



# wwPDB X-ray Structure Validation Summary Report

Jun 17, 2014 – 02:11 AM 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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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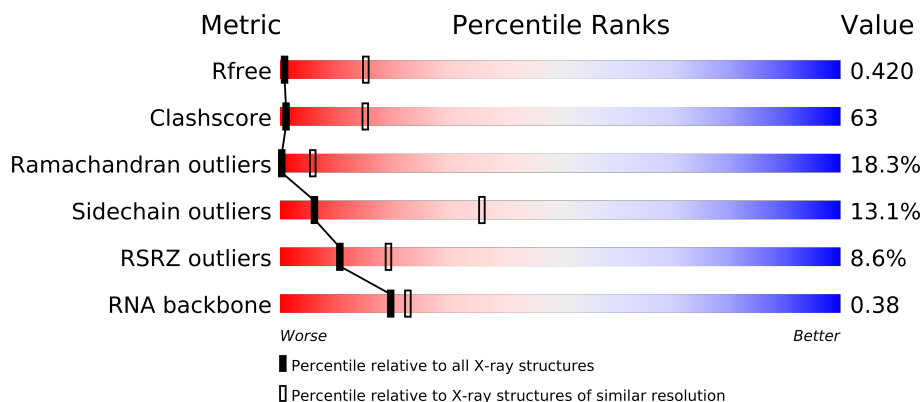
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable23397
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23397

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1106 (11.50-3.50)
Clashscore	79885	1010 (15.00-3.54)
Ramachandran outliers	78287	1304 (15.00-3.50)
Sidechain outliers	78261	1278 (15.00-3.50)
RSRZ outliers	66119	1105 (11.50-3.50)
RNA backbone	1838	1055 (11.50-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1526	
1	CA	1526	
1	EA	1526	
1	GA	1526	
1	IA	1526	
2	AB	234	
2	CB	234	
2	EB	234	
2	GB	234	
2	IB	234	
3	AC	206	
3	CC	206	

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Mol	Chain	Length	Quality of chain
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	
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	

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Mol	Chain	Length	Quality of chain
11	IK	119	
12	AL	124	
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	
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	

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Mol	Chain	Length	Quality of chain
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	
22	DB	2825	
22	FB	2825	
22	HB	2825	
22	JB	2825	
23	BA	119	
23	DA	119	
23	FA	119	
23	HA	119	
23	JA	119	
24	BD	270	
24	DD	270	
24	FD	270	
24	HD	270	
24	JD	270	
25	BE	205	
25	DE	205	
25	FE	205	
25	HE	205	
25	JE	205	
26	BF	198	
26	DF	198	
26	FF	198	
26	HF	198	
26	JF	198	
27	BG	178	
27	DG	178	
27	FG	178	
27	HG	178	
27	JG	178	
28	BH	177	
28	DH	177	
28	FH	177	

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Mol	Chain	Length	Quality of chain
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	
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	

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Mol	Chain	Length	Quality of chain
37	BQ	125	
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	
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	

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Mol	Chain	Length	Quality of chain
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	
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	
52	D6	35	
52	F6	35	
52	H6	35	
52	J6	35	
53	B7	217	
53	D7	217	
53	F7	217	
53	H7	217	

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Mol	Chain	Length	Quality of chain
53	J7	217	 A horizontal bar chart representing the quality of chain J7. The bar is divided into four segments: a red segment (approx. 10%), a green segment (approx. 10%), a yellow segment (approx. 70%), and an orange segment (approx. 10%).

## 2 Entry composition

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

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 834	C 512	N 168	O 154	8	0	0
36	HP	111	Total 834	C 512	N 168	O 154	8	0	0
36	JP	111	Total 834	C 512	N 168	O 154	8	0	0

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

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

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

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

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

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

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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			

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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			

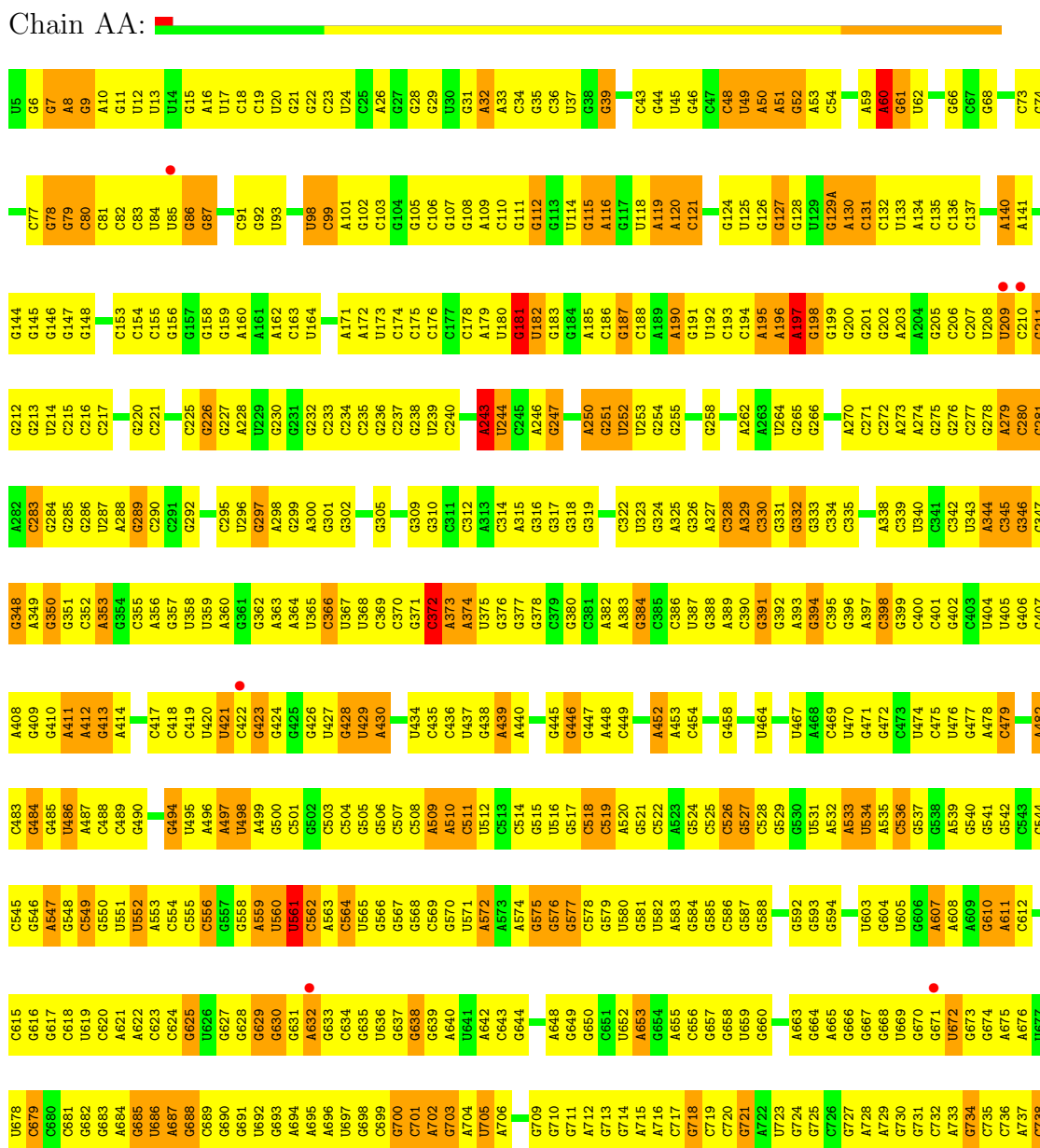
- Molecule 53 is a protein called 50S ribosomal protein L1P.

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S ribosomal RNA

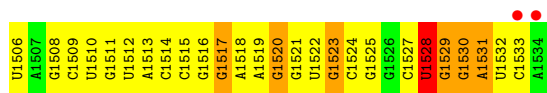






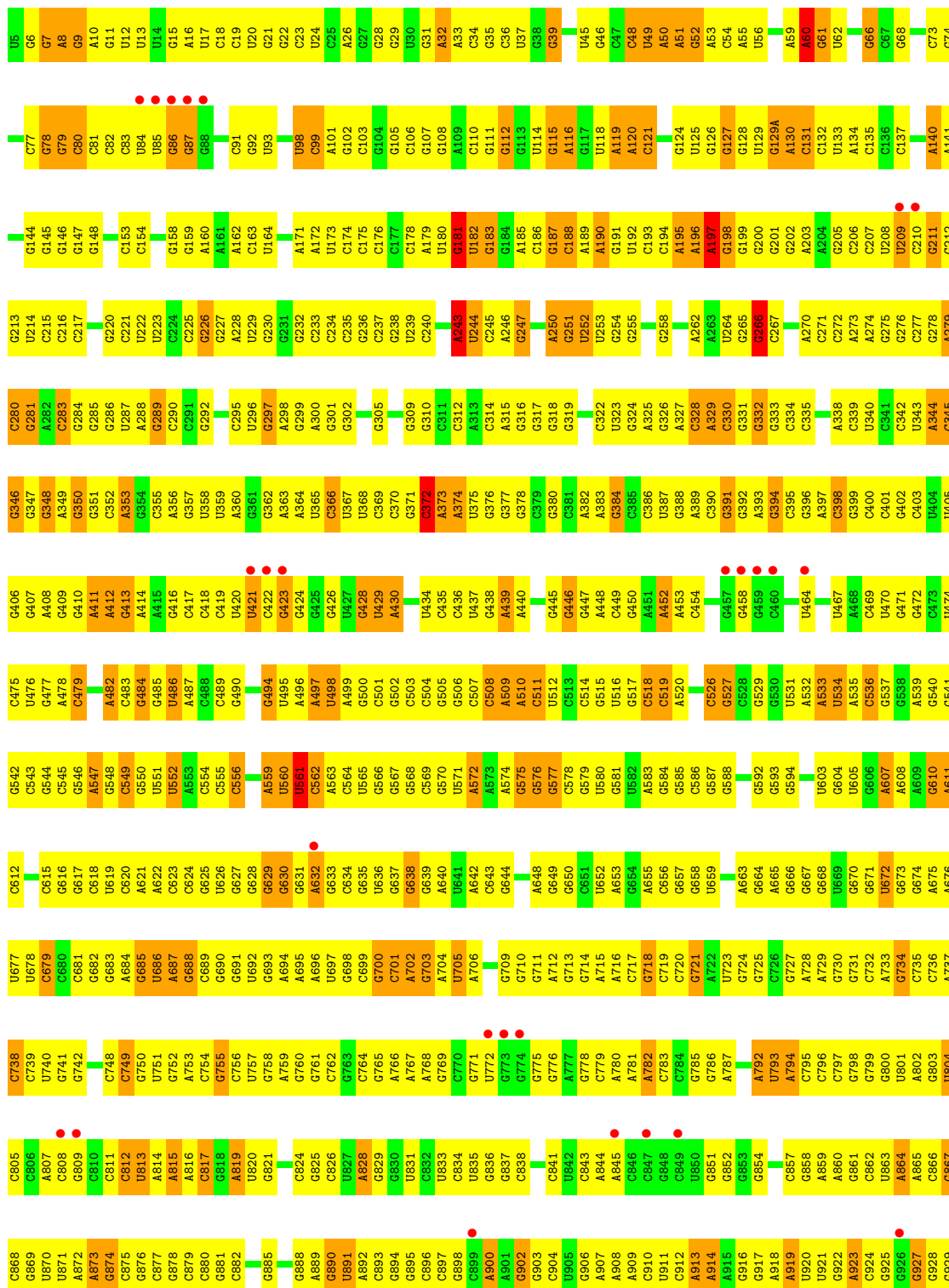


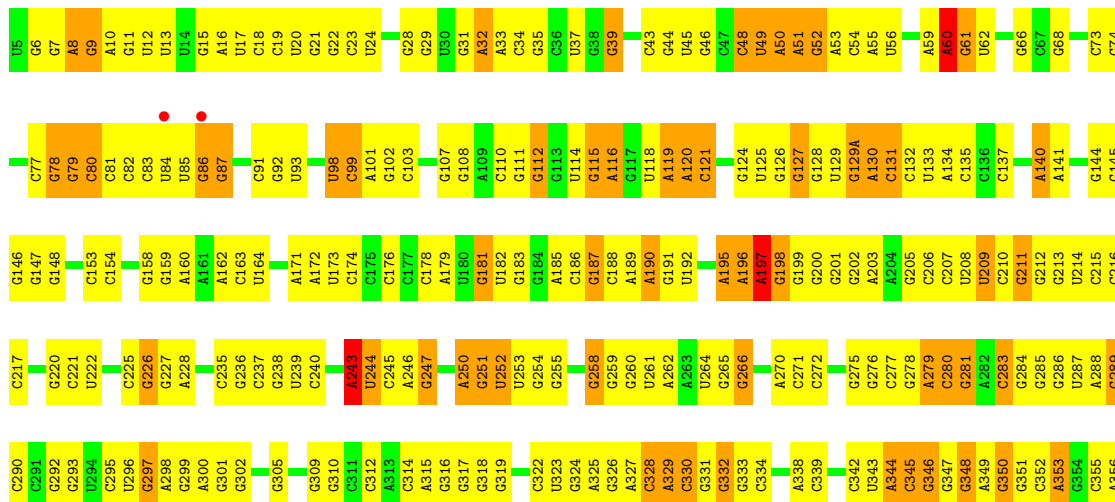
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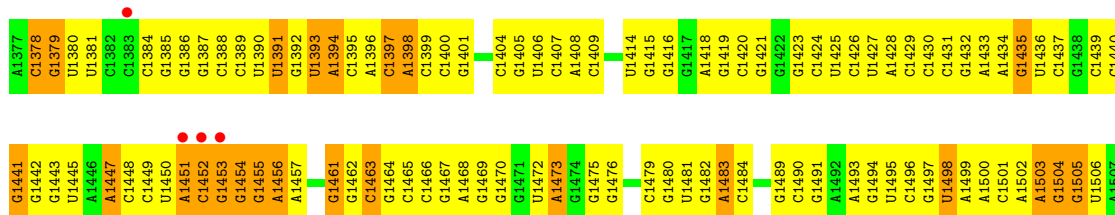
• Molecule 1: 16S ribosomal RNA

Chain GA:



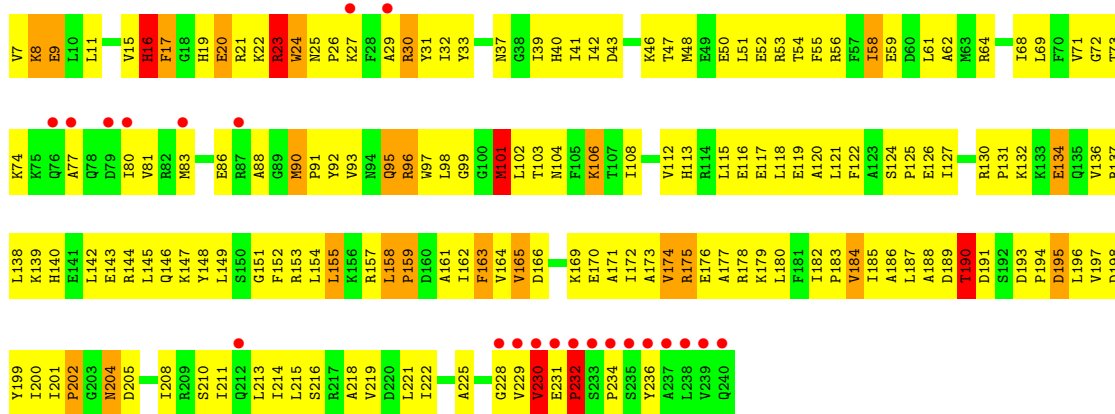


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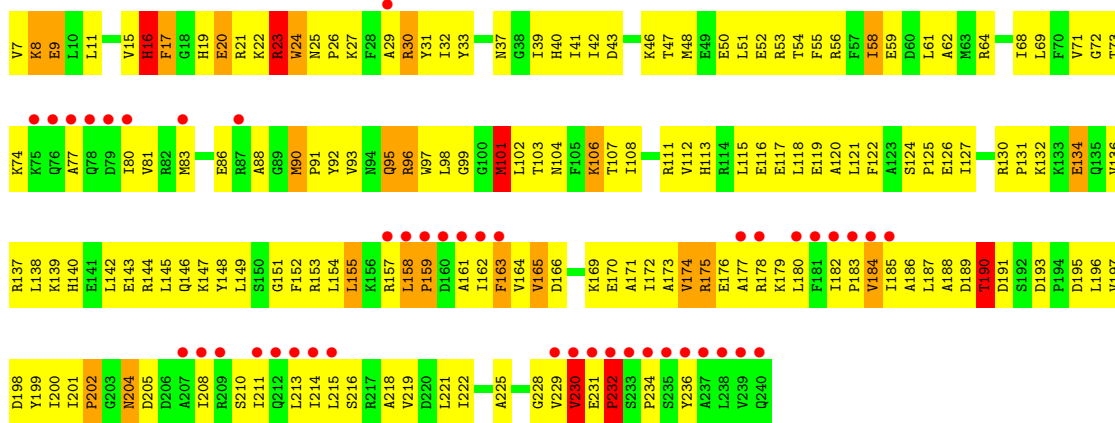
• Molecule 2: 30S ribosomal protein S2

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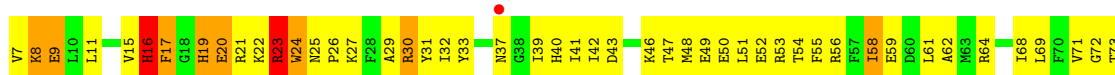
• Molecule 2: 30S ribosomal protein S2

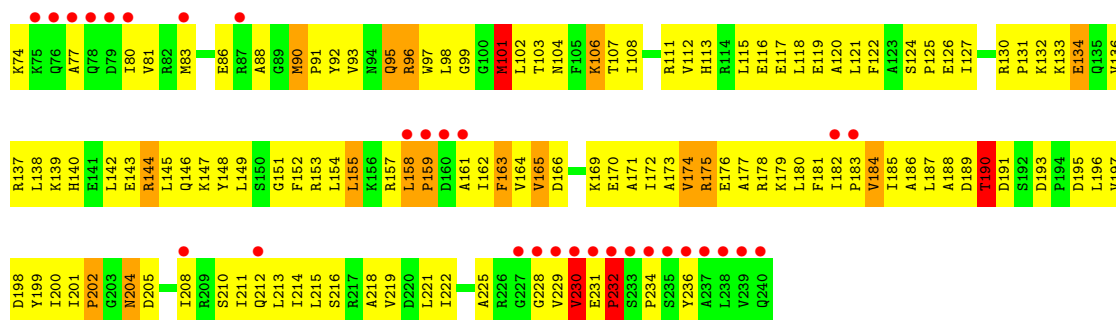
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• Molecule 2: 30S ribosomal protein S2

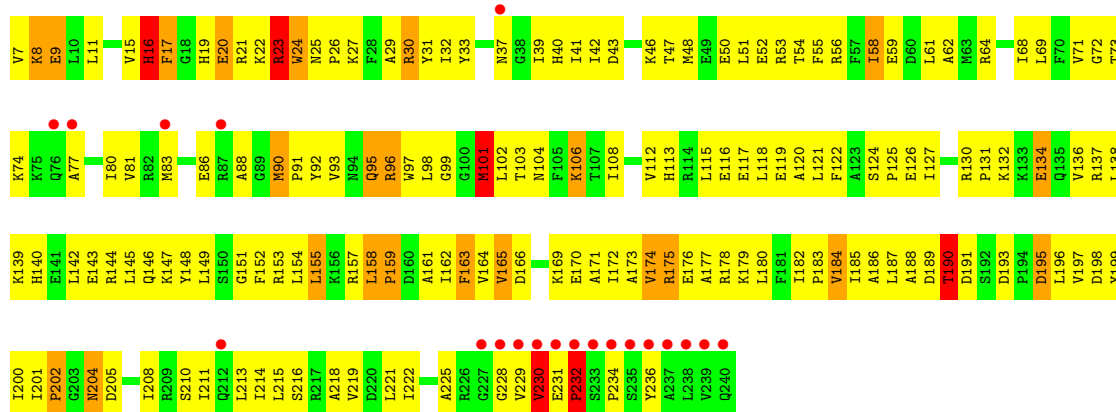
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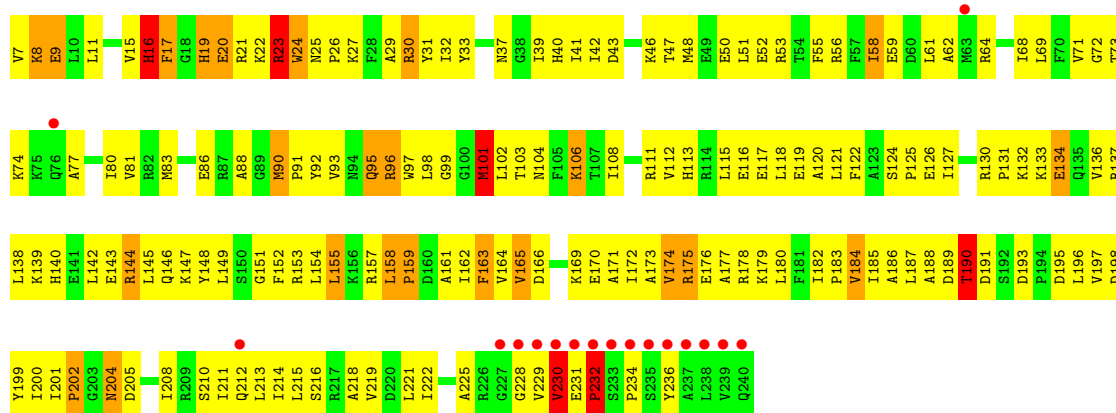
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Chain GB:



• Molecule 2: 30S ribosomal protein S2

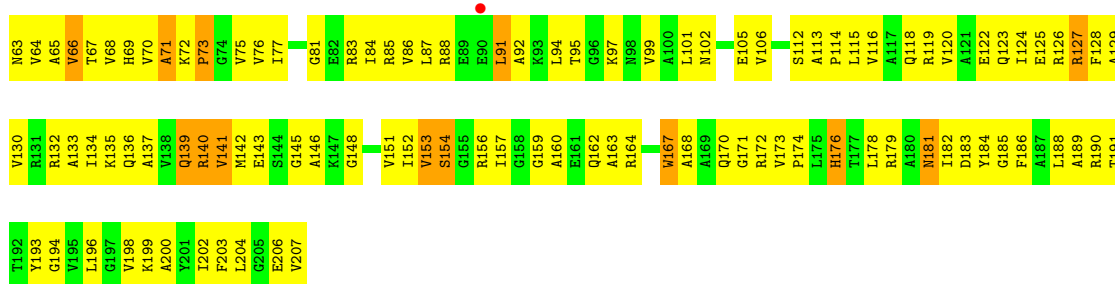
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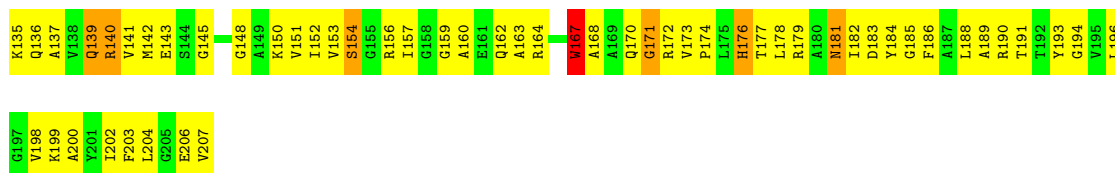


• Molecule 3: 30S ribosomal protein S3

Chain AC:

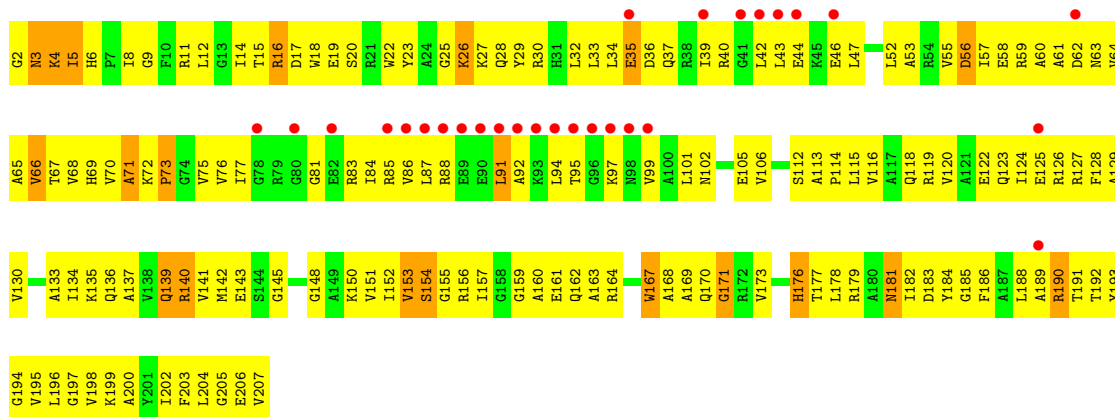






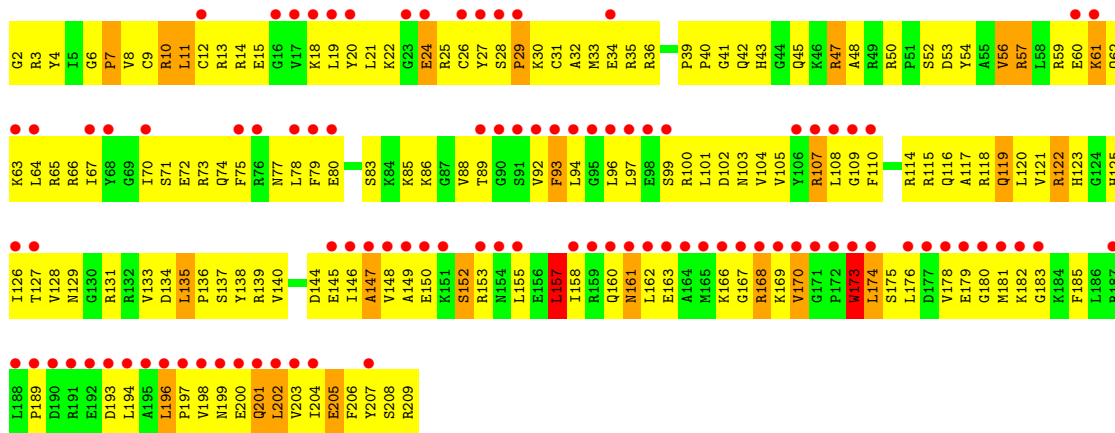
• Molecule 3: 30S ribosomal protein S3

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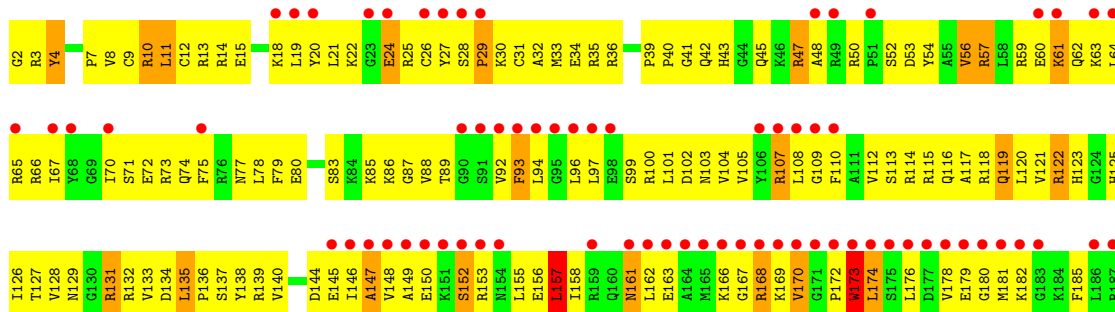
• Molecule 4: 30S ribosomal protein S4

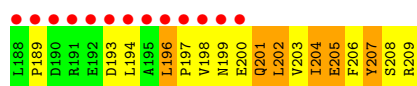
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• Molecule 4: 30S ribosomal protein S4

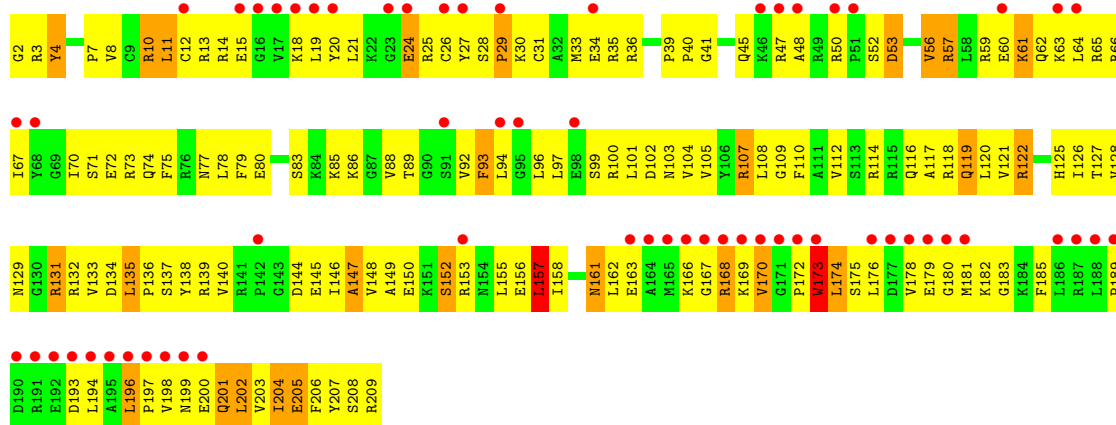
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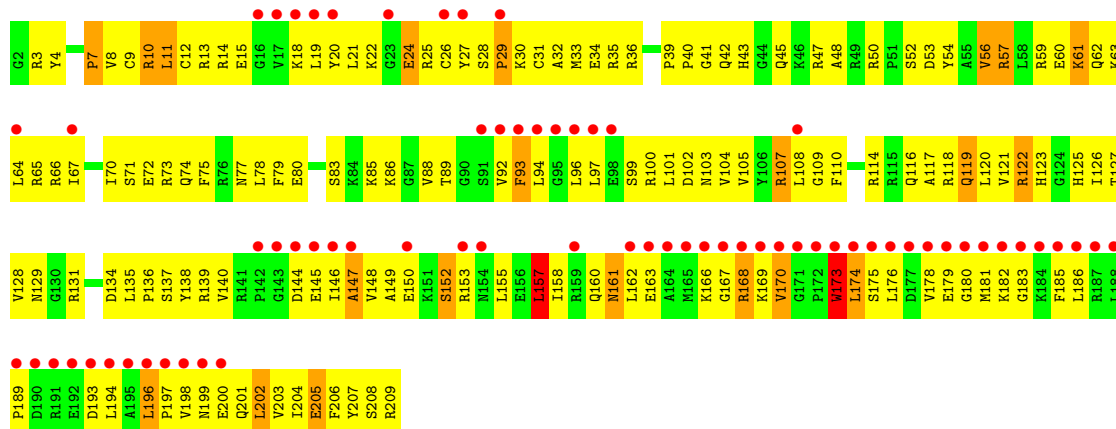
• Molecule 4: 30S ribosomal protein S4

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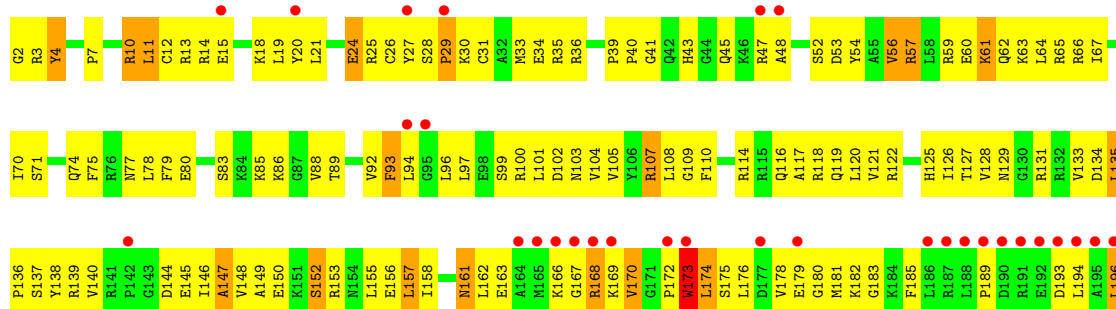
• Molecule 4: 30S ribosomal protein S4

Chain GD:



• Molecule 4: 30S ribosomal protein S4

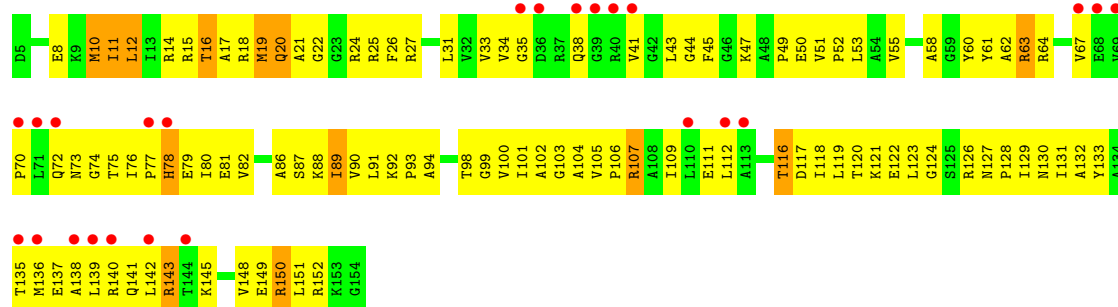
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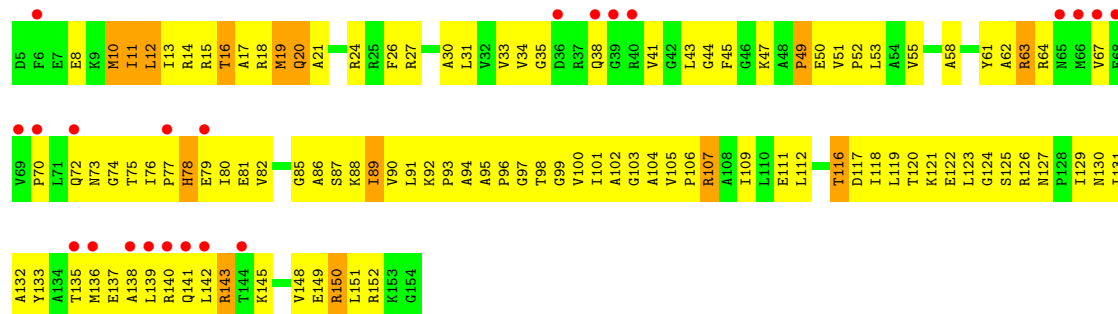
• Molecule 5: 30S ribosomal protein S5

Chain AE:



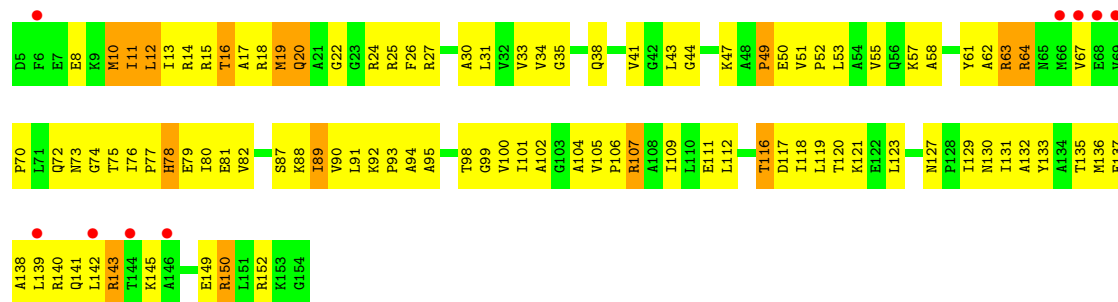
• Molecule 5: 30S ribosomal protein S5

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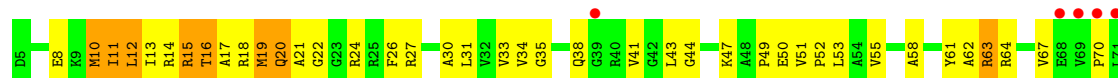
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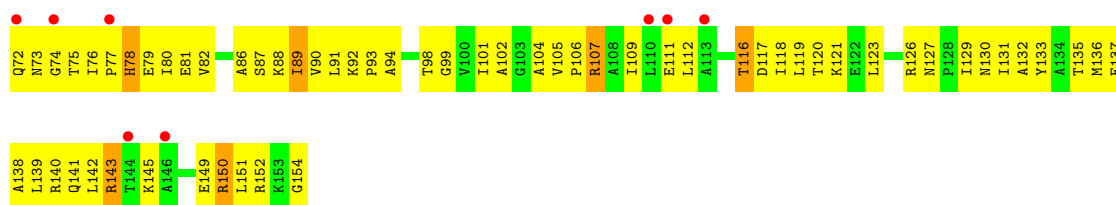
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• Molecule 5: 30S ribosomal protein S5

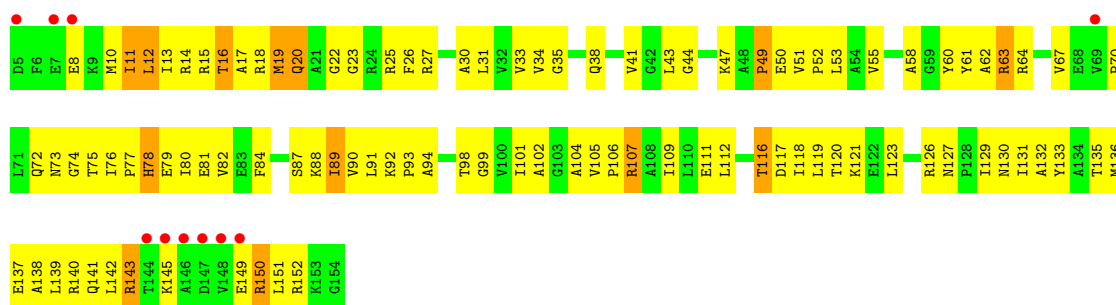
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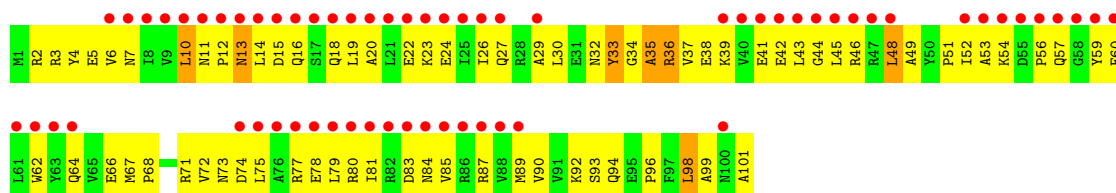
• Molecule 5: 30S ribosomal protein S5

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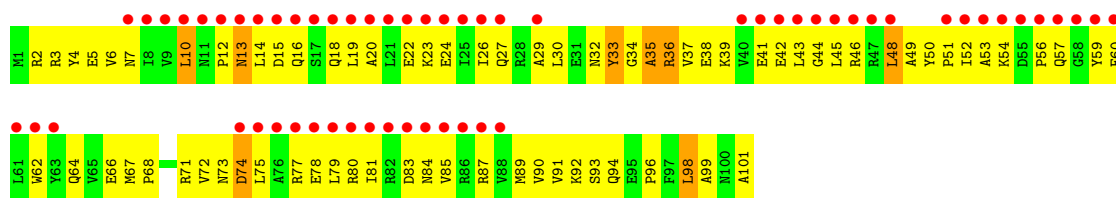
• Molecule 6: 30S ribosomal protein S6

Chain AF:



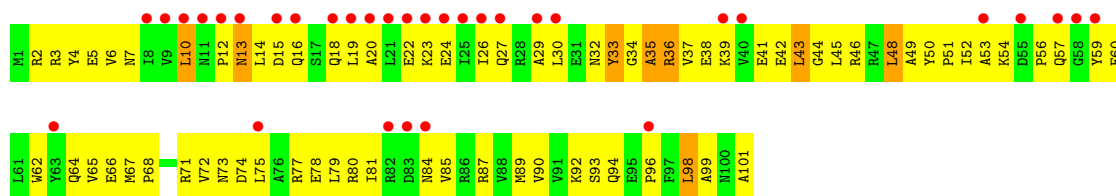
• Molecule 6: 30S ribosomal protein S6

Chain CF:



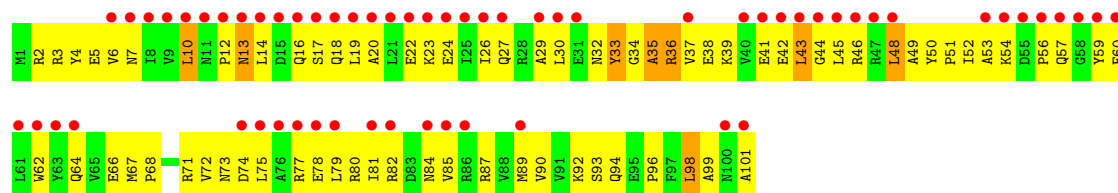
• Molecule 6: 30S ribosomal protein S6

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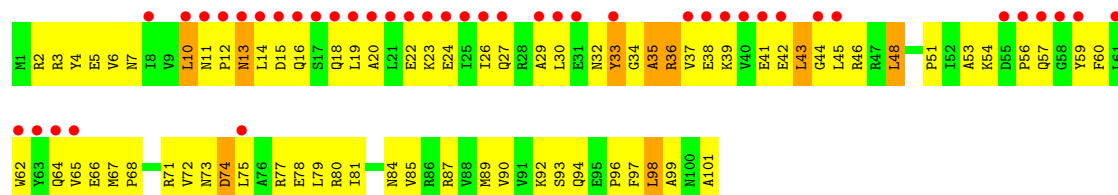
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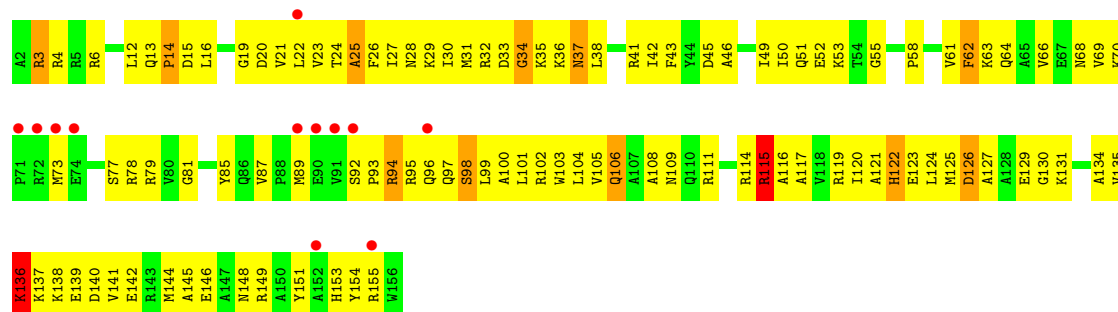
- Molecule 6: 30S ribosomal protein S6

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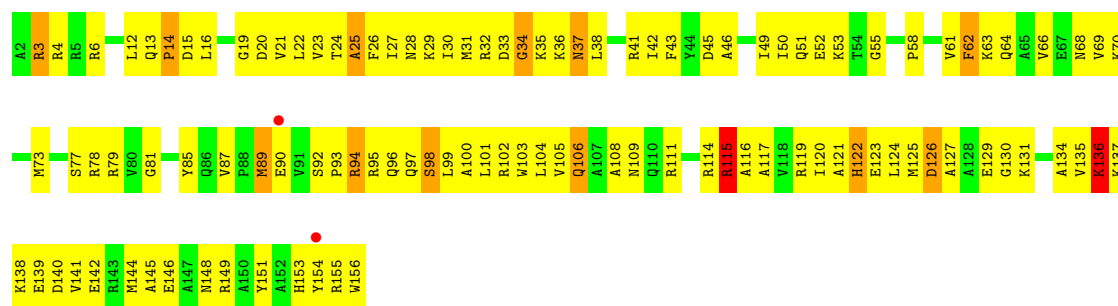
- Molecule 7: 30S ribosomal protein S7

Chain AG: 



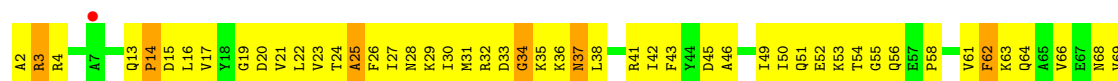
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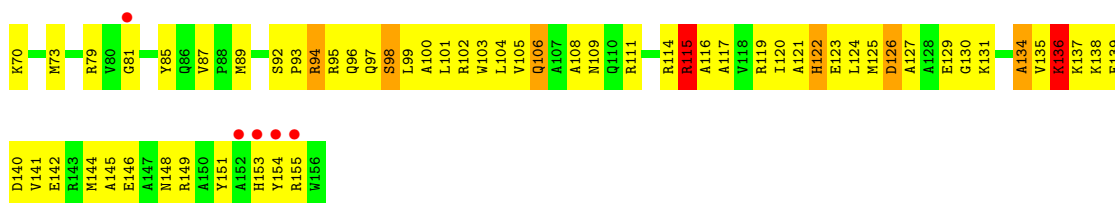
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- Molecule 7: 30S ribosomal protein S7

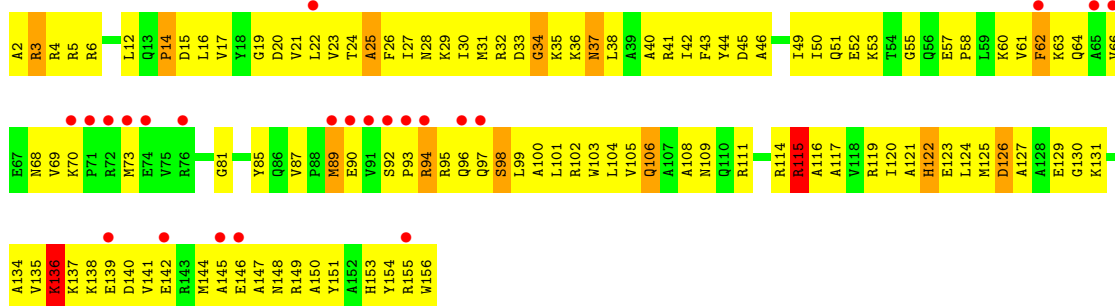
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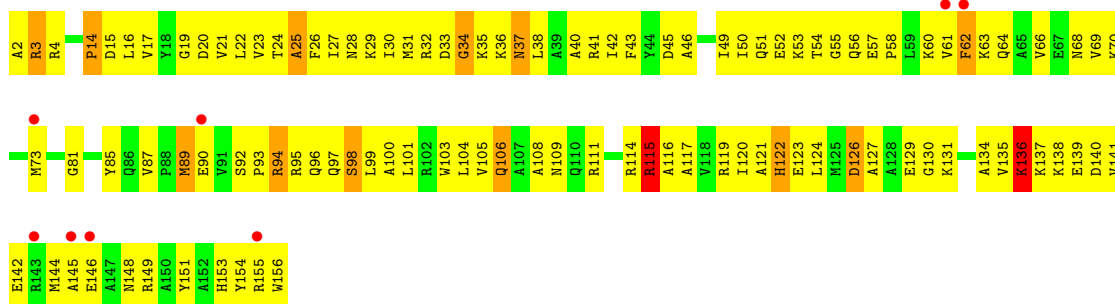
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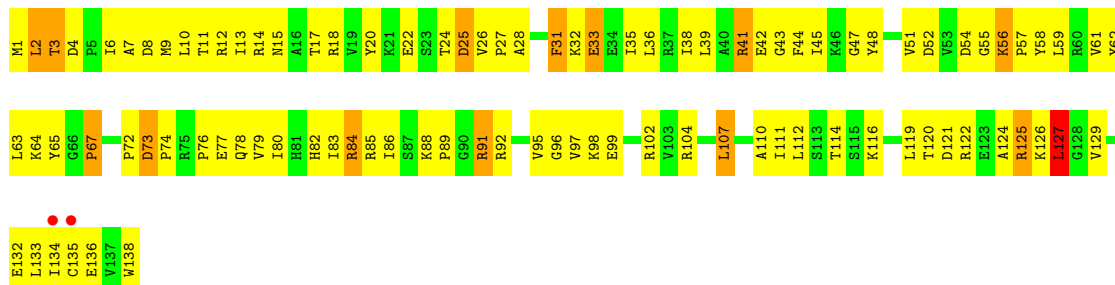
• Molecule 7: 30S ribosomal protein S7

Chain IG:



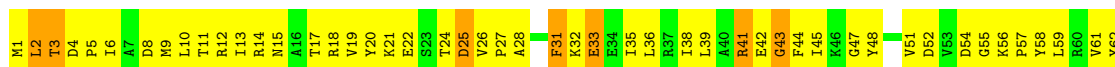
• Molecule 8: 30S ribosomal protein S8

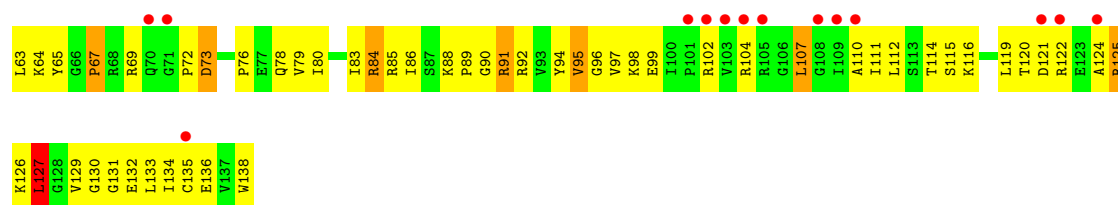
Chain AH:



• Molecule 8: 30S ribosomal protein S8

Chain CH:





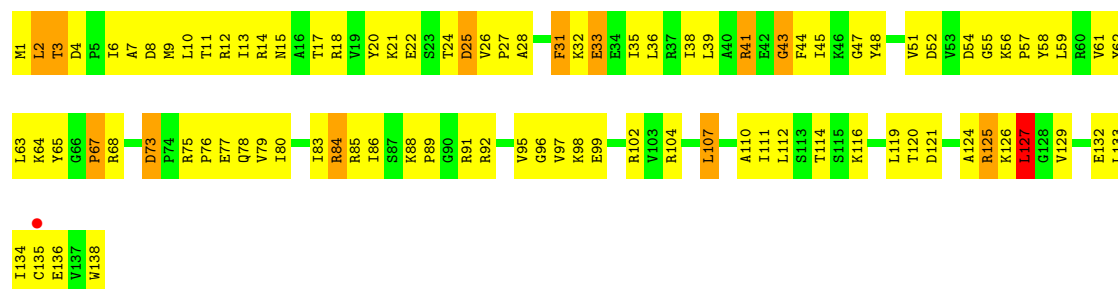
• Molecule 8: 30S ribosomal protein S8

Chain EH:



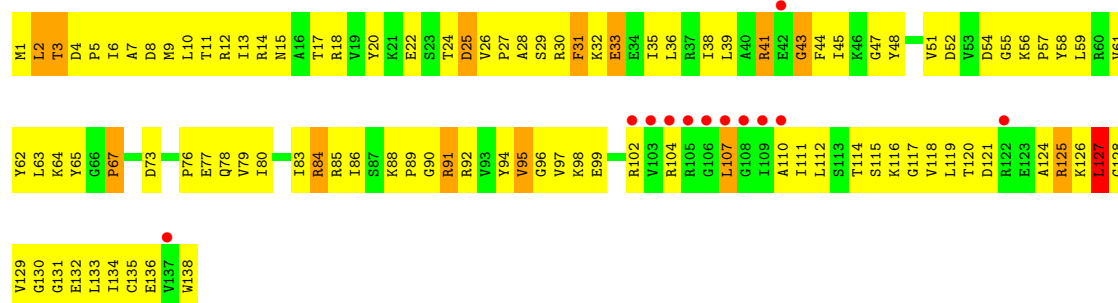
• Molecule 8: 30S ribosomal protein S8

Chain GH:



• Molecule 8: 30S ribosomal protein S8

Chain IH:



• Molecule 9: 30S ribosomal protein S9

Chain AI:





• Molecule 9: 30S ribosomal protein S9

Chain CI:



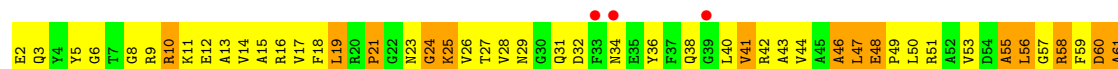
• Molecule 9: 30S ribosomal protein S9

Chain EI:



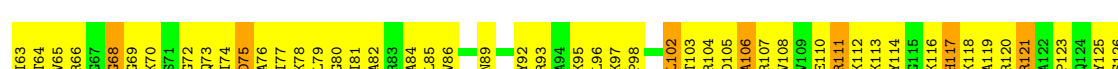
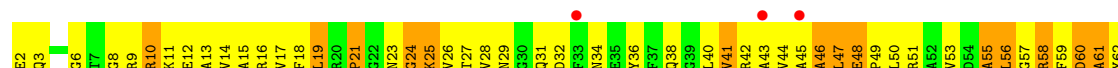
• Molecule 9: 30S ribosomal protein S9

Chain GI:



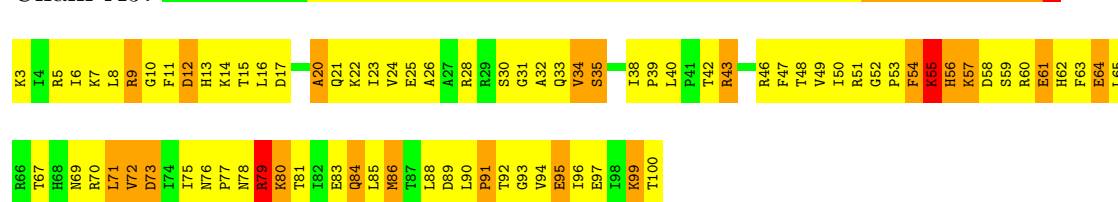
• Molecule 9: 30S ribosomal protein S9

Chain II:



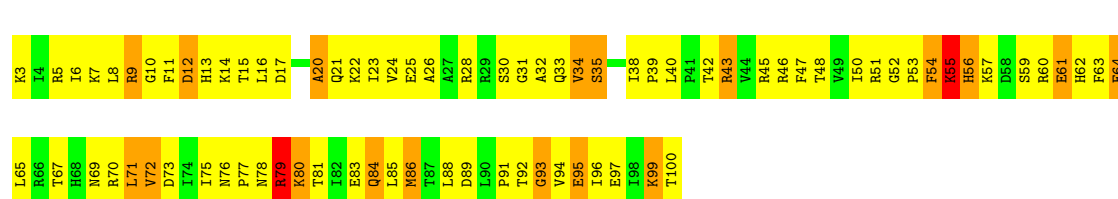
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



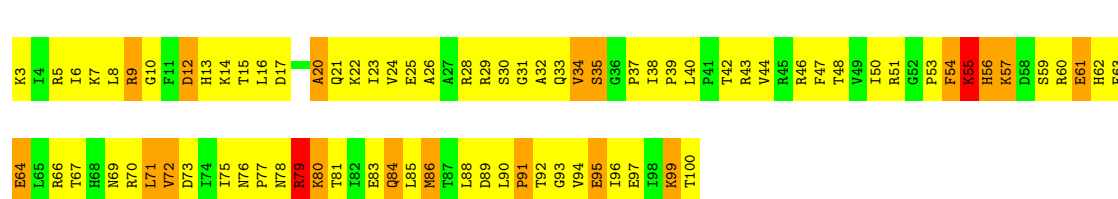
- Molecule 10: 30S ribosomal protein S10

Chain CJ:



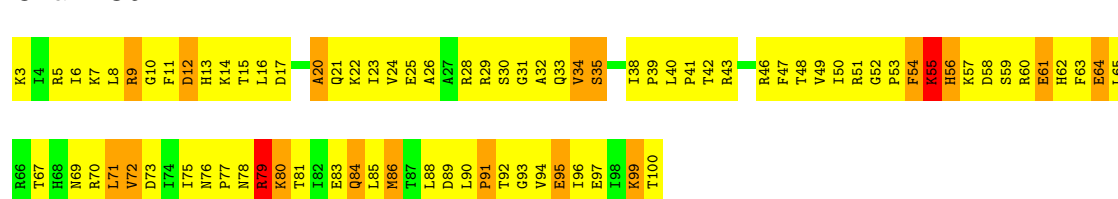
- Molecule 10: 30S ribosomal protein S10

Chain EJ:



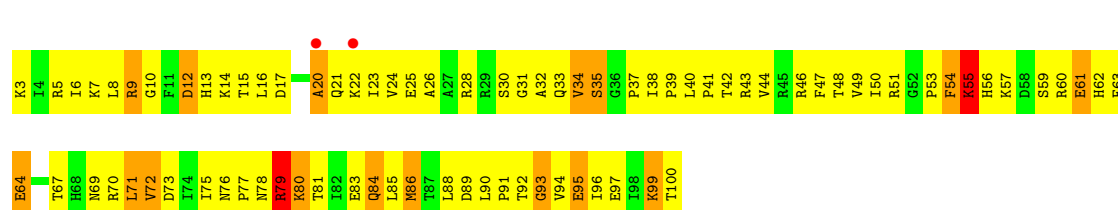
- Molecule 10: 30S ribosomal protein S10

Chain GJ:



- Molecule 10: 30S ribosomal protein S10

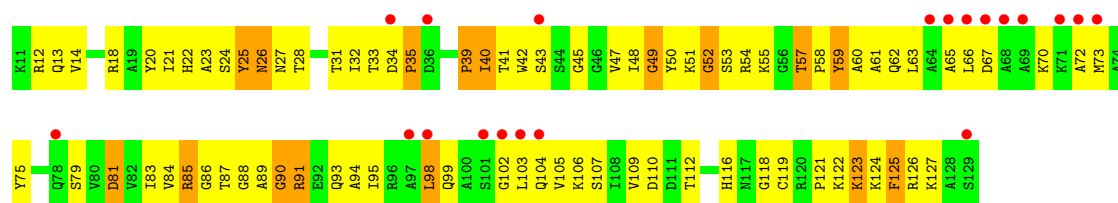
Chain IJ:



- Molecule 11: 30S ribosomal protein S11

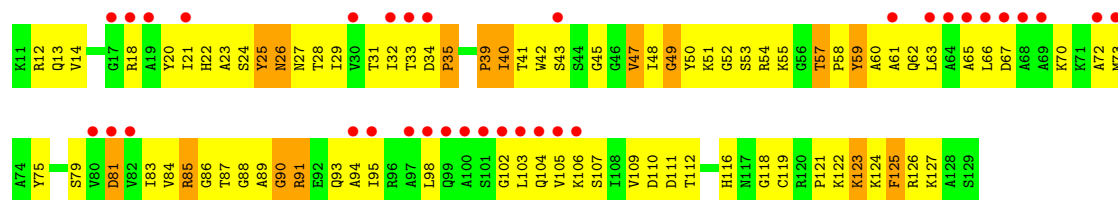
Chain AK:





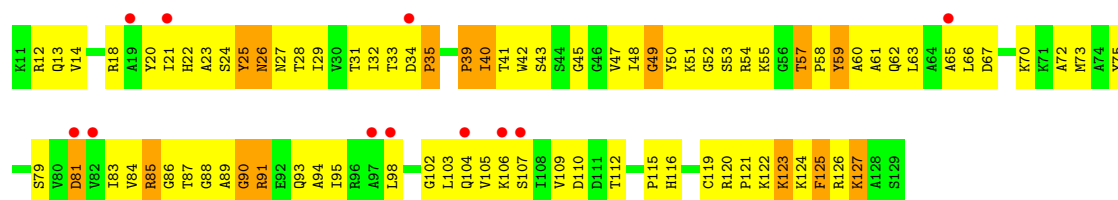
- Molecule 11: 30S ribosomal protein S11

Chain CK:



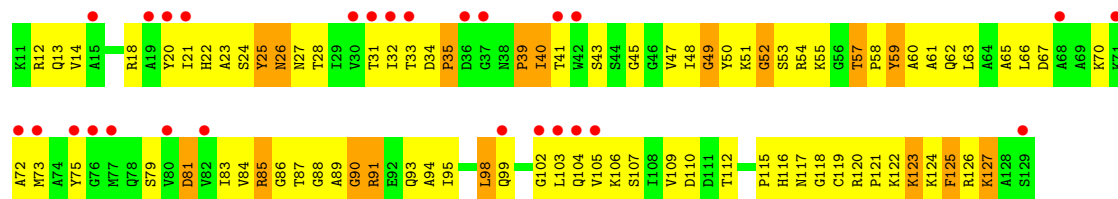
- Molecule 11: 30S ribosomal protein S11

Chain EK:



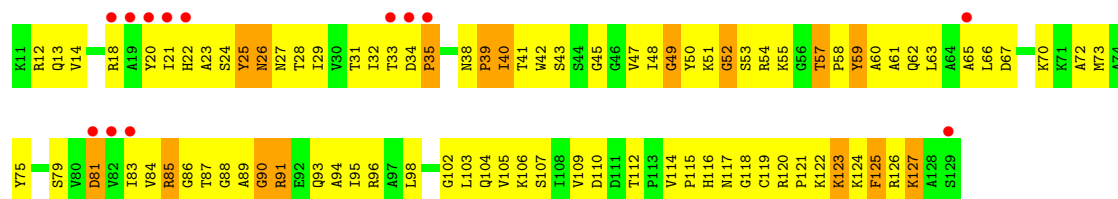
- Molecule 11: 30S ribosomal protein S11

Chain GK:



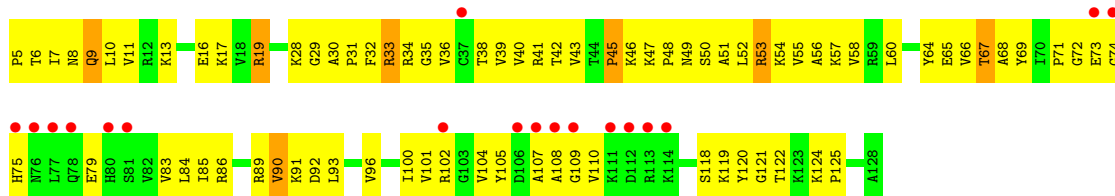
- Molecule 11: 30S ribosomal protein S11

Chain IK:



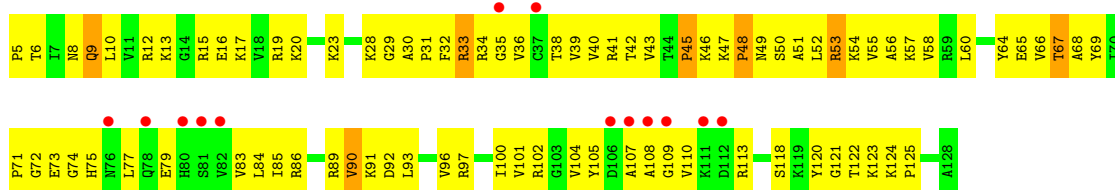
- Molecule 12: 30S ribosomal protein S12

Chain AL:



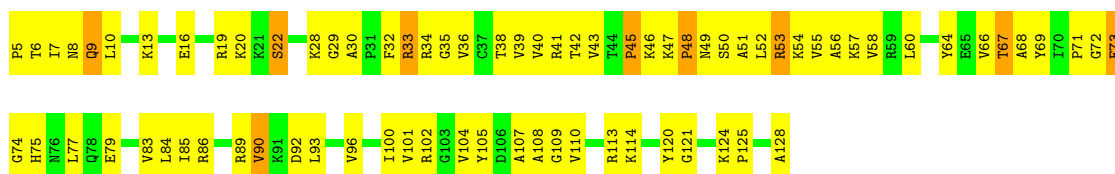
• Molecule 12: 30S ribosomal protein S12

Chain CL:



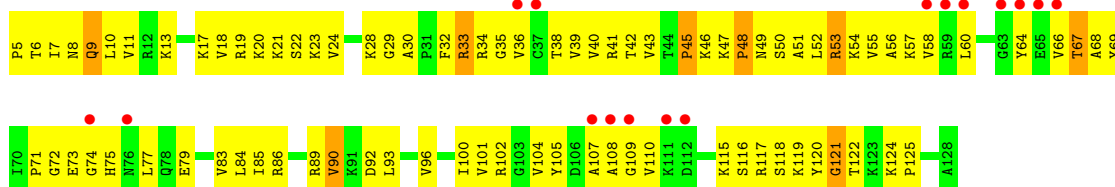
• Molecule 12: 30S ribosomal protein S12

Chain EL:



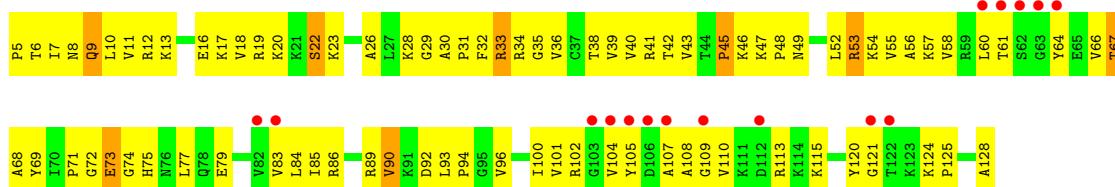
• Molecule 12: 30S ribosomal protein S12

Chain GL:



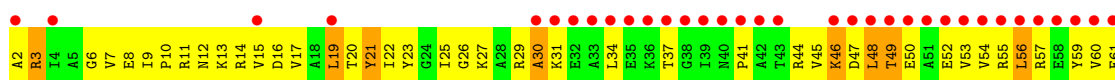
• Molecule 12: 30S ribosomal protein S12

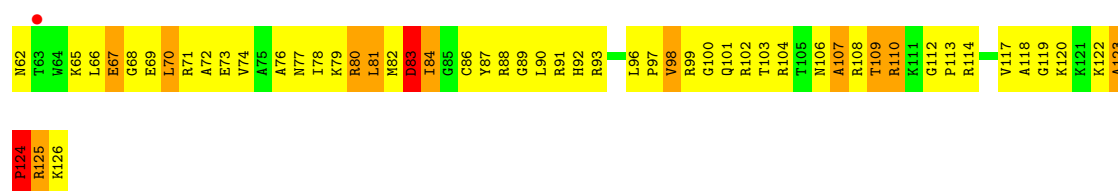
Chain IL:



• Molecule 13: 30S ribosomal protein S13

Chain AM:





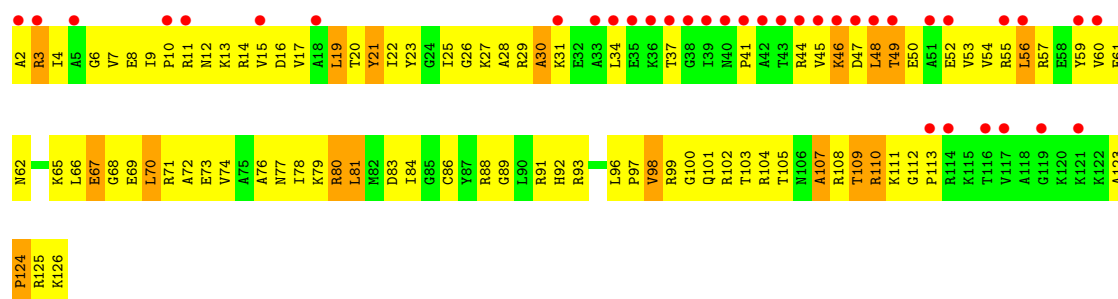
- Molecule 13: 30S ribosomal protein S13

Chain CM:



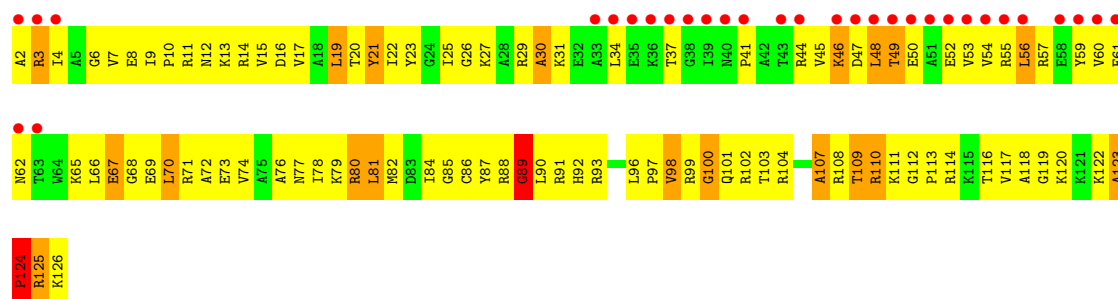
- Molecule 13: 30S ribosomal protein S13

Chain EM:



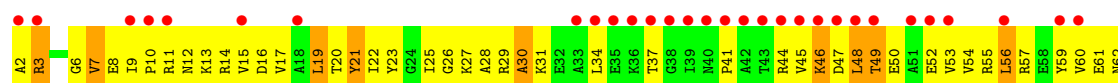
- Molecule 13: 30S ribosomal protein S13

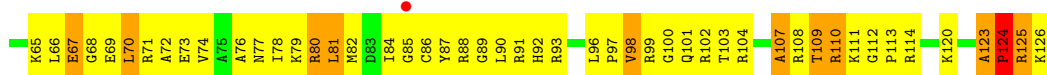
Chain GM:



- Molecule 13: 30S ribosomal protein S13

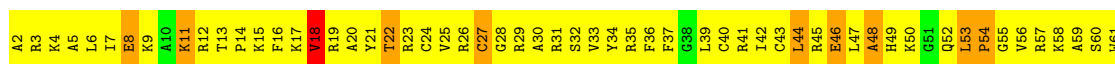
Chain IM:





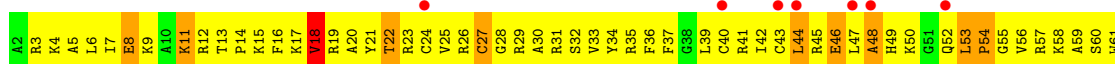
- Molecule 14: 30S ribosomal protein S14

Chain AN:



- Molecule 14: 30S ribosomal protein S14

Chain CN:



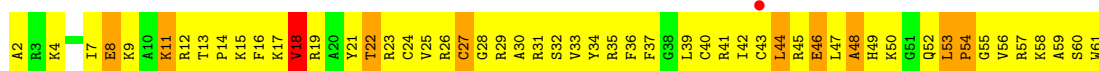
- Molecule 14: 30S ribosomal protein S14

Chain EN:



- Molecule 14: 30S ribosomal protein S14

Chain GN:



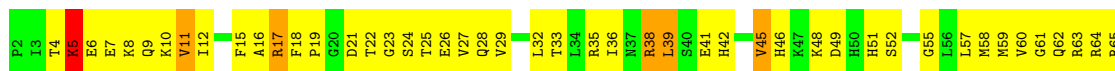
- Molecule 14: 30S ribosomal protein S14

Chain IN:



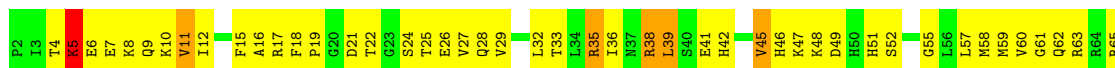
- Molecule 15: 30S ribosomal protein S15

Chain AO:



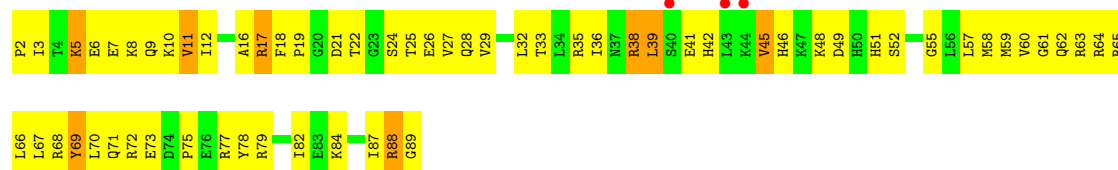
- Molecule 15: 30S ribosomal protein S15

Chain CO:

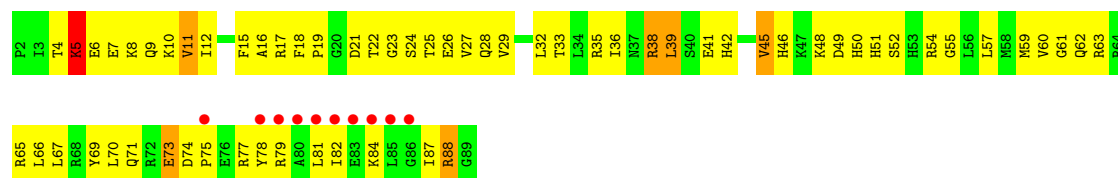




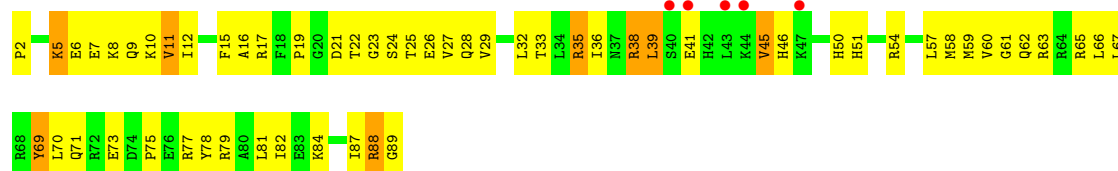
• Molecule 15: 30S ribosomal protein S15



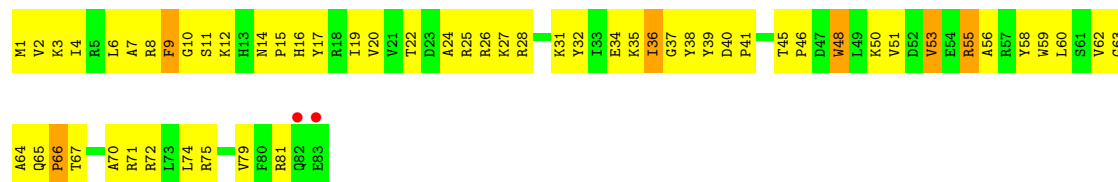
• Molecule 15: 30S ribosomal protein S15



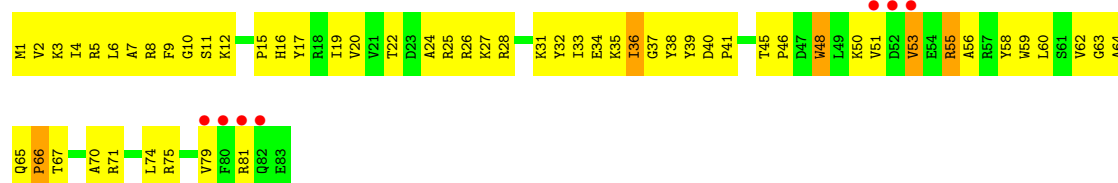
• Molecule 15: 30S ribosomal protein S15



• Molecule 16: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S16



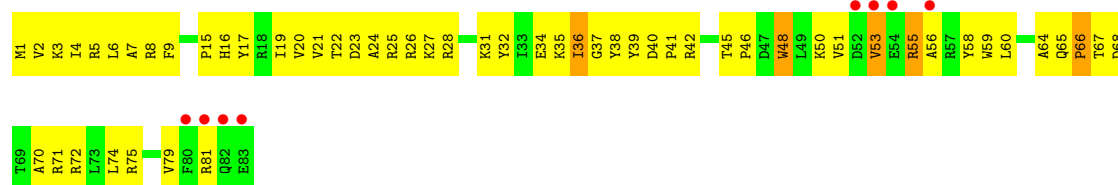
- Molecule 16: 30S ribosomal protein S16

Chain EP:



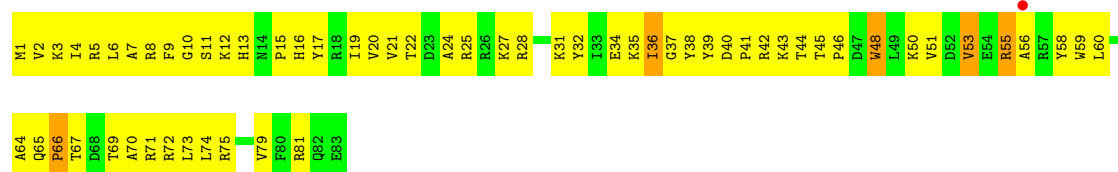
- Molecule 16: 30S ribosomal protein S16

Chain GP:



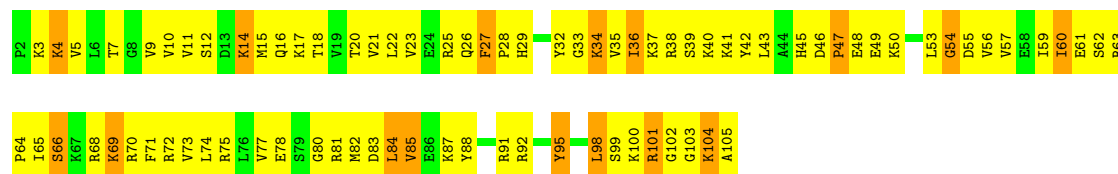
- Molecule 16: 30S ribosomal protein S16

Chain IP:



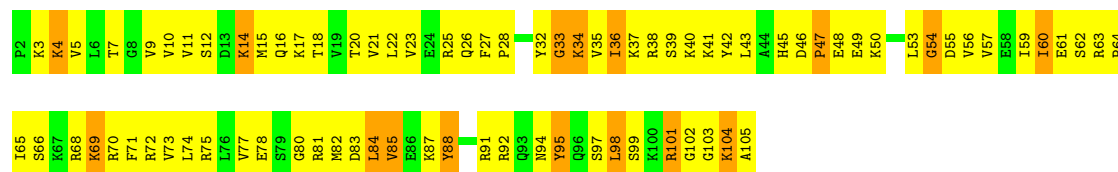
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



- Molecule 17: 30S ribosomal protein S17

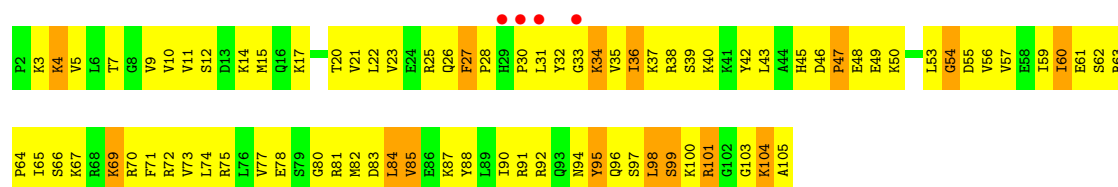
Chain CQ:



- Molecule 17: 30S ribosomal protein S17

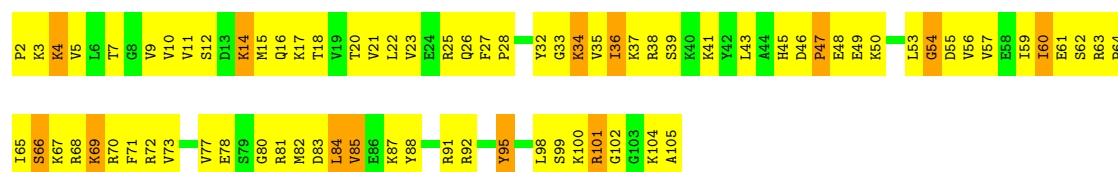
Chain EQ:





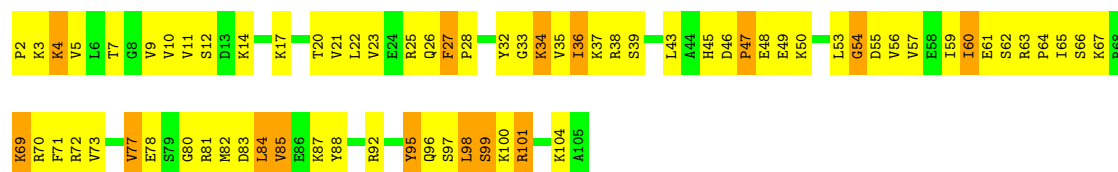
• Molecule 17: 30S ribosomal protein S17

Chain GQ:



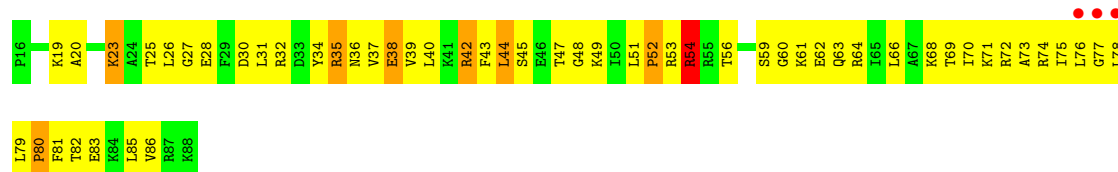
• Molecule 17: 30S ribosomal protein S17

Chain IQ:



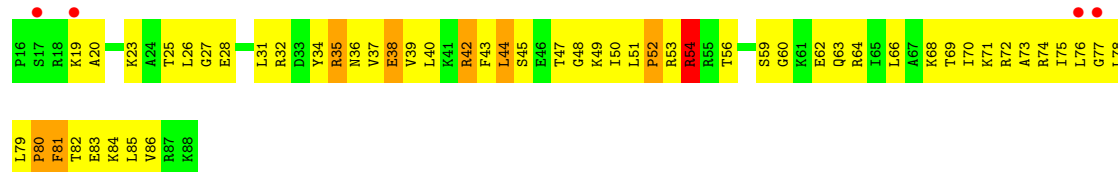
• Molecule 18: 30S ribosomal protein S18

Chain AR:



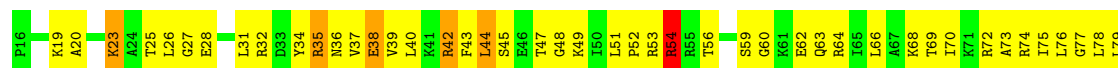
• Molecule 18: 30S ribosomal protein S18

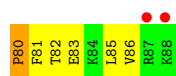
Chain CR:



• Molecule 18: 30S ribosomal protein S18

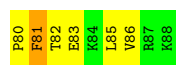
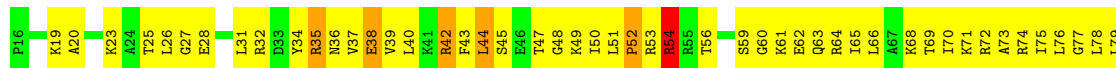
Chain ER:





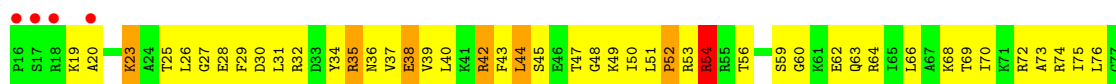
- Molecule 18: 30S ribosomal protein S18

Chain GR:



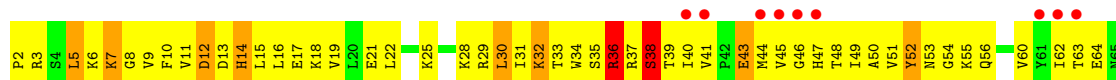
- Molecule 18: 30S ribosomal protein S18

Chain IR:



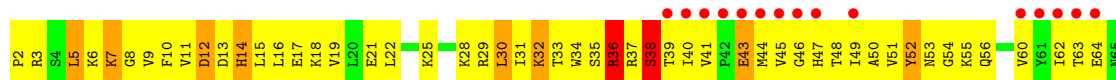
- Molecule 19: 30S ribosomal protein S19

Chain AS:



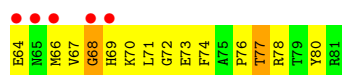
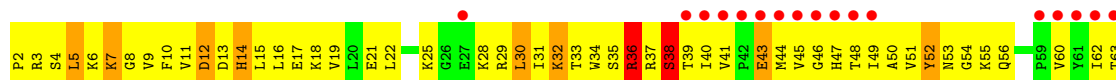
- Molecule 19: 30S ribosomal protein S19

Chain CS:

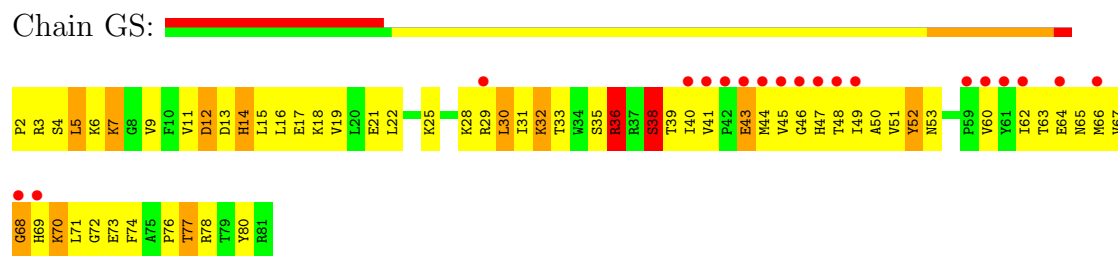


- Molecule 19: 30S ribosomal protein S19

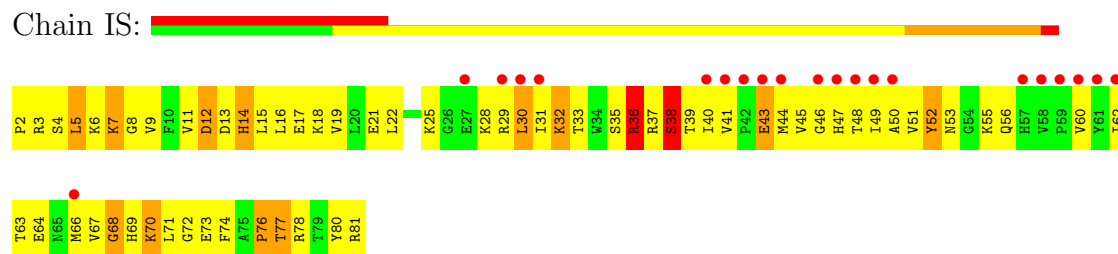
Chain ES:



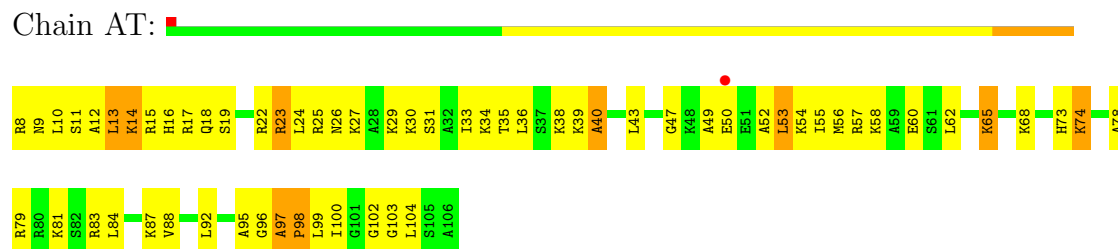
- Molecule 19: 30S ribosomal protein S19



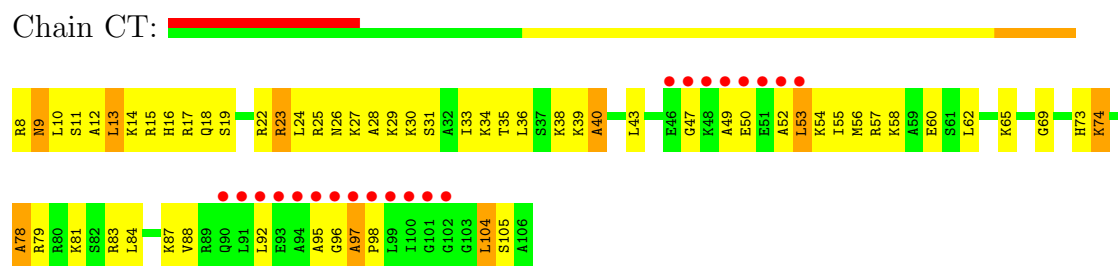
- Molecule 19: 30S ribosomal protein S19



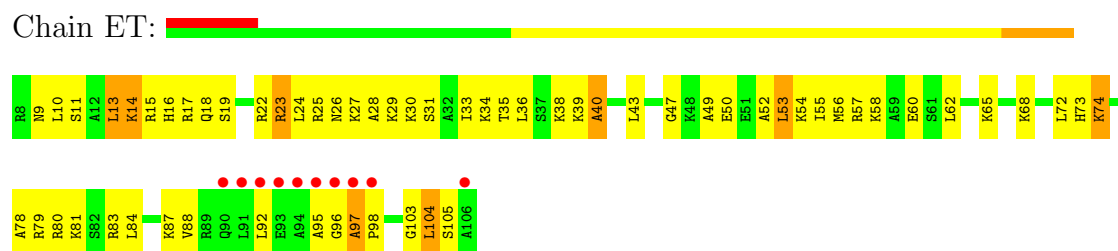
- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20

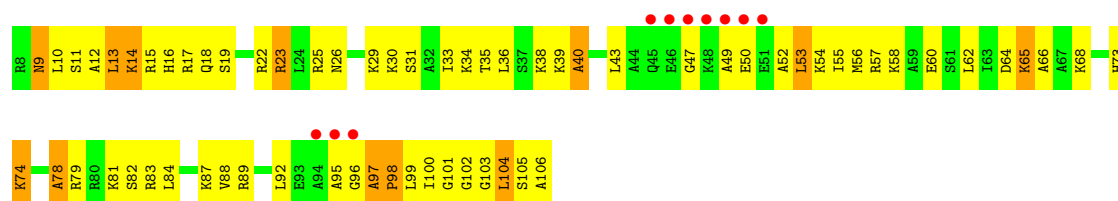


- Molecule 20: 30S ribosomal protein S20



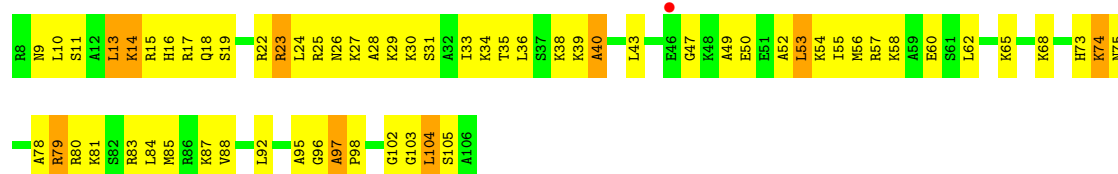
- Molecule 20: 30S ribosomal protein S20





- Molecule 20: 30S ribosomal protein S20

Chain IT:



- Molecule 21: protein Y

Chain Aa:



- Molecule 21: protein Y

Chain Ca:



- Molecule 21: protein Y

Chain Ea:



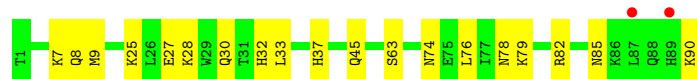
- Molecule 21: protein Y

Chain Ga:



- Molecule 21: protein Y

Chain Ia:

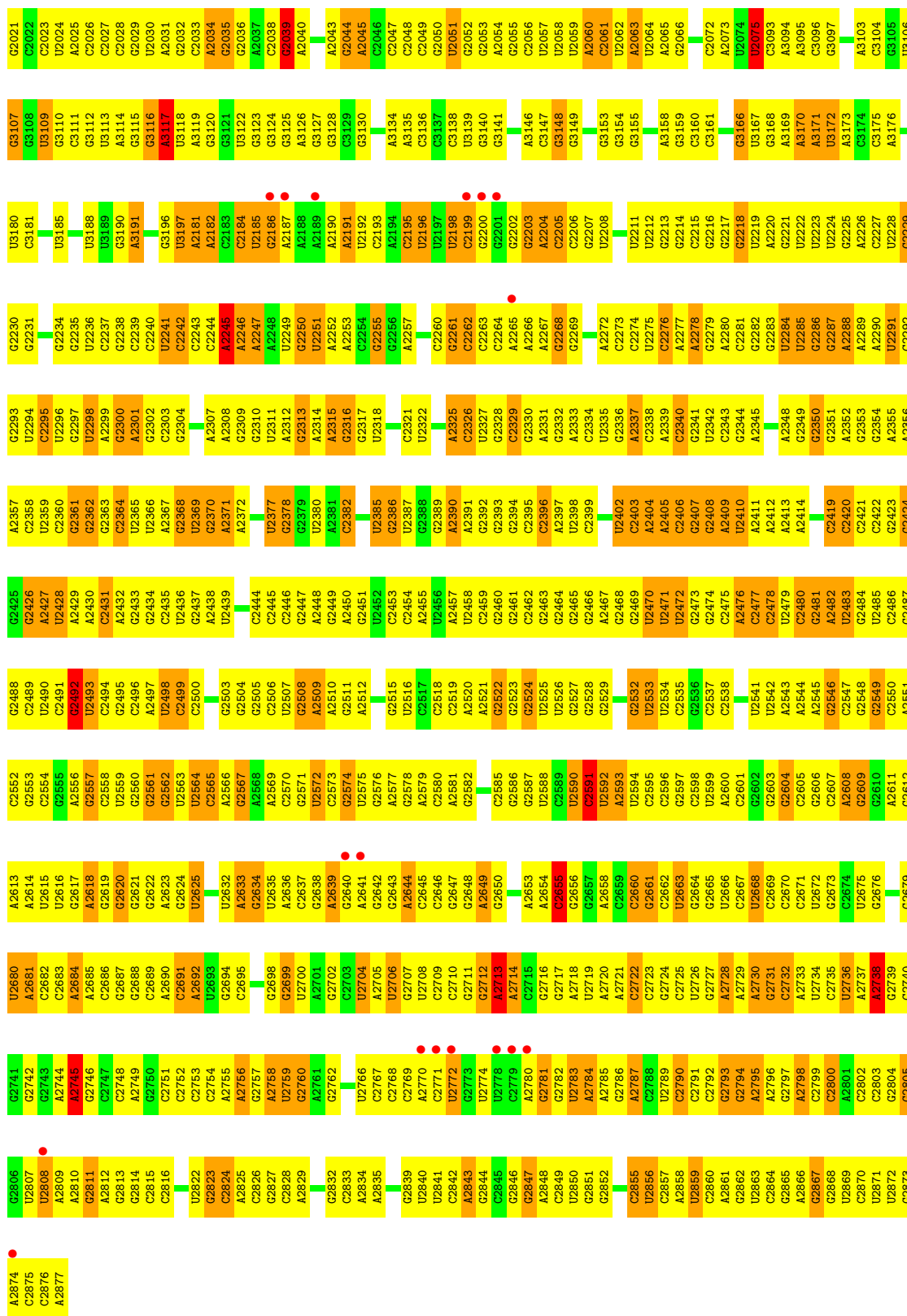


- Molecule 22: 23S RIBOSOMAL RNA

Chain BB: 

G1	G2	U3	C4	A5	A6	C7	A8	U9	G10	G11	U12	U13	A14	G15	G16	G17	U18	C19	G20	A21	G22	G23	G24	U25	G26	G27	U29	G35	G36	C37	G38	C39	U40	G41	G42	A43	G44	G45	C46	G47	A48	U49	G50	A51	A52	G53	G54	A55	C56	U57	G58	G59	A60	U61	G62	A63	C64																																																																		
C65	U66	C68	G69	A70	A71	A72	A73	G74	C75	G76	C77	C78	G79	A80	C81	G82	A83	C84	C85	A86	G87	G88	G89	A89	G90	A91	U92	A93	C94	G95	C96	U99	G100	A101	C102	G103	C104	A103	G104	G105	C106	U107	A108	G107	U110	G111	U112	A113	A114	A115	A116	A117	U118	C119	G120	G121	C122	G123	A124	U125	A126	C127																																																													
G128	A129	C130	G131	U132	C133	G134	U135	A136	A137	G138	A139	G140	G141	U142	A143	U144	C145	G146	G147	A148	C149	A150	G151	G152	A153	U154	G155	G156	G157	A158	U159	C160	G161	A162	A163	G164	G165	C166	A167	G168	U173	A174	C175	U176	A177	C178	U179	A180	U181	G182	U183	A184	C185	G186	A187	U188	A189	C190																																																																	
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A807	C808	C809	U810	C811	G812	A813	A814	C815	U816	A817	G818	C819	U820	A821	G822	U823	U824	C825	U826	C827	C828	C829	G830	G831	A832	A833	G836	U837	G838	U839	U840	G841	A842	G843	G844	U845	A846	C851	U852	U853	U854	A855	U856	C857	U858	A859	U860	C861	C862	C863	C864	A865	U867	C868	U869	C870	U871	G872	U873	A874																																																															
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G938	C939	G940	A1004	U1005	U1006	U1007	U1008	G1009	U1010	U1011	A1012	G1013	G1014	U1015	C1016	G1017	A1018	G1019	A1020	A1021	A1022	U1023	G1024	A1025	G1028	C1029	U1030	G1031	A1032	G1033	U1034	U1035	G1036	U1037	U1038	A1039	U1040	G1041	U1042	U1043	U1044	G1045	U1046	A1047	U1048	C1049	G1050	U1051	C1052	G1053	C1054	U1055	A1056	U1057	A1058	C1059	A1060	U1061	C1062	C1063	A1064																																																														

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A1960	G1784	G1847	A1785	A1658	A1590	G1527	U1459	C1396	A1334	U1268	G1200	A1138	G1069
A1961	A1901	G1848	A1786	G1659	U1591	C1528	U1460	A1397	A1335	G1269	G1201	A1139	U1071
	C1902	G1849	U1787	G1660	G1592	C1529	C1461	C1398	G1336	C1270	U1202	A1140	U1072
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U1965	G1904	G1851	G1789	G1662	U1594	C1531	A1463	A1400	G1338	G1272	G1204	G1142	U1074
C1966	U1906	G1852	G1790	G1663	A1596	U1532	A1464	A1401	U1339		G1205	G1143	U1075
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G1972	A1911	G1730		G1668	U1600	U1537	U1470	G1407	C1344	A1282		G1148	U1080
C1973	U1912	G1731		A1669	U1601	A1538	G1471	A1408	G1345		G1214	G1149	A1081
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C1977	G1916	U1735		C1674	C1614	U1544	C1476	U1413	G1351	A1287	G1223	G1155	
U1978	C1917	G1739		C1675	G1615	A1544	C1477	A1414	G1352	A1288	A1224		C1087
C1979	G1918	G1740			C1616	G1546	U1478	C1415	A1353	A1290	G1225		A1088
A1980	G1919	G1741		G1678	C1616	C1546	G1479	A1416	A1354	G1291	A1226		C1089
A1981	A1920	G1742		U1679	G1617	U1547	G1480	C1417	A1355	A1292	A1227		C1090
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A1984	A1922	G1745		A1682	C1620	C1550	G1483	A1420	C1358	U1295			U1093
G1985	C1924	U1746		G1683	C1621	U1551	U1484	U1421	G1359	G1296	U1232		A1095
U1986	G1925	G1747		G1684	G1622	U1552	U1485	C1422	G1360	A1297	A1233		
C1987	U1926	U1748		A1685	C1623	G1553	G1486	A1423	G1361	G1298	C1234		
A1988	U1927	G1749		A1686	A1624	G1554	C1487	U1424	A1362	A1299	C1235		
G1989	G1928	A1750		G1687	A1625	U1555	C1488	G1425	A1363	A1300	G1236		
U1990	U1929	A1751		U1688	A1626	A1556	C1489	U1426		U1301	G1237		G1100
C1991	G1930	U1752		U1689	C1627		U1490	G1427	A1366	C1302	G1238		U1101
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C1993	G1932	A1754		G1691	G1629	A1561	A1492	A1429	G1368	U1304	G1240		C1103
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G1995	U1934			A1693	C1631		G1494		U1370	U1306	A1242		A1109
A1996	A1935	A1759		A1694	A1632	G1565	G1495	A1433	G1371	U1307	G1243		G1110
A1997	A1936	G1760		U1695	C1633	G1566	G1496	U1434	A1372	C1308	U1244		C1111
U1998	G1937	G1761		C1696	A1634	U1567	C1497	G1435	G1373	G1309	G1245		U1112
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U2000	U1939	G1763		C1698	U1637	A1569		A1437	C1375	C1311	U1247		C1114
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A2002	C1941	C1765			U1639	G1571	G1502	G1439	G1377	U1313	A1249		U1116
A2003	U1942	U1766		C1702	C1639	C1572	G1503	G1440	A1378	A1180	C1250		G1117
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U2005	G1882	U1768		G1704	C1642	A1574	U1505	C1442	C1380	A1315	G1252		U1119
G2006	C1945	U1769		U1705	A1643	C1575	C1506	G1443	G1381	G1184	C1253		C1120
G2007	A1885	U1770		A1706	G1644	G1576	A1507		G1382	G1254	G1254		G1121
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U2009	G1831	C1772		C1708	U1646	U1578	A1509	U1447	G1384	A1186	C1256		C1127
G2010		C1773		U1709	U1647	C1579	U1510	A1448	C1385	A1187	U1257		C1128
A2015	C1950	A1774		U1710	C1648	U1580	A1511	C1449	A1386	G1189	G1258		A1129
	G1951	A1775		C1711	A1649	C1581	A1512	G1450	G1387	C1190	A1259		U1130
G2016	A1952	A1776		G1712	U1651	U1582	U1513	C1451	C1388	G1191	A1260		G1131
U2017	A1953	A1777		G1713	U1651	A1583	C1514	U1452	C1389		C1261		G1132
G2018	A1954	U1778		A1714	G1652	G1584	A1453	A1454	G1390		U1262		G1133
C2019	A1895	G1779		A1715	C1653	U1585	C1522	U1454	A1391		G1263		G1134
G2020	G1956	A1780		A1586	A1654	A1586	C1523	U1455	U1392		G1264		C1135
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• Molecule 22: 23S RIBOSOMAL RNA

Chain DB:

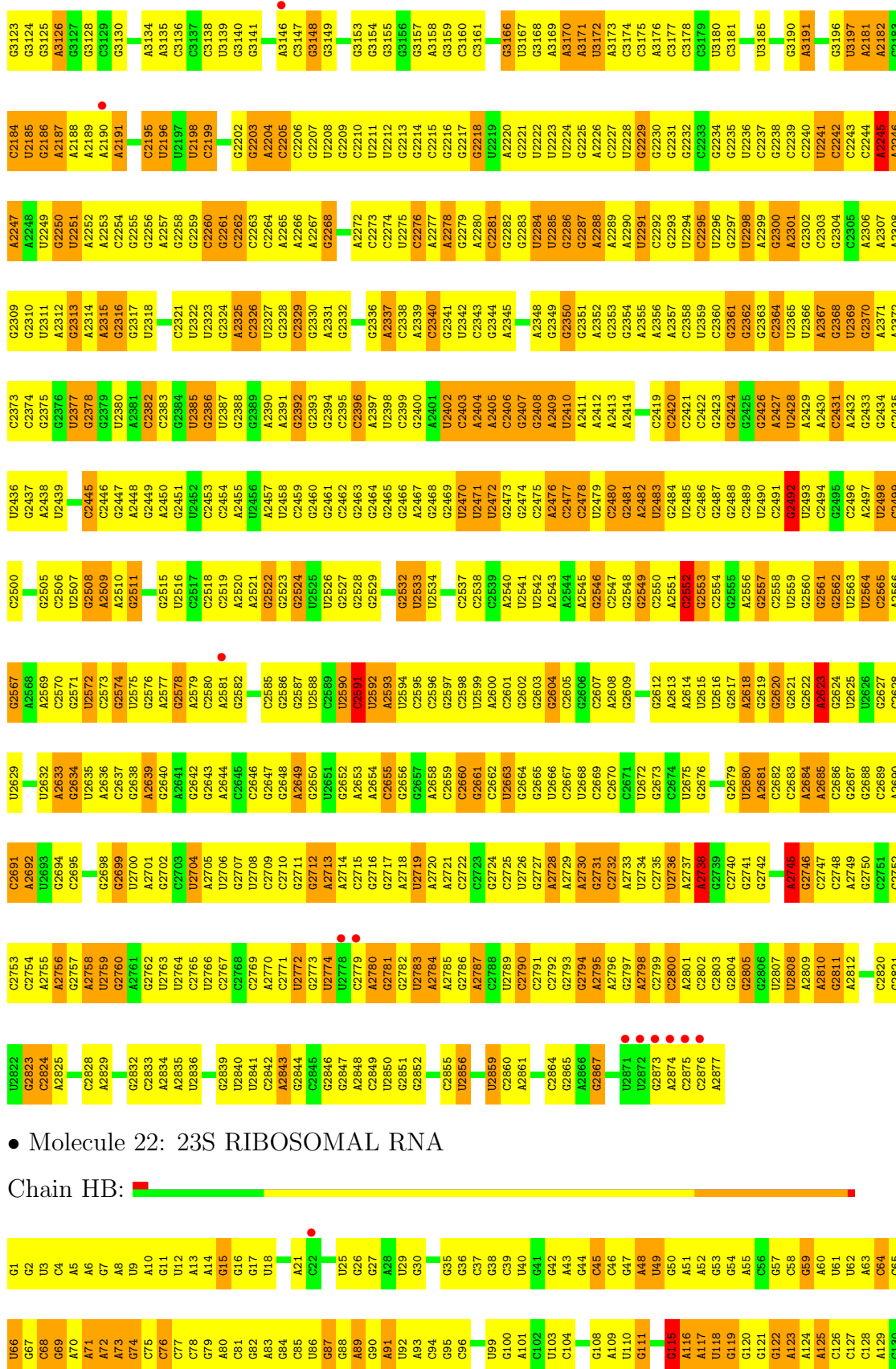
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A1006	A1007	A999	G875	C808	G746	C685	A502	G437	A503	C298	G193	C129	U66	U3
A1008	A1009	C937	A876	C809	A747	C686	G504	C438	G505	C299	G194	C130	G67	C4
A1010	A1011	G938	G877	U810	A748	C687	G506		G507	C300	A195	C131	C68	A5
A1012	A1013	C939	C878	G811	A749	A688	G508	A441	G509	C301	A196	U132	G69	A6
A1014	A1015	G940	A879	G812	C750	A689	G510	A442	G511	U302	G197	C133	A70	G7
A1016	A1017	U941	C880	A813	G751	A690	G512	A443	G513	C302	A198	C134	A71	A8
A1018	A1019	U942	U881	G814	G752	C691	G514	A444	G515	C303	A199	G135	A72	U9
A1020	A1021	U943	C882	A815	U753	C692	G516	U445	G517	A304	A200	A136	G73	G11
A1022	A1023	G945	A883	U816	G754	A693	G518	C446	G519	A305	G201	A137	G74	G12
A1024	A1025	U946	C884	A817	C755	G694	G520	U447	G521	A306	A202	C138	C75	U13
A1026	A1027	C947	A885	G818	C756	G695	G522	C448	G523	C307	G203	C139	C76	U14
A1028	A1029	G950	A886	C819	U757	U696	G524		G525	C308	A204	G140	C77	A14
A1030	A1031	U950	G887	U820	G758	G697	G526	G452	G527	A373	U205	G141	C78	G15
A1032	A1033	G951	U888	A821	C759	A698	G528	U453	G529	A374	A206	U142	C79	G16
A1034	A1035	U952	C889	G822	U760	A699	G530	G454	G531	A375	U207	U143	C80	G17
A1036	A1037	G953	U890	U823	G761	C700	G532	A455	G533	G388	C208	U144	C81	U18
A1038	A1039	U954	A891	U824	A762	U701	G534	C456	G535	A322	G209	U145	C82	C19
A1040	A1041	G955	A892	C825	A763	A702	G536	C457	G537	C324	A210	G146	A83	C20
A1042	A1043	U956	G893	U826	A764	A703	G538	C458	G539	U325	U211	G147	G84	A21
A1044	A1045	G957	G894	C827	C765	G704	G540	U459	G541	A320	U212	C148	C85	C22
A1046	A1047	U958	G895	C828	A766	C705	G542	A461	G543	A321	C213	A149	U86	G23
A1048	A1049	G959	G896	C829	G767	A706	G544	C462	G545	A322	C214	A150	G87	G24
A1050	A1051	U960	C898	C830	U768	G707	G546	C463	G547	U326	G215	G151	G88	U25
A1052	A1053	G960	U900	G831	C771	A709	G548	C464	G549	U327		G152	A89	G26
A1054	A1055	U961	A900A	A832	G772	C710	G550	C465	G551	U328	A218	A153	G90	G27
A1056	A1057	G962	U901	A833	G773	A711	G552	C466	G553	A326	G219	U154	A91	A28
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A1060	A1061	G964	U903	U837	G775	A713	G556	C468	G557	A328	A221	G156	A93	G30
A1062	A1063	U965	G904	A838	G776	G714	G558	C469	G559	C329	G222	G157	C94	
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A1066	A1067	U967	U906	U840	G778	A716	G562	C471	G563	U331	G224	A159	G96	G36
A1068	A1069	G968	U907	G841	G779	C717	G564	C472	G565	A332	G225	C160	G37	C37
A1070	A1071	U969	C908	A842	G780	A718	G566		G567	A333	G226	U161	G38	C39
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A1074	A1075	U971	U910	U844	G782	A720	G570	C474	G571	A335	A228	A163	G102	G41
A1076	A1077	G972	U911	G845	G783	C721	G572	C475	G573	A336	G229	G164	U103	G42
A1078	A1079	U973	A912	U846	G784	C722	G574	C476	G575	G337	G230	G165	U104	A43
A1080	A1081	G974	A913	A847	G785	C723	G576	C477	G577	U338	G231	A167	G105	G44
A1082	A1083	U975	C914	G848	G786	G723	G578	C478	G579	U339	A232	A168	G106	C45
A1084	A1085	G976	C915	U849	G787	C724	G580	C479	G581	A340	G233	G107	G107	C46
A1086	A1087	U977	U916	C851	G788	U726	G582	C480	G583	A341	C234	A173	G47	G47
A1088	A1089	G978	U917	U852	G789	G727	G584	C481	G585	U342	G235	A174	A48	A48
A1090	A1091	U979	U918	U853	G790	G728	G586	C482	G587	U343	G236	C175	U49	U49
A1092	A1093	G980	A918	U854	G791	A729	G588	C483	G589	U344	G237	C176	G50	G50
A1094	A1095	U980	U919	G855	G792	C730	G590	C484	G591	U345	G238	U177	C114	A51
A1096	A1097	G981	A920	U856	G793	A731	G592	C485	G593	C420	G239	G178	G115	A52
A1098	A1099	U981	A921	G857	G794	G732	G594	C486	G595	G421	U240	U179	A116	A53
A1100	A1101	G982	U922	A861	A795	G733	G596	C487	G597	C422	C241	C180	G117	G54
A1102	A1103	U982	A923	G862	A796	G734	G598	C488	G599	G423	A242	G181	U118	A55
A1104	A1105	G983	U923	C863	G797	G735	G600	C489	G601	G424	G243	G182	C56	G56
A1106	A1107	U983	U924	G864	A797	G736	G602	C490	G603	A425	C244	G183	G57	G57
A1108	A1109	G984	A924	U865	G798	G737	G604	C491	G605	C426	C245	U184	G120	C58
A1110	A1111	U984	U925	U866	G799	C737	G606	C492	G607	C427	G246	G185	G121	G59
A1112	A1113	G985	G926	U867	U800	G738	G608	C493	G609	C428	A247	C186	A60	A60
A1114	A1115	U985	U927	U868	G801	G739	G610	C494	G611		A248	U187	U61	U61
A1116	A1117	G986	A928	U869	A801	G740	G612	C495	G613	C432	A292	C188	A123	A63
A1118	A1119	U987	U929	C870	A802	A741	G614	C496	G615	A335	G248	A124	A125	U62
A1120	A1121	G988	A930	U871	C803	G742	G616	C497	G617	A336	A292	A126	C126	
A1122	A1123	U989	G931	U872	C804	G743	G618	C498	G619	C358	G295			
A1124	A1125	G990	U932	U873	G805	A743	G620	C499	G621					
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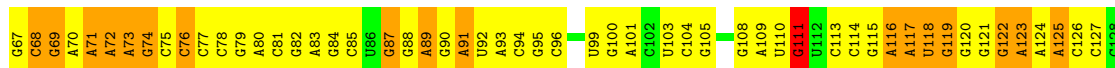
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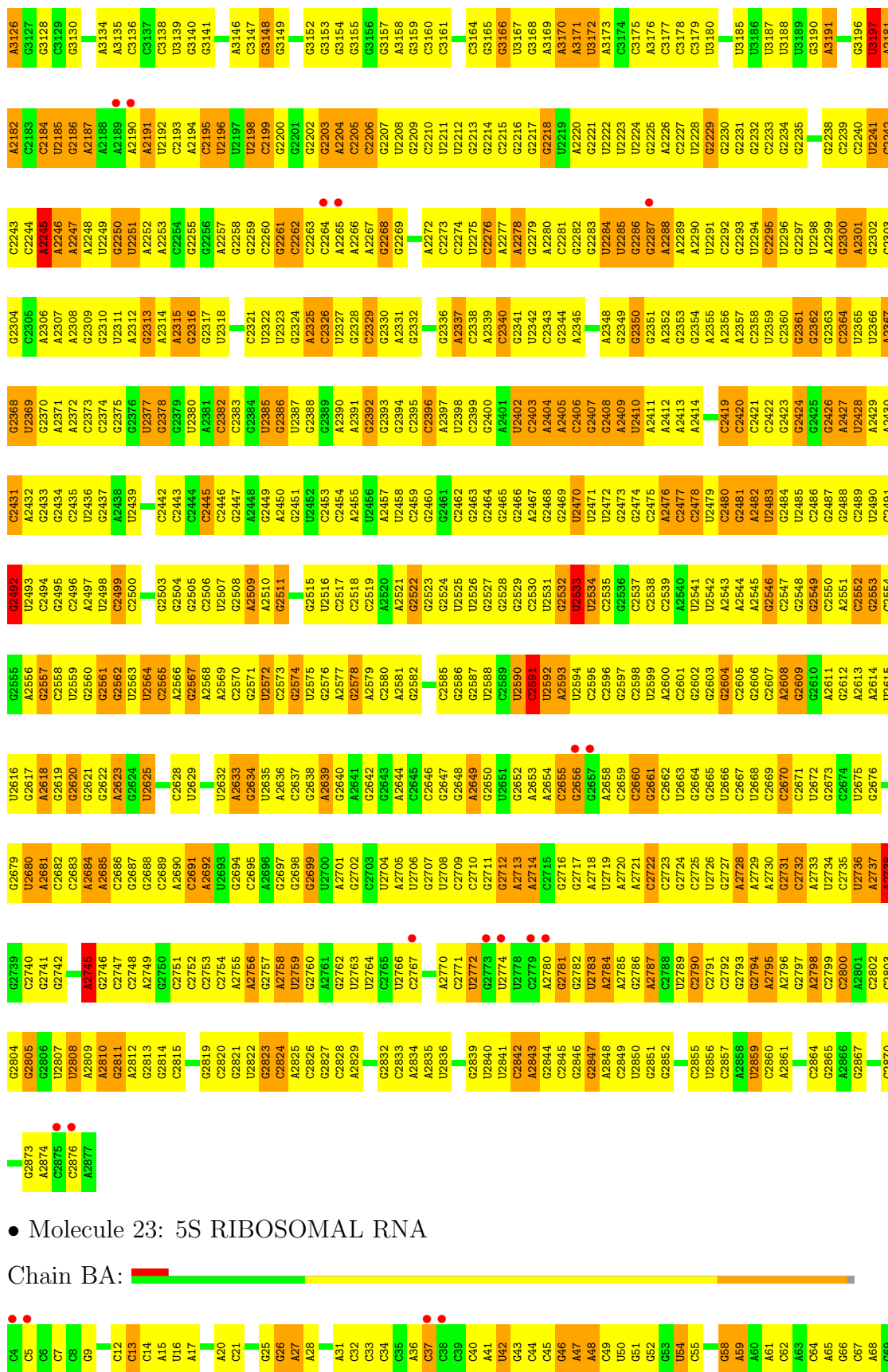
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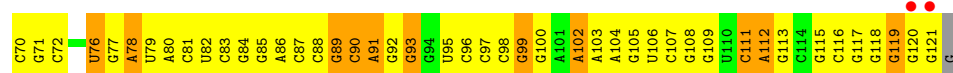
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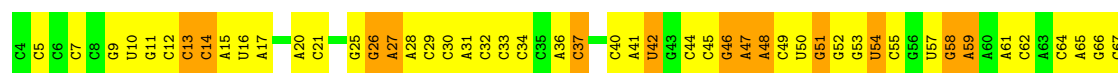
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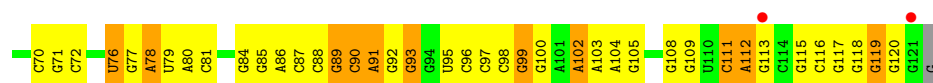
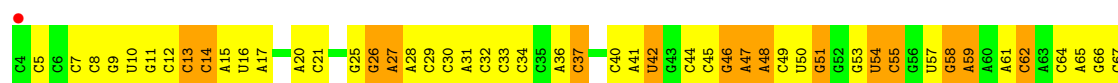
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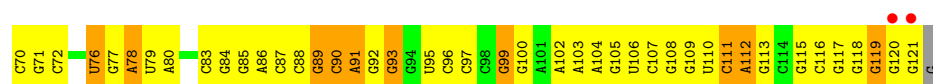
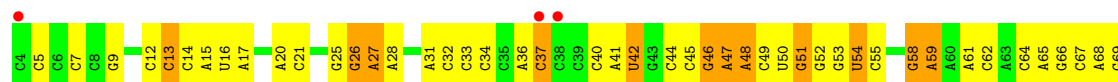
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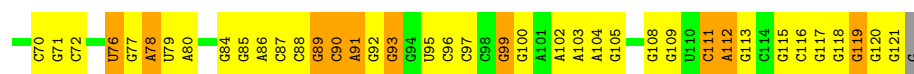
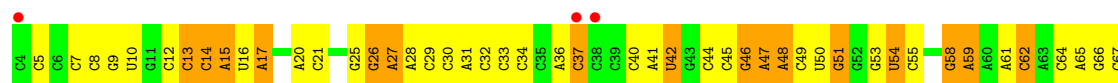
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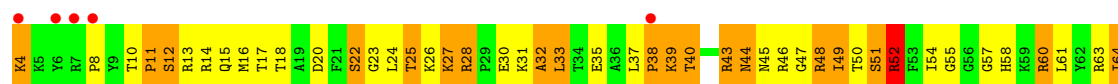
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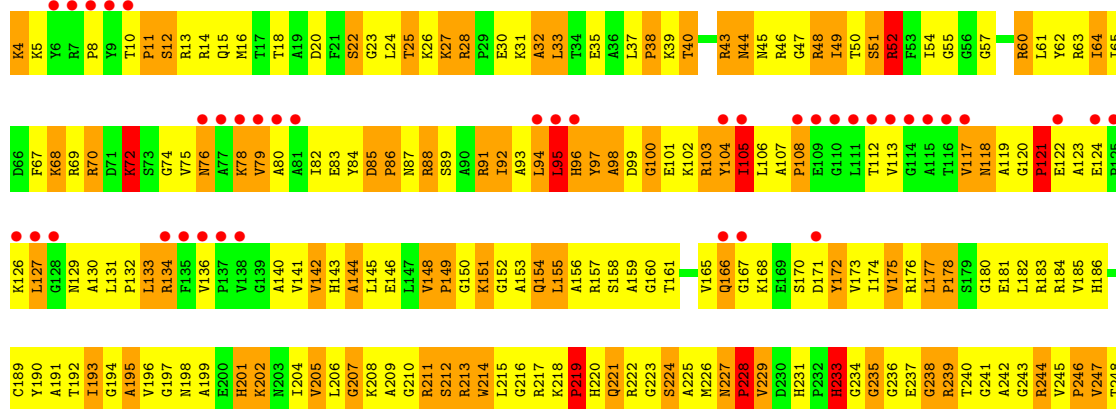
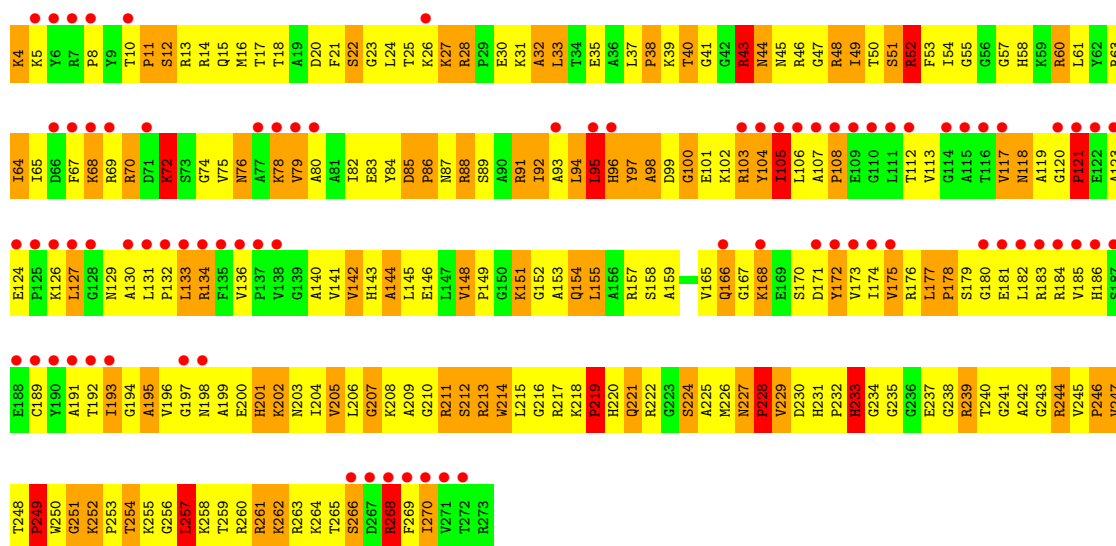
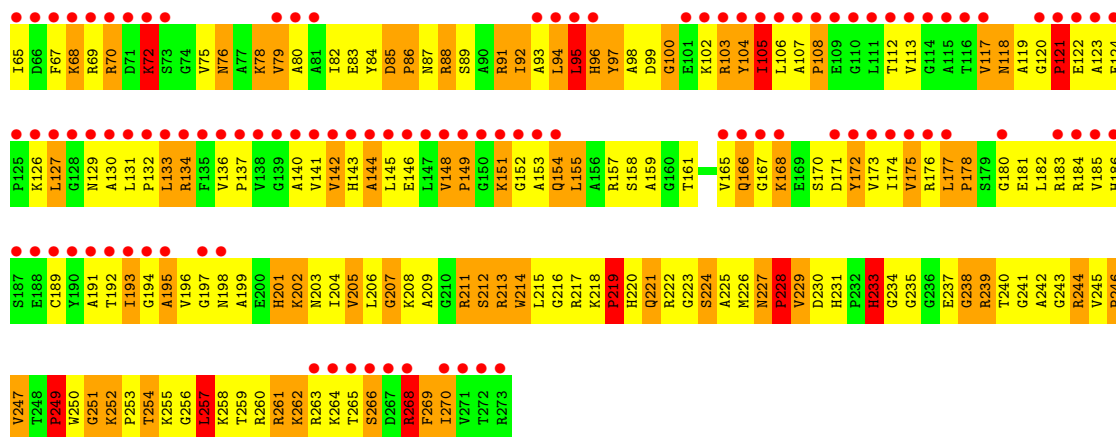
Chain JA:



• Molecule 24: 50S ribosomal protein L2

Chain BD:

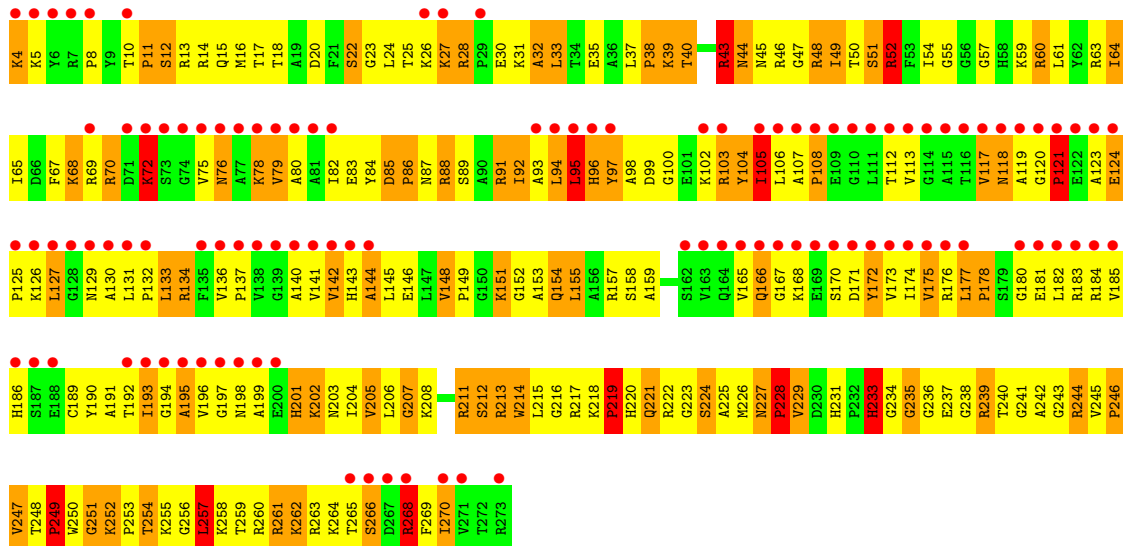






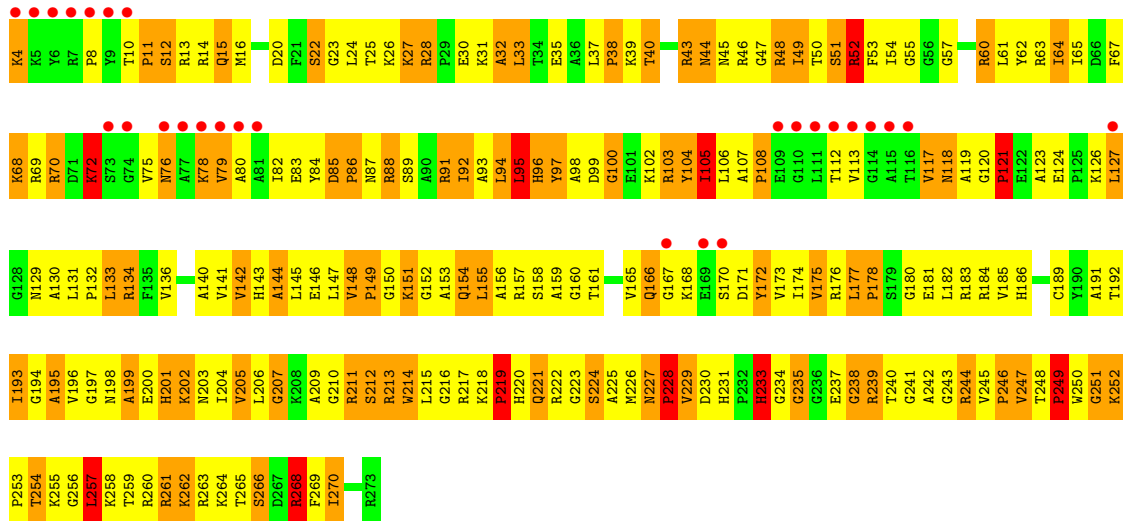
• Molecule 24: 50S ribosomal protein L2

Chain HD:



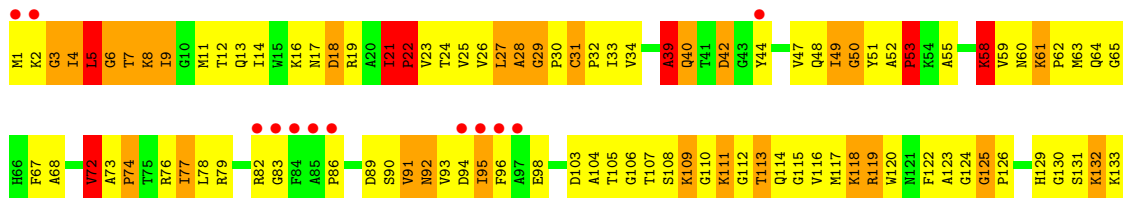
• Molecule 24: 50S ribosomal protein L2

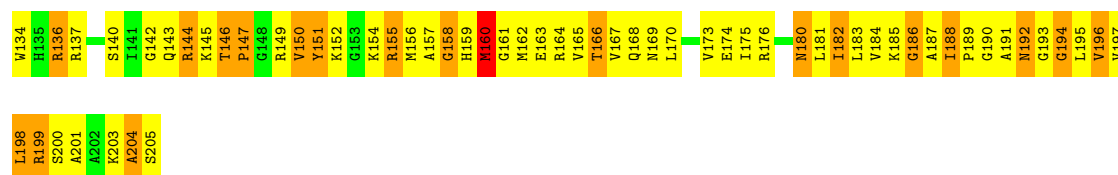
Chain JD:



• Molecule 25: 50S ribosomal protein L3

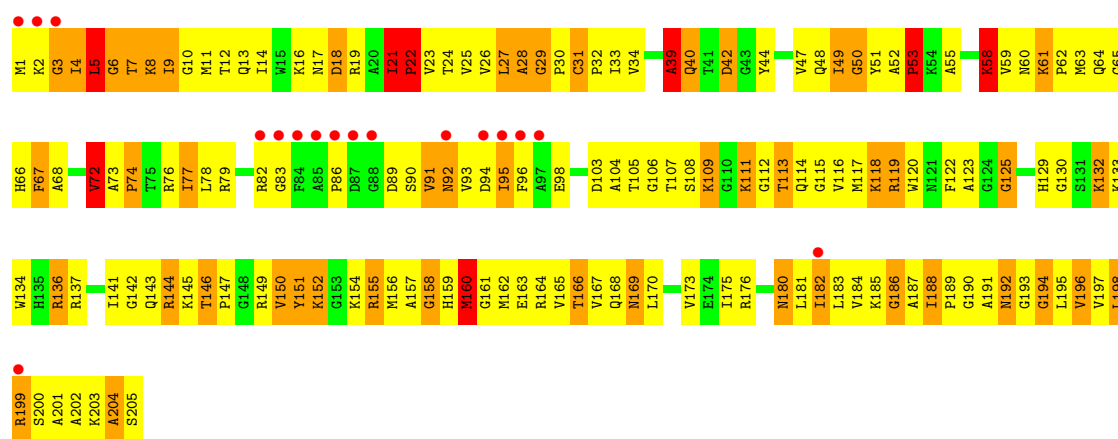
Chain BE:





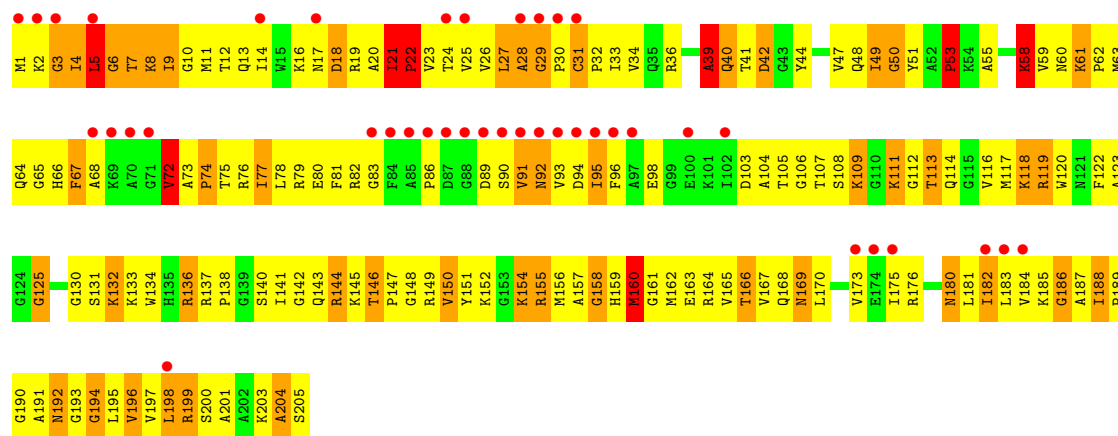
• Molecule 25: 50S ribosomal protein L3

Chain DE:



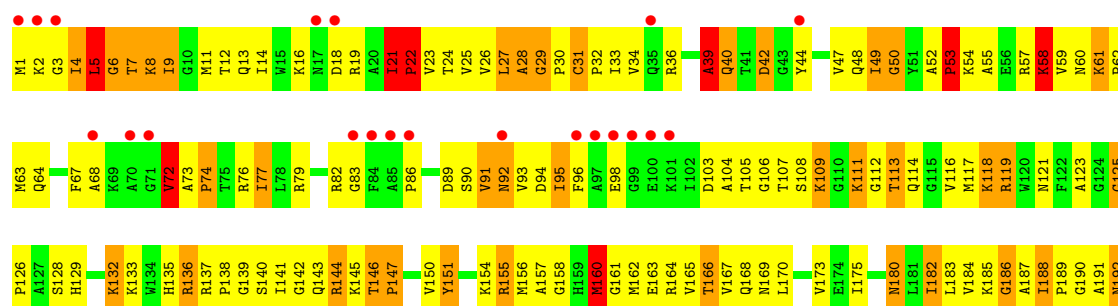
• Molecule 25: 50S ribosomal protein L3

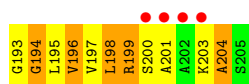
Chain FE:



• Molecule 25: 50S ribosomal protein L3

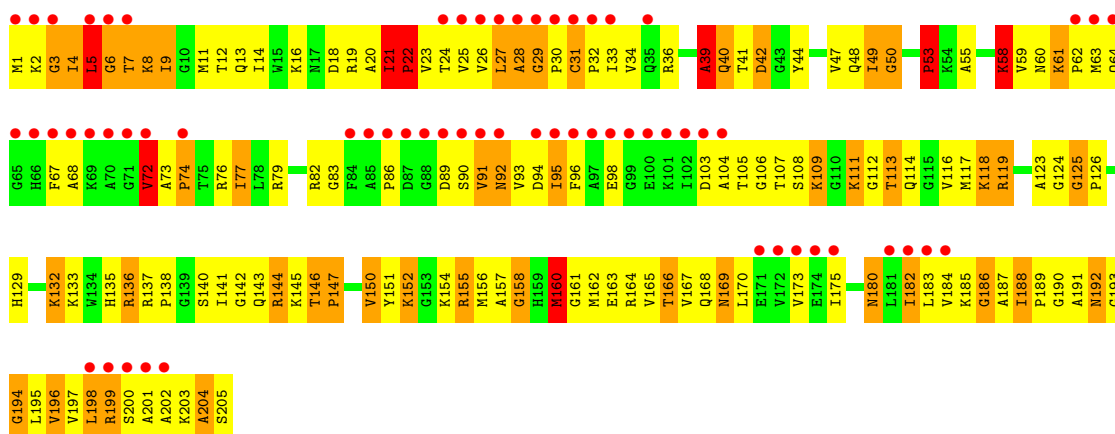
Chain HE:





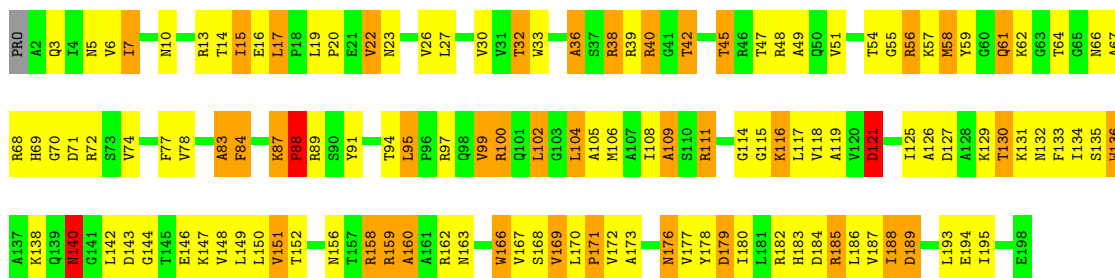
• Molecule 25: 50S ribosomal protein L3

Chain JE:



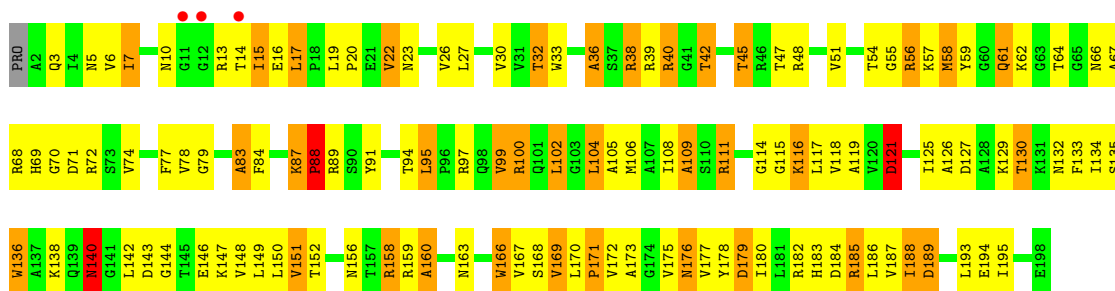
• Molecule 26: 50S ribosomal protein L4

Chain BF:



• Molecule 26: 50S ribosomal protein L4

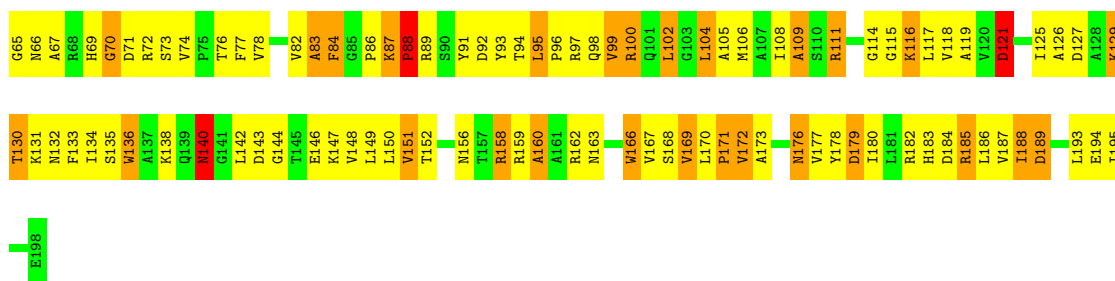
Chain DF:



• Molecule 26: 50S ribosomal protein L4

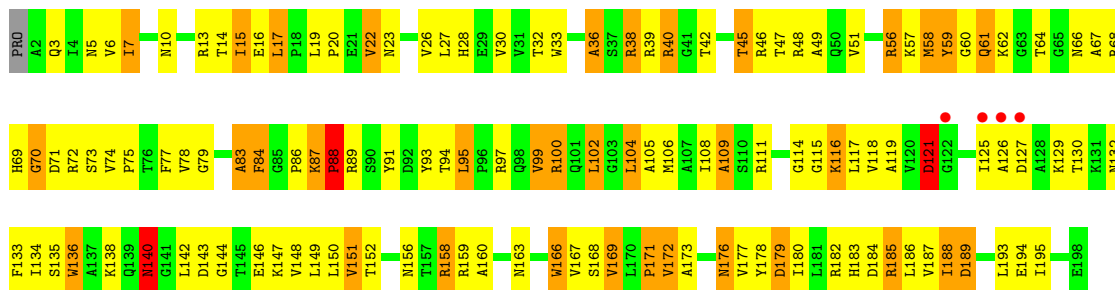
Chain FF:





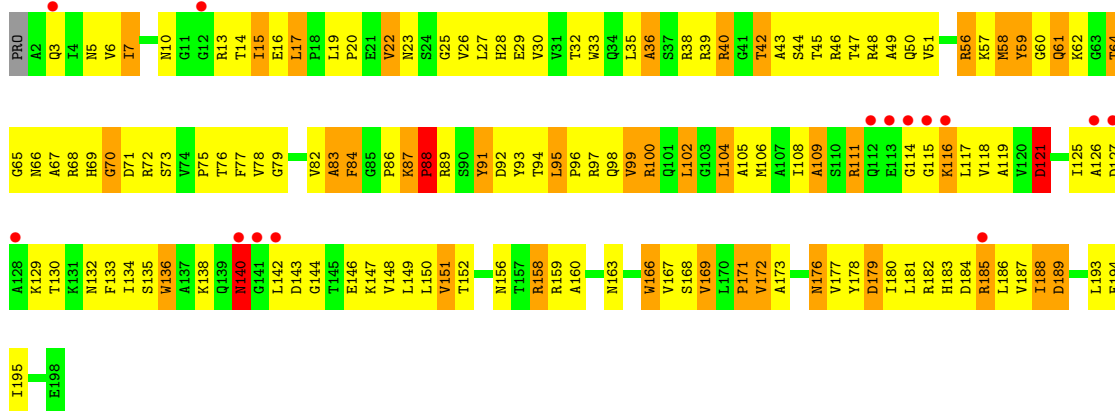
• Molecule 26: 50S ribosomal protein L4

Chain HF:



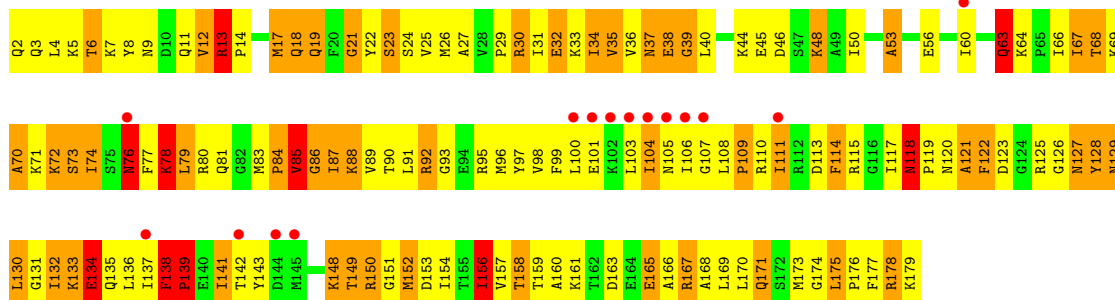
• Molecule 26: 50S ribosomal protein L4

Chain JF:



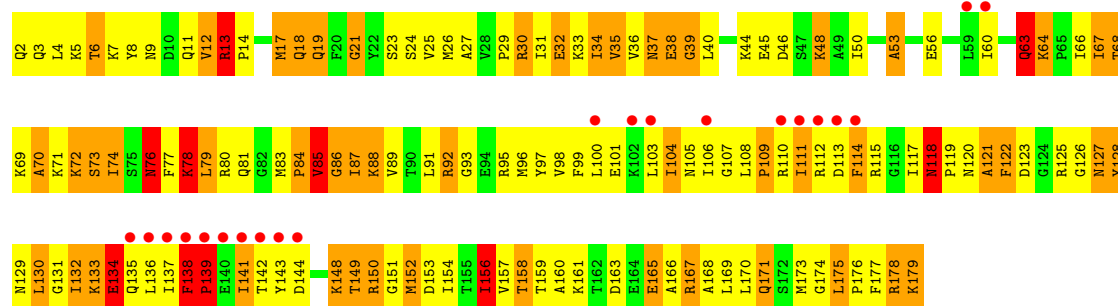
• Molecule 27: 50S ribosomal protein L5

Chain BG:



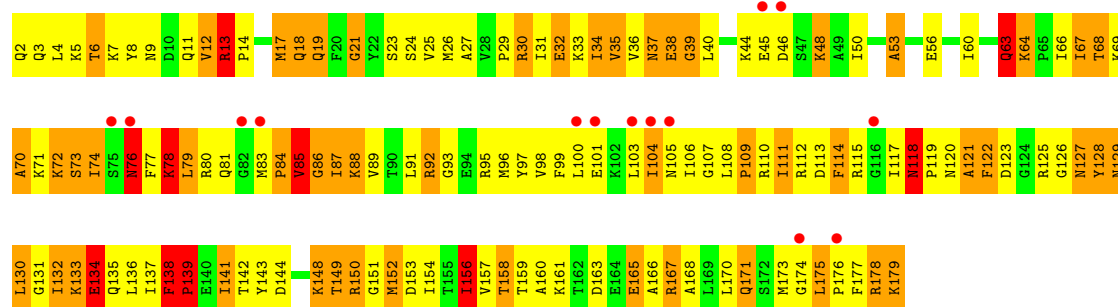
- Molecule 27: 50S ribosomal protein L5

Chain DG:



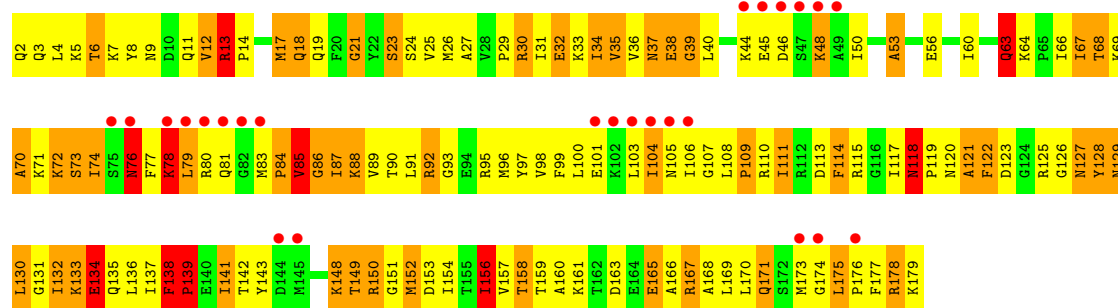
- Molecule 27: 50S ribosomal protein L5

Chain FG:



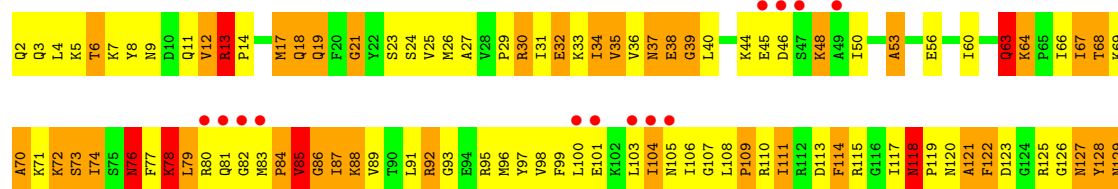
- Molecule 27: 50S ribosomal protein L5

Chain HG:



- Molecule 27: 50S ribosomal protein L5

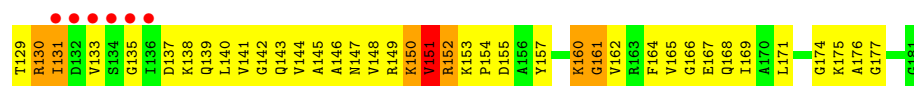
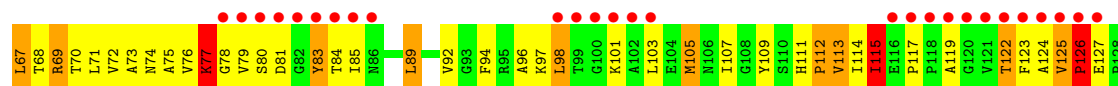
Chain JG:





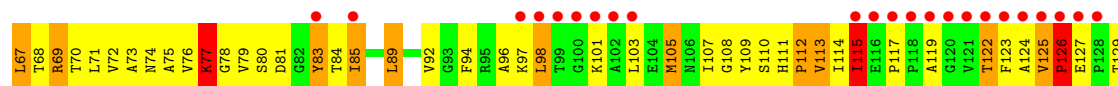
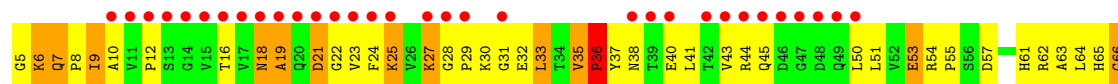
• Molecule 28: 50S ribosomal protein L6

Chain BH:



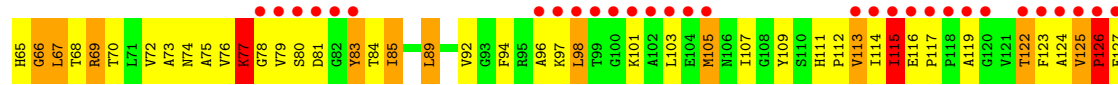
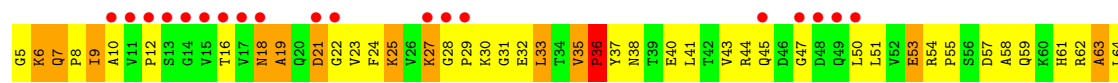
• Molecule 28: 50S ribosomal protein L6

Chain DH:



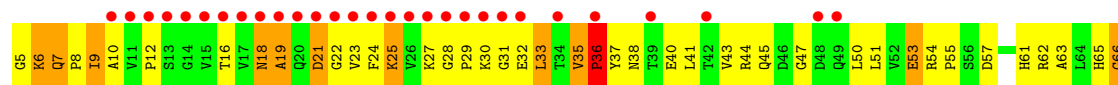
• Molecule 28: 50S ribosomal protein L6

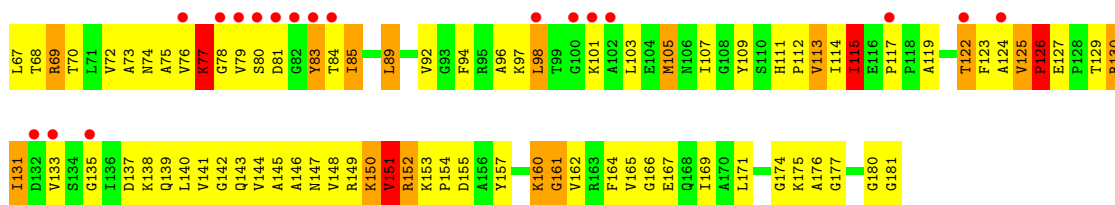
Chain FH:



• Molecule 28: 50S ribosomal protein L6

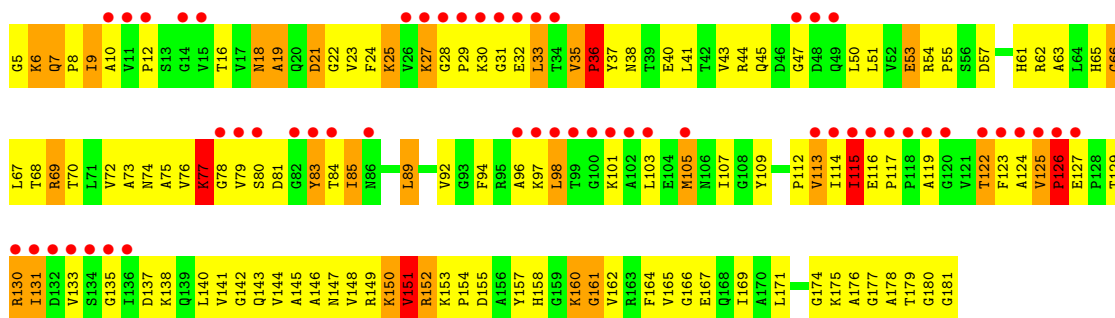
Chain HH:





• Molecule 28: 50S ribosomal protein L6

Chain JH:



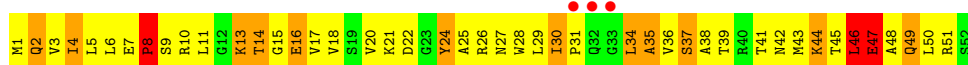
• Molecule 29: 50S ribosomal protein L9

Chain BI:



• Molecule 29: 50S ribosomal protein L9

Chain DI:



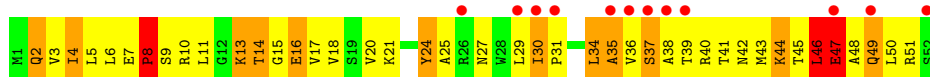
• Molecule 29: 50S ribosomal protein L9

Chain FI:



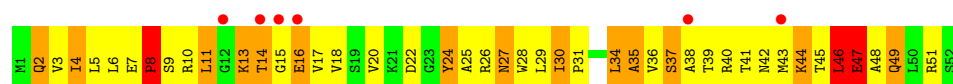
• Molecule 29: 50S ribosomal protein L9

Chain HI:



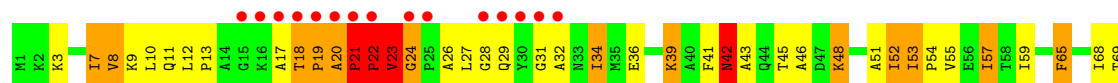
• Molecule 29: 50S ribosomal protein L9

Chain JI:



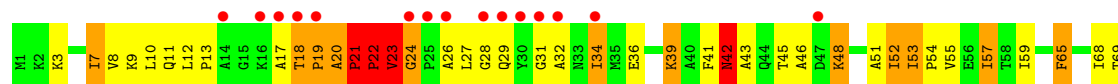
- Molecule 30: 50S ribosomal protein L11

Chain BJ:



- Molecule 30: 50S ribosomal protein L11

Chain DJ:



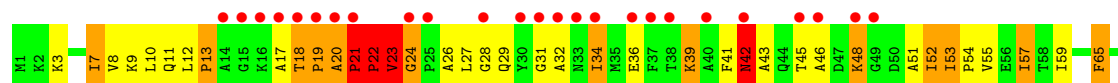
- Molecule 30: 50S ribosomal protein L11

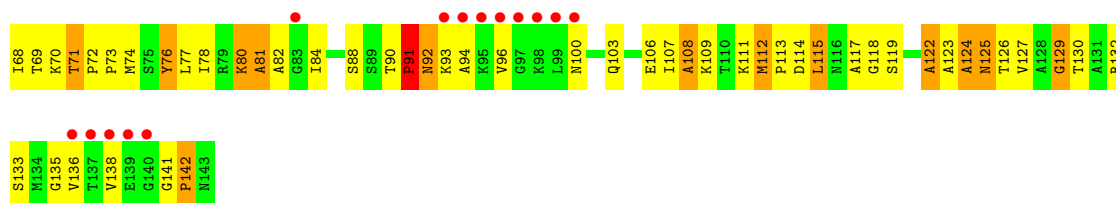
Chain FJ:



- Molecule 30: 50S ribosomal protein L11

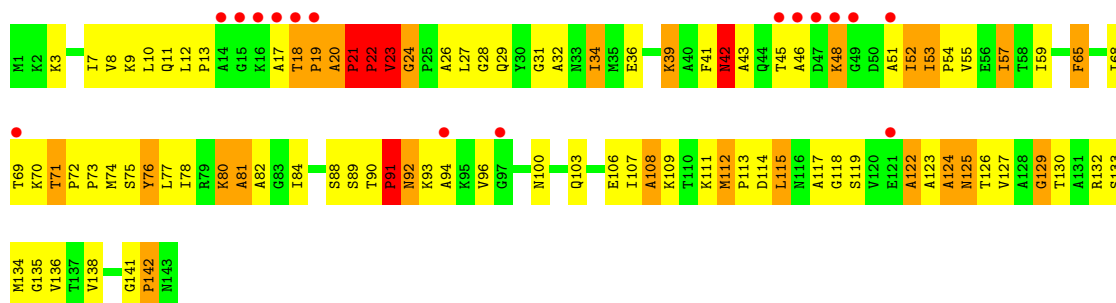
Chain HJ:





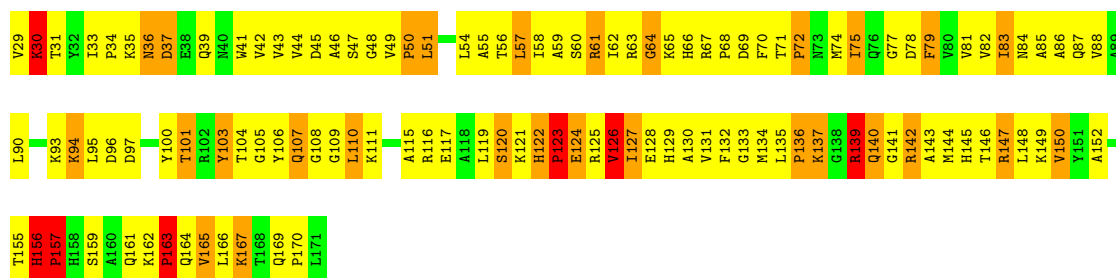
• Molecule 30: 50S ribosomal protein L11

Chain JJ:



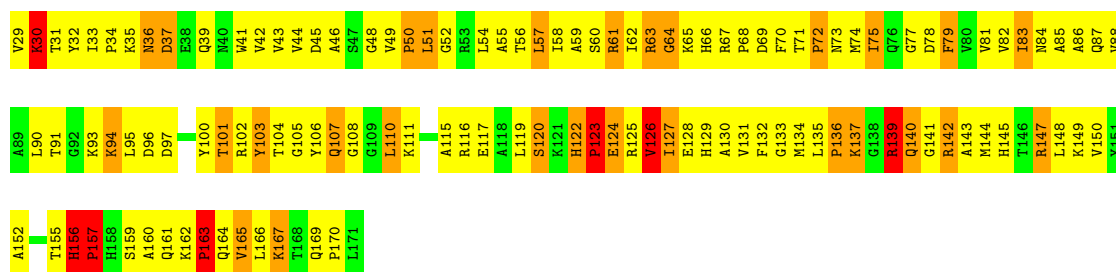
• Molecule 31: 50S ribosomal protein L13

Chain BK:



• Molecule 31: 50S ribosomal protein L13

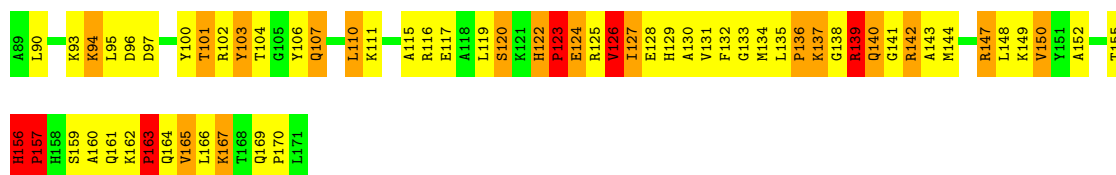
Chain DK:



• Molecule 31: 50S ribosomal protein L13

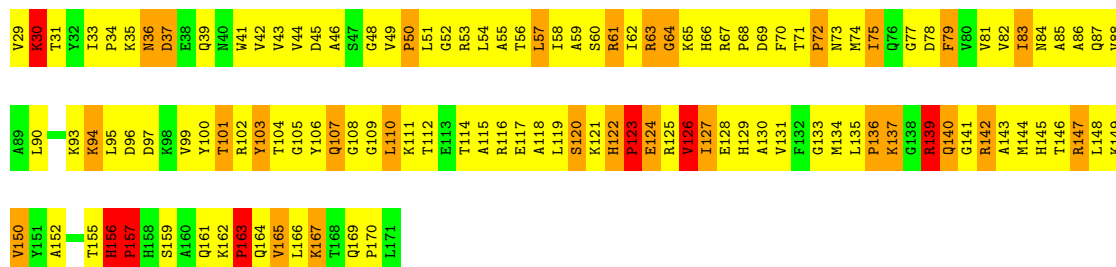
Chain FK:





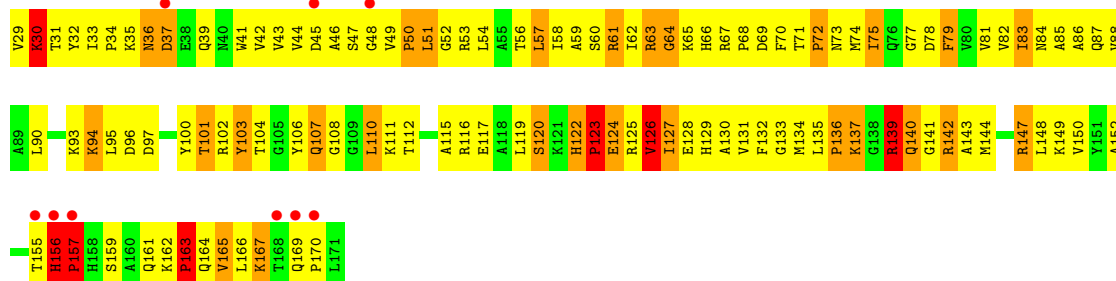
- Molecule 31: 50S ribosomal protein L13

Chain HK:



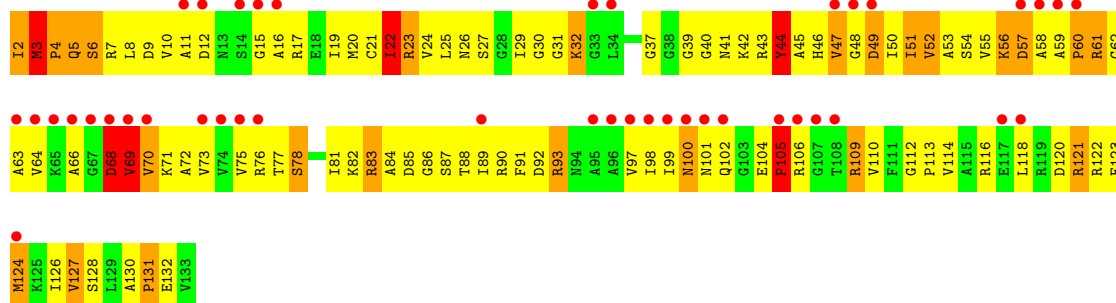
- Molecule 31: 50S ribosomal protein L13

Chain JK:



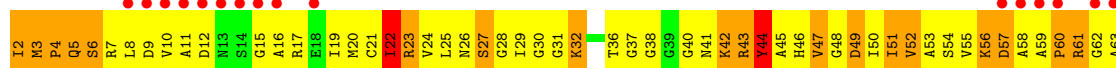
- Molecule 32: 50S ribosomal protein L14

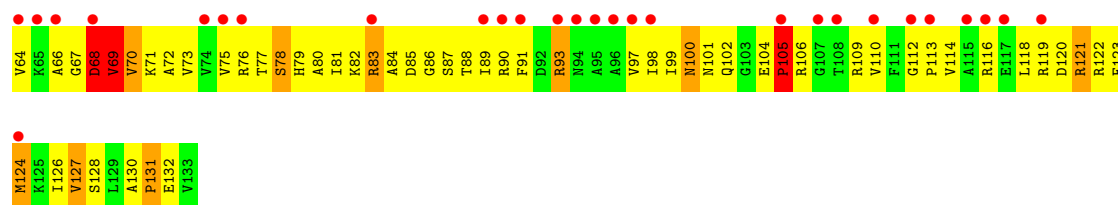
Chain BL:



- Molecule 32: 50S ribosomal protein L14

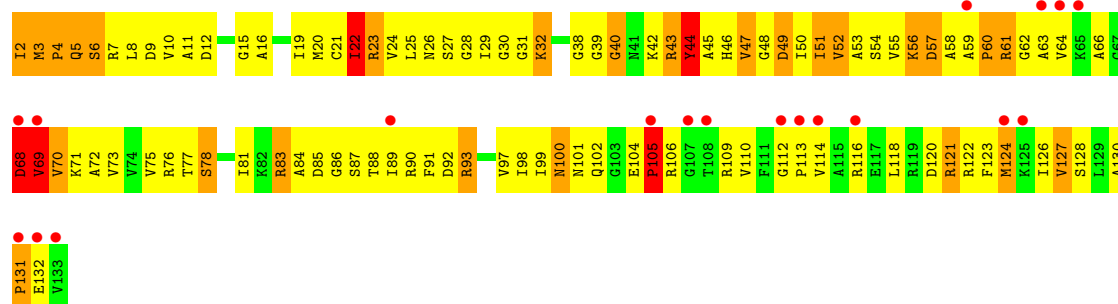
Chain DL:





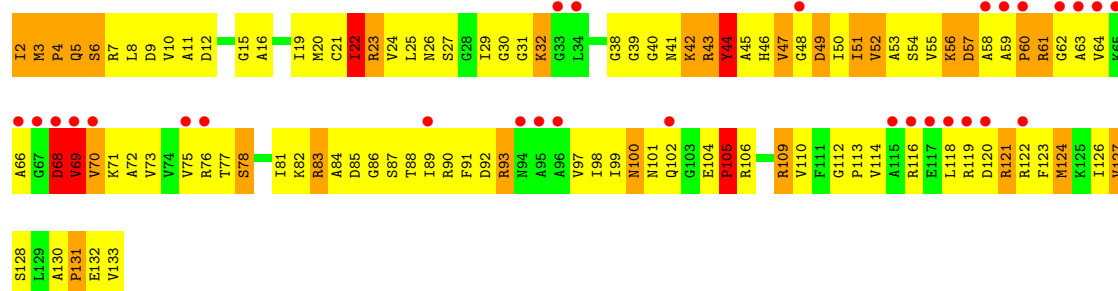
• Molecule 32: 50S ribosomal protein L14

Chain FL:



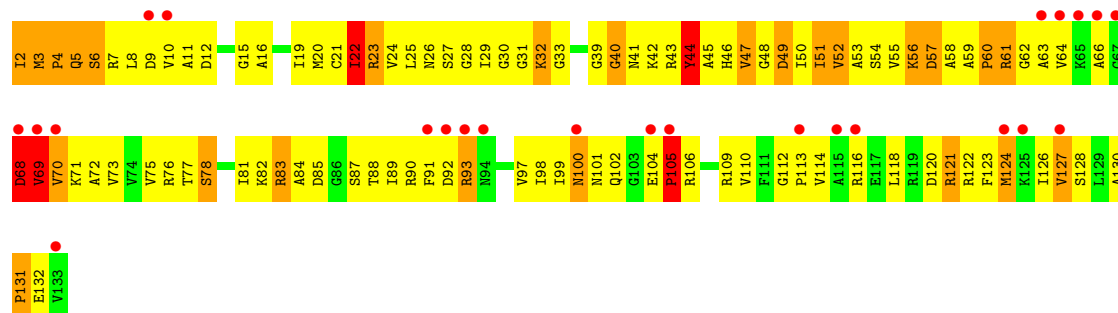
• Molecule 32: 50S ribosomal protein L14

Chain HL:



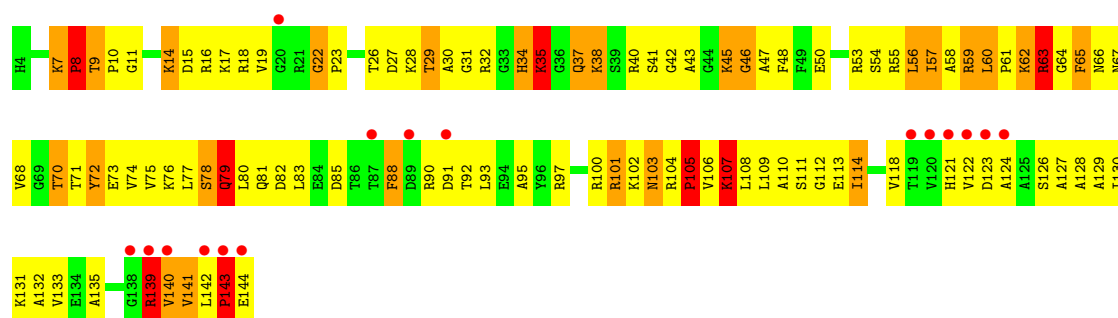
• Molecule 32: 50S ribosomal protein L14

Chain JL:



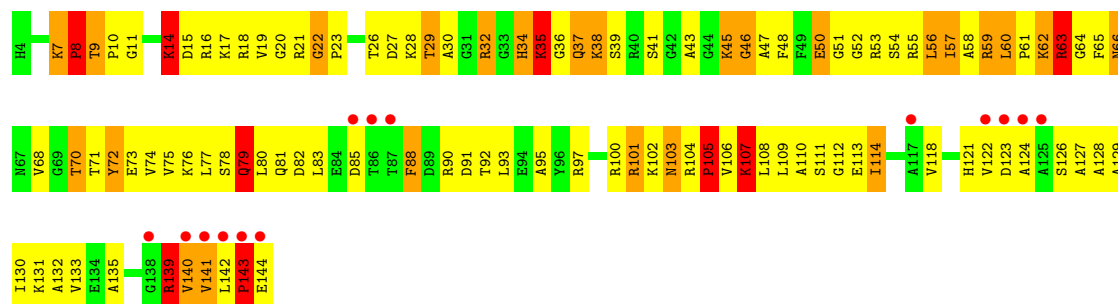
• Molecule 33: 50S ribosomal protein L15

Chain BM:



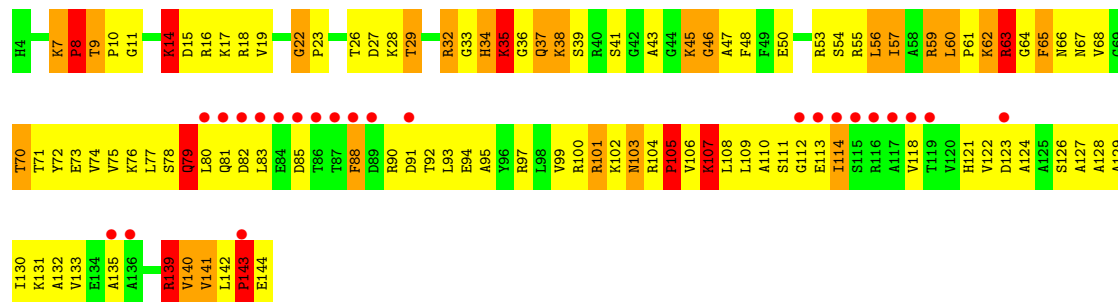
- Molecule 33: 50S ribosomal protein L15

Chain DM:



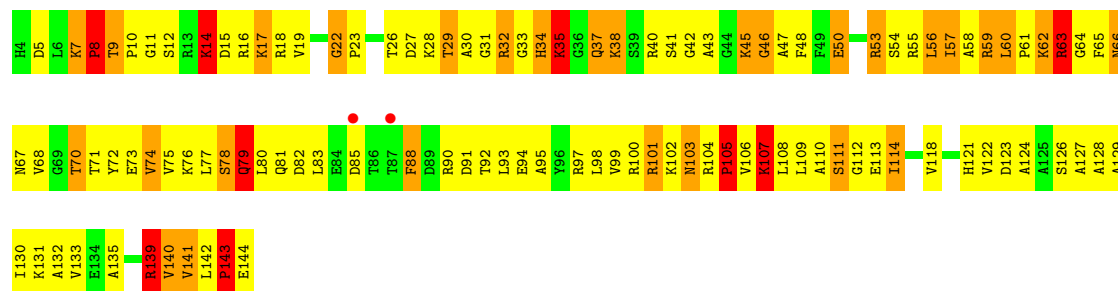
- Molecule 33: 50S ribosomal protein L15

Chain FM:



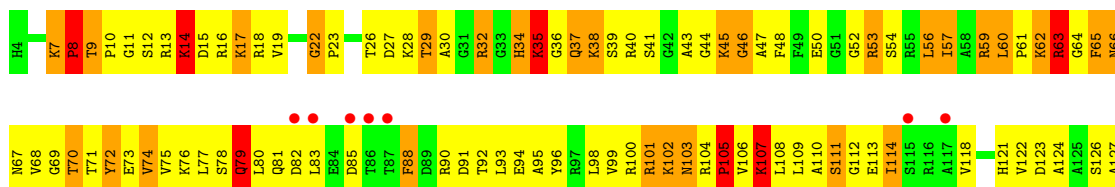
- Molecule 33: 50S ribosomal protein L15

Chain HM:



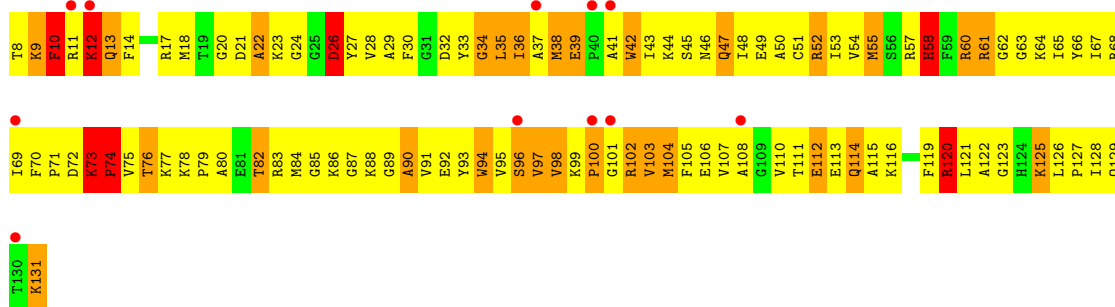
- Molecule 33: 50S ribosomal protein L15

Chain JM:



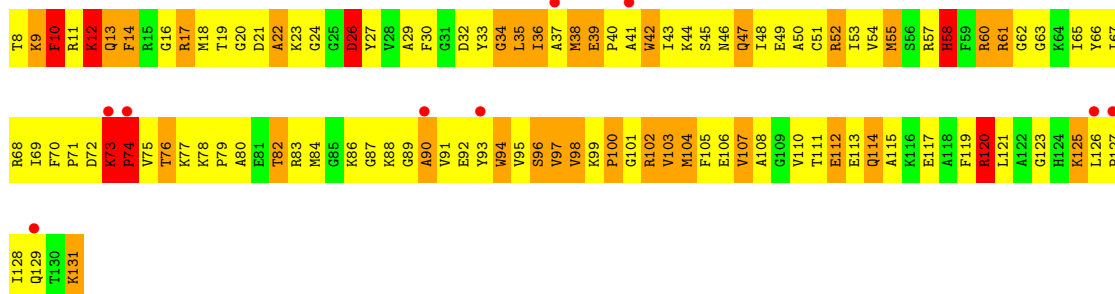
• Molecule 34: 50S ribosomal protein L16

Chain BN:



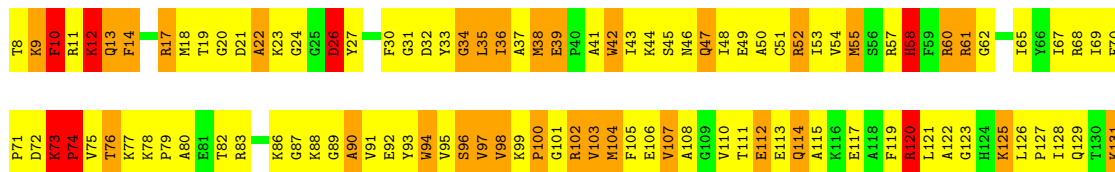
• Molecule 34: 50S ribosomal protein L16

Chain DN:



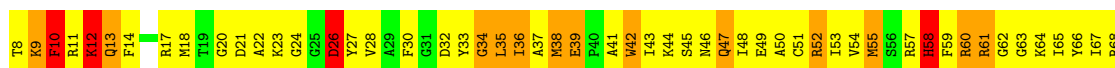
• Molecule 34: 50S ribosomal protein L16

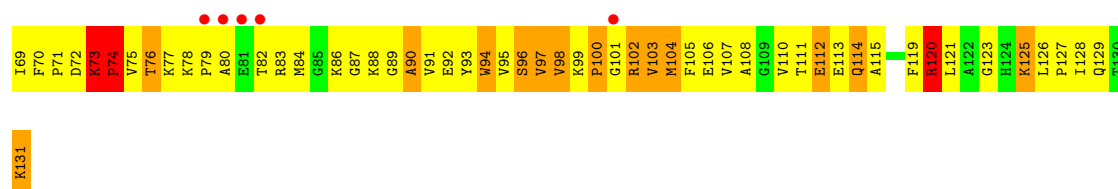
Chain FN:



• Molecule 34: 50S ribosomal protein L16

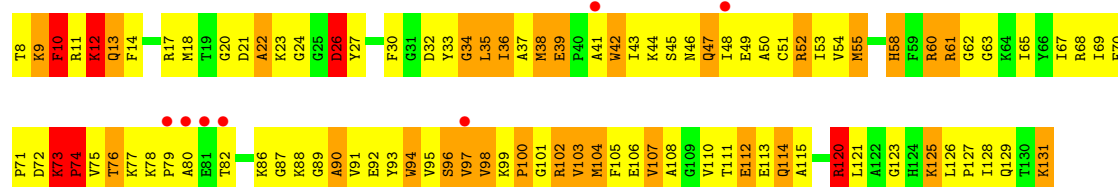
Chain HN:





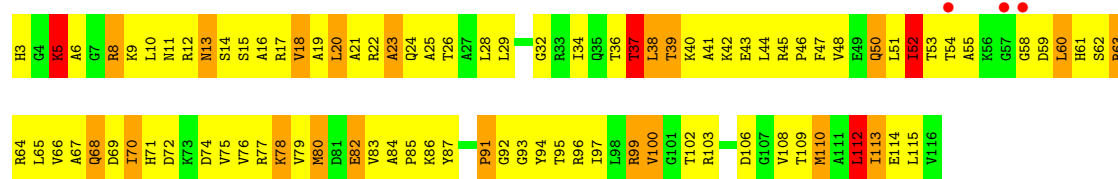
- Molecule 34: 50S ribosomal protein L16

Chain JN:



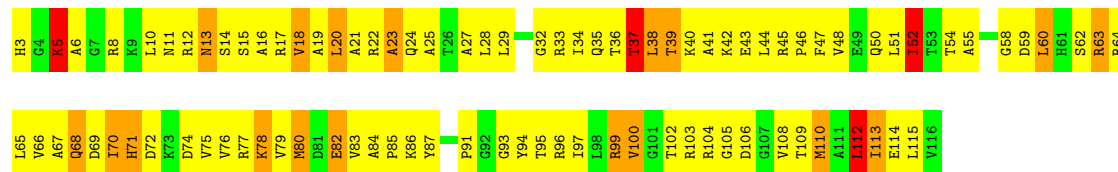
- Molecule 35: 50S ribosomal protein L17

Chain BO:



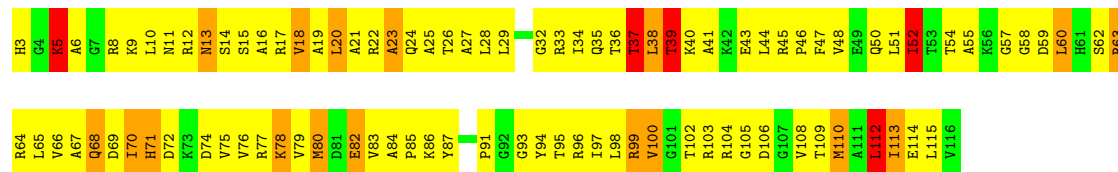
- Molecule 35: 50S ribosomal protein L17

Chain DO:



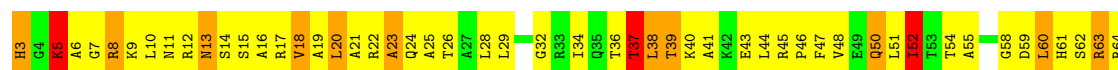
- Molecule 35: 50S ribosomal protein L17

Chain FO:



- Molecule 35: 50S ribosomal protein L17

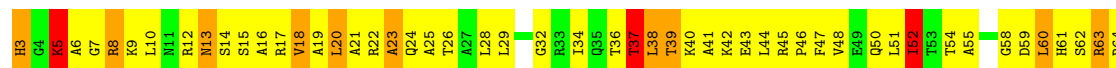
Chain HO:





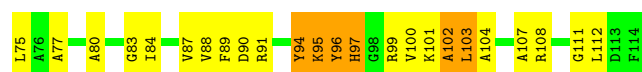
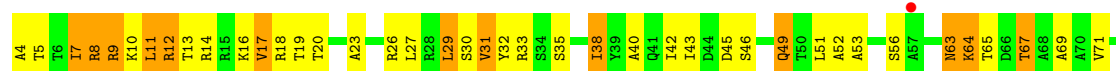
- Molecule 35: 50S ribosomal protein L17

Chain JO:



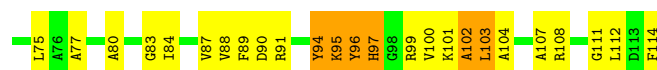
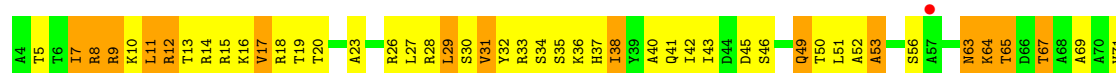
- Molecule 36: 50S ribosomal protein L18

Chain BP:



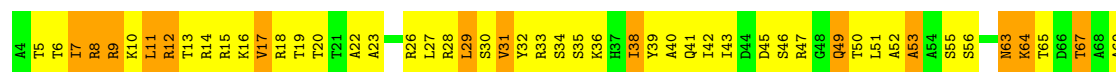
- Molecule 36: 50S ribosomal protein L18

Chain DP:



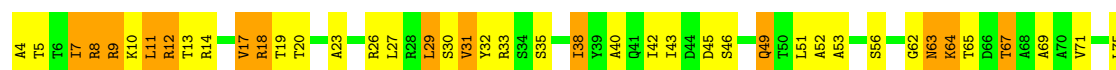
- Molecule 36: 50S ribosomal protein L18

Chain FP:



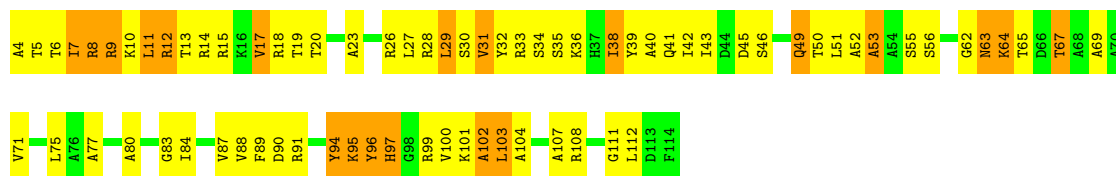
- Molecule 36: 50S ribosomal protein L18

Chain HP:



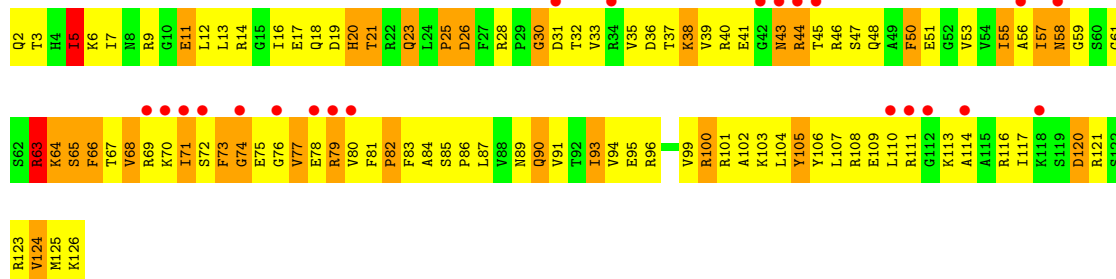
- Molecule 36: 50S ribosomal protein L18

Chain JP:



• Molecule 37: 50S ribosomal protein L19

Chain BQ:



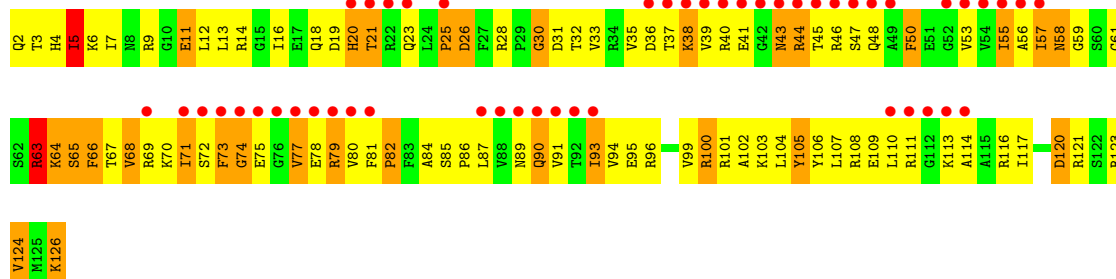
• Molecule 37: 50S ribosomal protein L19

Chain DQ:



• Molecule 37: 50S ribosomal protein L19

Chain FQ:



• Molecule 37: 50S ribosomal protein L19

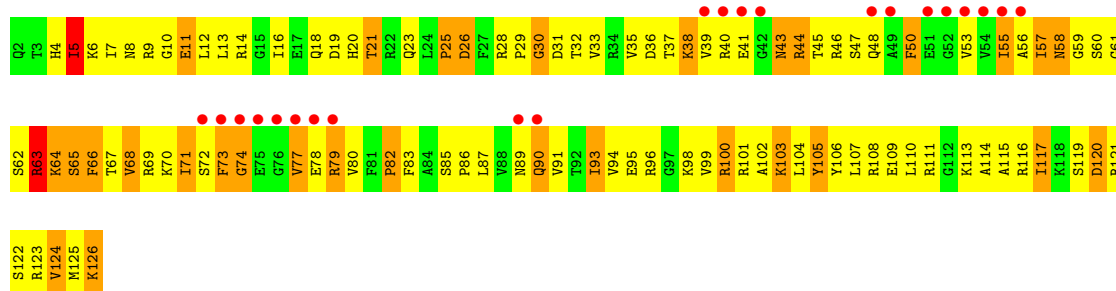
Chain HQ:





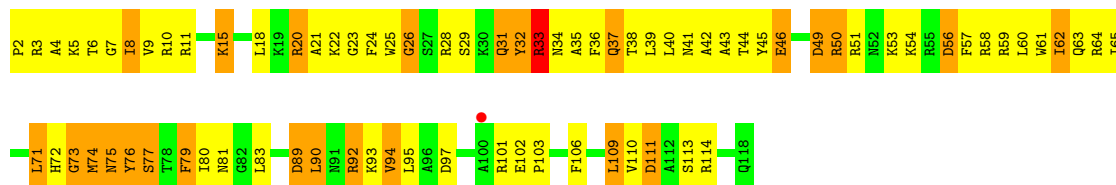
- Molecule 37: 50S ribosomal protein L19

Chain JQ:



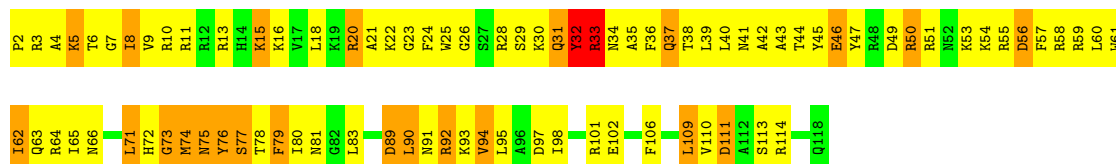
- Molecule 38: 50S ribosomal protein L20

Chain BR:



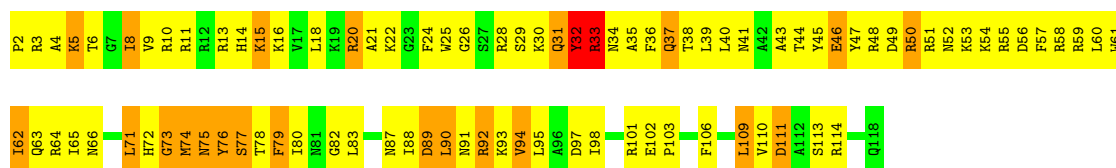
- Molecule 38: 50S ribosomal protein L20

Chain DR:



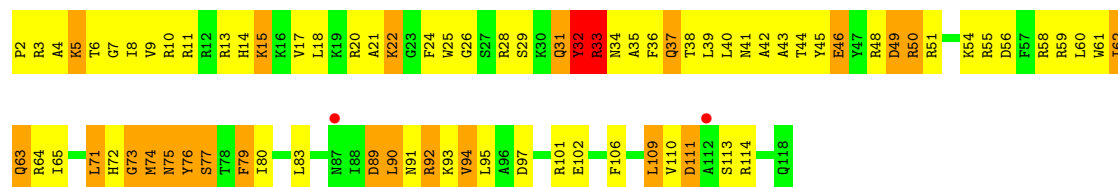
- Molecule 38: 50S ribosomal protein L20

Chain FR:



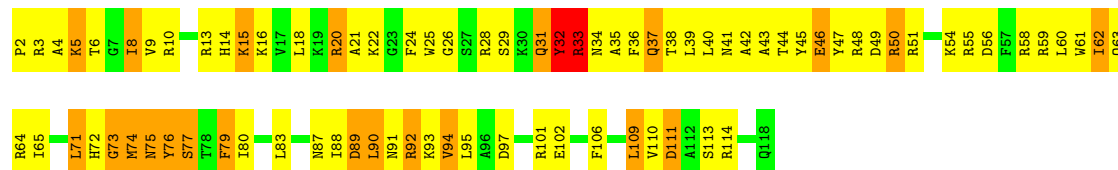
- Molecule 38: 50S ribosomal protein L20

Chain HR: 



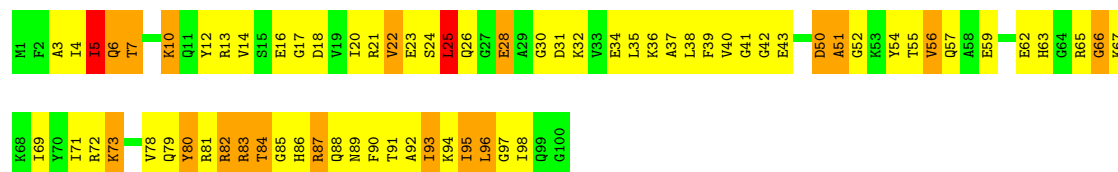
- Molecule 38: 50S ribosomal protein L20

Chain JR: 



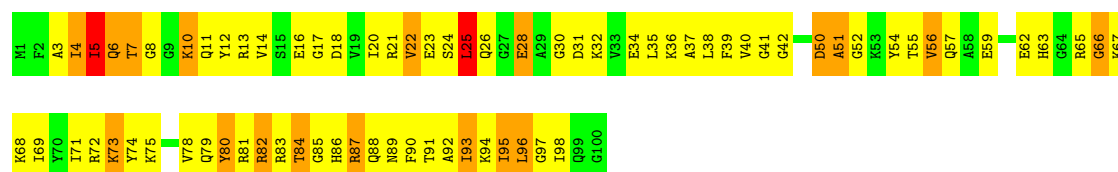
- Molecule 39: 50S ribosomal protein L21

Chain BS: 



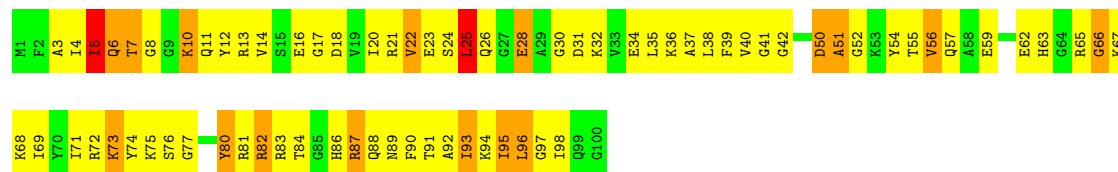
- Molecule 39: 50S ribosomal protein L21

Chain DS: 



- Molecule 39: 50S ribosomal protein L21

Chain FS: 



- Molecule 39: 50S ribosomal protein L21

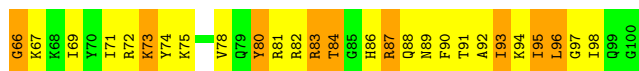
Chain HS: 





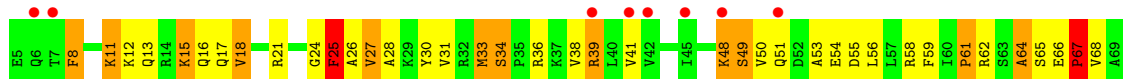
- Molecule 39: 50S ribosomal protein L21

Chain JS:



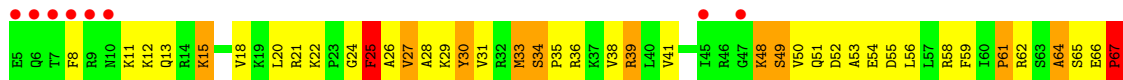
- Molecule 40: 50S ribosomal protein L22

Chain BT:



- Molecule 40: 50S ribosomal protein L22

Chain DT:



- Molecule 40: 50S ribosomal protein L22

Chain FT:





Chain FU: 



- Molecule 41: 50S ribosomal protein L23

Chain HU: 



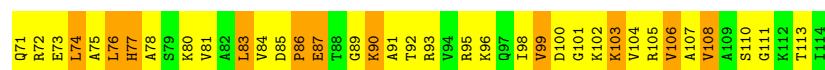
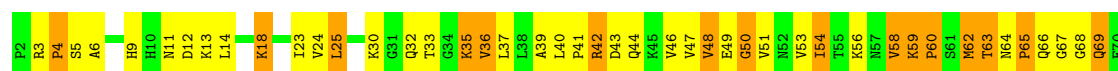
- Molecule 41: 50S ribosomal protein L23

Chain JU: 



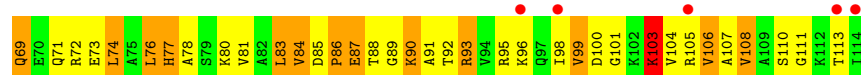
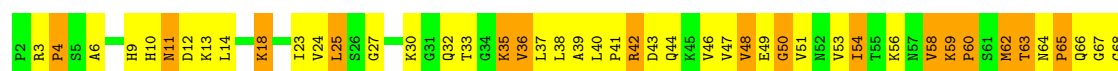
- Molecule 42: 50S ribosomal protein L24

Chain BV: 



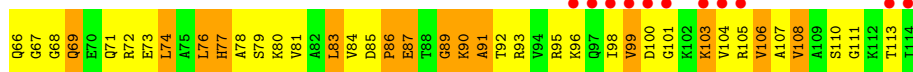
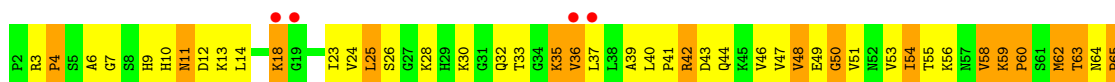
- Molecule 42: 50S ribosomal protein L24

Chain DV: 

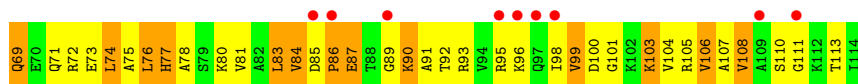
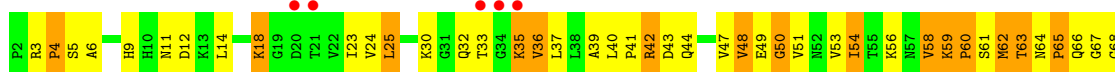


- Molecule 42: 50S ribosomal protein L24

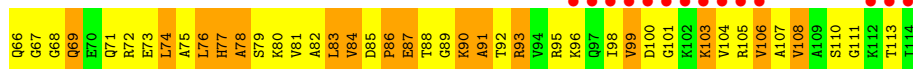
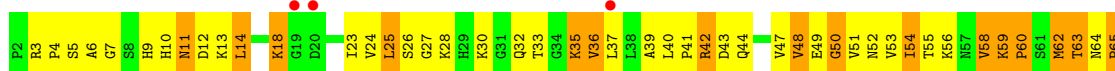
Chain FV: 



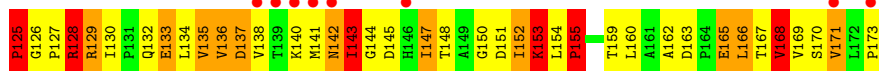
• Molecule 42: 50S ribosomal protein L24



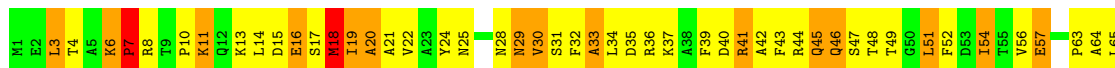
• Molecule 42: 50S ribosomal protein L24



• Molecule 43: general stress protein Ctc



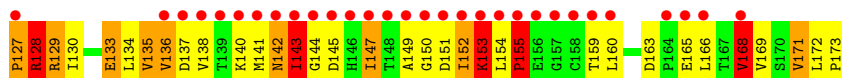
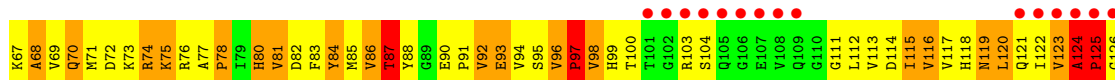
• Molecule 43: general stress protein Ctc





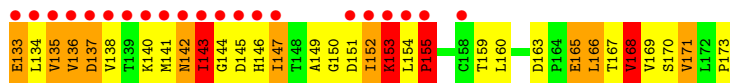
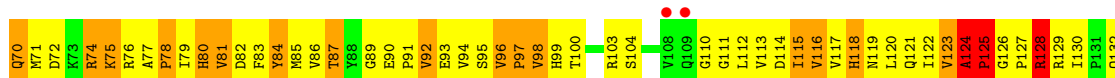
- Molecule 43: general stress protein Ctc

Chain FW:



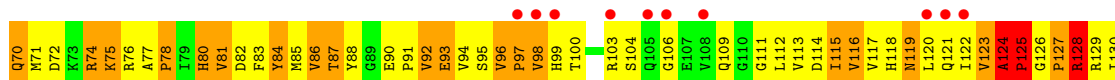
- Molecule 43: general stress protein Ctc

Chain HW:



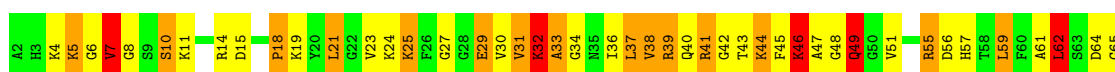
- Molecule 43: general stress protein Ctc

Chain JW:

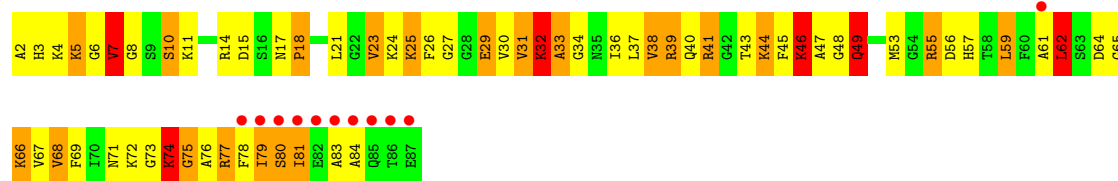


- Molecule 44: 50S ribosomal protein L27

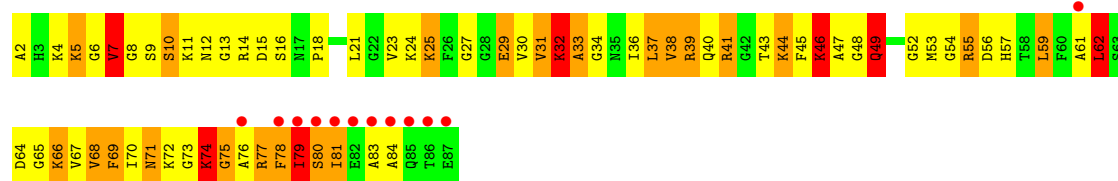
Chain BX:



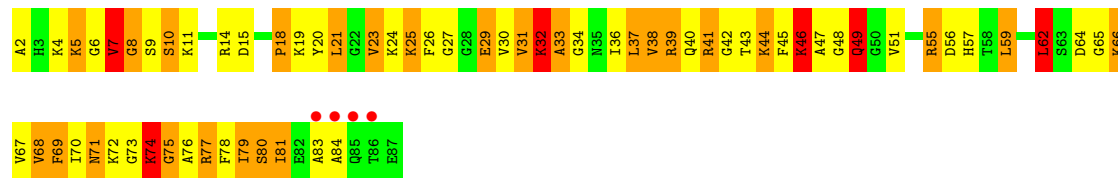
- Molecule 44: 50S ribosomal protein L27

Chain DX: 

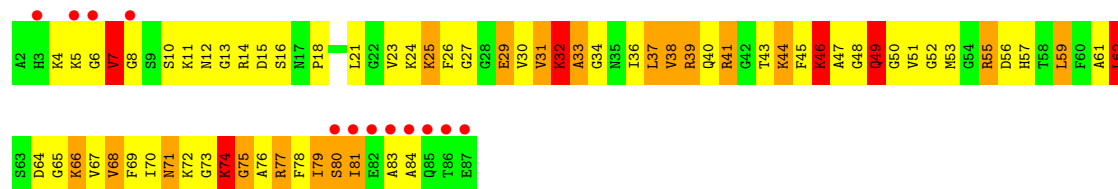
- Molecule 44: 50S ribosomal protein L27

Chain FX: 

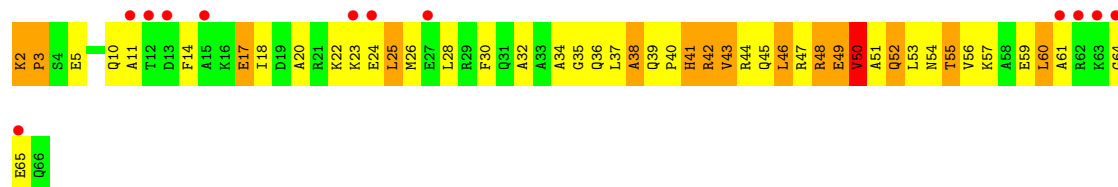
- Molecule 44: 50S ribosomal protein L27

Chain HX: 

- Molecule 44: 50S ribosomal protein L27

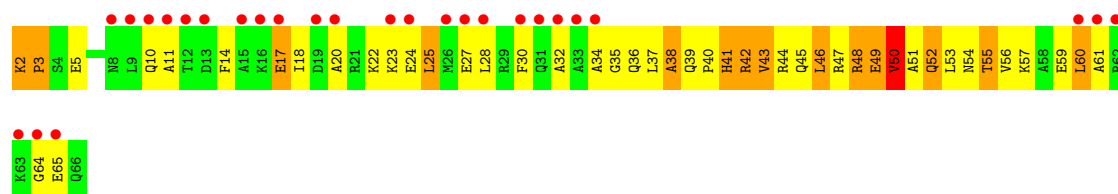
Chain JX: 

- Molecule 45: 50S ribosomal protein L29

Chain BY: 

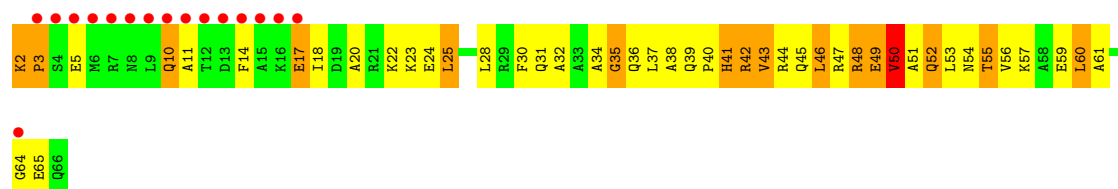
- Molecule 45: 50S ribosomal protein L29

Chain DY: 



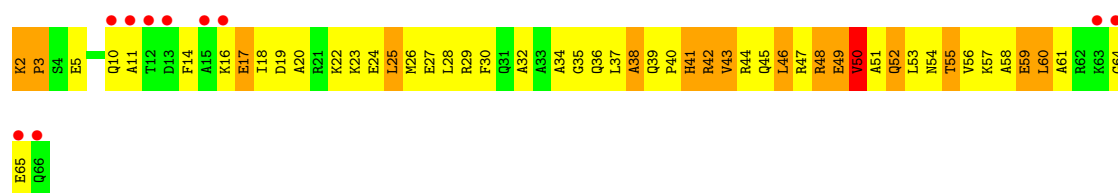
- Molecule 45: 50S ribosomal protein L29

Chain FY:



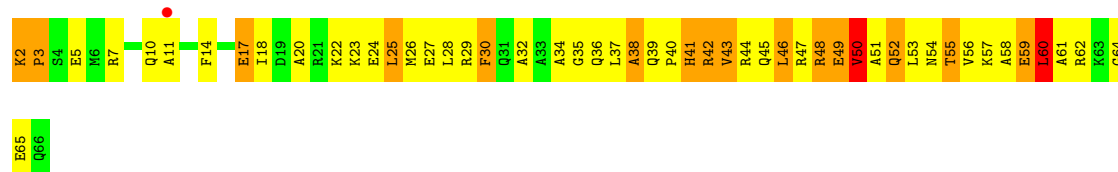
- Molecule 45: 50S ribosomal protein L29

Chain HY:



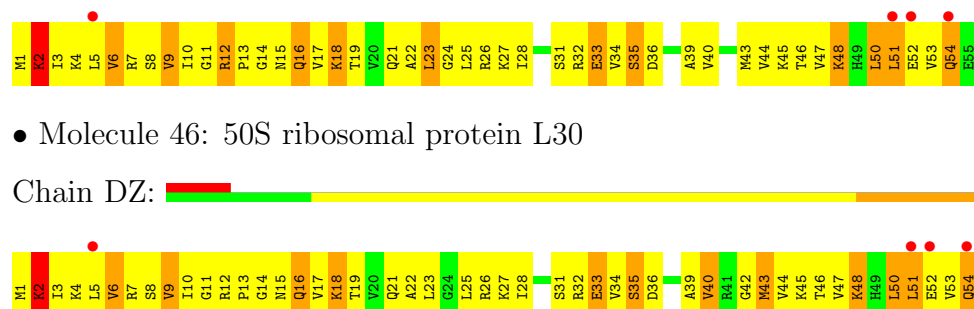
- Molecule 45: 50S ribosomal protein L29

Chain JY:



- Molecule 46: 50S ribosomal protein L30

Chain BZ:



- Molecule 46: 50S ribosomal protein L30

Chain FZ:



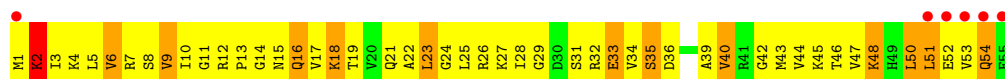
- Molecule 46: 50S ribosomal protein L30

Chain HZ:



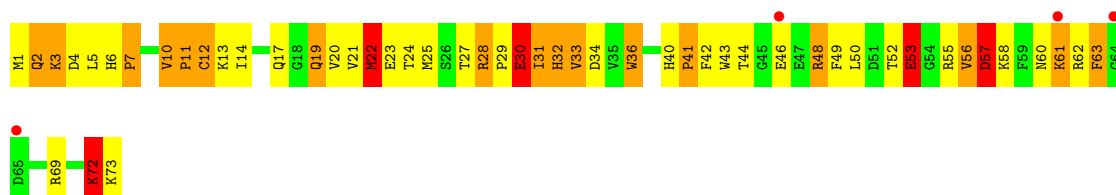
- Molecule 46: 50S ribosomal protein L30

Chain JZ:



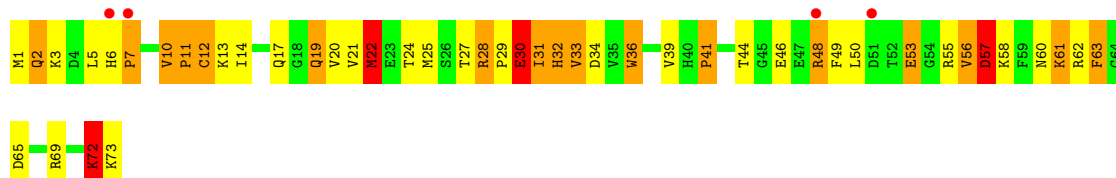
- Molecule 47: 50S ribosomal protein L31

Chain B1:



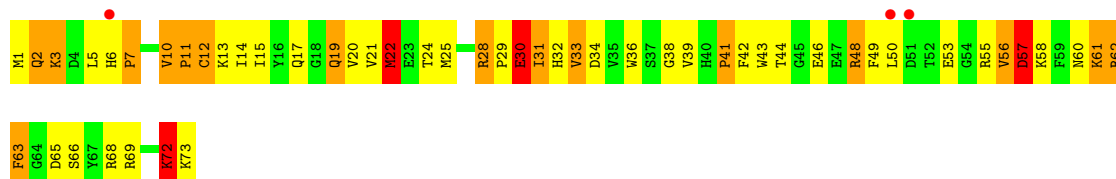
- Molecule 47: 50S ribosomal protein L31

Chain D1:



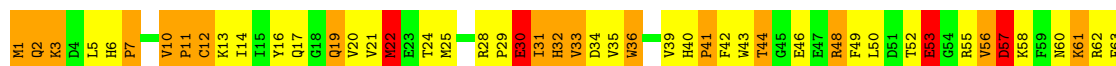
- Molecule 47: 50S ribosomal protein L31

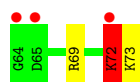
Chain F1:



- Molecule 47: 50S ribosomal protein L31

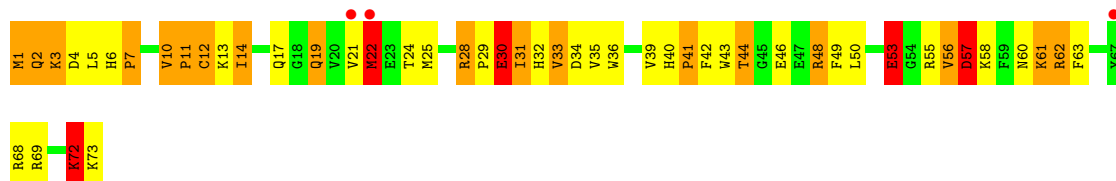
Chain H1:





- Molecule 47: 50S ribosomal protein L31

Chain J1:



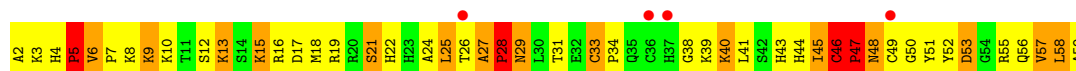
- Molecule 48: 50S ribosomal protein L32

Chain B2:



- Molecule 48: 50S ribosomal protein L32

Chain D2:



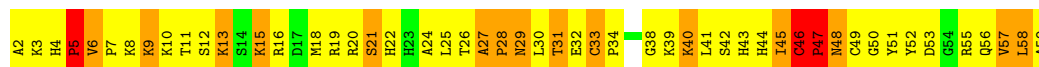
- Molecule 48: 50S ribosomal protein L32

Chain F2:



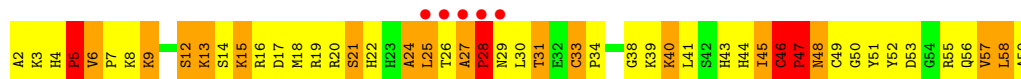
- Molecule 48: 50S ribosomal protein L32

Chain H2:



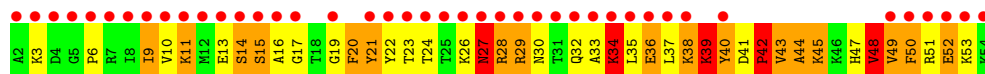
- Molecule 48: 50S ribosomal protein L32

Chain J2:

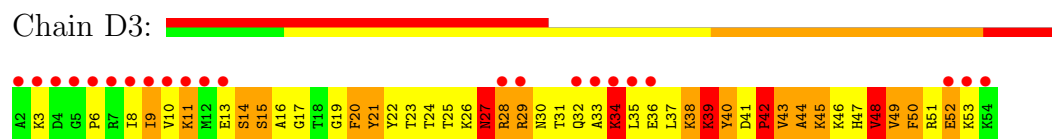


- Molecule 49: 50S ribosomal protein L33

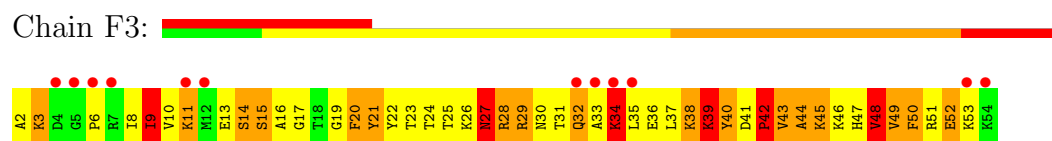
Chain B3:



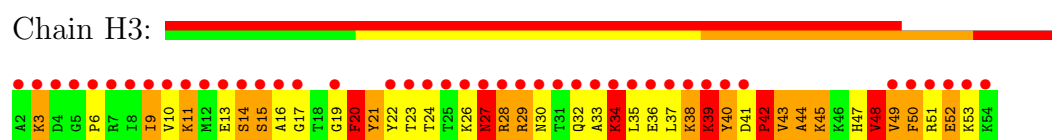
- Molecule 49: 50S ribosomal protein L33



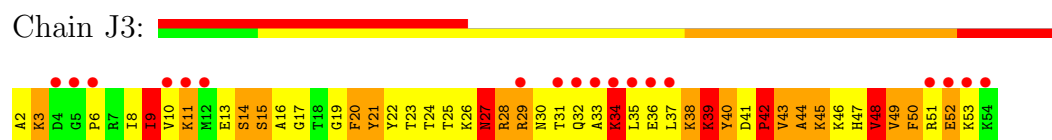
- Molecule 49: 50S ribosomal protein L33



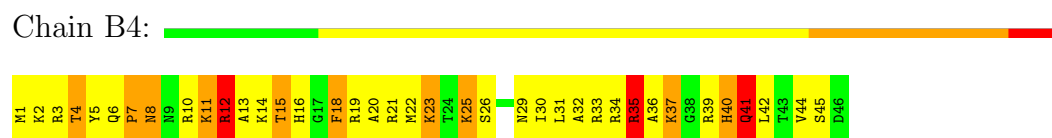
- Molecule 49: 50S ribosomal protein L33



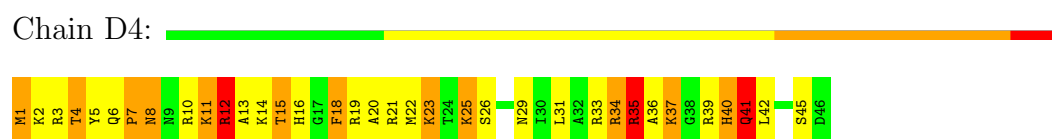
- Molecule 49: 50S ribosomal protein L33



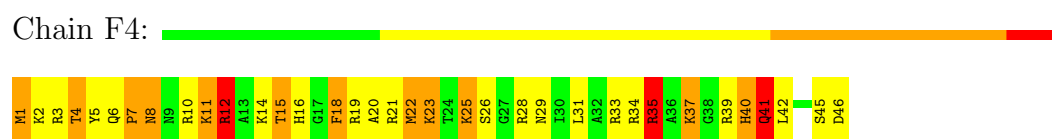
- Molecule 50: 50S ribosomal protein L34



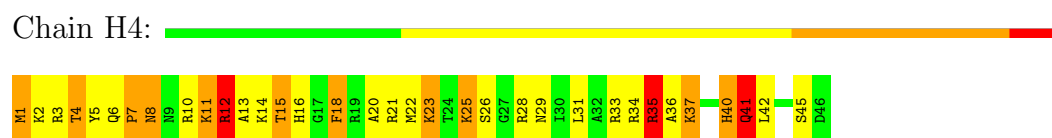
- Molecule 50: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L34



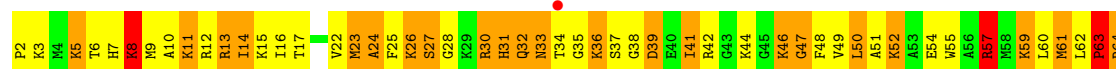
- Molecule 50: 50S ribosomal protein L34

Chain J4:



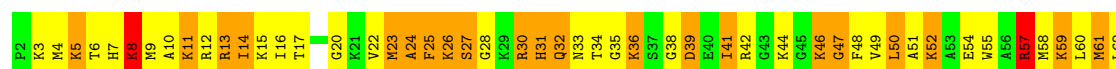
- Molecule 51: 50S ribosomal protein L35

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:



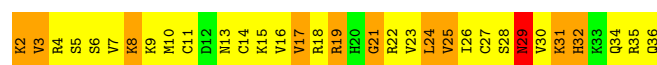
- Molecule 51: 50S ribosomal protein L35

Chain J5:



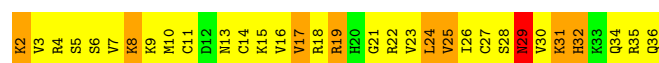
- Molecule 52: 50S ribosomal protein L36

Chain B6:



- Molecule 52: 50S ribosomal protein L36

Chain D6:



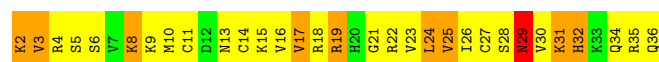
- Molecule 52: 50S ribosomal protein L36

Chain F6:



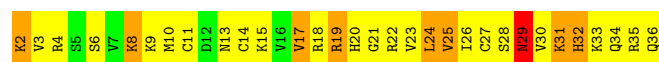
- Molecule 52: 50S ribosomal protein L36

Chain H6:



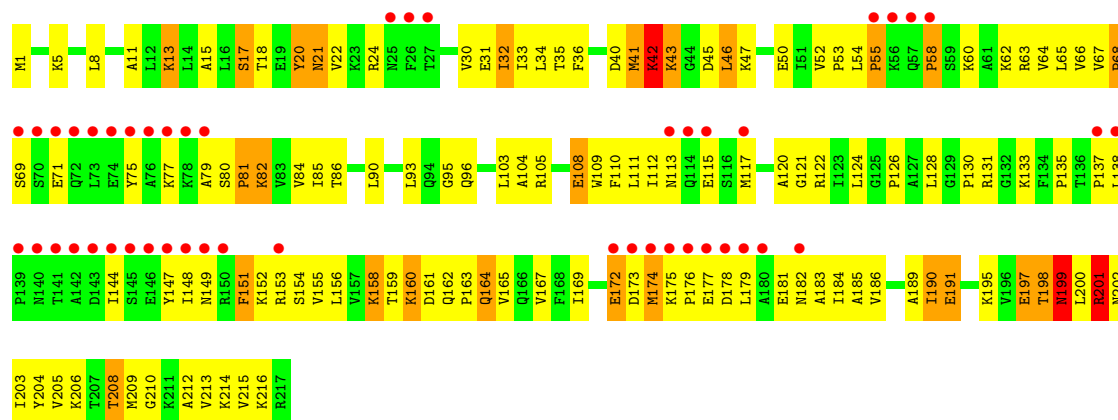
- Molecule 52: 50S ribosomal protein L36

Chain J6:



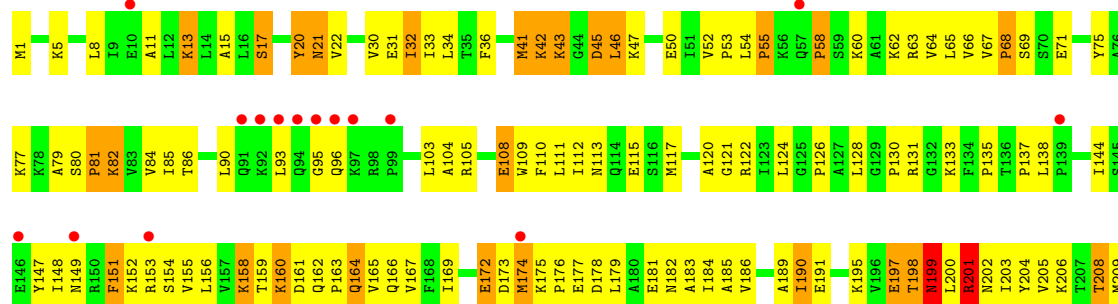
- Molecule 53: 50S ribosomal protein L1P

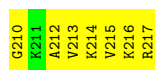
Chain B7:



- Molecule 53: 50S ribosomal protein L1P

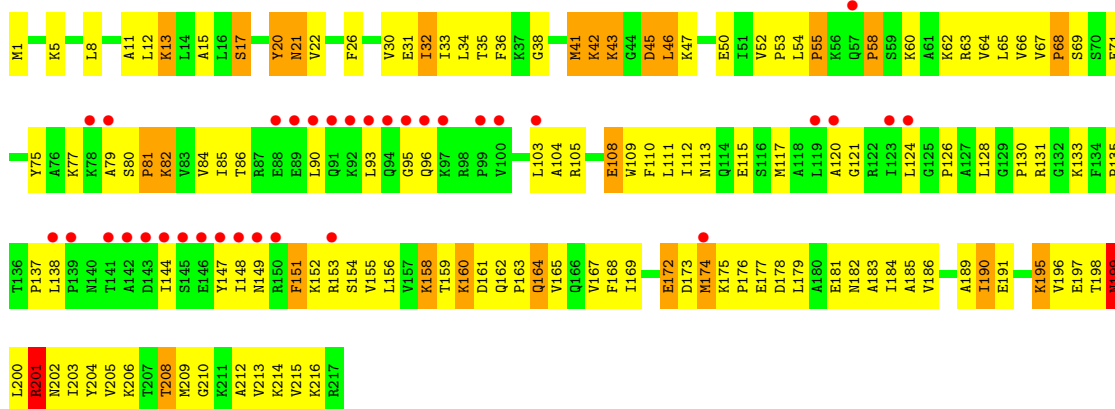
Chain D7:





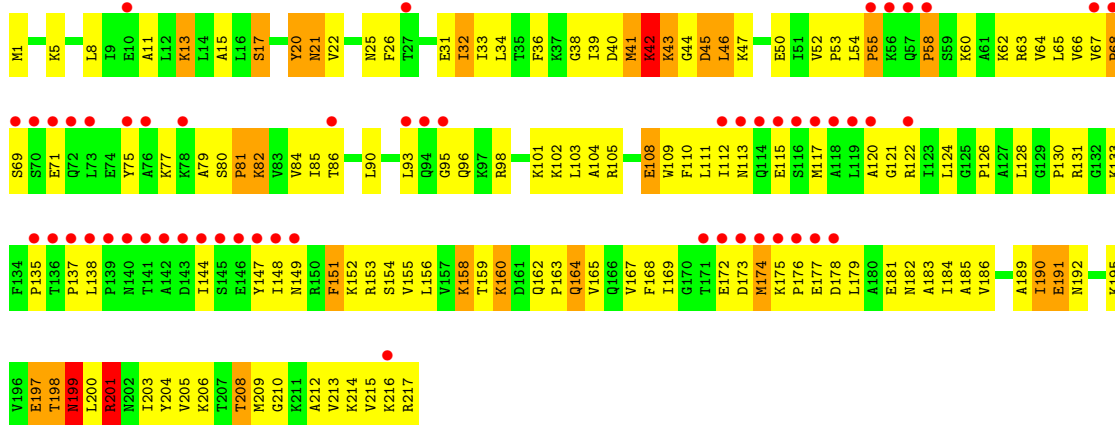
• Molecule 53: 50S ribosomal protein L1P

Chain F7:



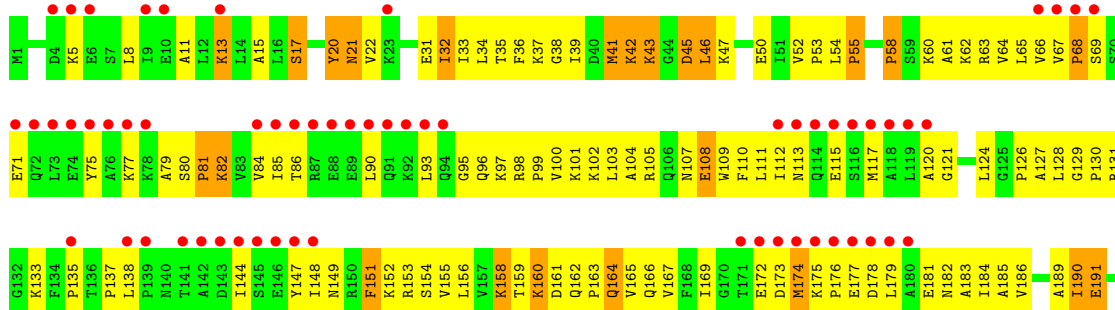
• Molecule 53: 50S ribosomal protein L1P

Chain H7:



• Molecule 53: 50S ribosomal protein L1P

Chain J7:



K195	V196	E197	T198	R199	L200	R201	N202	I203	Y204	V205	K206	T207	T208	M209	G210	R211	A212	V213	K214	V215	K216	R217
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



## 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 0.411 , 0.420	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
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> )	0.12 , 661.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Outliers	(Not available)	Xtriage
$F_o, F_c$ correlation	0.89	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)*

## 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 Close contacts ⓘ

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

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	IH	1116	0	1168	368	0
9	AI	1011	0	1036	313	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	CQ	857	0	916	300	0
17	EQ	857	0	920	289	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	HE	1540	0	1597	338	0
25	JE	1540	0	1600	367	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	BN	986	0	1010	489	0
34	DN	986	0	1006	542	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	FV	852	0	908	201	0
42	HV	852	0	908	132	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	J4	384	0	401	167	0
51	B5	496	0	547	162	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 63.

The worst 5 of 75816 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	1	14
2	CB	232/234 (99%)	128 (55%)	75 (32%)	29 (12%)	1	14
2	EB	232/234 (99%)	127 (55%)	76 (33%)	29 (12%)	1	14
2	GB	232/234 (99%)	129 (56%)	74 (32%)	29 (12%)	1	14
2	IB	232/234 (99%)	128 (55%)	75 (32%)	29 (12%)	1	14
3	AC	204/206 (99%)	125 (61%)	60 (29%)	19 (9%)	1	24
3	CC	204/206 (99%)	124 (61%)	61 (30%)	19 (9%)	1	24
3	EC	204/206 (99%)	125 (61%)	60 (29%)	19 (9%)	1	24
3	GC	204/206 (99%)	124 (61%)	61 (30%)	19 (9%)	1	24
3	IC	204/206 (99%)	124 (61%)	61 (30%)	19 (9%)	1	24
4	AD	206/208 (99%)	130 (63%)	56 (27%)	20 (10%)	1	22
4	CD	206/208 (99%)	129 (63%)	57 (28%)	20 (10%)	1	22
4	ED	206/208 (99%)	130 (63%)	56 (27%)	20 (10%)	1	22
4	GD	206/208 (99%)	128 (62%)	58 (28%)	20 (10%)	1	22
4	ID	206/208 (99%)	129 (63%)	57 (28%)	20 (10%)	1	22
5	AE	148/150 (99%)	93 (63%)	43 (29%)	12 (8%)	1	27
5	CE	148/150 (99%)	91 (62%)	45 (30%)	12 (8%)	1	27
5	EE	148/150 (99%)	92 (62%)	44 (30%)	12 (8%)	1	27
5	GE	148/150 (99%)	92 (62%)	44 (30%)	12 (8%)	1	27
5	IE	148/150 (99%)	92 (62%)	44 (30%)	12 (8%)	1	27
6	AF	99/101 (98%)	67 (68%)	25 (25%)	7 (7%)	2	32
6	CF	99/101 (98%)	67 (68%)	25 (25%)	7 (7%)	2	32
6	EF	99/101 (98%)	67 (68%)	25 (25%)	7 (7%)	2	32
6	GF	99/101 (98%)	67 (68%)	25 (25%)	7 (7%)	2	32
6	IF	99/101 (98%)	67 (68%)	25 (25%)	7 (7%)	2	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	153/155 (99%)	94 (61%)	47 (31%)	12 (8%)	1	29
7	CG	153/155 (99%)	94 (61%)	47 (31%)	12 (8%)	1	29
7	EG	153/155 (99%)	93 (61%)	48 (31%)	12 (8%)	1	29
7	GG	153/155 (99%)	94 (61%)	47 (31%)	12 (8%)	1	29
7	IG	153/155 (99%)	94 (61%)	47 (31%)	12 (8%)	1	29
8	AH	136/138 (99%)	83 (61%)	38 (28%)	15 (11%)	1	17
8	CH	136/138 (99%)	83 (61%)	37 (27%)	16 (12%)	1	15
8	EH	136/138 (99%)	83 (61%)	37 (27%)	16 (12%)	1	15
8	GH	136/138 (99%)	83 (61%)	37 (27%)	16 (12%)	1	15
8	IH	136/138 (99%)	83 (61%)	37 (27%)	16 (12%)	1	15
9	AI	125/127 (98%)	68 (54%)	43 (34%)	14 (11%)	1	16
9	CI	125/127 (98%)	68 (54%)	43 (34%)	14 (11%)	1	16
9	EI	125/127 (98%)	68 (54%)	43 (34%)	14 (11%)	1	16
9	GI	125/127 (98%)	68 (54%)	43 (34%)	14 (11%)	1	16
9	II	125/127 (98%)	68 (54%)	43 (34%)	14 (11%)	1	16
10	AJ	96/98 (98%)	52 (54%)	22 (23%)	22 (23%)	0	3
10	CJ	96/98 (98%)	53 (55%)	21 (22%)	22 (23%)	0	3
10	EJ	96/98 (98%)	52 (54%)	22 (23%)	22 (23%)	0	3
10	GJ	96/98 (98%)	52 (54%)	22 (23%)	22 (23%)	0	3
10	IJ	96/98 (98%)	52 (54%)	22 (23%)	22 (23%)	0	3
11	AK	117/119 (98%)	72 (62%)	32 (27%)	13 (11%)	1	17
11	CK	117/119 (98%)	74 (63%)	30 (26%)	13 (11%)	1	17
11	EK	117/119 (98%)	73 (62%)	31 (26%)	13 (11%)	1	17
11	GK	117/119 (98%)	73 (62%)	31 (26%)	13 (11%)	1	17
11	IK	117/119 (98%)	73 (62%)	31 (26%)	13 (11%)	1	17
12	AL	118/124 (95%)	77 (65%)	34 (29%)	7 (6%)	2	38
12	CL	116/124 (94%)	76 (66%)	32 (28%)	8 (7%)	2	33
12	EL	118/124 (95%)	76 (64%)	34 (29%)	8 (7%)	2	33
12	GL	116/124 (94%)	77 (66%)	31 (27%)	8 (7%)	2	33
12	IL	118/124 (95%)	78 (66%)	33 (28%)	7 (6%)	2	38
13	AM	121/125 (97%)	77 (64%)	32 (26%)	12 (10%)	1	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	CM	119/125 (95%)	77 (65%)	32 (27%)	10 (8%)	1	26
13	EM	119/125 (95%)	77 (65%)	32 (27%)	10 (8%)	1	26
13	GM	121/125 (97%)	77 (64%)	32 (26%)	12 (10%)	1	21
13	IM	119/125 (95%)	78 (66%)	30 (25%)	11 (9%)	1	24
14	AN	58/60 (97%)	22 (38%)	27 (47%)	9 (16%)	0	8
14	CN	58/60 (97%)	23 (40%)	26 (45%)	9 (16%)	0	8
14	EN	58/60 (97%)	22 (38%)	27 (47%)	9 (16%)	0	8
14	GN	58/60 (97%)	22 (38%)	27 (47%)	9 (16%)	0	8
14	IN	58/60 (97%)	22 (38%)	27 (47%)	9 (16%)	0	8
15	AO	86/88 (98%)	59 (69%)	19 (22%)	8 (9%)	1	24
15	CO	86/88 (98%)	59 (69%)	20 (23%)	7 (8%)	1	27
15	EO	86/88 (98%)	59 (69%)	19 (22%)	8 (9%)	1	24
15	GO	86/88 (98%)	59 (69%)	20 (23%)	7 (8%)	1	27
15	IO	86/88 (98%)	59 (69%)	19 (22%)	8 (9%)	1	24
16	AP	81/83 (98%)	48 (59%)	29 (36%)	4 (5%)	3	43
16	CP	81/83 (98%)	48 (59%)	29 (36%)	4 (5%)	3	43
16	EP	81/83 (98%)	48 (59%)	29 (36%)	4 (5%)	3	43
16	GP	81/83 (98%)	48 (59%)	29 (36%)	4 (5%)	3	43
16	IP	81/83 (98%)	49 (60%)	28 (35%)	4 (5%)	3	43
17	AQ	102/104 (98%)	53 (52%)	34 (33%)	15 (15%)	0	10
17	CQ	102/104 (98%)	53 (52%)	34 (33%)	15 (15%)	0	10
17	EQ	102/104 (98%)	53 (52%)	34 (33%)	15 (15%)	0	10
17	GQ	102/104 (98%)	53 (52%)	34 (33%)	15 (15%)	0	10
17	IQ	102/104 (98%)	53 (52%)	34 (33%)	15 (15%)	0	10
18	AR	71/73 (97%)	43 (61%)	20 (28%)	8 (11%)	1	16
18	CR	71/73 (97%)	43 (61%)	20 (28%)	8 (11%)	1	16
18	ER	71/73 (97%)	43 (61%)	20 (28%)	8 (11%)	1	16
18	GR	71/73 (97%)	43 (61%)	20 (28%)	8 (11%)	1	16
18	IR	71/73 (97%)	43 (61%)	20 (28%)	8 (11%)	1	16
19	AS	78/80 (98%)	48 (62%)	22 (28%)	8 (10%)	1	19
19	CS	78/80 (98%)	49 (63%)	21 (27%)	8 (10%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	ES	78/80 (98%)	48 (62%)	22 (28%)	8 (10%)	1	19
19	GS	78/80 (98%)	49 (63%)	20 (26%)	9 (12%)	1	15
19	IS	78/80 (98%)	48 (62%)	21 (27%)	9 (12%)	1	15
20	AT	97/99 (98%)	65 (67%)	20 (21%)	12 (12%)	1	14
20	CT	97/99 (98%)	64 (66%)	21 (22%)	12 (12%)	1	14
20	ET	97/99 (98%)	64 (66%)	21 (22%)	12 (12%)	1	14
20	GT	97/99 (98%)	64 (66%)	21 (22%)	12 (12%)	1	14
20	IT	97/99 (98%)	64 (66%)	21 (22%)	12 (12%)	1	14
21	Aa	88/90 (98%)	77 (88%)	10 (11%)	1 (1%)	21	78
21	Ca	88/90 (98%)	77 (88%)	10 (11%)	1 (1%)	21	78
21	Ea	88/90 (98%)	77 (88%)	10 (11%)	1 (1%)	21	78
21	Ga	88/90 (98%)	77 (88%)	10 (11%)	1 (1%)	21	78
21	Ia	88/90 (98%)	77 (88%)	10 (11%)	1 (1%)	21	78
24	BD	268/270 (99%)	96 (36%)	93 (35%)	79 (30%)	0	1
24	DD	268/270 (99%)	98 (37%)	92 (34%)	78 (29%)	0	1
24	FD	268/270 (99%)	97 (36%)	93 (35%)	78 (29%)	0	1
24	HD	268/270 (99%)	97 (36%)	93 (35%)	78 (29%)	0	1
24	JD	268/270 (99%)	96 (36%)	95 (35%)	77 (29%)	0	1
25	BE	203/205 (99%)	85 (42%)	74 (36%)	44 (22%)	0	4
25	DE	203/205 (99%)	85 (42%)	74 (36%)	44 (22%)	0	4
25	FE	203/205 (99%)	85 (42%)	73 (36%)	45 (22%)	0	3
25	HE	203/205 (99%)	85 (42%)	73 (36%)	45 (22%)	0	3
25	JE	203/205 (99%)	86 (42%)	73 (36%)	44 (22%)	0	4
26	BF	195/198 (98%)	90 (46%)	59 (30%)	46 (24%)	0	3
26	DF	195/198 (98%)	90 (46%)	59 (30%)	46 (24%)	0	3
26	FF	195/198 (98%)	90 (46%)	59 (30%)	46 (24%)	0	3
26	HF	195/198 (98%)	90 (46%)	59 (30%)	46 (24%)	0	3
26	JF	195/198 (98%)	90 (46%)	59 (30%)	46 (24%)	0	3
27	BG	176/178 (99%)	75 (43%)	59 (34%)	42 (24%)	0	3
27	DG	176/178 (99%)	75 (43%)	59 (34%)	42 (24%)	0	3
27	FG	176/178 (99%)	74 (42%)	60 (34%)	42 (24%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	HG	176/178 (99%)	75 (43%)	59 (34%)	42 (24%)	0	3
27	JG	176/178 (99%)	75 (43%)	58 (33%)	43 (24%)	0	2
28	BH	175/177 (99%)	84 (48%)	55 (31%)	36 (21%)	0	4
28	DH	175/177 (99%)	83 (47%)	56 (32%)	36 (21%)	0	4
28	FH	175/177 (99%)	83 (47%)	56 (32%)	36 (21%)	0	4
28	HH	175/177 (99%)	84 (48%)	55 (31%)	36 (21%)	0	4
28	JH	175/177 (99%)	83 (47%)	56 (32%)	36 (21%)	0	4
29	BI	50/52 (96%)	16 (32%)	19 (38%)	15 (30%)	0	1
29	DI	50/52 (96%)	16 (32%)	19 (38%)	15 (30%)	0	1
29	FI	50/52 (96%)	16 (32%)	19 (38%)	15 (30%)	0	1
29	HI	50/52 (96%)	16 (32%)	19 (38%)	15 (30%)	0	1
29	JI	50/52 (96%)	16 (32%)	19 (38%)	15 (30%)	0	1
30	BJ	141/143 (99%)	56 (40%)	47 (33%)	38 (27%)	0	2
30	DJ	141/143 (99%)	56 (40%)	47 (33%)	38 (27%)	0	2
30	FJ	141/143 (99%)	56 (40%)	47 (33%)	38 (27%)	0	2
30	HJ	141/143 (99%)	56 (40%)	47 (33%)	38 (27%)	0	2
30	JJ	141/143 (99%)	56 (40%)	47 (33%)	38 (27%)	0	2
31	BK	141/143 (99%)	55 (39%)	58 (41%)	28 (20%)	0	5
31	DK	141/143 (99%)	55 (39%)	58 (41%)	28 (20%)	0	5
31	FK	141/143 (99%)	55 (39%)	58 (41%)	28 (20%)	0	5
31	HK	141/143 (99%)	55 (39%)	58 (41%)	28 (20%)	0	5
31	JK	141/143 (99%)	55 (39%)	58 (41%)	28 (20%)	0	5
32	BL	130/132 (98%)	56 (43%)	37 (28%)	37 (28%)	0	1
32	DL	130/132 (98%)	56 (43%)	37 (28%)	37 (28%)	0	1
32	FL	130/132 (98%)	56 (43%)	37 (28%)	37 (28%)	0	1
32	HL	130/132 (98%)	56 (43%)	37 (28%)	37 (28%)	0	1
32	JL	130/132 (98%)	56 (43%)	37 (28%)	37 (28%)	0	1
33	BM	139/141 (99%)	60 (43%)	43 (31%)	36 (26%)	0	2
33	DM	139/141 (99%)	60 (43%)	43 (31%)	36 (26%)	0	2
33	FM	139/141 (99%)	60 (43%)	43 (31%)	36 (26%)	0	2
33	HM	139/141 (99%)	60 (43%)	43 (31%)	36 (26%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	JM	139/141 (99%)	60 (43%)	43 (31%)	36 (26%)	0	2
34	BN	122/124 (98%)	60 (49%)	35 (29%)	27 (22%)	0	3
34	DN	122/124 (98%)	61 (50%)	34 (28%)	27 (22%)	0	3
34	FN	122/124 (98%)	61 (50%)	34 (28%)	27 (22%)	0	3
34	HN	122/124 (98%)	61 (50%)	34 (28%)	27 (22%)	0	3
34	JN	122/124 (98%)	61 (50%)	34 (28%)	27 (22%)	0	3
35	BO	112/114 (98%)	52 (46%)	38 (34%)	22 (20%)	0	5
35	DO	112/114 (98%)	52 (46%)	38 (34%)	22 (20%)	0	5
35	FO	112/114 (98%)	52 (46%)	37 (33%)	23 (20%)	0	5
35	HO	112/114 (98%)	52 (46%)	38 (34%)	22 (20%)	0	5
35	JO	112/114 (98%)	51 (46%)	39 (35%)	22 (20%)	0	5
36	BP	109/111 (98%)	52 (48%)	37 (34%)	20 (18%)	0	6
36	DP	109/111 (98%)	52 (48%)	37 (34%)	20 (18%)	0	6
36	FP	109/111 (98%)	52 (48%)	37 (34%)	20 (18%)	0	6
36	HP	109/111 (98%)	52 (48%)	37 (34%)	20 (18%)	0	6
36	JP	109/111 (98%)	52 (48%)	37 (34%)	20 (18%)	0	6
37	BQ	123/125 (98%)	50 (41%)	47 (38%)	26 (21%)	0	4
37	DQ	123/125 (98%)	50 (41%)	48 (39%)	25 (20%)	0	5
37	FQ	123/125 (98%)	50 (41%)	47 (38%)	26 (21%)	0	4
37	HQ	123/125 (98%)	50 (41%)	48 (39%)	25 (20%)	0	5
37	JQ	123/125 (98%)	50 (41%)	47 (38%)	26 (21%)	0	4
38	BR	115/117 (98%)	55 (48%)	41 (36%)	19 (16%)	0	7
38	DR	115/117 (98%)	55 (48%)	41 (36%)	19 (16%)	0	7
38	FR	115/117 (98%)	55 (48%)	41 (36%)	19 (16%)	0	7
38	HR	115/117 (98%)	55 (48%)	40 (35%)	20 (17%)	0	6
38	JR	115/117 (98%)	55 (48%)	41 (36%)	19 (16%)	0	7
39	BS	98/100 (98%)	39 (40%)	37 (38%)	22 (22%)	0	3
39	DS	98/100 (98%)	38 (39%)	38 (39%)	22 (22%)	0	3
39	FS	98/100 (98%)	39 (40%)	37 (38%)	22 (22%)	0	3
39	HS	98/100 (98%)	39 (40%)	37 (38%)	22 (22%)	0	3
39	JS	98/100 (98%)	39 (40%)	37 (38%)	22 (22%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BT	128/130 (98%)	52 (41%)	51 (40%)	25 (20%)	0	5
40	DT	128/130 (98%)	52 (41%)	51 (40%)	25 (20%)	0	5
40	FT	128/130 (98%)	52 (41%)	51 (40%)	25 (20%)	0	5
40	HT	128/130 (98%)	52 (41%)	51 (40%)	25 (20%)	0	5
40	JT	128/130 (98%)	53 (41%)	50 (39%)	25 (20%)	0	5
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	1
42	DV	111/113 (98%)	43 (39%)	36 (32%)	32 (29%)	0	1
42	FV	111/113 (98%)	43 (39%)	36 (32%)	32 (29%)	0	1
42	HV	111/113 (98%)	43 (39%)	35 (32%)	33 (30%)	0	1
42	JV	111/113 (98%)	43 (39%)	36 (32%)	32 (29%)	0	1
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	1
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	1
43	JW	168/173 (97%)	44 (26%)	70 (42%)	54 (32%)	0	1
44	BX	84/86 (98%)	31 (37%)	29 (34%)	24 (29%)	0	1
44	DX	84/86 (98%)	31 (37%)	29 (34%)	24 (29%)	0	1
44	FX	84/86 (98%)	31 (37%)	29 (34%)	24 (29%)	0	1
44	HX	84/86 (98%)	31 (37%)	29 (34%)	24 (29%)	0	1
44	JX	84/86 (98%)	31 (37%)	29 (34%)	24 (29%)	0	1
45	BY	63/65 (97%)	35 (56%)	16 (25%)	12 (19%)	0	5
45	DY	63/65 (97%)	35 (56%)	16 (25%)	12 (19%)	0	5
45	FY	63/65 (97%)	35 (56%)	16 (25%)	12 (19%)	0	5
45	HY	63/65 (97%)	35 (56%)	16 (25%)	12 (19%)	0	5
45	JY	63/65 (97%)	35 (56%)	16 (25%)	12 (19%)	0	5
46	BZ	53/55 (96%)	25 (47%)	19 (36%)	9 (17%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	DZ	53/55 (96%)	25 (47%)	19 (36%)	9 (17%)	0	7
46	FZ	53/55 (96%)	25 (47%)	19 (36%)	9 (17%)	0	7
46	HZ	53/55 (96%)	25 (47%)	19 (36%)	9 (17%)	0	7
46	JZ	53/55 (96%)	25 (47%)	19 (36%)	9 (17%)	0	7
47	B1	71/73 (97%)	26 (37%)	24 (34%)	21 (30%)	0	1
47	D1	71/73 (97%)	26 (37%)	24 (34%)	21 (30%)	0	1
47	F1	71/73 (97%)	26 (37%)	25 (35%)	20 (28%)	0	1
47	H1	71/73 (97%)	26 (37%)	24 (34%)	21 (30%)	0	1
47	J1	71/73 (97%)	26 (37%)	24 (34%)	21 (30%)	0	1
48	B2	56/58 (97%)	19 (34%)	23 (41%)	14 (25%)	0	2
48	D2	56/58 (97%)	19 (34%)	23 (41%)	14 (25%)	0	2
48	F2	56/58 (97%)	19 (34%)	23 (41%)	14 (25%)	0	2
48	H2	56/58 (97%)	19 (34%)	23 (41%)	14 (25%)	0	2
48	J2	56/58 (97%)	19 (34%)	23 (41%)	14 (25%)	0	2
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	5
50	D4	44/46 (96%)	20 (46%)	15 (34%)	9 (20%)	0	5
50	F4	44/46 (96%)	20 (46%)	15 (34%)	9 (20%)	0	5
50	H4	44/46 (96%)	20 (46%)	15 (34%)	9 (20%)	0	5
50	J4	44/46 (96%)	20 (46%)	15 (34%)	9 (20%)	0	5
51	B5	61/63 (97%)	26 (43%)	19 (31%)	16 (26%)	0	2
51	D5	61/63 (97%)	27 (44%)	19 (31%)	15 (25%)	0	2
51	F5	61/63 (97%)	26 (43%)	20 (33%)	15 (25%)	0	2
51	H5	61/63 (97%)	26 (43%)	20 (33%)	15 (25%)	0	2
51	J5	61/63 (97%)	26 (43%)	20 (33%)	15 (25%)	0	2
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%)	1	16
53	D7	215/217 (99%)	113 (53%)	78 (36%)	24 (11%)	1	16
53	F7	215/217 (99%)	114 (53%)	77 (36%)	24 (11%)	1	16
53	H7	215/217 (99%)	113 (53%)	78 (36%)	24 (11%)	1	16
53	J7	215/217 (99%)	112 (52%)	79 (37%)	24 (11%)	1	16
All	All	29701/30260 (98%)	14747 (50%)	9520 (32%)	5434 (18%)	0	6

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%)	8	42
2	CB	202/202 (100%)	179 (89%)	23 (11%)	8	42
2	EB	202/202 (100%)	179 (89%)	23 (11%)	8	42
2	GB	202/202 (100%)	179 (89%)	23 (11%)	8	42
2	IB	202/202 (100%)	179 (89%)	23 (11%)	8	42
3	AC	160/160 (100%)	150 (94%)	10 (6%)	25	72
3	CC	160/160 (100%)	150 (94%)	10 (6%)	25	72
3	EC	160/160 (100%)	150 (94%)	10 (6%)	25	72
3	GC	160/160 (100%)	150 (94%)	10 (6%)	25	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	IC	160/160 (100%)	150 (94%)	10 (6%)	25	72
4	AD	180/180 (100%)	157 (87%)	23 (13%)	6	37
4	CD	180/180 (100%)	157 (87%)	23 (13%)	6	37
4	ED	180/180 (100%)	157 (87%)	23 (13%)	6	37
4	GD	180/180 (100%)	157 (87%)	23 (13%)	6	37
4	ID	180/180 (100%)	157 (87%)	23 (13%)	6	37
5	AE	115/115 (100%)	106 (92%)	9 (8%)	18	63
5	CE	115/115 (100%)	106 (92%)	9 (8%)	18	63
5	EE	115/115 (100%)	106 (92%)	9 (8%)	18	63
5	GE	115/115 (100%)	106 (92%)	9 (8%)	18	63
5	IE	115/115 (100%)	106 (92%)	9 (8%)	18	63
6	AF	90/90 (100%)	82 (91%)	8 (9%)	14	57
6	CF	90/90 (100%)	81 (90%)	9 (10%)	11	50
6	EF	90/90 (100%)	82 (91%)	8 (9%)	14	57
6	GF	90/90 (100%)	82 (91%)	8 (9%)	14	57
6	IF	90/90 (100%)	81 (90%)	9 (10%)	11	50
7	AG	126/126 (100%)	115 (91%)	11 (9%)	15	58
7	CG	126/126 (100%)	115 (91%)	11 (9%)	15	58
7	EG	126/126 (100%)	115 (91%)	11 (9%)	15	58
7	GG	126/126 (100%)	115 (91%)	11 (9%)	15	58
7	IG	126/126 (100%)	115 (91%)	11 (9%)	15	58
8	AH	119/119 (100%)	113 (95%)	6 (5%)	34	78
8	CH	119/119 (100%)	113 (95%)	6 (5%)	34	78
8	EH	119/119 (100%)	113 (95%)	6 (5%)	34	78
8	GH	119/119 (100%)	113 (95%)	6 (5%)	34	78
8	IH	119/119 (100%)	113 (95%)	6 (5%)	34	78
9	AI	98/98 (100%)	87 (89%)	11 (11%)	9	44
9	CI	98/98 (100%)	87 (89%)	11 (11%)	9	44
9	EI	98/98 (100%)	88 (90%)	10 (10%)	11	49
9	GI	98/98 (100%)	87 (89%)	11 (11%)	9	44
9	II	98/98 (100%)	87 (89%)	11 (11%)	9	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AJ	88/88 (100%)	81 (92%)	7 (8%)	17	62
10	CJ	88/88 (100%)	81 (92%)	7 (8%)	17	62
10	EJ	88/88 (100%)	81 (92%)	7 (8%)	17	62
10	GJ	88/88 (100%)	81 (92%)	7 (8%)	17	62
10	IJ	88/88 (100%)	81 (92%)	7 (8%)	17	62
11	AK	90/90 (100%)	80 (89%)	10 (11%)	9	45
11	CK	90/90 (100%)	80 (89%)	10 (11%)	9	45
11	EK	90/90 (100%)	80 (89%)	10 (11%)	9	45
11	GK	90/90 (100%)	80 (89%)	10 (11%)	9	45
11	IK	90/90 (100%)	80 (89%)	10 (11%)	9	45
12	AL	104/104 (100%)	98 (94%)	6 (6%)	28	74
12	CL	104/104 (100%)	98 (94%)	6 (6%)	28	74
12	EL	104/104 (100%)	98 (94%)	6 (6%)	28	74
12	GL	104/104 (100%)	98 (94%)	6 (6%)	28	74
12	IL	104/104 (100%)	98 (94%)	6 (6%)	28	74
13	AM	100/100 (100%)	86 (86%)	14 (14%)	5	33
13	CM	100/100 (100%)	86 (86%)	14 (14%)	5	33
13	EM	100/100 (100%)	86 (86%)	14 (14%)	5	33
13	GM	100/100 (100%)	86 (86%)	14 (14%)	5	33
13	IM	100/100 (100%)	86 (86%)	14 (14%)	5	33
14	AN	49/49 (100%)	44 (90%)	5 (10%)	11	49
14	CN	49/49 (100%)	44 (90%)	5 (10%)	11	49
14	EN	49/49 (100%)	44 (90%)	5 (10%)	11	49
14	GN	49/49 (100%)	44 (90%)	5 (10%)	11	49
14	IN	49/49 (100%)	44 (90%)	5 (10%)	11	49
15	AO	79/79 (100%)	75 (95%)	4 (5%)	33	78
15	CO	79/79 (100%)	75 (95%)	4 (5%)	33	78
15	EO	79/79 (100%)	75 (95%)	4 (5%)	33	78
15	GO	79/79 (100%)	75 (95%)	4 (5%)	33	78
15	IO	79/79 (100%)	75 (95%)	4 (5%)	33	78
16	AP	72/72 (100%)	68 (94%)	4 (6%)	30	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	CP	72/72 (100%)	68 (94%)	4 (6%)	30	76
16	EP	72/72 (100%)	68 (94%)	4 (6%)	30	76
16	GP	72/72 (100%)	68 (94%)	4 (6%)	30	76
16	IP	72/72 (100%)	68 (94%)	4 (6%)	30	76
17	AQ	96/96 (100%)	88 (92%)	8 (8%)	16	60
17	CQ	96/96 (100%)	88 (92%)	8 (8%)	16	60
17	EQ	96/96 (100%)	88 (92%)	8 (8%)	16	60
17	GQ	96/96 (100%)	88 (92%)	8 (8%)	16	60
17	IQ	96/96 (100%)	88 (92%)	8 (8%)	16	60
18	AR	64/64 (100%)	57 (89%)	7 (11%)	9	46
18	CR	64/64 (100%)	57 (89%)	7 (11%)	9	46
18	ER	64/64 (100%)	57 (89%)	7 (11%)	9	46
18	GR	64/64 (100%)	57 (89%)	7 (11%)	9	46
18	IR	64/64 (100%)	57 (89%)	7 (11%)	9	46
19	AS	71/71 (100%)	62 (87%)	9 (13%)	6	37
19	CS	71/71 (100%)	62 (87%)	9 (13%)	6	37
19	ES	71/71 (100%)	62 (87%)	9 (13%)	6	37
19	GS	71/71 (100%)	62 (87%)	9 (13%)	6	37
19	IS	71/71 (100%)	62 (87%)	9 (13%)	6	37
20	AT	76/76 (100%)	73 (96%)	3 (4%)	43	84
20	CT	76/76 (100%)	73 (96%)	3 (4%)	43	84
20	ET	76/76 (100%)	73 (96%)	3 (4%)	43	84
20	GT	76/76 (100%)	73 (96%)	3 (4%)	43	84
20	IT	76/76 (100%)	73 (96%)	3 (4%)	43	84
21	Aa	80/80 (100%)	62 (78%)	18 (22%)	1	10
21	Ca	80/80 (100%)	62 (78%)	18 (22%)	1	10
21	Ea	80/80 (100%)	62 (78%)	18 (22%)	1	10
21	Ga	80/80 (100%)	62 (78%)	18 (22%)	1	10
21	Ia	80/80 (100%)	62 (78%)	18 (22%)	1	10
24	BD	212/212 (100%)	168 (79%)	44 (21%)	2	12
24	DD	212/212 (100%)	168 (79%)	44 (21%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	FD	212/212 (100%)	168 (79%)	44 (21%)	2	12
24	HD	212/212 (100%)	168 (79%)	44 (21%)	2	12
24	JD	212/212 (100%)	168 (79%)	44 (21%)	2	12
25	BE	155/155 (100%)	130 (84%)	25 (16%)	3	26
25	DE	155/155 (100%)	130 (84%)	25 (16%)	3	26
25	FE	155/155 (100%)	131 (84%)	24 (16%)	4	27
25	HE	155/155 (100%)	131 (84%)	24 (16%)	4	27
25	JE	155/155 (100%)	130 (84%)	25 (16%)	3	26
26	BF	157/158 (99%)	139 (88%)	18 (12%)	8	42
26	DF	157/158 (99%)	139 (88%)	18 (12%)	8	42
26	FF	157/158 (99%)	139 (88%)	18 (12%)	8	42
26	HF	157/158 (99%)	139 (88%)	18 (12%)	8	42
26	JF	157/158 (99%)	139 (88%)	18 (12%)	8	42
27	BG	154/154 (100%)	122 (79%)	32 (21%)	2	12
27	DG	154/154 (100%)	122 (79%)	32 (21%)	2	12
27	FG	154/154 (100%)	122 (79%)	32 (21%)	2	12
27	HG	154/154 (100%)	122 (79%)	32 (21%)	2	12
27	JG	154/154 (100%)	122 (79%)	32 (21%)	2	12
28	BH	137/137 (100%)	116 (85%)	21 (15%)	4	28
28	DH	137/137 (100%)	116 (85%)	21 (15%)	4	28
28	FH	137/137 (100%)	116 (85%)	21 (15%)	4	28
28	HH	137/137 (100%)	116 (85%)	21 (15%)	4	28
28	JH	137/137 (100%)	116 (85%)	21 (15%)	4	28
29	BI	44/44 (100%)	39 (89%)	5 (11%)	8	42
29	DI	44/44 (100%)	39 (89%)	5 (11%)	8	42
29	FI	44/44 (100%)	39 (89%)	5 (11%)	8	42
29	HI	44/44 (100%)	39 (89%)	5 (11%)	8	42
29	JI	44/44 (100%)	39 (89%)	5 (11%)	8	42
30	BJ	107/107 (100%)	95 (89%)	12 (11%)	9	44
30	DJ	107/107 (100%)	95 (89%)	12 (11%)	9	44
30	FJ	107/107 (100%)	95 (89%)	12 (11%)	9	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	HJ	107/107 (100%)	95 (89%)	12 (11%)	9	44
30	JJ	107/107 (100%)	95 (89%)	12 (11%)	9	44
31	BK	119/119 (100%)	102 (86%)	17 (14%)	5	32
31	DK	119/119 (100%)	102 (86%)	17 (14%)	5	32
31	FK	119/119 (100%)	102 (86%)	17 (14%)	5	32
31	HK	119/119 (100%)	102 (86%)	17 (14%)	5	32
31	JK	119/119 (100%)	102 (86%)	17 (14%)	5	32
32	BL	101/101 (100%)	88 (87%)	13 (13%)	6	37
32	DL	101/101 (100%)	88 (87%)	13 (13%)	6	37
32	FL	101/101 (100%)	88 (87%)	13 (13%)	6	37
32	HL	101/101 (100%)	88 (87%)	13 (13%)	6	37
32	JL	101/101 (100%)	88 (87%)	13 (13%)	6	37
33	BM	108/108 (100%)	88 (82%)	20 (18%)	2	17
33	DM	108/108 (100%)	88 (82%)	20 (18%)	2	17
33	FM	108/108 (100%)	88 (82%)	20 (18%)	2	17
33	HM	108/108 (100%)	88 (82%)	20 (18%)	2	17
33	JM	108/108 (100%)	88 (82%)	20 (18%)	2	17
34	BN	99/99 (100%)	75 (76%)	24 (24%)	1	8
34	DN	99/99 (100%)	75 (76%)	24 (24%)	1	8
34	FN	99/99 (100%)	75 (76%)	24 (24%)	1	8
34	HN	99/99 (100%)	75 (76%)	24 (24%)	1	8
34	JN	99/99 (100%)	75 (76%)	24 (24%)	1	8
35	BO	91/91 (100%)	78 (86%)	13 (14%)	5	32
35	DO	91/91 (100%)	78 (86%)	13 (14%)	5	32
35	FO	91/91 (100%)	78 (86%)	13 (14%)	5	32
35	HO	91/91 (100%)	78 (86%)	13 (14%)	5	32
35	JO	91/91 (100%)	78 (86%)	13 (14%)	5	32
36	BP	80/80 (100%)	71 (89%)	9 (11%)	9	43
36	DP	80/80 (100%)	71 (89%)	9 (11%)	9	43
36	FP	80/80 (100%)	71 (89%)	9 (11%)	9	43
36	HP	80/80 (100%)	71 (89%)	9 (11%)	9	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	JP	80/80 (100%)	71 (89%)	9 (11%)	9	43
37	BQ	108/108 (100%)	92 (85%)	16 (15%)	4	30
37	DQ	108/108 (100%)	92 (85%)	16 (15%)	4	30
37	FQ	108/108 (100%)	92 (85%)	16 (15%)	4	30
37	HQ	108/108 (100%)	92 (85%)	16 (15%)	4	30
37	JQ	108/108 (100%)	92 (85%)	16 (15%)	4	30
38	BR	96/96 (100%)	82 (85%)	14 (15%)	5	30
38	DR	96/96 (100%)	82 (85%)	14 (15%)	5	30
38	FR	96/96 (100%)	82 (85%)	14 (15%)	5	30
38	HR	96/96 (100%)	82 (85%)	14 (15%)	5	30
38	JR	96/96 (100%)	82 (85%)	14 (15%)	5	30
39	BS	79/79 (100%)	70 (89%)	9 (11%)	8	42
39	DS	79/79 (100%)	70 (89%)	9 (11%)	8	42
39	FS	79/79 (100%)	70 (89%)	9 (11%)	8	42
39	HS	79/79 (100%)	70 (89%)	9 (11%)	8	42
39	JS	79/79 (100%)	70 (89%)	9 (11%)	8	42
40	BT	112/112 (100%)	99 (88%)	13 (12%)	8	42
40	DT	112/112 (100%)	99 (88%)	13 (12%)	8	42
40	FT	112/112 (100%)	99 (88%)	13 (12%)	8	42
40	HT	112/112 (100%)	99 (88%)	13 (12%)	8	42
40	JT	112/112 (100%)	99 (88%)	13 (12%)	8	42
41	BU	75/75 (100%)	69 (92%)	6 (8%)	17	62
41	DU	75/75 (100%)	69 (92%)	6 (8%)	17	62
41	FU	75/75 (100%)	69 (92%)	6 (8%)	17	62
41	HU	75/75 (100%)	68 (91%)	7 (9%)	13	54
41	JU	75/75 (100%)	68 (91%)	7 (9%)	13	54
42	BV	94/94 (100%)	86 (92%)	8 (8%)	15	60
42	DV	94/94 (100%)	86 (92%)	8 (8%)	15	60
42	FV	94/94 (100%)	86 (92%)	8 (8%)	15	60
42	HV	94/94 (100%)	86 (92%)	8 (8%)	15	60
42	JV	94/94 (100%)	86 (92%)	8 (8%)	15	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BW	147/147 (100%)	125 (85%)	22 (15%)	4	29
43	DW	147/147 (100%)	125 (85%)	22 (15%)	4	29
43	FW	147/147 (100%)	125 (85%)	22 (15%)	4	29
43	HW	147/147 (100%)	125 (85%)	22 (15%)	4	29
43	JW	147/147 (100%)	125 (85%)	22 (15%)	4	29
44	BX	64/64 (100%)	49 (77%)	15 (23%)	1	9
44	DX	64/64 (100%)	49 (77%)	15 (23%)	1	9
44	FX	64/64 (100%)	48 (75%)	16 (25%)	1	8
44	HX	64/64 (100%)	48 (75%)	16 (25%)	1	8
44	JX	64/64 (100%)	49 (77%)	15 (23%)	1	9
45	BY	53/53 (100%)	44 (83%)	9 (17%)	3	22
45	DY	53/53 (100%)	44 (83%)	9 (17%)	3	22
45	FY	53/53 (100%)	44 (83%)	9 (17%)	3	22
45	HY	53/53 (100%)	44 (83%)	9 (17%)	3	22
45	JY	53/53 (100%)	44 (83%)	9 (17%)	3	22
46	BZ	48/48 (100%)	38 (79%)	10 (21%)	2	12
46	DZ	48/48 (100%)	38 (79%)	10 (21%)	2	12
46	FZ	48/48 (100%)	38 (79%)	10 (21%)	2	12
46	HZ	48/48 (100%)	38 (79%)	10 (21%)	2	12
46	JZ	48/48 (100%)	38 (79%)	10 (21%)	2	12
47	B1	66/66 (100%)	53 (80%)	13 (20%)	2	15
47	D1	66/66 (100%)	53 (80%)	13 (20%)	2	15
47	F1	66/66 (100%)	53 (80%)	13 (20%)	2	15
47	H1	66/66 (100%)	53 (80%)	13 (20%)	2	15
47	J1	66/66 (100%)	53 (80%)	13 (20%)	2	15
48	B2	51/51 (100%)	39 (76%)	12 (24%)	1	9
48	D2	51/51 (100%)	39 (76%)	12 (24%)	1	9
48	F2	51/51 (100%)	39 (76%)	12 (24%)	1	9
48	H2	51/51 (100%)	39 (76%)	12 (24%)	1	9
48	J2	51/51 (100%)	39 (76%)	12 (24%)	1	9
49	B3	46/46 (100%)	33 (72%)	13 (28%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	D3	46/46 (100%)	33 (72%)	13 (28%)	0	5
49	F3	46/46 (100%)	33 (72%)	13 (28%)	0	5
49	H3	46/46 (100%)	33 (72%)	13 (28%)	0	5
49	J3	46/46 (100%)	33 (72%)	13 (28%)	0	5
50	B4	39/39 (100%)	28 (72%)	11 (28%)	0	5
50	D4	39/39 (100%)	28 (72%)	11 (28%)	0	5
50	F4	39/39 (100%)	28 (72%)	11 (28%)	0	5
50	H4	39/39 (100%)	28 (72%)	11 (28%)	0	5
50	J4	39/39 (100%)	28 (72%)	11 (28%)	0	5
51	B5	50/50 (100%)	35 (70%)	15 (30%)	0	5
51	D5	50/50 (100%)	35 (70%)	15 (30%)	0	5
51	F5	50/50 (100%)	35 (70%)	15 (30%)	0	5
51	H5	50/50 (100%)	35 (70%)	15 (30%)	0	5
51	J5	50/50 (100%)	35 (70%)	15 (30%)	0	5
52	B6	34/34 (100%)	30 (88%)	4 (12%)	8	41
52	D6	34/34 (100%)	30 (88%)	4 (12%)	8	41
52	F6	34/34 (100%)	30 (88%)	4 (12%)	8	41
52	H6	34/34 (100%)	30 (88%)	4 (12%)	8	41
52	J6	34/34 (100%)	30 (88%)	4 (12%)	8	41
53	B7	191/187 (102%)	179 (94%)	12 (6%)	25	72
53	D7	191/187 (102%)	179 (94%)	12 (6%)	25	72
53	F7	191/187 (102%)	179 (94%)	12 (6%)	25	72
53	H7	191/187 (102%)	179 (94%)	12 (6%)	25	72
53	J7	191/187 (102%)	179 (94%)	12 (6%)	25	72
All	All	24880/24865 (100%)	21622 (87%)	3258 (13%)	6	36

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
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

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Mol	Chain	Res	Type
22	JB	181	A
1	EA	975	A
1	EA	1397	C

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	FB	43
22	BB	42
22	JB	41
22	HB	39
22	DB	37
1	CA	4
1	GA	4
1	EA	4
1	AA	4
1	IA	4
12	GL	3
12	IL	3
12	CL	3

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

The worst 5 of 253 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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1526/1526 (100%)	-0.32	28 (1%) 65 56	521, 521, 521, 521	0
1	CA	1526/1526 (100%)	-0.40	20 (1%) 74 63	607, 607, 607, 607	0
1	EA	1526/1526 (100%)	-0.39	16 (1%) 79 68	628, 628, 628, 628	0
1	GA	1526/1526 (100%)	-0.28	36 (2%) 56 48	669, 669, 669, 669	0
1	IA	1526/1526 (100%)	-0.34	22 (1%) 72 61	743, 743, 743, 743	0
2	AB	234/234 (100%)	0.80	22 (9%) 9 18	521, 521, 521, 521	0
2	CB	234/234 (100%)	1.03	44 (18%) 2 7	607, 607, 607, 607	0
2	EB	234/234 (100%)	0.92	31 (13%) 4 11	628, 628, 628, 628	0
2	GB	234/234 (100%)	0.55	20 (8%) 11 19	669, 669, 669, 669	0
2	IB	234/234 (100%)	0.50	17 (7%) 15 22	743, 743, 743, 743	0
3	AC	206/206 (100%)	0.40	9 (4%) 33 34	521, 521, 521, 521	0
3	CC	206/206 (100%)	0.29	9 (4%) 33 34	607, 607, 607, 607	0
3	EC	206/206 (100%)	0.54	18 (8%) 10 19	628, 628, 628, 628	0
3	GC	206/206 (100%)	0.67	25 (12%) 5 13	669, 669, 669, 669	0
3	IC	206/206 (100%)	0.76	28 (13%) 4 11	743, 743, 743, 743	0
4	AD	208/208 (100%)	2.16	97 (46%) 1 4	521, 521, 521, 521	0
4	CD	208/208 (100%)	1.99	84 (40%) 1 4	607, 607, 607, 607	0
4	ED	208/208 (100%)	1.43	61 (29%) 1 5	628, 628, 628, 628	0
4	GD	208/208 (100%)	1.69	69 (33%) 1 5	669, 669, 669, 669	0
4	ID	208/208 (100%)	0.90	33 (15%) 3 9	743, 743, 743, 743	0
5	AE	150/150 (100%)	0.77	24 (16%) 3 9	521, 521, 521, 521	0
5	CE	150/150 (100%)	0.72	22 (14%) 3 10	607, 607, 607, 607	0
5	EE	150/150 (100%)	0.27	9 (6%) 21 27	628, 628, 628, 628	0
5	GE	150/150 (100%)	0.56	13 (8%) 10 19	669, 669, 669, 669	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
5	IE	150/150 (100%)	0.25	10 (6%)	17 25	743, 743, 743, 743	0
6	AF	101/101 (100%)	2.58	63 (62%)	0 4	521, 521, 521, 521	0
6	CF	101/101 (100%)	2.33	59 (58%)	0 4	607, 607, 607, 607	0
6	EF	101/101 (100%)	1.54	33 (32%)	1 5	628, 628, 628, 628	0
6	GF	101/101 (100%)	2.96	61 (60%)	0 4	669, 669, 669, 669	0
6	IF	101/101 (100%)	1.94	42 (41%)	1 4	743, 743, 743, 743	0
7	AG	155/155 (100%)	0.58	12 (7%)	13 21	521, 521, 521, 521	0
7	CG	155/155 (100%)	0.34	2 (1%)	74 63	607, 607, 607, 607	0
7	EG	155/155 (100%)	0.36	6 (3%)	37 36	628, 628, 628, 628	0
7	GG	155/155 (100%)	0.71	23 (14%)	3 10	669, 669, 669, 669	0
7	IG	155/155 (100%)	0.49	8 (5%)	26 29	743, 743, 743, 743	0
8	AH	138/138 (100%)	0.43	2 (1%)	72 61	521, 521, 521, 521	0
8	CH	138/138 (100%)	0.66	14 (10%)	7 16	607, 607, 607, 607	0
8	EH	138/138 (100%)	0.29	6 (4%)	34 34	628, 628, 628, 628	0
8	GH	138/138 (100%)	0.15	1 (0%)	84 75	669, 669, 669, 669	0
8	IH	138/138 (100%)	0.24	12 (8%)	10 19	743, 743, 743, 743	0
9	AI	127/127 (100%)	-0.14	0	100 100	521, 521, 521, 521	0
9	CI	127/127 (100%)	-0.10	0	100 100	607, 607, 607, 607	0
9	EI	127/127 (100%)	0.07	0	100 100	628, 628, 628, 628	0
9	GI	127/127 (100%)	-0.02	3 (2%)	56 48	669, 669, 669, 669	0
9	II	127/127 (100%)	0.06	3 (2%)	56 48	743, 743, 743, 743	0
10	AJ	98/98 (100%)	0.01	0	100 100	521, 521, 521, 521	0
10	CJ	98/98 (100%)	0.02	0	100 100	607, 607, 607, 607	0
10	EJ	98/98 (100%)	-0.01	0	100 100	628, 628, 628, 628	0
10	GJ	98/98 (100%)	0.15	0	100 100	669, 669, 669, 669	0
10	IJ	98/98 (100%)	0.20	2 (2%)	62 52	743, 743, 743, 743	0
11	AK	119/119 (100%)	1.01	20 (16%)	2 8	521, 521, 521, 521	0
11	CK	119/119 (100%)	1.41	34 (28%)	1 5	607, 607, 607, 607	0
11	EK	119/119 (100%)	0.75	11 (9%)	9 18	628, 628, 628, 628	0
11	GK	119/119 (100%)	1.06	27 (22%)	1 6	669, 669, 669, 669	0
11	IK	119/119 (100%)	0.78	13 (10%)	6 15	743, 743, 743, 743	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
12	AL	124/124 (100%)	0.58	18 (14%) 3 10	521, 521, 521, 521	0
12	CL	124/124 (100%)	0.49	13 (10%) 7 15	607, 607, 607, 607	0
12	EL	124/124 (100%)	0.28	0 100 100	628, 628, 628, 628	0
12	GL	124/124 (100%)	0.65	16 (12%) 4 12	669, 669, 669, 669	0
12	IL	124/124 (100%)	0.63	16 (12%) 4 12	743, 743, 743, 743	0
13	AM	125/125 (100%)	0.92	35 (28%) 1 5	521, 521, 521, 521	0
13	CM	125/125 (100%)	1.43	45 (36%) 1 5	607, 607, 607, 607	0
13	EM	125/125 (100%)	1.36	37 (29%) 1 5	628, 628, 628, 628	0
13	GM	125/125 (100%)	0.74	31 (24%) 1 6	669, 669, 669, 669	0
13	IM	125/125 (100%)	0.95	31 (24%) 1 6	743, 743, 743, 743	0
14	AN	60/60 (100%)	0.01	0 100 100	521, 521, 521, 521	0
14	CN	60/60 (100%)	0.47	7 (11%) 5 14	607, 607, 607, 607	0
14	EN	60/60 (100%)	0.62	7 (11%) 5 14	628, 628, 628, 628	0
14	GN	60/60 (100%)	0.14	1 (1%) 67 57	669, 669, 669, 669	0
14	IN	60/60 (100%)	0.34	4 (6%) 17 25	743, 743, 743, 743	0
15	AO	88/88 (100%)	0.09	4 (4%) 32 33	521, 521, 521, 521	0
15	CO	88/88 (100%)	0.07	3 (3%) 43 40	607, 607, 607, 607	0
15	EO	88/88 (100%)	-0.05	3 (3%) 43 40	628, 628, 628, 628	0
15	GO	88/88 (100%)	0.17	10 (11%) 6 14	669, 669, 669, 669	0
15	IO	88/88 (100%)	-0.08	5 (5%) 23 28	743, 743, 743, 743	0
16	AP	83/83 (100%)	-0.06	2 (2%) 56 48	521, 521, 521, 521	0
16	CP	83/83 (100%)	0.16	7 (8%) 11 20	607, 607, 607, 607	0
16	EP	83/83 (100%)	-0.03	1 (1%) 75 64	628, 628, 628, 628	0
16	GP	83/83 (100%)	0.23	8 (9%) 8 17	669, 669, 669, 669	0
16	IP	83/83 (100%)	-0.14	1 (1%) 75 64	743, 743, 743, 743	0
17	AQ	104/104 (100%)	-0.20	0 100 100	521, 521, 521, 521	0
17	CQ	104/104 (100%)	-0.30	0 100 100	607, 607, 607, 607	0
17	EQ	104/104 (100%)	-0.21	4 (3%) 38 37	628, 628, 628, 628	0
17	GQ	104/104 (100%)	-0.06	0 100 100	669, 669, 669, 669	0
17	IQ	104/104 (100%)	-0.12	0 100 100	743, 743, 743, 743	0
18	AR	73/73 (100%)	0.33	3 (4%) 35 35	521, 521, 521, 521	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
18	CR	73/73 (100%)	0.14	4 (5%) 24 28	607, 607, 607, 607	0
18	ER	73/73 (100%)	0.02	2 (2%) 52 46	628, 628, 628, 628	0
18	GR	73/73 (100%)	0.28	0 100 100	669, 669, 669, 669	0
18	IR	73/73 (100%)	-0.09	5 (6%) 17 24	743, 743, 743, 743	0
19	AS	80/80 (100%)	0.46	11 (13%) 4 11	521, 521, 521, 521	0
19	CS	80/80 (100%)	0.92	18 (22%) 1 6	607, 607, 607, 607	0
19	ES	80/80 (100%)	1.20	22 (27%) 1 6	628, 628, 628, 628	0
19	GS	80/80 (100%)	0.89	19 (23%) 1 6	669, 669, 669, 669	0
19	IS	80/80 (100%)	1.12	21 (26%) 1 6	743, 743, 743, 743	0
20	AT	99/99 (100%)	-0.13	1 (1%) 79 68	521, 521, 521, 521	0
20	CT	99/99 (100%)	0.79	21 (21%) 1 6	607, 607, 607, 607	0
20	ET	99/99 (100%)	0.55	10 (10%) 7 16	628, 628, 628, 628	0
20	GT	99/99 (100%)	0.12	10 (10%) 7 16	669, 669, 669, 669	0
20	IT	99/99 (100%)	-0.03	1 (1%) 79 68	743, 743, 743, 743	0
21	Aa	90/90 (100%)	0.16	3 (3%) 44 41	4, 4, 4, 4	90 (100%)
21	Ca	90/90 (100%)	-0.06	1 (1%) 77 66	4, 4, 4, 4	90 (100%)
21	Ea	90/90 (100%)	0.14	1 (1%) 77 66	4, 4, 4, 4	90 (100%)
21	Ga	90/90 (100%)	0.43	7 (7%) 13 21	4, 4, 4, 4	90 (100%)
21	Ia	90/90 (100%)	0.11	2 (2%) 59 50	4, 4, 4, 4	90 (100%)
22	BB	2825/2825 (100%)	-0.42	58 (2%) 60 51	849, 855, 857, 859	0
22	DB	2825/2825 (100%)	-0.44	51 (1%) 65 56	895, 902, 903, 904	0
22	FB	2825/2825 (100%)	-0.44	61 (2%) 59 50	896, 902, 905, 905	0
22	HB	2825/2825 (100%)	-0.45	48 (1%) 67 57	894, 902, 903, 903	0
22	JB	2825/2825 (100%)	-0.38	66 (2%) 57 49	897, 902, 906, 908	0
23	BA	118/119 (99%)	0.27	6 (5%) 27 30	846, 846, 846, 846	0
23	DA	118/119 (99%)	0.03	2 (1%) 67 57	893, 893, 893, 893	0
23	FA	118/119 (99%)	-0.10	3 (2%) 54 48	896, 896, 896, 896	0
23	HA	118/119 (99%)	0.07	5 (4%) 35 34	894, 894, 894, 894	0
23	JA	118/119 (99%)	0.04	3 (2%) 54 48	894, 894, 894, 894	0
24	BD	270/270 (100%)	1.48	110 (40%) 1 4	904, 904, 904, 904	0
24	DD	270/270 (100%)	1.03	80 (29%) 1 5	950, 950, 950, 950	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
24	FD	270/270 (100%)	0.54	40 (14%) 3 10	950, 950, 950, 950	0
24	HD	270/270 (100%)	1.68	108 (40%) 1 4	950, 950, 950, 950	0
24	JD	270/270 (100%)	0.42	27 (10%) 8 16	950, 950, 950, 950	0
25	BE	205/205 (100%)	0.35	12 (5%) 22 27	904, 904, 904, 904	0
25	DE	205/205 (100%)	0.54	17 (8%) 11 20	950, 950, 950, 950	0
25	FE	205/205 (100%)	0.76	40 (19%) 2 7	950, 950, 950, 950	0
25	HE	205/205 (100%)	0.68	25 (12%) 5 13	950, 950, 950, 950	0
25	JE	205/205 (100%)	1.03	63 (30%) 1 5	950, 950, 950, 950	0
26	BF	197/198 (99%)	-0.12	0 100 100	904, 904, 904, 904	0
26	DF	197/198 (99%)	0.02	3 (1%) 70 59	950, 950, 950, 950	0
26	FF	197/198 (99%)	-0.05	1 (0%) 88 80	950, 950, 950, 950	0
26	HF	197/198 (99%)	0.19	4 (2%) 62 52	950, 950, 950, 950	0
26	JF	197/198 (99%)	0.34	14 (7%) 16 23	950, 950, 950, 950	0
27	BG	178/178 (100%)	0.50	15 (8%) 11 20	904, 904, 904, 904	0
27	DG	178/178 (100%)	0.55	21 (11%) 5 14	950, 950, 950, 950	0
27	FG	178/178 (100%)	0.55	14 (7%) 13 21	950, 950, 950, 950	0
27	HG	178/178 (100%)	0.63	25 (14%) 3 10	950, 950, 950, 950	0
27	JG	178/178 (100%)	0.73	19 (10%) 6 15	950, 950, 950, 950	0
28	BH	177/177 (100%)	1.47	64 (36%) 1 5	904, 904, 904, 904	0
28	DH	177/177 (100%)	1.23	60 (33%) 1 5	950, 950, 950, 950	0
28	FH	177/177 (100%)	1.25	55 (31%) 1 5	950, 950, 950, 950	0
28	HH	177/177 (100%)	1.03	47 (26%) 1 6	950, 950, 950, 950	0
28	JH	177/177 (100%)	1.02	54 (30%) 1 5	950, 950, 950, 950	0
29	BI	52/52 (100%)	0.88	1 (1%) 64 54	904, 904, 904, 904	0
29	DI	52/52 (100%)	0.44	3 (5%) 22 27	950, 950, 950, 950	0
29	FI	52/52 (100%)	0.35	2 (3%) 38 37	950, 950, 950, 950	0
29	HI	52/52 (100%)	1.40	12 (23%) 1 6	950, 950, 950, 950	0
29	JI	52/52 (100%)	1.13	6 (11%) 5 14	950, 950, 950, 950	0
30	BJ	143/143 (100%)	1.34	38 (26%) 1 6	904, 904, 904, 904	0
30	DJ	143/143 (100%)	1.06	32 (22%) 1 6	950, 950, 950, 950	0
30	FJ	143/143 (100%)	0.82	22 (15%) 3 10	950, 950, 950, 950	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
30	HJ	143/143 (100%)	1.20	39 (27%) 1 6	950, 950, 950, 950	0
30	JJ	143/143 (100%)	0.78	16 (11%) 6 14	950, 950, 950, 950	0
31	BK	143/143 (100%)	-0.47	0 100 100	904, 904, 904, 904	0
31	DK	143/143 (100%)	-0.37	0 100 100	950, 950, 950, 950	0
31	FK	143/143 (100%)	-0.46	0 100 100	950, 950, 950, 950	0
31	HK	143/143 (100%)	-0.38	0 100 100	950, 950, 950, 950	0
31	JK	143/143 (100%)	0.12	9 (6%) 19 26	950, 950, 950, 950	0
32	BL	132/132 (100%)	1.47	42 (31%) 1 5	904, 904, 904, 904	0
32	DL	132/132 (100%)	1.43	44 (33%) 1 5	950, 950, 950, 950	0
32	FL	132/132 (100%)	0.81	19 (14%) 3 10	950, 950, 950, 950	0
32	HL	132/132 (100%)	1.28	29 (21%) 1 6	950, 950, 950, 950	0
32	JL	132/132 (100%)	0.82	24 (18%) 2 7	950, 950, 950, 950	0
33	BM	141/141 (100%)	0.30	16 (11%) 6 14	904, 904, 904, 904	0
33	DM	141/141 (100%)	0.32	14 (9%) 8 16	950, 950, 950, 950	0
33	FM	141/141 (100%)	0.58	23 (16%) 2 9	950, 950, 950, 950	0
33	HM	141/141 (100%)	0.04	2 (1%) 72 61	950, 950, 950, 950	0
33	JM	141/141 (100%)	0.08	7 (4%) 28 30	950, 950, 950, 950	0
34	BN	124/124 (100%)	0.60	11 (8%) 10 19	904, 904, 904, 904	0
34	DN	124/124 (100%)	0.68	9 (7%) 15 22	950, 950, 950, 950	0
34	FN	124/124 (100%)	0.24	0 100 100	950, 950, 950, 950	0
34	HN	124/124 (100%)	0.50	5 (4%) 36 36	950, 950, 950, 950	0
34	JN	124/124 (100%)	0.50	7 (5%) 24 28	950, 950, 950, 950	0
35	BO	114/114 (100%)	-0.01	3 (2%) 53 46	904, 904, 904, 904	0
35	DO	114/114 (100%)	-0.14	0 100 100	950, 950, 950, 950	0
35	FO	114/114 (100%)	-0.26	0 100 100	950, 950, 950, 950	0
35	HO	114/114 (100%)	-0.25	0 100 100	950, 950, 950, 950	0
35	JO	114/114 (100%)	-0.39	0 100 100	950, 950, 950, 950	0
36	BP	111/111 (100%)	-0.21	1 (0%) 81 71	904, 904, 904, 904	7 (6%)
36	DP	111/111 (100%)	-0.24	1 (0%) 81 71	950, 950, 950, 950	7 (6%)
36	FP	111/111 (100%)	-0.26	0 100 100	950, 950, 950, 950	7 (6%)
36	HP	111/111 (100%)	-0.16	0 100 100	950, 950, 950, 950	7 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
36	JP	111/111 (100%)	-0.18	0	100	100	950, 950, 950, 950	7 (6%)
37	BQ	125/125 (100%)	1.06	22 (17%)	2	8	904, 904, 904, 904	0
37	DQ	125/125 (100%)	1.24	28 (22%)	1	6	950, 950, 950, 950	0
37	FQ	125/125 (100%)	1.81	49 (39%)	1	4	950, 950, 950, 950	0
37	HQ	125/125 (100%)	0.77	21 (16%)	2	8	950, 950, 950, 950	0
37	JQ	125/125 (100%)	0.73	22 (17%)	2	8	950, 950, 950, 950	0
38	BR	117/117 (100%)	-0.25	1 (0%)	81	71	904, 904, 904, 904	9 (7%)
38	DR	117/117 (100%)	-0.34	0	100	100	950, 950, 950, 950	9 (7%)
38	FR	117/117 (100%)	-0.46	0	100	100	950, 950, 950, 950	9 (7%)
38	HR	117/117 (100%)	-0.19	2 (1%)	67	57	950, 950, 950, 950	9 (7%)
38	JR	117/117 (100%)	-0.53	0	100	100	950, 950, 950, 950	9 (7%)
39	BS	100/100 (100%)	-0.21	0	100	100	904, 904, 904, 904	0
39	DS	100/100 (100%)	-0.41	0	100	100	950, 950, 950, 950	0
39	FS	100/100 (100%)	-0.55	0	100	100	950, 950, 950, 950	0
39	HS	100/100 (100%)	0.66	13 (13%)	4	12	950, 950, 950, 950	0
39	JS	100/100 (100%)	-0.02	1 (1%)	79	68	950, 950, 950, 950	0
40	BT	130/130 (100%)	0.78	23 (17%)	2	8	904, 904, 904, 904	0
40	DT	130/130 (100%)	1.13	28 (21%)	1	6	950, 950, 950, 950	0
40	FT	130/130 (100%)	1.60	42 (32%)	1	5	950, 950, 950, 950	0
40	HT	130/130 (100%)	1.04	39 (30%)	1	5	950, 950, 950, 950	0
40	JT	130/130 (100%)	2.80	62 (47%)	1	4	950, 950, 950, 950	0
41	BU	93/93 (100%)	1.06	24 (25%)	1	6	904, 904, 904, 904	0
41	DU	93/93 (100%)	0.91	22 (23%)	1	6	950, 950, 950, 950	0
41	FU	93/93 (100%)	0.84	22 (23%)	1	6	950, 950, 950, 950	0
41	HU	93/93 (100%)	1.02	25 (26%)	1	6	950, 950, 950, 950	0
41	JU	93/93 (100%)	0.46	8 (8%)	11	19	950, 950, 950, 950	0
42	BV	113/113 (100%)	-0.19	0	100	100	904, 904, 904, 904	0
42	DV	113/113 (100%)	0.04	5 (4%)	33	34	950, 950, 950, 950	0
42	FV	113/113 (100%)	0.26	15 (13%)	4	11	950, 950, 950, 950	0
42	HV	113/113 (100%)	0.50	14 (12%)	5	13	950, 950, 950, 950	0
42	JV	113/113 (100%)	0.57	17 (15%)	3	10	950, 950, 950, 950	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BW	173/173 (100%)	0.41	17 (9%) 8 17	904, 904, 904, 904	0
43	DW	173/173 (100%)	0.65	22 (12%) 4 12	950, 950, 950, 950	0
43	FW	173/173 (100%)	0.94	45 (26%) 1 6	950, 950, 950, 950	0
43	HW	173/173 (100%)	0.68	23 (13%) 4 11	950, 950, 950, 950	0
43	JW	173/173 (100%)	0.76	35 (20%) 2 6	950, 950, 950, 950	0
44	BX	86/86 (100%)	-0.07	5 (5%) 22 27	904, 904, 904, 904	0
44	DX	86/86 (100%)	0.49	11 (12%) 4 12	950, 950, 950, 950	0
44	FX	86/86 (100%)	0.63	12 (13%) 3 10	950, 950, 950, 950	0
44	HX	86/86 (100%)	-0.15	4 (4%) 30 32	950, 950, 950, 950	0
44	JX	86/86 (100%)	0.50	12 (13%) 3 10	950, 950, 950, 950	0
45	BY	65/65 (100%)	0.80	12 (18%) 2 7	904, 904, 904, 904	0
45	DY	65/65 (100%)	1.73	27 (41%) 1 4	950, 950, 950, 950	0
45	FY	65/65 (100%)	1.15	16 (24%) 1 6	950, 950, 950, 950	0
45	HY	65/65 (100%)	0.50	10 (15%) 3 10	950, 950, 950, 950	0
45	JY	65/65 (100%)	-0.05	1 (1%) 70 59	950, 950, 950, 950	0
46	BZ	55/55 (100%)	0.30	4 (7%) 15 22	904, 904, 904, 904	3 (5%)
46	DZ	55/55 (100%)	0.34	4 (7%) 15 22	950, 950, 950, 950	3 (5%)
46	FZ	55/55 (100%)	0.47	8 (14%) 3 10	950, 950, 950, 950	3 (5%)
46	HZ	55/55 (100%)	-0.05	0 100 100	950, 950, 950, 950	3 (5%)
46	JZ	55/55 (100%)	0.23	6 (10%) 6 15	950, 950, 950, 950	3 (5%)
47	B1	73/73 (100%)	0.18	4 (5%) 24 28	904, 904, 904, 904	0
47	D1	73/73 (100%)	0.02	4 (5%) 24 28	950, 950, 950, 950	0
47	F1	73/73 (100%)	0.02	3 (4%) 35 35	950, 950, 950, 950	0
47	H1	73/73 (100%)	0.15	3 (4%) 35 35	950, 950, 950, 950	0
47	J1	73/73 (100%)	0.38	3 (4%) 35 35	950, 950, 950, 950	0
48	B2	58/58 (100%)	0.08	0 100 100	904, 904, 904, 904	0
48	D2	58/58 (100%)	0.39	4 (6%) 17 24	950, 950, 950, 950	0
48	F2	58/58 (100%)	0.39	6 (10%) 7 16	950, 950, 950, 950	0
48	H2	58/58 (100%)	-0.05	0 100 100	950, 950, 950, 950	0
48	J2	58/58 (100%)	0.30	5 (8%) 11 19	950, 950, 950, 950	0
49	B3	53/53 (100%)	4.66	42 (79%) 0 3	904, 904, 904, 904	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
49	D3	53/53 (100%)	1.74	22 (41%) 1 4	950, 950, 950, 950	0
49	F3	53/53 (100%)	0.76	12 (22%) 1 6	950, 950, 950, 950	0
49	H3	53/53 (100%)	3.91	43 (81%) 0 3	950, 950, 950, 950	0
49	J3	53/53 (100%)	1.60	18 (33%) 1 5	950, 950, 950, 950	0
50	B4	46/46 (100%)	-0.46	0 100 100	904, 904, 904, 904	0
50	D4	46/46 (100%)	-0.43	0 100 100	950, 950, 950, 950	0
50	F4	46/46 (100%)	-0.39	0 100 100	950, 950, 950, 950	0
50	H4	46/46 (100%)	-0.10	0 100 100	950, 950, 950, 950	0
50	J4	46/46 (100%)	-0.37	0 100 100	950, 950, 950, 950	0
51	B5	63/63 (100%)	-0.48	1 (1%) 68 58	904, 904, 904, 904	0
51	D5	63/63 (100%)	-0.43	0 100 100	950, 950, 950, 950	0
51	F5	63/63 (100%)	-0.47	0 100 100	950, 950, 950, 950	0
51	H5	63/63 (100%)	-0.45	0 100 100	950, 950, 950, 950	0
51	J5	63/63 (100%)	-0.57	0 100 100	950, 950, 950, 950	0
52	B6	35/35 (100%)	0.18	0 100 100	904, 904, 904, 904	0
52	D6	35/35 (100%)	-0.40	0 100 100	950, 950, 950, 950	0
52	F6	35/35 (100%)	-0.52	0 100 100	950, 950, 950, 950	0
52	H6	35/35 (100%)	-0.13	0 100 100	950, 950, 950, 950	0
52	J6	35/35 (100%)	-0.41	0 100 100	950, 950, 950, 950	0
53	B7	217/217 (100%)	1.10	47 (21%) 1 6	904, 904, 904, 904	0
53	D7	217/217 (100%)	0.39	15 (6%) 17 24	950, 950, 950, 950	0
53	F7	217/217 (100%)	0.88	34 (15%) 3 9	950, 950, 950, 950	0
53	H7	217/217 (100%)	0.91	54 (24%) 1 6	950, 950, 950, 950	0
53	J7	217/217 (100%)	1.14	61 (28%) 1 5	950, 950, 950, 950	0
All	All	52600/52610 (99%)	0.17	4513 (8%) 11 19	4, 900, 950, 950	545 (1%)

The worst 5 of 4513 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
40	JT	89	ARG	12.3
53	F7	95	GLY	11.9
49	B3	36	GLU	11.6
40	JT	49	SER	11.6
24	HD	111	LEU	11.3

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.