%)	49 (60%)	28 (35%)	4 (5%)	2	20
17	AQ	102/104 (98%)	53 (52%)	34 (33%)	15 (15%)	0	4
17	CQ	102/104 (98%)	53 (52%)	34 (33%)	15 (15%)	0	4
17	EQ	102/104 (98%)	53 (52%)	34 (33%)	15 (15%)	0	4
17	GQ	102/104 (98%)	53 (52%)	34 (33%)	15 (15%)	0	4
17	IQ	102/104 (98%)	53 (52%)	34 (33%)	15 (15%)	0	4
18	AR	71/73 (97%)	43 (61%)	20 (28%)	8 (11%)	0	7
18	CR	71/73 (97%)	43 (61%)	20 (28%)	8 (11%)	0	7
18	ER	71/73 (97%)	43 (61%)	20 (28%)	8 (11%)	0	7
18	GR	71/73 (97%)	43 (61%)	20 (28%)	8 (11%)	0	7
18	IR	71/73 (97%)	43 (61%)	20 (28%)	8 (11%)	0	7
19	AS	78/80 (98%)	48 (62%)	22 (28%)	8 (10%)	0	8
19	CS	78/80 (98%)	49 (63%)	21 (27%)	8 (10%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	ES	78/80 (98%)	48 (62%)	22 (28%)	8 (10%)	0	8
19	GS	78/80 (98%)	49 (63%)	20 (26%)	9 (12%)	0	6
19	IS	78/80 (98%)	48 (62%)	21 (27%)	9 (12%)	0	6
20	AT	97/99 (98%)	65 (67%)	20 (21%)	12 (12%)	0	5
20	CT	97/99 (98%)	64 (66%)	21 (22%)	12 (12%)	0	5
20	ET	97/99 (98%)	64 (66%)	21 (22%)	12 (12%)	0	5
20	GT	97/99 (98%)	64 (66%)	21 (22%)	12 (12%)	0	5
20	IT	97/99 (98%)	64 (66%)	21 (22%)	12 (12%)	0	5
21	Aa	88/90 (98%)	77 (88%)	10 (11%)	1 (1%)	14	52
21	Ca	88/90 (98%)	77 (88%)	10 (11%)	1 (1%)	14	52
21	Ea	88/90 (98%)	77 (88%)	10 (11%)	1 (1%)	14	52
21	Ga	88/90 (98%)	77 (88%)	10 (11%)	1 (1%)	14	52
21	Ia	88/90 (98%)	77 (88%)	10 (11%)	1 (1%)	14	52
24	BD	268/270 (99%)	96 (36%)	93 (35%)	79 (30%)	0	0
24	DD	268/270 (99%)	98 (37%)	92 (34%)	78 (29%)	0	0
24	FD	268/270 (99%)	97 (36%)	93 (35%)	78 (29%)	0	0
24	HD	268/270 (99%)	97 (36%)	93 (35%)	78 (29%)	0	0
24	JD	268/270 (99%)	96 (36%)	95 (35%)	77 (29%)	0	0
25	BE	203/205 (99%)	85 (42%)	74 (36%)	44 (22%)	0	2
25	DE	203/205 (99%)	85 (42%)	74 (36%)	44 (22%)	0	2
25	FE	203/205 (99%)	85 (42%)	73 (36%)	45 (22%)	0	1
25	HE	203/205 (99%)	85 (42%)	73 (36%)	45 (22%)	0	1
25	JE	203/205 (99%)	86 (42%)	73 (36%)	44 (22%)	0	2
26	BF	195/198 (98%)	90 (46%)	59 (30%)	46 (24%)	0	1
26	DF	195/198 (98%)	90 (46%)	59 (30%)	46 (24%)	0	1
26	FF	195/198 (98%)	90 (46%)	59 (30%)	46 (24%)	0	1
26	HF	195/198 (98%)	90 (46%)	59 (30%)	46 (24%)	0	1
26	JF	195/198 (98%)	90 (46%)	59 (30%)	46 (24%)	0	1
27	BG	176/178 (99%)	75 (43%)	59 (34%)	42 (24%)	0	1
27	DG	176/178 (99%)	75 (43%)	59 (34%)	42 (24%)	0	1
27	FG	176/178 (99%)	74 (42%)	60 (34%)	42 (24%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	HG	176/178 (99%)	75 (43%)	59 (34%)	42 (24%)	0	1
27	JG	176/178 (99%)	75 (43%)	58 (33%)	43 (24%)	0	1
28	BH	175/177 (99%)	84 (48%)	55 (31%)	36 (21%)	0	2
28	DH	175/177 (99%)	83 (47%)	56 (32%)	36 (21%)	0	2
28	FH	175/177 (99%)	83 (47%)	56 (32%)	36 (21%)	0	2
28	HH	175/177 (99%)	84 (48%)	55 (31%)	36 (21%)	0	2
28	JH	175/177 (99%)	83 (47%)	56 (32%)	36 (21%)	0	2
29	BI	50/52 (96%)	16 (32%)	19 (38%)	15 (30%)	0	0
29	DI	50/52 (96%)	16 (32%)	19 (38%)	15 (30%)	0	0
29	FI	50/52 (96%)	16 (32%)	19 (38%)	15 (30%)	0	0
29	HI	50/52 (96%)	16 (32%)	19 (38%)	15 (30%)	0	0
29	JI	50/52 (96%)	16 (32%)	19 (38%)	15 (30%)	0	0
30	BJ	141/143 (99%)	56 (40%)	47 (33%)	38 (27%)	0	0
30	DJ	141/143 (99%)	56 (40%)	47 (33%)	38 (27%)	0	0
30	FJ	141/143 (99%)	56 (40%)	47 (33%)	38 (27%)	0	0
30	HJ	141/143 (99%)	56 (40%)	47 (33%)	38 (27%)	0	0
30	JJ	141/143 (99%)	56 (40%)	47 (33%)	38 (27%)	0	0
31	BK	141/143 (99%)	55 (39%)	58 (41%)	28 (20%)	0	2
31	DK	141/143 (99%)	55 (39%)	58 (41%)	28 (20%)	0	2
31	FK	141/143 (99%)	55 (39%)	58 (41%)	28 (20%)	0	2
31	HK	141/143 (99%)	55 (39%)	58 (41%)	28 (20%)	0	2
31	JK	141/143 (99%)	55 (39%)	58 (41%)	28 (20%)	0	2
32	BL	130/132 (98%)	56 (43%)	37 (28%)	37 (28%)	0	0
32	DL	130/132 (98%)	56 (43%)	37 (28%)	37 (28%)	0	0
32	FL	130/132 (98%)	56 (43%)	37 (28%)	37 (28%)	0	0
32	HL	130/132 (98%)	56 (43%)	37 (28%)	37 (28%)	0	0
32	JL	130/132 (98%)	56 (43%)	37 (28%)	37 (28%)	0	0
33	BM	139/141 (99%)	60 (43%)	43 (31%)	36 (26%)	0	1
33	DM	139/141 (99%)	60 (43%)	43 (31%)	36 (26%)	0	1
33	FM	139/141 (99%)	60 (43%)	43 (31%)	36 (26%)	0	1
33	HM	139/141 (99%)	60 (43%)	43 (31%)	36 (26%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	JM	139/141 (99%)	60 (43%)	43 (31%)	36 (26%)	0	1
34	BN	122/124 (98%)	60 (49%)	35 (29%)	27 (22%)	0	1
34	DN	122/124 (98%)	61 (50%)	34 (28%)	27 (22%)	0	1
34	FN	122/124 (98%)	61 (50%)	34 (28%)	27 (22%)	0	1
34	HN	122/124 (98%)	61 (50%)	34 (28%)	27 (22%)	0	1
34	JN	122/124 (98%)	61 (50%)	34 (28%)	27 (22%)	0	1
35	BO	112/114 (98%)	52 (46%)	38 (34%)	22 (20%)	0	2
35	DO	112/114 (98%)	52 (46%)	38 (34%)	22 (20%)	0	2
35	FO	112/114 (98%)	52 (46%)	37 (33%)	23 (20%)	0	2
35	HO	112/114 (98%)	52 (46%)	38 (34%)	22 (20%)	0	2
35	JO	112/114 (98%)	51 (46%)	39 (35%)	22 (20%)	0	2
36	BP	109/111 (98%)	52 (48%)	37 (34%)	20 (18%)	0	3
36	DP	109/111 (98%)	52 (48%)	37 (34%)	20 (18%)	0	3
36	FP	109/111 (98%)	52 (48%)	37 (34%)	20 (18%)	0	3
36	HP	109/111 (98%)	52 (48%)	37 (34%)	20 (18%)	0	3
36	JP	109/111 (98%)	52 (48%)	37 (34%)	20 (18%)	0	3
37	BQ	123/125 (98%)	50 (41%)	47 (38%)	26 (21%)	0	2
37	DQ	123/125 (98%)	50 (41%)	48 (39%)	25 (20%)	0	2
37	FQ	123/125 (98%)	50 (41%)	47 (38%)	26 (21%)	0	2
37	HQ	123/125 (98%)	50 (41%)	48 (39%)	25 (20%)	0	2
37	JQ	123/125 (98%)	50 (41%)	47 (38%)	26 (21%)	0	2
38	BR	115/117 (98%)	55 (48%)	41 (36%)	19 (16%)	0	3
38	DR	115/117 (98%)	55 (48%)	41 (36%)	19 (16%)	0	3
38	FR	115/117 (98%)	55 (48%)	41 (36%)	19 (16%)	0	3
38	HR	115/117 (98%)	55 (48%)	40 (35%)	20 (17%)	0	3
38	JR	115/117 (98%)	55 (48%)	41 (36%)	19 (16%)	0	3
39	BS	98/100 (98%)	39 (40%)	37 (38%)	22 (22%)	0	1
39	DS	98/100 (98%)	38 (39%)	38 (39%)	22 (22%)	0	1
39	FS	98/100 (98%)	39 (40%)	37 (38%)	22 (22%)	0	1
39	HS	98/100 (98%)	39 (40%)	37 (38%)	22 (22%)	0	1
39	JS	98/100 (98%)	39 (40%)	37 (38%)	22 (22%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BT	128/130 (98%)	52 (41%)	51 (40%)	25 (20%)	0	2
40	DT	128/130 (98%)	52 (41%)	51 (40%)	25 (20%)	0	2
40	FT	128/130 (98%)	52 (41%)	51 (40%)	25 (20%)	0	2
40	HT	128/130 (98%)	52 (41%)	51 (40%)	25 (20%)	0	2
40	JT	128/130 (98%)	53 (41%)	50 (39%)	25 (20%)	0	2
41	BU	91/93 (98%)	29 (32%)	30 (33%)	32 (35%)	0	0
41	DU	91/93 (98%)	29 (32%)	30 (33%)	32 (35%)	0	0
41	FU	91/93 (98%)	28 (31%)	31 (34%)	32 (35%)	0	0
41	HU	91/93 (98%)	29 (32%)	30 (33%)	32 (35%)	0	0
41	JU	91/93 (98%)	28 (31%)	31 (34%)	32 (35%)	0	0
42	BV	111/113 (98%)	43 (39%)	35 (32%)	33 (30%)	0	0
42	DV	111/113 (98%)	43 (39%)	36 (32%)	32 (29%)	0	0
42	FV	111/113 (98%)	43 (39%)	36 (32%)	32 (29%)	0	0
42	HV	111/113 (98%)	43 (39%)	35 (32%)	33 (30%)	0	0
42	JV	111/113 (98%)	43 (39%)	36 (32%)	32 (29%)	0	0
43	BW	169/173 (98%)	45 (27%)	69 (41%)	55 (32%)	0	0
43	DW	168/173 (97%)	44 (26%)	70 (42%)	54 (32%)	0	0
43	FW	168/173 (97%)	44 (26%)	69 (41%)	55 (33%)	0	0
43	HW	168/173 (97%)	44 (26%)	70 (42%)	54 (32%)	0	0
43	JW	168/173 (97%)	44 (26%)	70 (42%)	54 (32%)	0	0
44	BX	84/86 (98%)	31 (37%)	29 (34%)	24 (29%)	0	0
44	DX	84/86 (98%)	31 (37%)	29 (34%)	24 (29%)	0	0
44	FX	84/86 (98%)	31 (37%)	29 (34%)	24 (29%)	0	0
44	HX	84/86 (98%)	31 (37%)	29 (34%)	24 (29%)	0	0
44	JX	84/86 (98%)	31 (37%)	29 (34%)	24 (29%)	0	0
45	BY	63/65 (97%)	35 (56%)	16 (25%)	12 (19%)	0	2
45	DY	63/65 (97%)	35 (56%)	16 (25%)	12 (19%)	0	2
45	FY	63/65 (97%)	35 (56%)	16 (25%)	12 (19%)	0	2
45	HY	63/65 (97%)	35 (56%)	16 (25%)	12 (19%)	0	2
45	JY	63/65 (97%)	35 (56%)	16 (25%)	12 (19%)	0	2
46	BZ	53/55 (96%)	25 (47%)	19 (36%)	9 (17%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	DZ	53/55 (96%)	25 (47%)	19 (36%)	9 (17%)	0	3
46	FZ	53/55 (96%)	25 (47%)	19 (36%)	9 (17%)	0	3
46	HZ	53/55 (96%)	25 (47%)	19 (36%)	9 (17%)	0	3
46	JZ	53/55 (96%)	25 (47%)	19 (36%)	9 (17%)	0	3
47	B1	71/73 (97%)	26 (37%)	24 (34%)	21 (30%)	0	0
47	D1	71/73 (97%)	26 (37%)	24 (34%)	21 (30%)	0	0
47	F1	71/73 (97%)	26 (37%)	25 (35%)	20 (28%)	0	0
47	H1	71/73 (97%)	26 (37%)	24 (34%)	21 (30%)	0	0
47	J1	71/73 (97%)	26 (37%)	24 (34%)	21 (30%)	0	0
48	B2	56/58 (97%)	19 (34%)	23 (41%)	14 (25%)	0	1
48	D2	56/58 (97%)	19 (34%)	23 (41%)	14 (25%)	0	1
48	F2	56/58 (97%)	19 (34%)	23 (41%)	14 (25%)	0	1
48	H2	56/58 (97%)	19 (34%)	23 (41%)	14 (25%)	0	1
48	J2	56/58 (97%)	19 (34%)	23 (41%)	14 (25%)	0	1
49	B3	51/53 (96%)	13 (26%)	18 (35%)	20 (39%)	0	0
49	D3	51/53 (96%)	13 (26%)	18 (35%)	20 (39%)	0	0
49	F3	51/53 (96%)	13 (26%)	18 (35%)	20 (39%)	0	0
49	H3	51/53 (96%)	13 (26%)	18 (35%)	20 (39%)	0	0
49	J3	51/53 (96%)	13 (26%)	18 (35%)	20 (39%)	0	0
50	B4	44/46 (96%)	20 (46%)	15 (34%)	9 (20%)	0	2
50	D4	44/46 (96%)	20 (46%)	15 (34%)	9 (20%)	0	2
50	F4	44/46 (96%)	20 (46%)	15 (34%)	9 (20%)	0	2
50	H4	44/46 (96%)	20 (46%)	15 (34%)	9 (20%)	0	2
50	J4	44/46 (96%)	20 (46%)	15 (34%)	9 (20%)	0	2
51	B5	61/63 (97%)	26 (43%)	19 (31%)	16 (26%)	0	1
51	D5	61/63 (97%)	27 (44%)	19 (31%)	15 (25%)	0	1
51	F5	61/63 (97%)	26 (43%)	20 (33%)	15 (25%)	0	1
51	H5	61/63 (97%)	26 (43%)	20 (33%)	15 (25%)	0	1
51	J5	61/63 (97%)	26 (43%)	20 (33%)	15 (25%)	0	1
52	B6	33/35 (94%)	12 (36%)	10 (30%)	11 (33%)	0	0
52	D6	33/35 (94%)	12 (36%)	10 (30%)	11 (33%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	F6	33/35 (94%)	12 (36%)	10 (30%)	11 (33%)	0	0
52	H6	33/35 (94%)	12 (36%)	10 (30%)	11 (33%)	0	0
52	J6	33/35 (94%)	12 (36%)	10 (30%)	11 (33%)	0	0
53	B7	215/217 (99%)	112 (52%)	79 (37%)	24 (11%)	0	7
53	D7	215/217 (99%)	113 (53%)	78 (36%)	24 (11%)	0	7
53	F7	215/217 (99%)	114 (53%)	77 (36%)	24 (11%)	0	7
53	H7	215/217 (99%)	113 (53%)	78 (36%)	24 (11%)	0	7
53	J7	215/217 (99%)	112 (52%)	79 (37%)	24 (11%)	0	7
All	All	29701/30260 (98%)	14747 (50%)	9520 (32%)	5434 (18%)	0	3

5 of 5434 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	19	HIS
2	AB	24	TRP
2	AB	165	VAL
2	AB	195	ASP
3	AC	4	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/202 (100%)	179 (89%)	23 (11%)	5	21
2	CB	202/202 (100%)	179 (89%)	23 (11%)	5	21
2	EB	202/202 (100%)	179 (89%)	23 (11%)	5	21
2	GB	202/202 (100%)	179 (89%)	23 (11%)	5	21
2	IB	202/202 (100%)	179 (89%)	23 (11%)	5	21
3	AC	160/160 (100%)	150 (94%)	10 (6%)	18	43
3	CC	160/160 (100%)	150 (94%)	10 (6%)	18	43
3	EC	160/160 (100%)	150 (94%)	10 (6%)	18	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	GC	160/160 (100%)	150 (94%)	10 (6%)	18	43
3	IC	160/160 (100%)	150 (94%)	10 (6%)	18	43
4	AD	180/180 (100%)	157 (87%)	23 (13%)	4	18
4	CD	180/180 (100%)	157 (87%)	23 (13%)	4	18
4	ED	180/180 (100%)	157 (87%)	23 (13%)	4	18
4	GD	180/180 (100%)	157 (87%)	23 (13%)	4	18
4	ID	180/180 (100%)	157 (87%)	23 (13%)	4	18
5	AE	115/115 (100%)	106 (92%)	9 (8%)	12	36
5	CE	115/115 (100%)	106 (92%)	9 (8%)	12	36
5	EE	115/115 (100%)	106 (92%)	9 (8%)	12	36
5	GE	115/115 (100%)	106 (92%)	9 (8%)	12	36
5	IE	115/115 (100%)	106 (92%)	9 (8%)	12	36
6	AF	90/90 (100%)	82 (91%)	8 (9%)	9	30
6	CF	90/90 (100%)	81 (90%)	9 (10%)	7	26
6	EF	90/90 (100%)	82 (91%)	8 (9%)	9	30
6	GF	90/90 (100%)	82 (91%)	8 (9%)	9	30
6	IF	90/90 (100%)	81 (90%)	9 (10%)	7	26
7	AG	126/126 (100%)	115 (91%)	11 (9%)	10	31
7	CG	126/126 (100%)	115 (91%)	11 (9%)	10	31
7	EG	126/126 (100%)	115 (91%)	11 (9%)	10	31
7	GG	126/126 (100%)	115 (91%)	11 (9%)	10	31
7	IG	126/126 (100%)	115 (91%)	11 (9%)	10	31
8	AH	119/119 (100%)	113 (95%)	6 (5%)	24	49
8	CH	119/119 (100%)	113 (95%)	6 (5%)	24	49
8	EH	119/119 (100%)	113 (95%)	6 (5%)	24	49
8	GH	119/119 (100%)	113 (95%)	6 (5%)	24	49
8	IH	119/119 (100%)	113 (95%)	6 (5%)	24	49
9	AI	98/98 (100%)	87 (89%)	11 (11%)	6	22
9	CI	98/98 (100%)	87 (89%)	11 (11%)	6	22
9	EI	98/98 (100%)	88 (90%)	10 (10%)	7	25
9	GI	98/98 (100%)	87 (89%)	11 (11%)	6	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	II	98/98 (100%)	87 (89%)	11 (11%)	6	22
10	AJ	88/88 (100%)	81 (92%)	7 (8%)	12	35
10	CJ	88/88 (100%)	81 (92%)	7 (8%)	12	35
10	EJ	88/88 (100%)	81 (92%)	7 (8%)	12	35
10	GJ	88/88 (100%)	81 (92%)	7 (8%)	12	35
10	IJ	88/88 (100%)	81 (92%)	7 (8%)	12	35
11	AK	90/90 (100%)	80 (89%)	10 (11%)	6	22
11	CK	90/90 (100%)	80 (89%)	10 (11%)	6	22
11	EK	90/90 (100%)	80 (89%)	10 (11%)	6	22
11	GK	90/90 (100%)	80 (89%)	10 (11%)	6	22
11	IK	90/90 (100%)	80 (89%)	10 (11%)	6	22
12	AL	104/104 (100%)	98 (94%)	6 (6%)	20	45
12	CL	104/104 (100%)	98 (94%)	6 (6%)	20	45
12	EL	104/104 (100%)	98 (94%)	6 (6%)	20	45
12	GL	104/104 (100%)	98 (94%)	6 (6%)	20	45
12	IL	104/104 (100%)	98 (94%)	6 (6%)	20	45
13	AM	100/100 (100%)	86 (86%)	14 (14%)	3	17
13	CM	100/100 (100%)	86 (86%)	14 (14%)	3	17
13	EM	100/100 (100%)	86 (86%)	14 (14%)	3	17
13	GM	100/100 (100%)	86 (86%)	14 (14%)	3	17
13	IM	100/100 (100%)	86 (86%)	14 (14%)	3	17
14	AN	49/49 (100%)	44 (90%)	5 (10%)	7	25
14	CN	49/49 (100%)	44 (90%)	5 (10%)	7	25
14	EN	49/49 (100%)	44 (90%)	5 (10%)	7	25
14	GN	49/49 (100%)	44 (90%)	5 (10%)	7	25
14	IN	49/49 (100%)	44 (90%)	5 (10%)	7	25
15	AO	79/79 (100%)	75 (95%)	4 (5%)	24	48
15	CO	79/79 (100%)	75 (95%)	4 (5%)	24	48
15	EO	79/79 (100%)	75 (95%)	4 (5%)	24	48
15	GO	79/79 (100%)	75 (95%)	4 (5%)	24	48
15	IO	79/79 (100%)	75 (95%)	4 (5%)	24	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AP	72/72 (100%)	68 (94%)	4 (6%)	21	46
16	CP	72/72 (100%)	68 (94%)	4 (6%)	21	46
16	EP	72/72 (100%)	68 (94%)	4 (6%)	21	46
16	GP	72/72 (100%)	68 (94%)	4 (6%)	21	46
16	IP	72/72 (100%)	68 (94%)	4 (6%)	21	46
17	AQ	96/96 (100%)	88 (92%)	8 (8%)	11	34
17	CQ	96/96 (100%)	88 (92%)	8 (8%)	11	34
17	EQ	96/96 (100%)	88 (92%)	8 (8%)	11	34
17	GQ	96/96 (100%)	88 (92%)	8 (8%)	11	34
17	IQ	96/96 (100%)	88 (92%)	8 (8%)	11	34
18	AR	64/64 (100%)	57 (89%)	7 (11%)	6	23
18	CR	64/64 (100%)	57 (89%)	7 (11%)	6	23
18	ER	64/64 (100%)	57 (89%)	7 (11%)	6	23
18	GR	64/64 (100%)	57 (89%)	7 (11%)	6	23
18	IR	64/64 (100%)	57 (89%)	7 (11%)	6	23
19	AS	71/71 (100%)	62 (87%)	9 (13%)	4	18
19	CS	71/71 (100%)	62 (87%)	9 (13%)	4	18
19	ES	71/71 (100%)	62 (87%)	9 (13%)	4	18
19	GS	71/71 (100%)	62 (87%)	9 (13%)	4	18
19	IS	71/71 (100%)	62 (87%)	9 (13%)	4	18
20	AT	76/76 (100%)	73 (96%)	3 (4%)	32	56
20	CT	76/76 (100%)	73 (96%)	3 (4%)	32	56
20	ET	76/76 (100%)	73 (96%)	3 (4%)	32	56
20	GT	76/76 (100%)	73 (96%)	3 (4%)	32	56
20	IT	76/76 (100%)	73 (96%)	3 (4%)	32	56
21	Aa	80/80 (100%)	62 (78%)	18 (22%)	1	5
21	Ca	80/80 (100%)	62 (78%)	18 (22%)	1	5
21	Ea	80/80 (100%)	62 (78%)	18 (22%)	1	5
21	Ga	80/80 (100%)	62 (78%)	18 (22%)	1	5
21	Ia	80/80 (100%)	62 (78%)	18 (22%)	1	5
24	BD	212/212 (100%)	168 (79%)	44 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	DD	212/212 (100%)	168 (79%)	44 (21%)	1	6
24	FD	212/212 (100%)	168 (79%)	44 (21%)	1	6
24	HD	212/212 (100%)	168 (79%)	44 (21%)	1	6
24	JD	212/212 (100%)	168 (79%)	44 (21%)	1	6
25	BE	155/155 (100%)	130 (84%)	25 (16%)	2	13
25	DE	155/155 (100%)	130 (84%)	25 (16%)	2	13
25	FE	155/155 (100%)	131 (84%)	24 (16%)	2	14
25	HE	155/155 (100%)	131 (84%)	24 (16%)	2	14
25	JE	155/155 (100%)	130 (84%)	25 (16%)	2	13
26	BF	157/158 (99%)	139 (88%)	18 (12%)	5	21
26	DF	157/158 (99%)	139 (88%)	18 (12%)	5	21
26	FF	157/158 (99%)	139 (88%)	18 (12%)	5	21
26	HF	157/158 (99%)	139 (88%)	18 (12%)	5	21
26	JF	157/158 (99%)	139 (88%)	18 (12%)	5	21
27	BG	154/154 (100%)	122 (79%)	32 (21%)	1	6
27	DG	154/154 (100%)	122 (79%)	32 (21%)	1	6
27	FG	154/154 (100%)	122 (79%)	32 (21%)	1	6
27	HG	154/154 (100%)	122 (79%)	32 (21%)	1	6
27	JG	154/154 (100%)	122 (79%)	32 (21%)	1	6
28	BH	137/137 (100%)	116 (85%)	21 (15%)	2	14
28	DH	137/137 (100%)	116 (85%)	21 (15%)	2	14
28	FH	137/137 (100%)	116 (85%)	21 (15%)	2	14
28	HH	137/137 (100%)	116 (85%)	21 (15%)	2	14
28	JH	137/137 (100%)	116 (85%)	21 (15%)	2	14
29	BI	44/44 (100%)	39 (89%)	5 (11%)	5	21
29	DI	44/44 (100%)	39 (89%)	5 (11%)	5	21
29	FI	44/44 (100%)	39 (89%)	5 (11%)	5	21
29	HI	44/44 (100%)	39 (89%)	5 (11%)	5	21
29	JI	44/44 (100%)	39 (89%)	5 (11%)	5	21
30	BJ	107/107 (100%)	95 (89%)	12 (11%)	6	22
30	DJ	107/107 (100%)	95 (89%)	12 (11%)	6	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	FJ	107/107 (100%)	95 (89%)	12 (11%)	6	22
30	HJ	107/107 (100%)	95 (89%)	12 (11%)	6	22
30	JJ	107/107 (100%)	95 (89%)	12 (11%)	6	22
31	BK	119/119 (100%)	102 (86%)	17 (14%)	3	16
31	DK	119/119 (100%)	102 (86%)	17 (14%)	3	16
31	FK	119/119 (100%)	102 (86%)	17 (14%)	3	16
31	HK	119/119 (100%)	102 (86%)	17 (14%)	3	16
31	JK	119/119 (100%)	102 (86%)	17 (14%)	3	16
32	BL	101/101 (100%)	88 (87%)	13 (13%)	4	18
32	DL	101/101 (100%)	88 (87%)	13 (13%)	4	18
32	FL	101/101 (100%)	88 (87%)	13 (13%)	4	18
32	HL	101/101 (100%)	88 (87%)	13 (13%)	4	18
32	JL	101/101 (100%)	88 (87%)	13 (13%)	4	18
33	BM	108/108 (100%)	88 (82%)	20 (18%)	1	9
33	DM	108/108 (100%)	88 (82%)	20 (18%)	1	9
33	FM	108/108 (100%)	88 (82%)	20 (18%)	1	9
33	HM	108/108 (100%)	88 (82%)	20 (18%)	1	9
33	JM	108/108 (100%)	88 (82%)	20 (18%)	1	9
34	BN	99/99 (100%)	75 (76%)	24 (24%)	0	4
34	DN	99/99 (100%)	75 (76%)	24 (24%)	0	4
34	FN	99/99 (100%)	75 (76%)	24 (24%)	0	4
34	HN	99/99 (100%)	75 (76%)	24 (24%)	0	4
34	JN	99/99 (100%)	75 (76%)	24 (24%)	0	4
35	BO	91/91 (100%)	78 (86%)	13 (14%)	3	16
35	DO	91/91 (100%)	78 (86%)	13 (14%)	3	16
35	FO	91/91 (100%)	78 (86%)	13 (14%)	3	16
35	HO	91/91 (100%)	78 (86%)	13 (14%)	3	16
35	JO	91/91 (100%)	78 (86%)	13 (14%)	3	16
36	BP	80/80 (100%)	71 (89%)	9 (11%)	6	21
36	DP	80/80 (100%)	71 (89%)	9 (11%)	6	21
36	FP	80/80 (100%)	71 (89%)	9 (11%)	6	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	HP	80/80 (100%)	71 (89%)	9 (11%)	6	21
36	JP	80/80 (100%)	71 (89%)	9 (11%)	6	21
37	BQ	108/108 (100%)	92 (85%)	16 (15%)	3	15
37	DQ	108/108 (100%)	92 (85%)	16 (15%)	3	15
37	FQ	108/108 (100%)	92 (85%)	16 (15%)	3	15
37	HQ	108/108 (100%)	92 (85%)	16 (15%)	3	15
37	JQ	108/108 (100%)	92 (85%)	16 (15%)	3	15
38	BR	96/96 (100%)	82 (85%)	14 (15%)	3	15
38	DR	96/96 (100%)	82 (85%)	14 (15%)	3	15
38	FR	96/96 (100%)	82 (85%)	14 (15%)	3	15
38	HR	96/96 (100%)	82 (85%)	14 (15%)	3	15
38	JR	96/96 (100%)	82 (85%)	14 (15%)	3	15
39	BS	79/79 (100%)	70 (89%)	9 (11%)	5	21
39	DS	79/79 (100%)	70 (89%)	9 (11%)	5	21
39	FS	79/79 (100%)	70 (89%)	9 (11%)	5	21
39	HS	79/79 (100%)	70 (89%)	9 (11%)	5	21
39	JS	79/79 (100%)	70 (89%)	9 (11%)	5	21
40	BT	112/112 (100%)	99 (88%)	13 (12%)	5	21
40	DT	112/112 (100%)	99 (88%)	13 (12%)	5	21
40	FT	112/112 (100%)	99 (88%)	13 (12%)	5	21
40	HT	112/112 (100%)	99 (88%)	13 (12%)	5	21
40	JT	112/112 (100%)	99 (88%)	13 (12%)	5	21
41	BU	75/75 (100%)	69 (92%)	6 (8%)	12	35
41	DU	75/75 (100%)	69 (92%)	6 (8%)	12	35
41	FU	75/75 (100%)	69 (92%)	6 (8%)	12	35
41	HU	75/75 (100%)	68 (91%)	7 (9%)	9	28
41	JU	75/75 (100%)	68 (91%)	7 (9%)	9	28
42	BV	94/94 (100%)	86 (92%)	8 (8%)	10	33
42	DV	94/94 (100%)	86 (92%)	8 (8%)	10	33
42	FV	94/94 (100%)	86 (92%)	8 (8%)	10	33
42	HV	94/94 (100%)	86 (92%)	8 (8%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	JV	94/94 (100%)	86 (92%)	8 (8%)	10	33
43	BW	147/147 (100%)	125 (85%)	22 (15%)	3	15
43	DW	147/147 (100%)	125 (85%)	22 (15%)	3	15
43	FW	147/147 (100%)	125 (85%)	22 (15%)	3	15
43	HW	147/147 (100%)	125 (85%)	22 (15%)	3	15
43	JW	147/147 (100%)	125 (85%)	22 (15%)	3	15
44	BX	64/64 (100%)	49 (77%)	15 (23%)	1	4
44	DX	64/64 (100%)	49 (77%)	15 (23%)	1	4
44	FX	64/64 (100%)	48 (75%)	16 (25%)	0	3
44	HX	64/64 (100%)	48 (75%)	16 (25%)	0	3
44	JX	64/64 (100%)	49 (77%)	15 (23%)	1	4
45	BY	53/53 (100%)	44 (83%)	9 (17%)	2	12
45	DY	53/53 (100%)	44 (83%)	9 (17%)	2	12
45	FY	53/53 (100%)	44 (83%)	9 (17%)	2	12
45	HY	53/53 (100%)	44 (83%)	9 (17%)	2	12
45	JY	53/53 (100%)	44 (83%)	9 (17%)	2	12
46	BZ	48/48 (100%)	38 (79%)	10 (21%)	1	6
46	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	6
46	FZ	48/48 (100%)	38 (79%)	10 (21%)	1	6
46	HZ	48/48 (100%)	38 (79%)	10 (21%)	1	6
46	JZ	48/48 (100%)	38 (79%)	10 (21%)	1	6
47	B1	66/66 (100%)	53 (80%)	13 (20%)	1	8
47	D1	66/66 (100%)	53 (80%)	13 (20%)	1	8
47	F1	66/66 (100%)	53 (80%)	13 (20%)	1	8
47	H1	66/66 (100%)	53 (80%)	13 (20%)	1	8
47	J1	66/66 (100%)	53 (80%)	13 (20%)	1	8
48	B2	51/51 (100%)	39 (76%)	12 (24%)	1	4
48	D2	51/51 (100%)	39 (76%)	12 (24%)	1	4
48	F2	51/51 (100%)	39 (76%)	12 (24%)	1	4
48	H2	51/51 (100%)	39 (76%)	12 (24%)	1	4
48	J2	51/51 (100%)	39 (76%)	12 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B3	46/46 (100%)	33 (72%)	13 (28%)	0	2
49	D3	46/46 (100%)	33 (72%)	13 (28%)	0	2
49	F3	46/46 (100%)	33 (72%)	13 (28%)	0	2
49	H3	46/46 (100%)	33 (72%)	13 (28%)	0	2
49	J3	46/46 (100%)	33 (72%)	13 (28%)	0	2
50	B4	39/39 (100%)	28 (72%)	11 (28%)	0	2
50	D4	39/39 (100%)	28 (72%)	11 (28%)	0	2
50	F4	39/39 (100%)	28 (72%)	11 (28%)	0	2
50	H4	39/39 (100%)	28 (72%)	11 (28%)	0	2
50	J4	39/39 (100%)	28 (72%)	11 (28%)	0	2
51	B5	50/50 (100%)	35 (70%)	15 (30%)	0	2
51	D5	50/50 (100%)	35 (70%)	15 (30%)	0	2
51	F5	50/50 (100%)	35 (70%)	15 (30%)	0	2
51	H5	50/50 (100%)	35 (70%)	15 (30%)	0	2
51	J5	50/50 (100%)	35 (70%)	15 (30%)	0	2
52	B6	34/34 (100%)	30 (88%)	4 (12%)	5	20
52	D6	34/34 (100%)	30 (88%)	4 (12%)	5	20
52	F6	34/34 (100%)	30 (88%)	4 (12%)	5	20
52	H6	34/34 (100%)	30 (88%)	4 (12%)	5	20
52	J6	34/34 (100%)	30 (88%)	4 (12%)	5	20
53	B7	191/187 (102%)	179 (94%)	12 (6%)	18	43
53	D7	191/187 (102%)	179 (94%)	12 (6%)	18	43
53	F7	191/187 (102%)	179 (94%)	12 (6%)	18	43
53	H7	191/187 (102%)	179 (94%)	12 (6%)	18	43
53	J7	191/187 (102%)	179 (94%)	12 (6%)	18	43
All	All	24880/24865 (100%)	21622 (87%)	3258 (13%)	4	18

5 of 3258 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	ES	36	ARG
43	FW	51	LEU
34	JN	12	LYS

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Mol	Chain	Res	Type
24	FD	118	ASN
31	FK	30	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 944 such sidechains are listed below:

Mol	Chain	Res	Type
15	EO	13	GLN
42	FV	32	GLN
32	JL	26	ASN
19	ES	56	GLN
28	FH	74	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1521/1526 (99%)	348 (22%)	56 (3%)
1	CA	1521/1526 (99%)	348 (22%)	57 (3%)
1	EA	1522/1526 (99%)	349 (22%)	57 (3%)
1	GA	1522/1526 (99%)	349 (22%)	56 (3%)
1	IA	1522/1526 (99%)	348 (22%)	57 (3%)
22	BB	2801/2825 (99%)	768 (27%)	35 (1%)
22	DB	2804/2825 (99%)	771 (27%)	36 (1%)
22	FB	2801/2825 (99%)	768 (27%)	38 (1%)
22	HB	2803/2825 (99%)	768 (27%)	36 (1%)
22	JB	2804/2825 (99%)	765 (27%)	37 (1%)
23	BA	117/119 (98%)	30 (25%)	1 (0%)
23	DA	117/119 (98%)	30 (25%)	1 (0%)
23	FA	117/119 (98%)	31 (26%)	1 (0%)
23	HA	117/119 (98%)	30 (25%)	1 (0%)
23	JA	117/119 (98%)	30 (25%)	1 (0%)
All	All	22206/22350 (99%)	5733 (25%)	470 (2%)

5 of 5733 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	31	G
1	AA	32	A

5 of 470 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	EA	687	A
22	FB	1710	U
22	JB	181	A
1	EA	975	A
1	EA	1397	C

## 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	FB	56
22	HB	55
22	JB	52
22	BB	51
22	DB	51
1	EA	5
1	CA	4
1	GA	4
1	AA	4
1	IA	4
12	GL	3

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Mol	Chain	Number of breaks
12	AL	3
12	IL	3
12	CL	3
43	HW	2
13	EM	2
13	GM	2
43	FW	2
12	EL	2
13	IM	2
43	DW	2
13	CM	2
43	JW	2
43	BW	2
13	AM	1

The worst 5 of 319 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	JB	373:A	O3'	387:A	P	28.29
1	HB	373:A	O3'	387:A	P	28.03
1	FB	373:A	O3'	387:A	P	28.01
1	DB	373:A	O3'	387:A	P	27.91
1	FB	248:A	O3'	292:A	P	27.80

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.