



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 07:09 AM EDT

PDB ID : 4V8A
Title : The structure of thermorubin in complex with the 70S ribosome from *Thermus thermophilus*.
Authors : Bulkley, D.; Johnson, F.A.; Steitz, T.A.
Deposited on : 2011-12-05
Resolution : 3.20 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

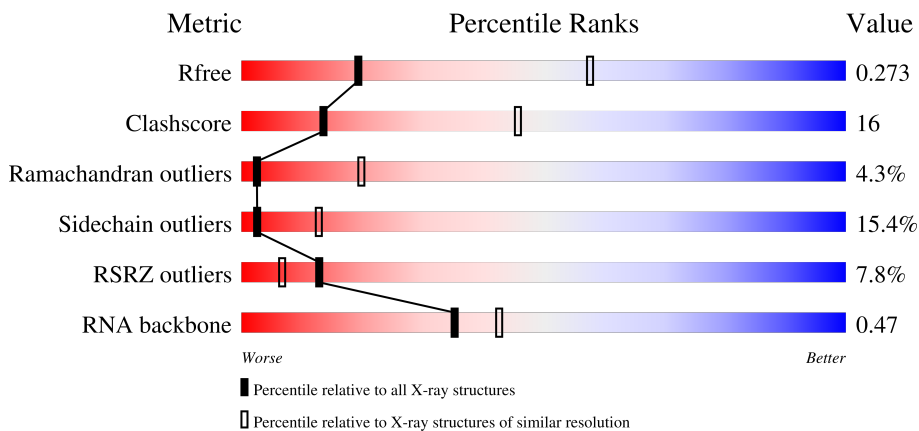
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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









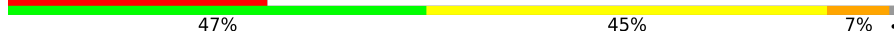




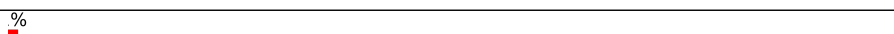













Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	AA	2915	
1	BA	2915	
2	AB	122	
2	BB	122	

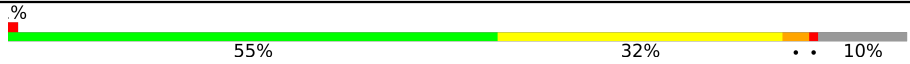




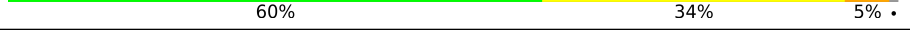
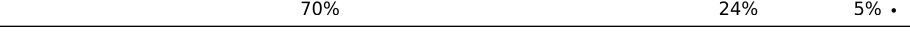
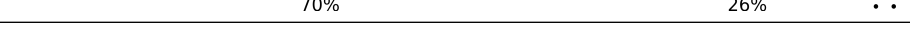
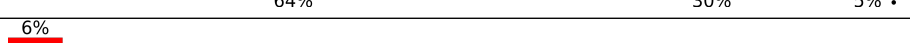
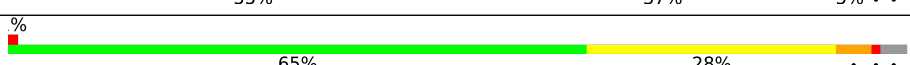



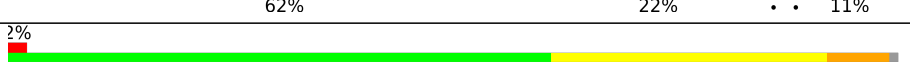



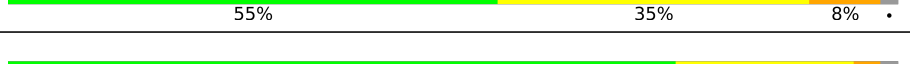
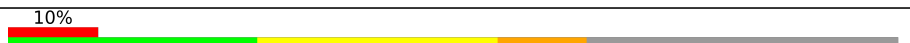
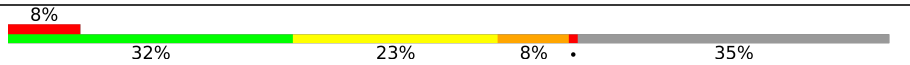





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Mol	Chain	Length	Quality of chain
3	AD	276	
3	BD	276	
4	AE	206	
4	BE	206	
5	AF	205	
5	BF	205	
6	AG	182	
6	BG	182	
7	AH	180	
7	BH	180	
8	AI	148	
8	BI	148	
9	AN	140	
9	BN	140	
10	AO	122	
10	BO	122	
11	AP	150	
11	BP	150	
12	AQ	141	
12	BQ	141	
13	AR	118	
13	BR	118	
14	AS	112	
14	BS	112	
15	AT	146	

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Mol	Chain	Length	Quality of chain
15	BT	146	
16	AU	118	
16	BU	118	
17	AV	101	
17	BV	101	
18	AW	113	
18	BW	113	
19	AX	96	
19	BX	96	
20	AY	110	
20	BY	110	
21	AZ	206	
21	BZ	206	
22	A0	85	
22	B0	85	
23	A1	98	
23	B1	98	
24	A2	72	
24	B2	72	
25	A3	60	
25	B3	60	
26	A4	71	
26	B4	71	
27	A5	60	
27	B5	60	

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Mol	Chain	Length	Quality of chain
28	A6	54	6% 44% 43% 9% ..
28	B6	54	50% 39% 9% .
29	A7	49	8% 53% 43% ..
29	B7	49	2% 57% 33% 8% .
30	A8	65	54% 42% ..
30	B8	65	66% 29% ..
31	CA	1521	12% 29% 53% 14% ..
31	DA	1521	12% 31% 51% 14% ..
32	CB	256	5% 38% 40% 11% 11%
32	DB	256	12% 38% 42% 9% 11%
33	CC	239	19% 54% 28% 5% 14%
33	DC	239	14% 47% 33% 6% 14%
34	CD	209	5% 48% 41% 9% .
34	DD	209	5% 51% 40% 8%
35	CE	162	2% 41% 42% 8% . 9%
35	DE	162	3% 44% 40% 6% . 9%
36	CF	101	5% 57% 35% 7% .
36	DF	101	3% 60% 31% 7% ..
37	CG	156	49% 57% 33% 8% ..
37	DG	156	48% 52% 42% ..
38	CH	138	3% 57% 35% 8% .
38	DH	138	2% 52% 37% 10% .
39	CI	128	39% 52% 38% 9% .
39	DI	128	55% 53% 37% 8% .
40	CJ	105	41% 54% 28% 9% . 9%

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Mol	Chain	Length	Quality of chain
40	DJ	105	44% 43% 38% 10% 9%
41	CK	129	56% 29% 12%
41	DK	129	3% 51% 33% 12%
42	CL	132	53% 31% 8% 8%
42	DL	132	53% 33% 6% 8%
43	CM	126	40% 50% 32% 9% 10%
43	DM	126	35% 43% 35% 12% 10%
44	CN	61	25% 33% 51% 15%
44	DN	61	34% 49% 34% 13%
45	CO	89	2% 49% 39% 10%
45	DO	89	6% 54% 36% 9%
46	CP	88	7% 47% 34% 13% 7%
46	DP	88	3% 44% 45% 7%
47	CQ	105	2% 54% 35% 5% 6%
47	DQ	105	3% 64% 25% 6% 6%
48	CR	88	10% 51% 23% 23%
48	DR	88	3% 53% 22% 23%
49	CS	93	47% 39% 34% 10% 16%
49	DS	93	56% 39% 42% 16%
50	CT	106	3% 40% 42% 8% 9%
50	DT	106	9% 52% 34% 9%
51	CU	27	44% 52% 26% 7% 15%
51	DU	27	48% 48% 30% 7% 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	T8B	AA	3001	-	-	X	-
52	T8B	BA	3001	-	-	X	-

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 279316 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	2827	Total	C	N	O	P	0	0	0
			60900	27102	11403	19569	2826			
1	BA	2827	Total	C	N	O	P	0	0	0
			60900	27102	11403	19569	2826			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	272A	G	U	CONFLICT	GB AP008226.1
BA	272A	G	U	CONFLICT	GB AP008226.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AB	120	Total	C	N	O	P	0	0	0
			2574	1146	476	833	119			
2	BB	120	Total	C	N	O	P	0	0	0
			2574	1146	476	833	119			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	120	G	A	CONFLICT	GB AP008226.1
BB	120	G	A	CONFLICT	GB AP008226.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			
4	BE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	203	Total	C	N	O	S	0	0	1
			1576	1005	297	272	2			
5	BF	203	Total	C	N	O	S	0	0	1
			1576	1005	297	272	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			
6	BG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			
7	BH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	145	Total	C	N	O	S	0	0	0
			1046	674	180	191	1			
8	BI	145	Total	C	N	O	S	0	0	0
			1046	674	180	191	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	110	GLU	ASP	CONFLICT	UNP Q5SLQ1

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Chain	Residue	Modelled	Actual	Comment	Reference
BI	110	GLU	ASP	CONFLICT	UNP Q5SLQ1

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			
9	BN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			
10	BO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AP	147	Total	C	N	O	S	0	0	0
			1119	695	227	194	3			
11	BP	147	Total	C	N	O	S	0	0	0
			1119	695	227	194	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AS	110	Total	C	N	O	0	0	0
			865	544	172	149			
14	BS	110	Total	C	N	O	0	0	0
			865	544	172	149			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			
15	BT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			
18	BW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			
19	BX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			
20	BY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			
21	BZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			
22	B0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	A1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			
23	B1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	B2	70	588	365	118	103	2	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	A3	59	458	293	87	78		0	0	0
25	B3	59	458	293	87	78		0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	A4	46	349	223	57	64	5	0	0	0
26	B4	46	349	223	57	64	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	A5	59	455	286	90	74	5	0	0	0
27	B5	59	455	286	90	74	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	A6	53	449	278	90	77	4	0	0	0
28	B6	53	449	278	90	77	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	A7	48	418	257	104	55	2	0	0	0
29	B7	48	418	257	104	55	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			
30	B8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CA	1498	Total	C	N	O	P	0	0	0
			32208	14334	5974	10402	1498			
31	DA	1498	Total	C	N	O	P	0	0	0
			32208	14334	5974	10402	1498			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	?	-	U	DELETION	GB AP008226.1
DA	?	-	U	DELETION	GB AP008226.1

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CB	229	Total	C	N	O	S	0	0	0
			1777	1134	318	320	5			
32	DB	229	Total	C	N	O	S	0	0	0
			1777	1134	318	320	5			

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			
33	DC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CD	208	Total	C	N	O	S	0	0	0
			1520	960	283	272	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	DD	208	1520	960	283	272	5	0	0	0

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	CE	148	1105	699	204	198	4	0	0	0
35	DE	148	1105	699	204	198	4	0	0	0

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	CF	100	781	495	137	146	3	0	0	0
36	DF	100	781	495	137	146	3	0	0	0

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	CG	155	1167	727	224	210	6	0	0	0
37	DG	155	1167	727	224	210	6	0	0	0

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	CH	138	1045	665	188	190	2	0	0	0
38	DH	138	1045	665	188	190	2	0	0	0

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
39	CI	125	852	533	163	156	0	0	0
39	DI	125	852	533	163	156	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	58	ARG	HIS	CONFLICT	UNP P80374
DI	58	ARG	HIS	CONFLICT	UNP P80374

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	CJ	96	Total	C	N	O	0	0	0
			659	408	131	120			
40	DJ	96	Total	C	N	O	0	0	0
			659	408	131	120			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CJ	75	LEU	ILE	CONFLICT	UNP Q5SHN7
DJ	75	LEU	ILE	CONFLICT	UNP Q5SHN7

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CK	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			
41	DK	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CL	122	Total	C	N	O	S	0	0	0
			909	570	179	159	1			
42	DL	122	Total	C	N	O	S	0	0	0
			909	570	179	159	1			

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CM	114	Total	C	N	O	S	0	0	0
			801	494	164	142	1			
43	DM	114	Total	C	N	O	S	0	0	0
			801	494	164	142	1			

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CN	60	Total	C	N	O	S	0	0	0
			478	303	99	72	4			
44	DN	60	Total	C	N	O	S	0	0	0
			478	303	99	72	4			

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			
45	DO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			
46	DP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
47	DQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	CR	68	Total	C	N	O	0	0	0
			514	329	98	87			
48	DR	68	Total	C	N	O	0	0	0
			514	329	98	87			

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	CS	78	Total 544	C 342	N 105	O 95	S 2	0	0	0
49	DS	78	Total 544	C 342	N 105	O 95	S 2	0	0	0

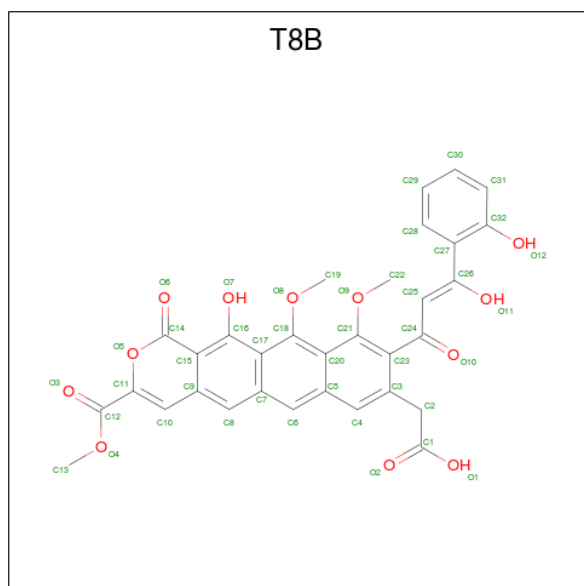
- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	CT	96	Total 708	C 435	N 151	O 120	S 2	0	0	0
50	DT	96	Total 708	C 435	N 151	O 120	S 2	0	0	0

- Molecule 51 is a protein called 30S ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
51	CU	23	Total 199	C 122	N 48	O 29	0	0	0
51	DU	23	Total 199	C 122	N 48	O 29	0	0	0

- Molecule 52 is Thermorubin (three-letter code: T8B) (formula: C₃₂H₂₄O₁₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
52	AA	1	Total 44	C 32	O 12	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
52	BA	1	Total	C	O	0	0
			44	32	12		

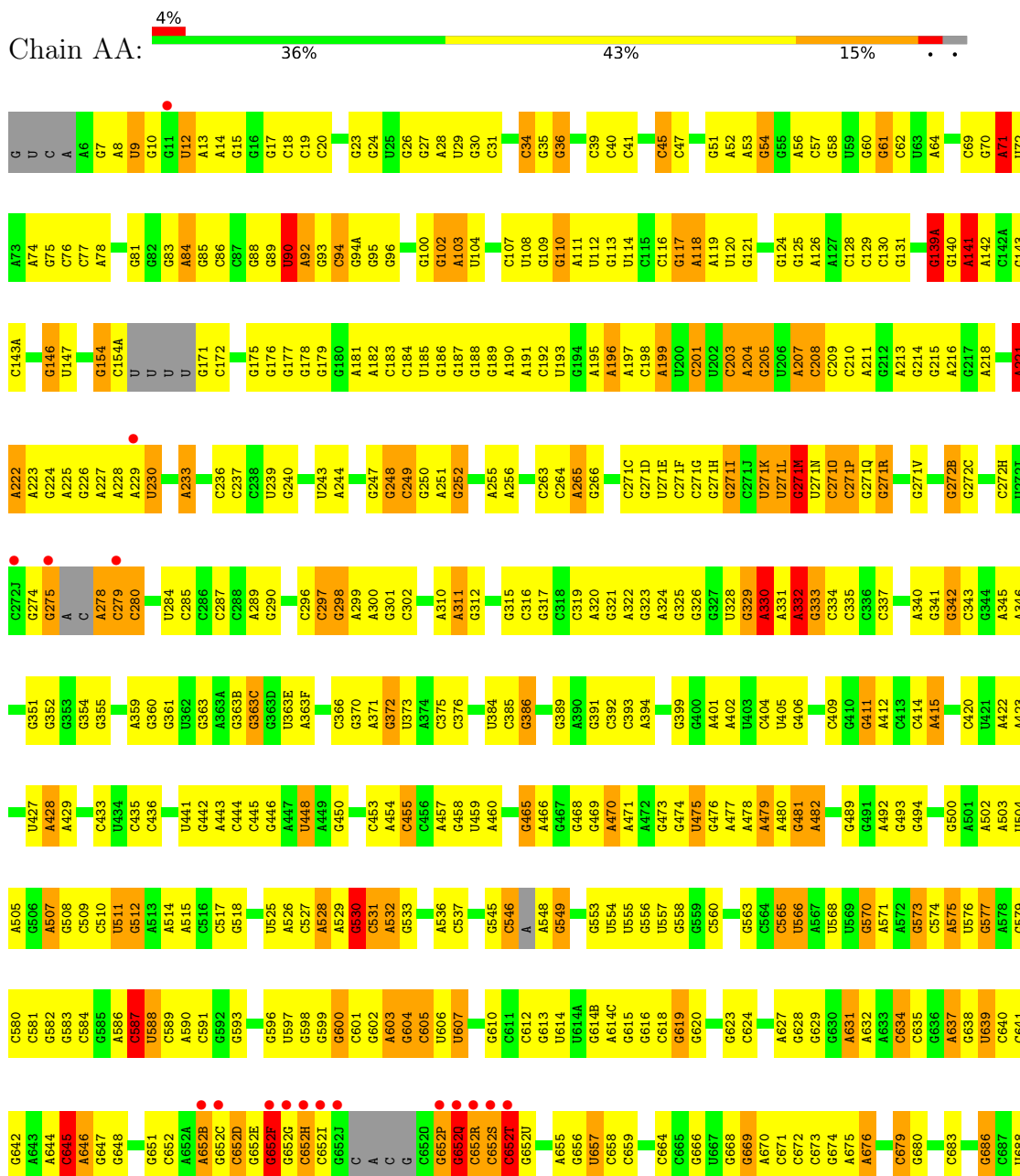
- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

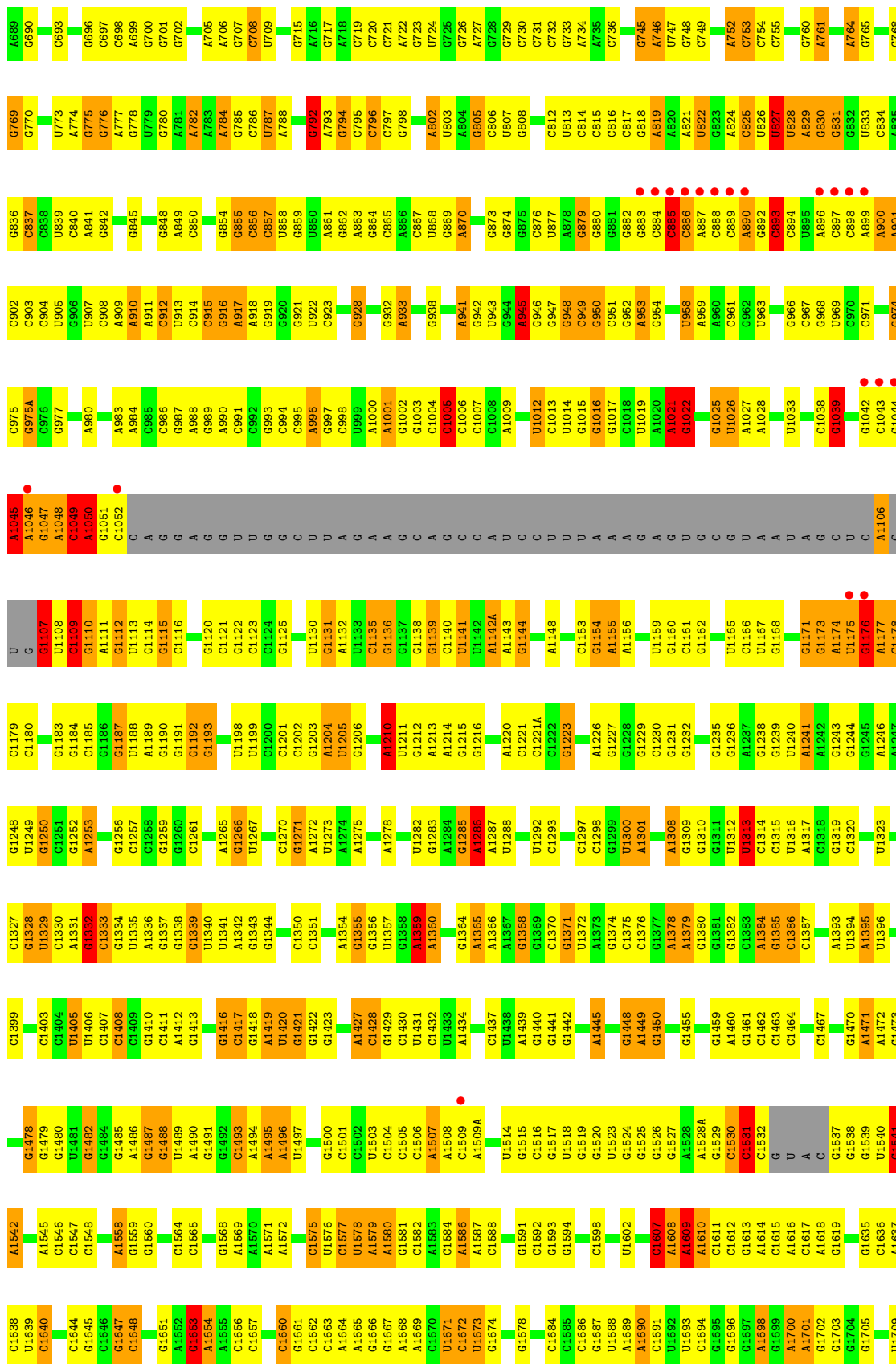
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	AA	2	Total	Mg	0	0
			2	2		
53	BA	2	Total	Mg	0	0
			2	2		

3 Residue-property plots

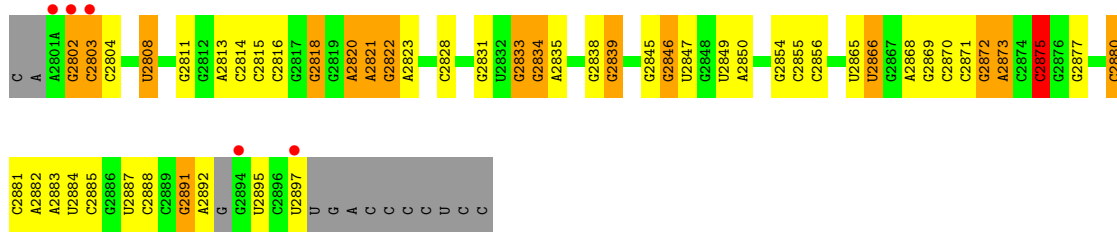
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S ribosomal RNA

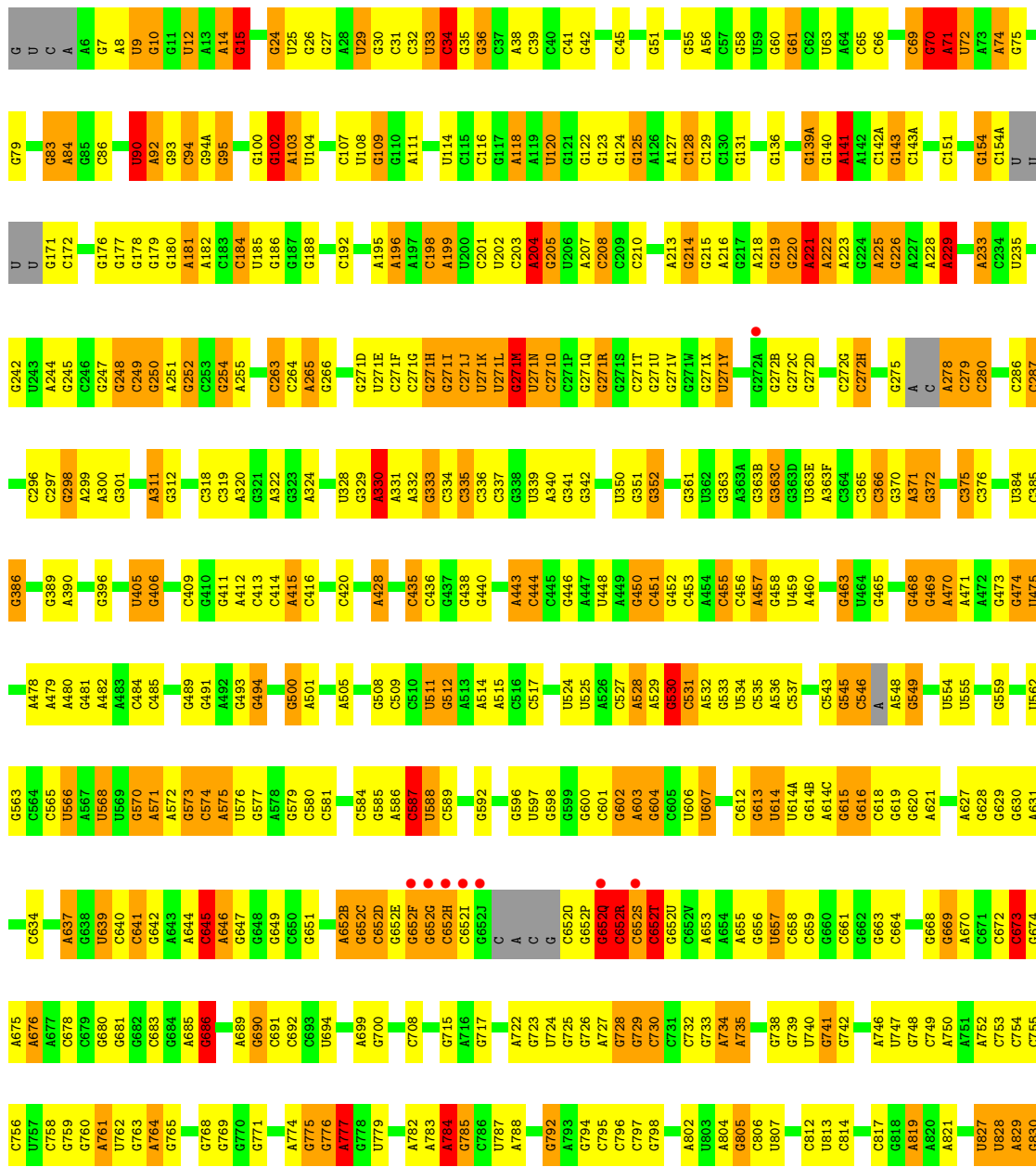


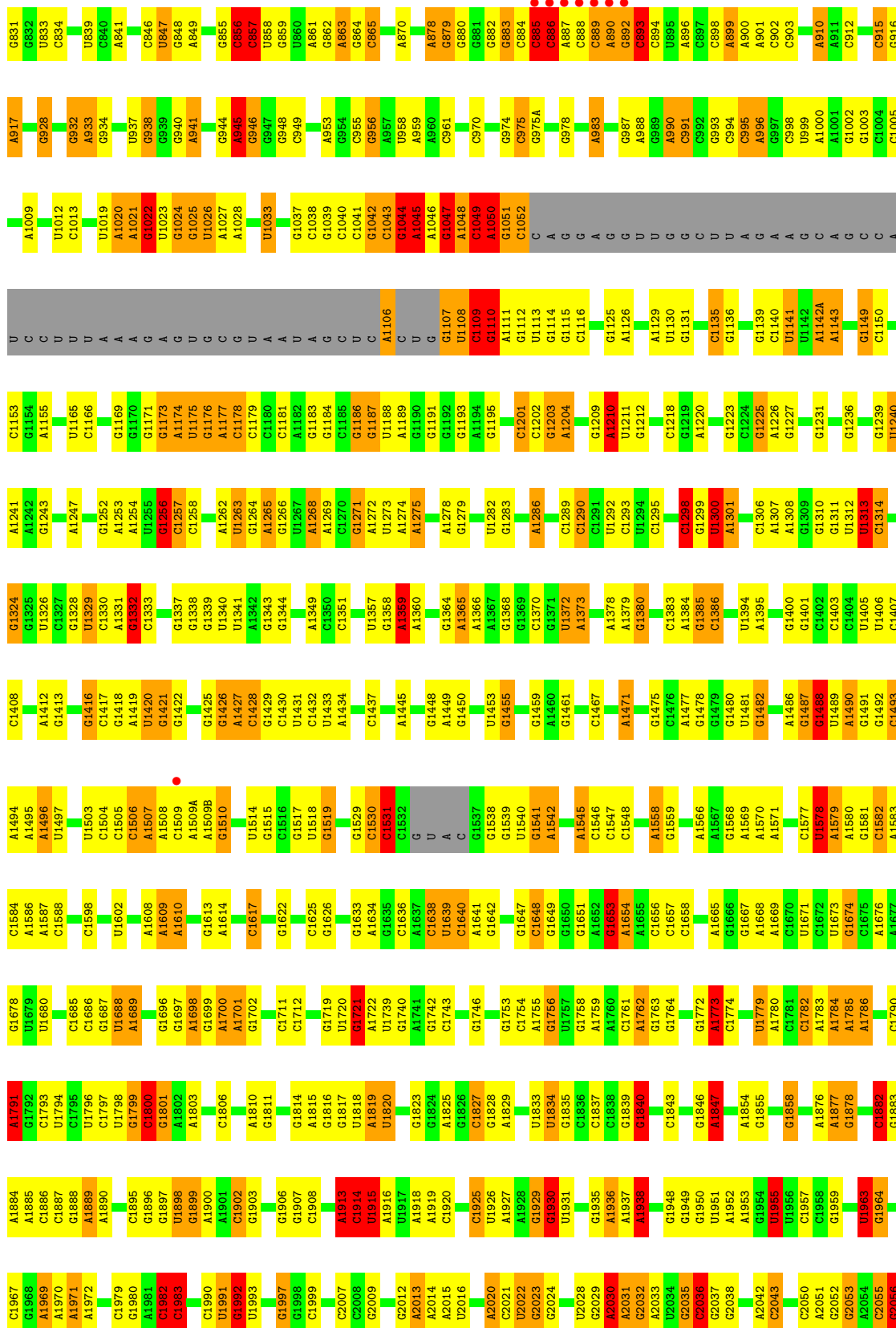


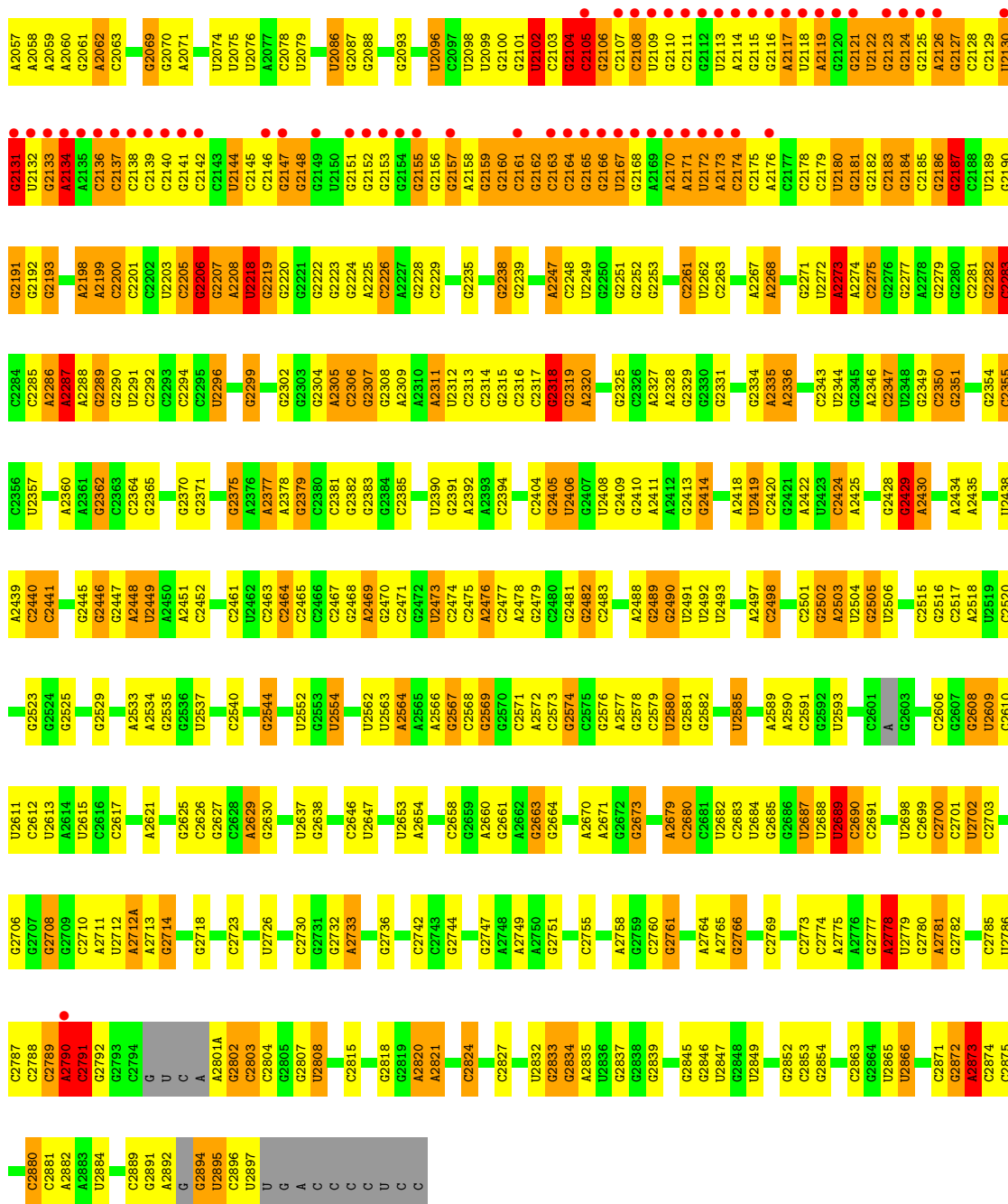
G2729	G2730	G2731	G2732	G2733	G2734	G2735	G2736	G2737	G2738	G2739	G2740	G2741	G2742	G2743	G2744	G2745	G2746	G2747	G2748	G2749	G2750	G2751	G2752	G2753	G2754	G2755	G2756	G2757	G2758	G2759	G2760	G2761	A2764	A2765	G2766	G2767	G2768	G2769	A2776	G2777	A2778	A2781	G2782	G2783	G2784	G2785	U2786	G2787	G2788	G2789	A2790	G2791	G2792	G2793	G2794	G	U
G2640	G2641	G2645	G2646	G2647	G2658	G2659	G2660	G2661	G2662	G2663	G2667	G2673	G2677	G2678	G2680	G2681	G2682	G2683	G2684	G2685	G2686	G2687	G2688	G2689	G2690	A2693	G2694	G2695	G2696	G2697	G2698	G2699	G2700	G2703	G2707	G2710	A2711	G2712	A2712A	A2713	G2714	A2721	G2722	G2723	U2726	G2727	U2728										
U2563	A2564	A2566	A2567	C2568	A2572	C2573	A2574	C2575	A2576	A2577	G2578	G2582	G2583	U2584	U2585	A2587	A2590	G2591	G2592	U2593	C2594	G2597	U2598	G2599	A2600	C2601	A	G2603	U2604	U2605	C2606	G2607	G2608	U2609	G2610	U2611	C2612	U2615	C2616	C2617	G2618	C2619	C2620	G2627	C2628	A2629	G2630	G2631	G2638	G2639	A2639						
G2490	U2493	G2494	G2495	G2496	G2497	G2498	G2499	U2500	C2501	G2502	A2503	U2504	G2505	U2506	G2507	G2508	C2512	G2513	U2514	C2515	G2516	C2517	A2518	U2519	C2520	C2521	U2522	G2523	G2524	G2525	C2526	G2529	G2530	A2531	G2535	G2536	U2537	C2538	C2539	A2542	G2543	G2544	G2550	G2551	U2552	G2553	U2554	G2558	C2559	U2560	U2562						
U2419	C2420	G2421	G2422	G2423	C2424	A2425	A2426	G2427	G2428	G2429	A2430	U2431	A2432	A2433	A2434	A2435	U2438	A2439	C2441	G2445	G2446	G2447	A2448	A2449	A2450	A2453	G2454	G2455	C2456	U2462	U2463	C2463	C2464	C2465	G2468	A2469	G2470	G2471	G2472	U2473	C2474	C2475	A2476	C2477	G2481	G2482	C2483	G2484	G2485	G2486	G2487	G2488	G2489				
C2350	G2351	A2352	G2353	G2354	C2355	C2356	U2357	C2358	G2359	U2360	A2361	G2362	C2363	G2364	A2366	G2367	G2371	A2376	A2377	A2378	G2379	C2380	C2381	C2382	G2383	G2384	C2385	C2386	U2387	A2388	G2389	U2390	G2391	C2392	C2393	C2394	C2395	G2396	G2399	G2400	C2403	G2404	G2405	U2406	G2407	U2408	G2409	G2410	A2411	G2414	G2415	G2416	G2417	G2418	G2419		
A2287	A2288	G2289	G2290	U2291	C2292	C2293	C2294	C2295	U2296	U2297	A2298	G2299	G2300	C2301	G2302	G2303	G2304	A2305	C2306	G2307	G2308	A2309	G2310	A2311	U2312	C2313	C2314	G2315	C2316	C2317	G2318	G2319	A2320	G2321	G2322	G2323	C2324	G2325	C2326	A2327	A2328	G2329	G2330	G2331	G2334	A2335	A2336	G2337	G2338	C2342	G2343	G2344	G2345	A2346	U2348	U2349	G2349
G2287	A2208	G2219	G2223	G2224	A2225	C2226	A2227	G2228	C2229	U2233	G2234	G2235	G2236	G2237	G2238	G2239	C2240	G2242	U2244	A2247	C2248	U2249	G2250	G2251	G2252	G2253	G2254	G2255	G2256	U2257	G2261	U2262	C2263	C2264	A2268	A2269	U2272	A2273	A2274	C2275	G2276	G2277	A2278	G2279	G2280	G2281	G2282	C2283	C2284	C2285	C2286	C2287	C2288	C2289	A2286		
U2074	U2075	C2076	G2077	G2078	G2079	C2081	A2082	G2083	C2085	U2086	G2089	C2095	U2096	C2097	U2098	U2099	G2100	C2102	C2103	G2104	C2105	G2106	C2107	C2108	U2109	G2110	C2111	G2112	U2113	C2114	G2115	G2116	A2117	U2118	A2119	C2120	U2122	G2123	G2124	G2125	A2126	G2127	U2130	U2132	G2133	A2134	A2135	C2136	C2137	C2138	C2139	C2140	G2141				
G1988	C1999	C2007	G2010	U2011	G2012	A2013	A2014	C2015	U2016	G2017	G2018	A2019	A2020	C2021	U2022	G2023	G2024	G2027	U2028	U2029	A2031	G2032	C2033	U2034	G2035	C2036	C2040	U2041	A2042	C2043	G2049	C2050	A2051	G2052	C2055	G2056	A2057	A2058	A2059	A2060	G2061	C2062	C2063	C2064	C2065	C2066	U2068	G2069	A2070	G2071							
C1944	U1945	A1916	U1917	A1918	U1919	C1920	A1927	A1928	U1929	G1930	U1931	C1934	U1935	A1936	U1937	A1938	U1939	U1940	C1942	U1946	C1947	G1948	U1955	C1962	U1963	G1964	C1965	A1966	C1967	G1968	A1969	A1970	A1971	C1972	U1973	A1974	C1975	U1976	A1977	C1982	A1986	C1987	A1988	A1989	C1992	U1993	C1994	G1997									
U1805	G1814	A1815	G1816	U1817	U1818	A1819	U1820	G1823	G1826	C1827	G1828	A1829	U1833	U1834	U1835	C1836	C1837	C1838	G1839	G1840	C1844	A1847	A1848	G1849	G1850	A1853	A1854	G1855	G1858	A1863	A1876	A1877	G1878	C1882	G1883	A1884	A1889	A1890	G1891	C1892	G1899	A1900	G1906	A1913													
C1710	C1711	C1712	U1720	G1721	U1722	U1739	G1740	A1741	G1742	C1743	G1746	G1753	A1754	U1755	G1756	U1757	G1758	C1761	G1762	G1763	G1764	C1765	C1766	C1767	A1773	U1775	U1779	A1780	C1781	C1782	A1783	A1784	A1785	A1786	A1787	C1788	A1789	C1790	A1791	G1792	C1793	U1794	C1795	U1796	C1797	U1798	C1800	G1801	A1802	C1804							



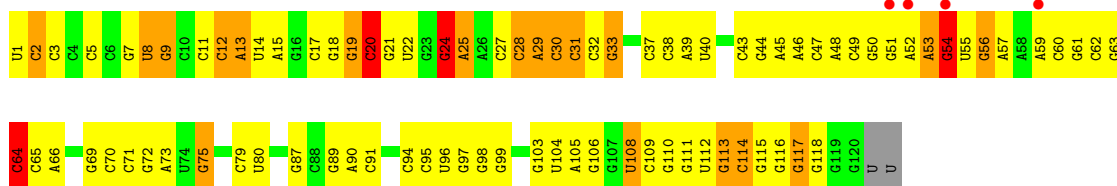
• Molecule 1: 23S ribosomal RNA





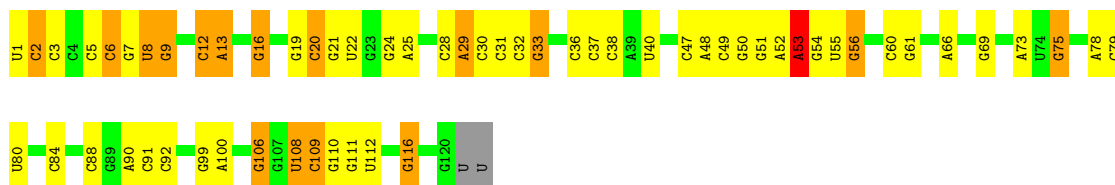


• Molecule 2: 5S ribosomal RNA



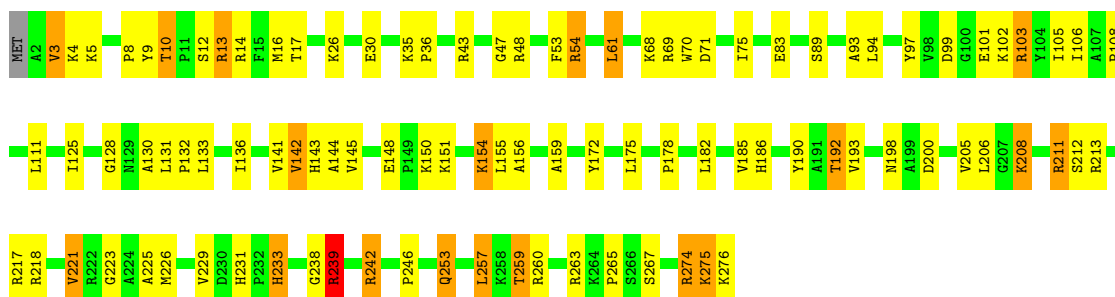
• Molecule 2: 5S ribosomal RNA

Chain BB: 



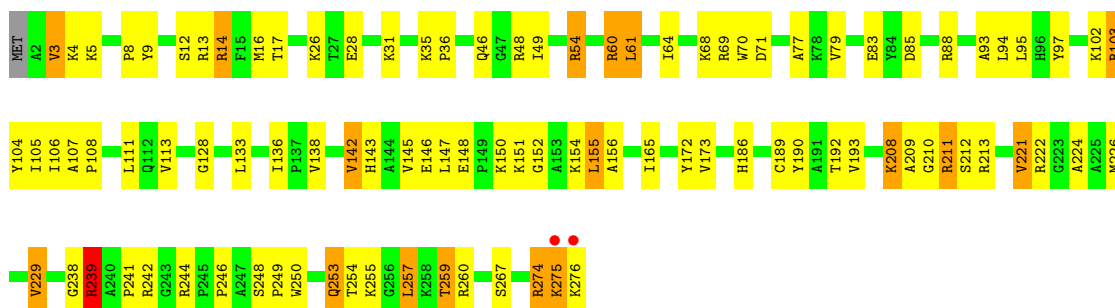
• Molecule 3: 50S ribosomal protein L2

Chain AD: 



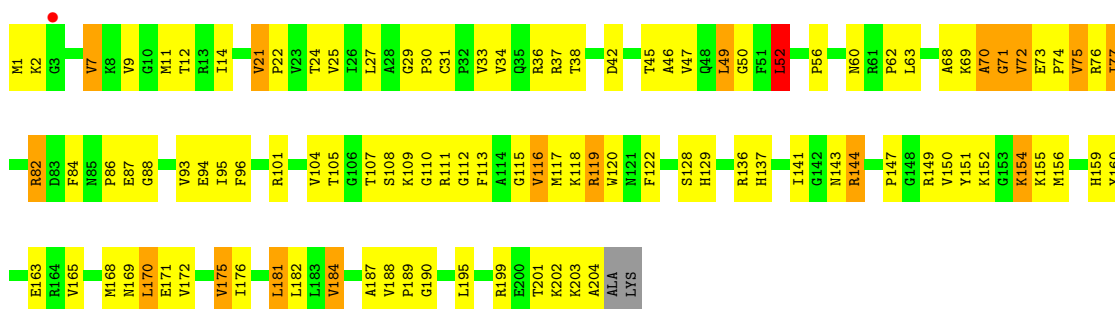
• Molecule 3: 50S ribosomal protein L2

Chain BD: 



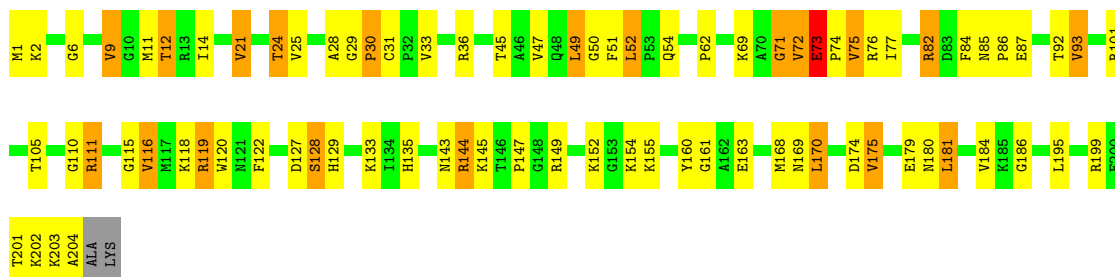
• Molecule 4: 50S ribosomal protein L3

Chain AE: 



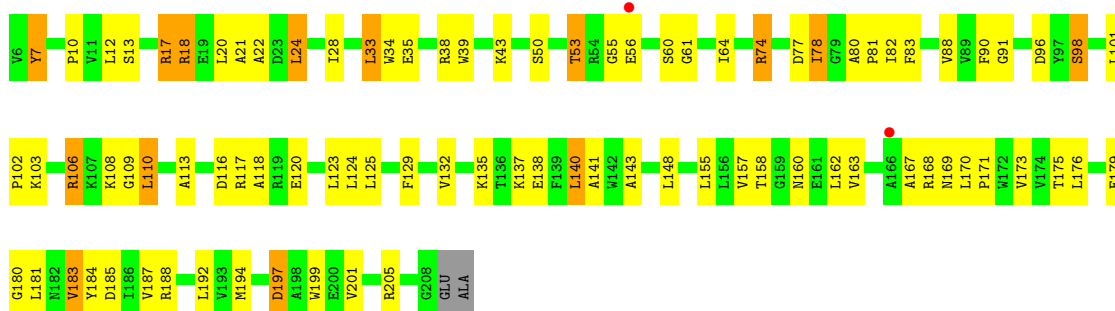
• Molecule 4: 50S ribosomal protein L3

Chain BE: 



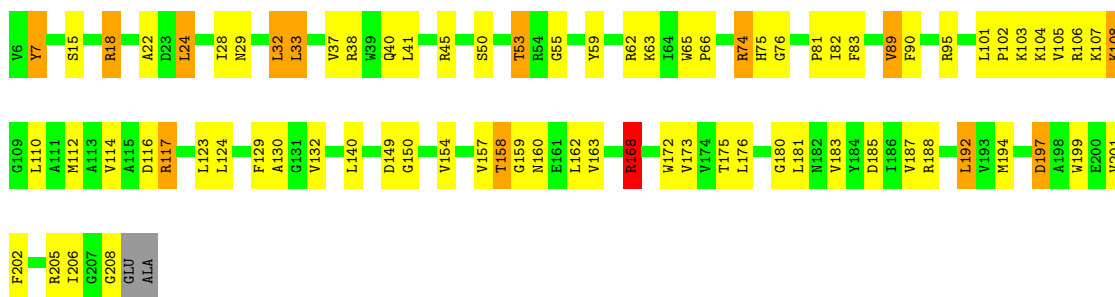
• Molecule 5: 50S ribosomal protein L4

Chain AF: 



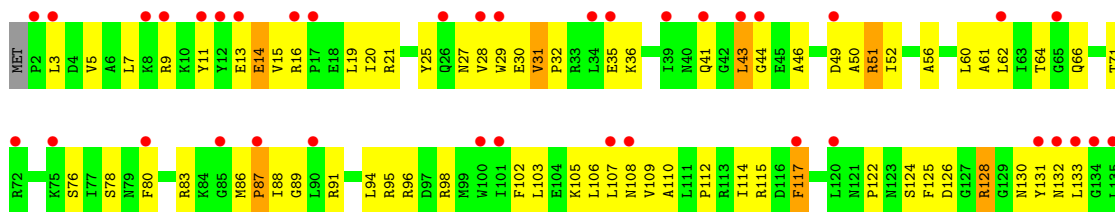
• Molecule 5: 50S ribosomal protein L4

Chain BF: 



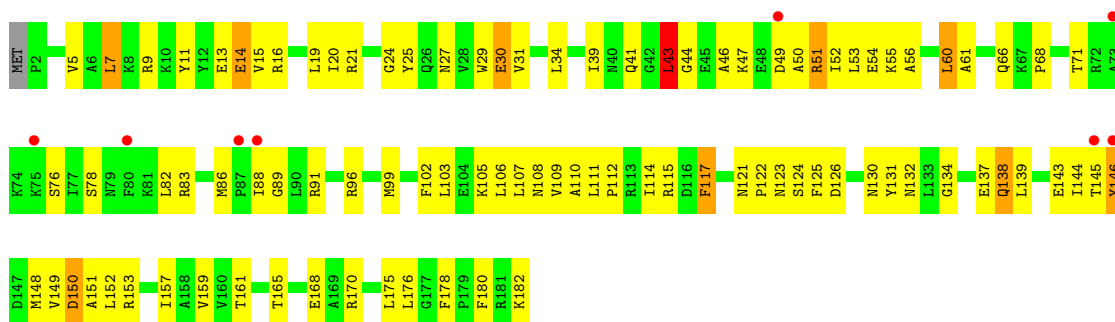
• Molecule 6: 50S ribosomal protein L5

Chain AG: 

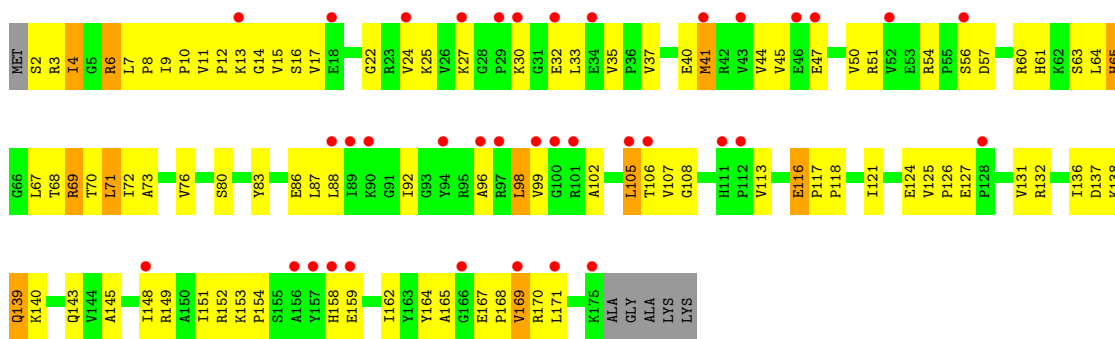




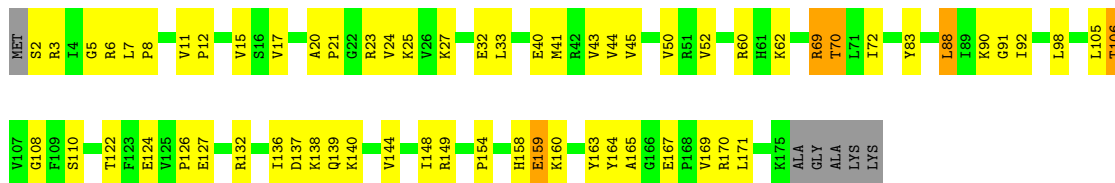
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6

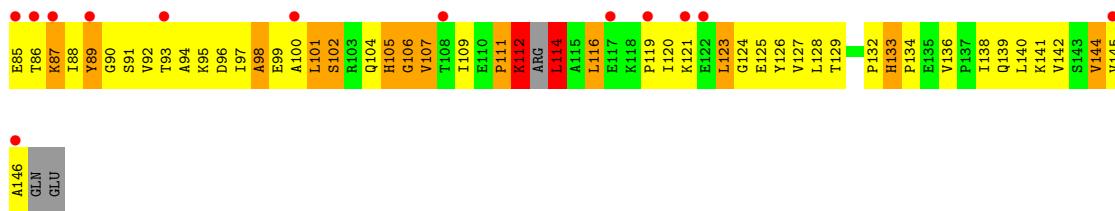


- Molecule 7: 50S ribosomal protein L6

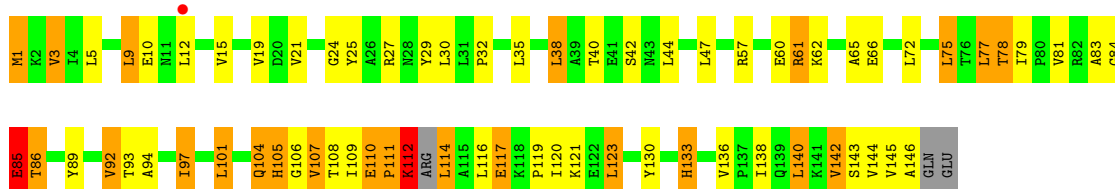


- Molecule 8: 50S ribosomal protein L9

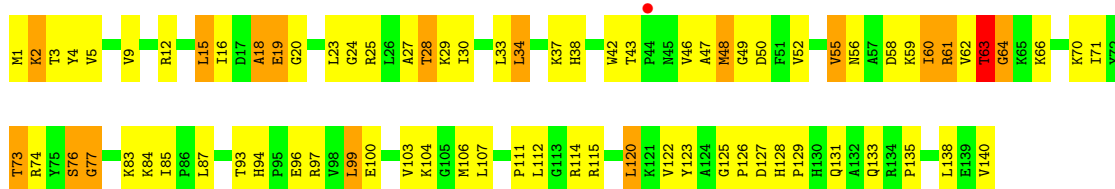




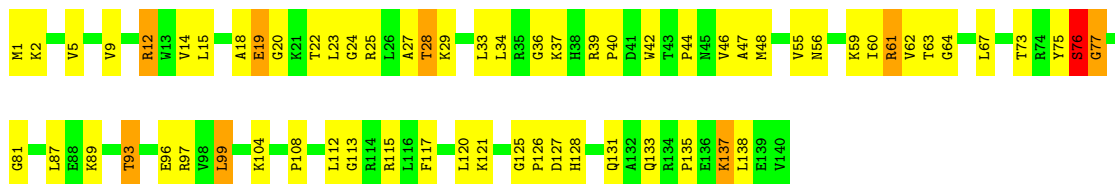
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



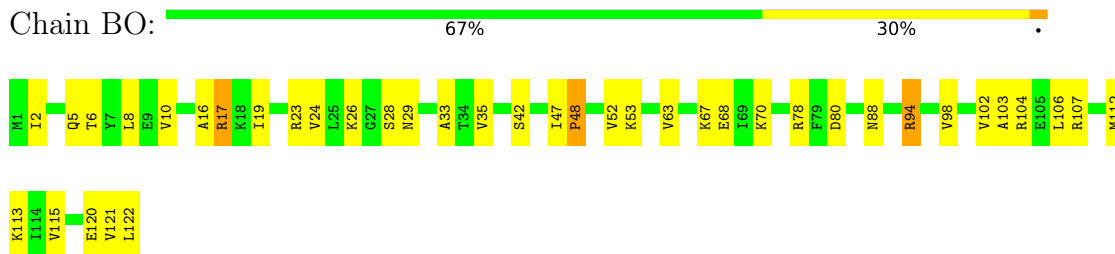
- Molecule 9: 50S ribosomal protein L13



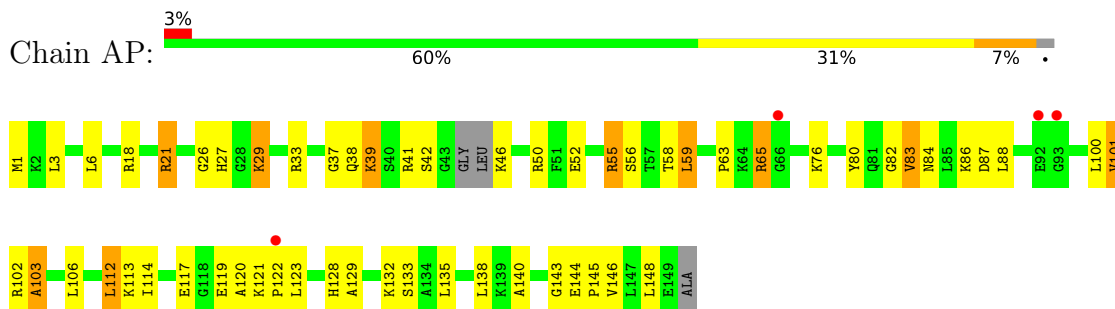
- Molecule 10: 50S ribosomal protein L14



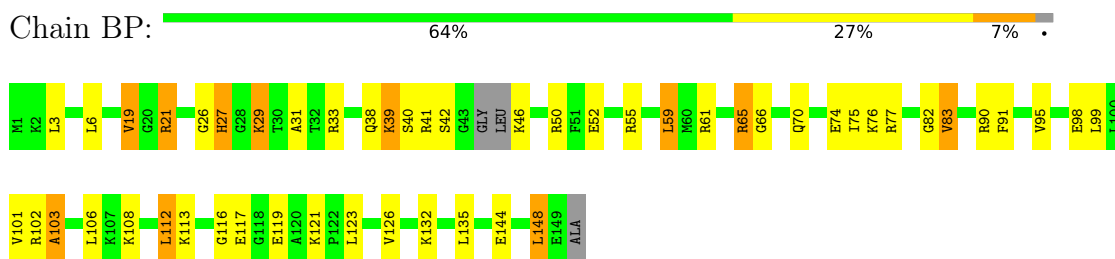
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



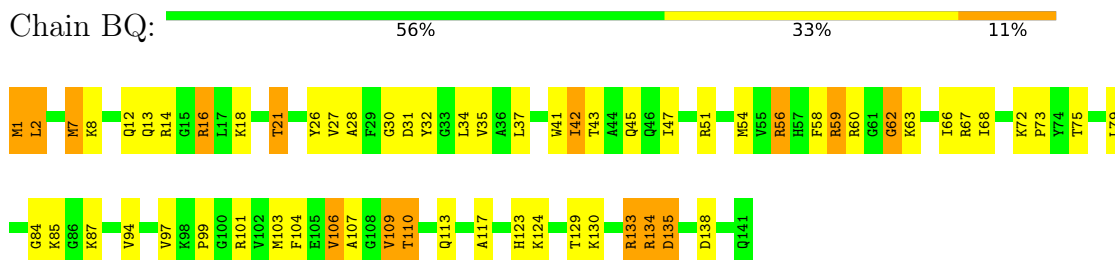
- Molecule 11: 50S ribosomal protein L15



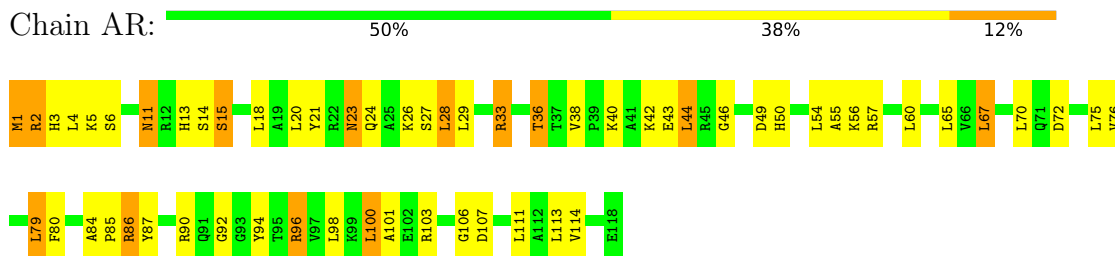
- Molecule 12: 50S ribosomal protein L16



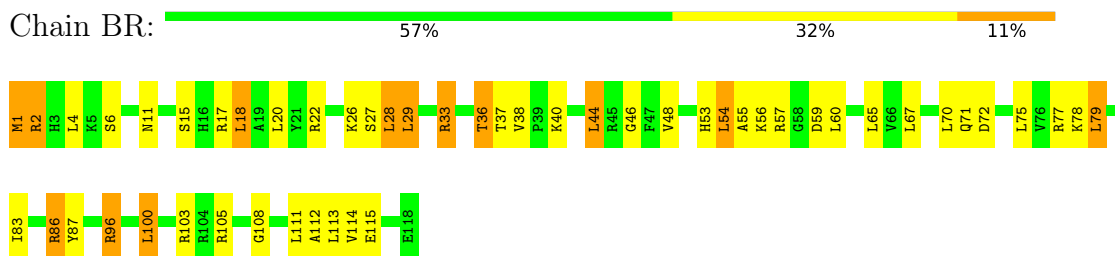
- Molecule 12: 50S ribosomal protein L16



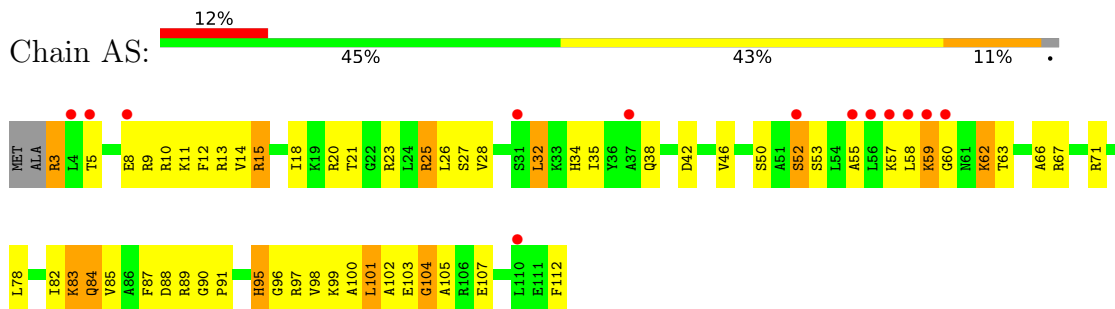
- Molecule 13: 50S ribosomal protein L17



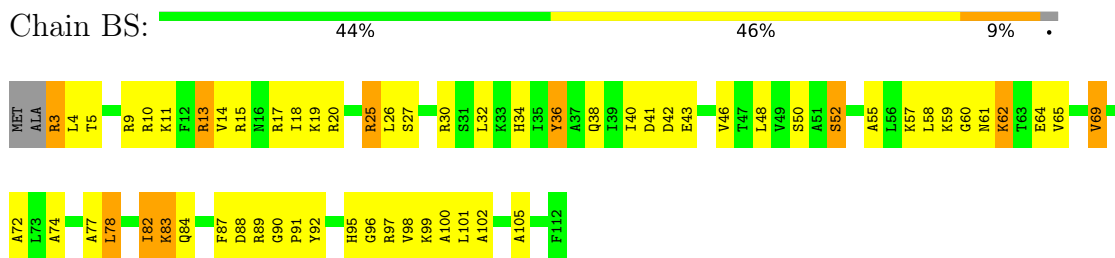
- Molecule 13: 50S ribosomal protein L17



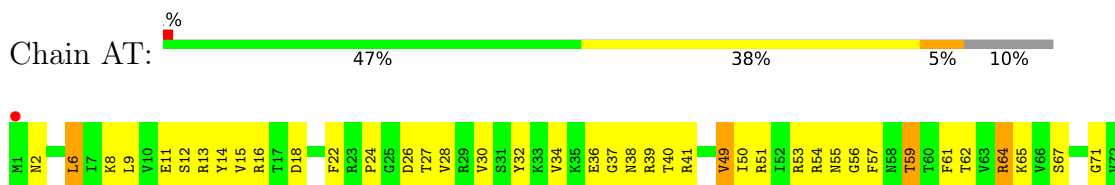
- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18

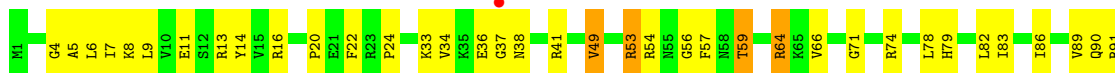


- Molecule 15: 50S ribosomal protein L19

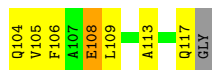




- Molecule 15: 50S ribosomal protein L19



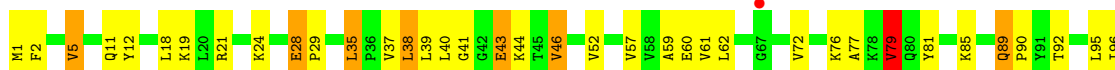
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



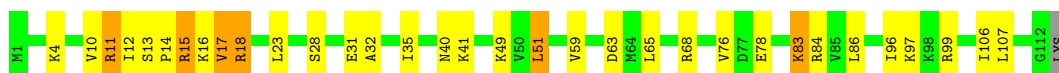
- Molecule 18: 50S ribosomal protein L22

Chain AW:  60% 34% 5%



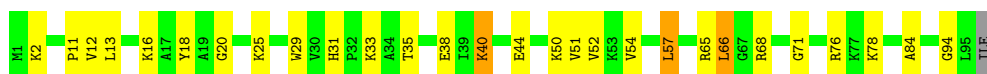
- Molecule 18: 50S ribosomal protein L22

Chain BW:  70% 24% 5%



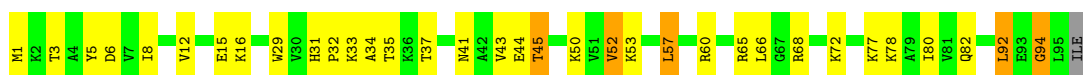
- Molecule 19: 50S ribosomal protein L23

Chain AX:  70% 26%



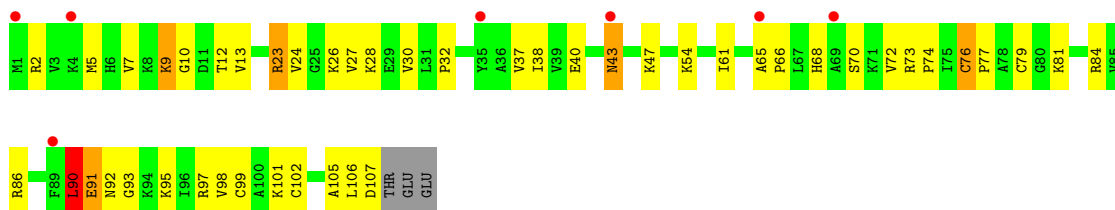
- Molecule 19: 50S ribosomal protein L23

Chain BX:  64% 30% 5%



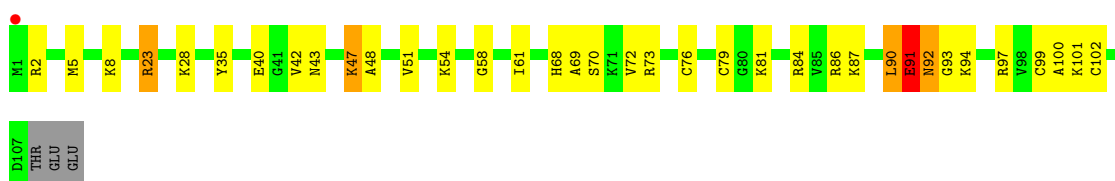
- Molecule 20: 50S ribosomal protein L24

Chain AY:  6% 55% 37% 5%

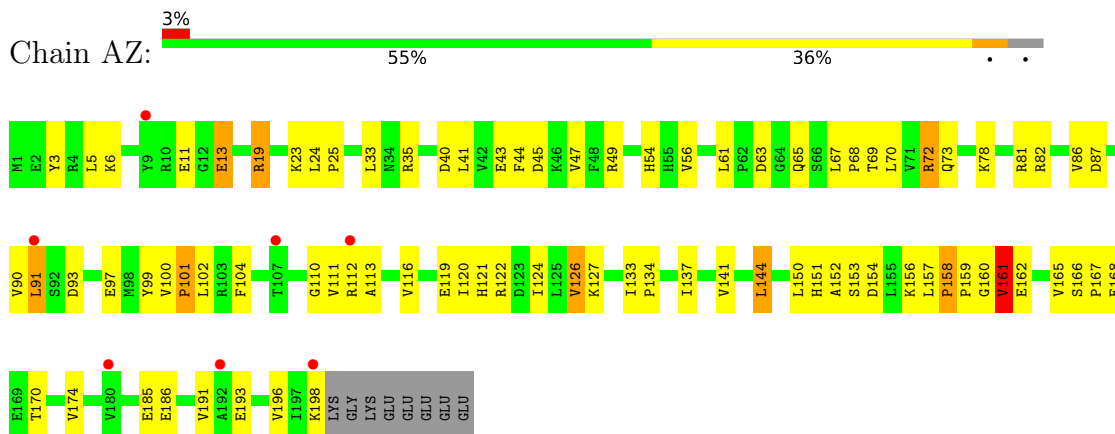


- Molecule 20: 50S ribosomal protein L24

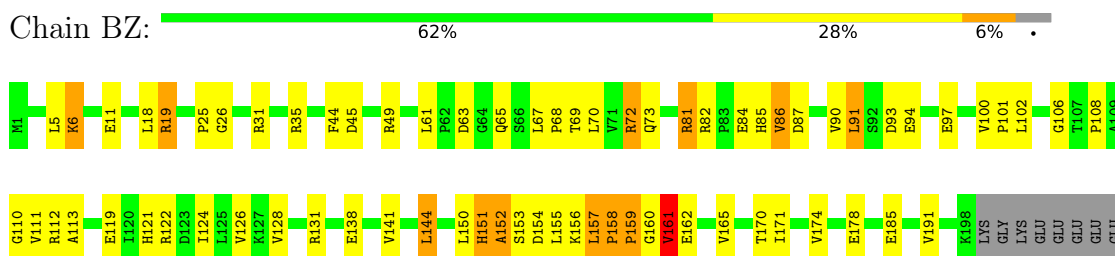
Chain BY:  65% 28%



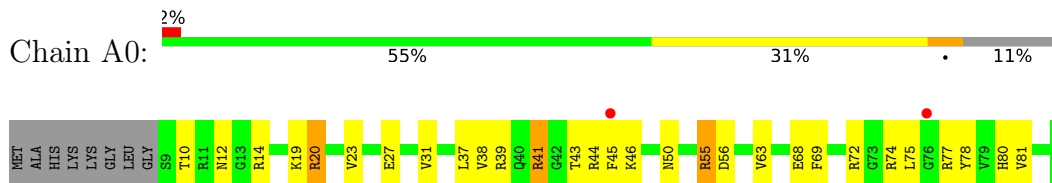
- Molecule 21: 50S ribosomal protein L25



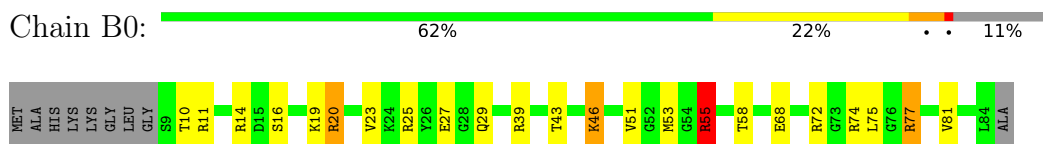
- Molecule 21: 50S ribosomal protein L25



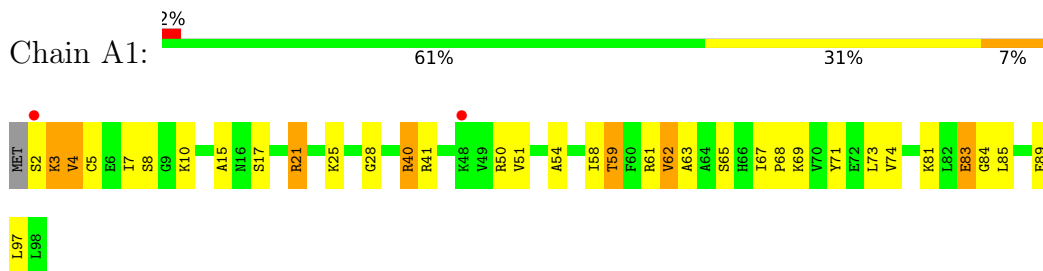
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27



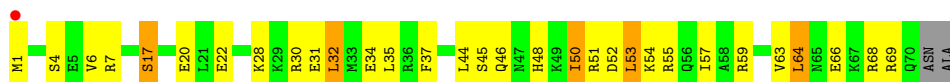
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



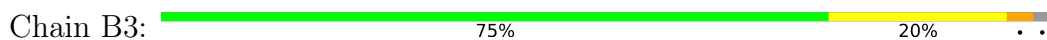
- Molecule 24: 50S ribosomal protein L29



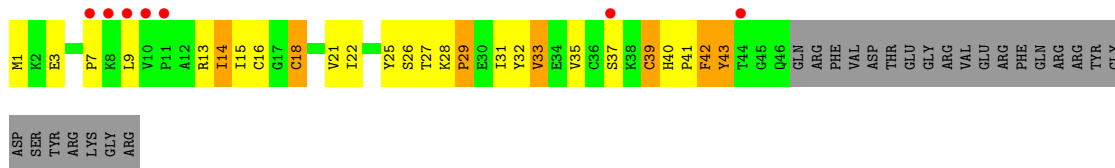
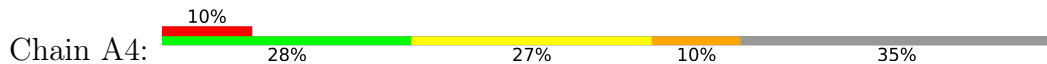
- Molecule 25: 50S ribosomal protein L30



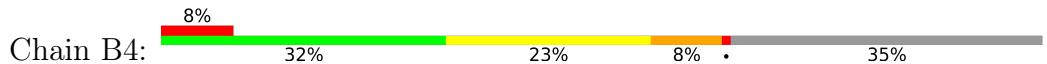
- Molecule 25: 50S ribosomal protein L30

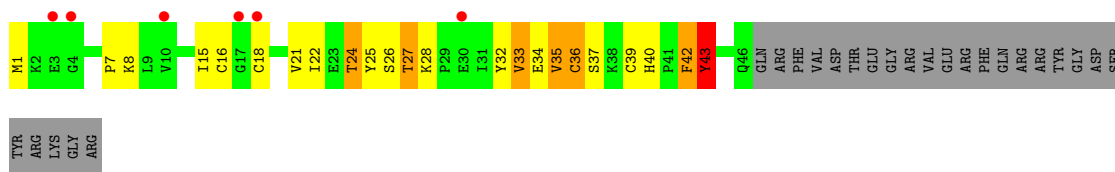


- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31

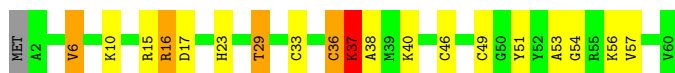




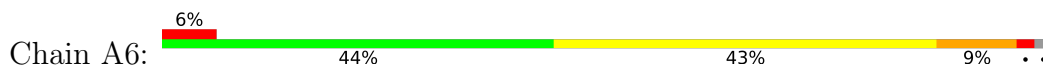
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



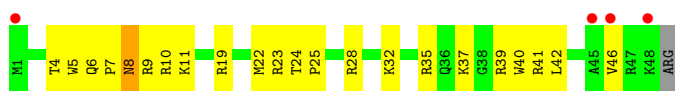
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



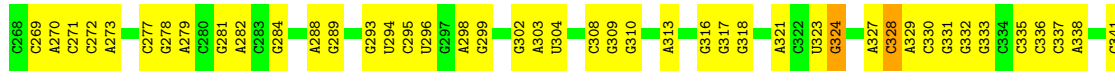
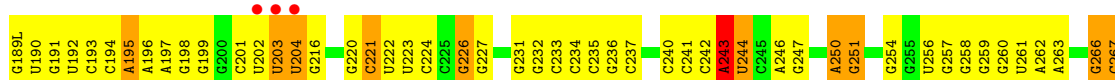
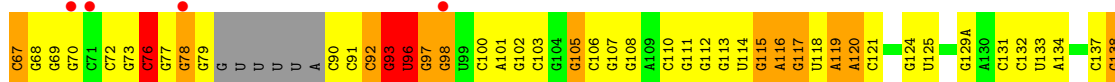
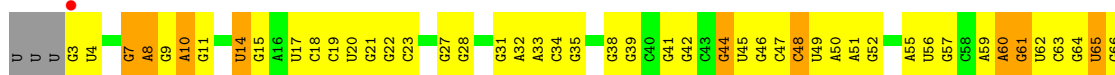
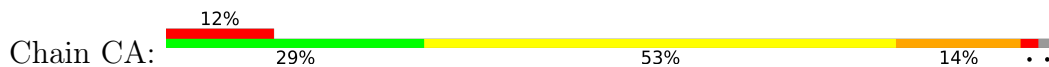
- Molecule 30: 50S ribosomal protein L35

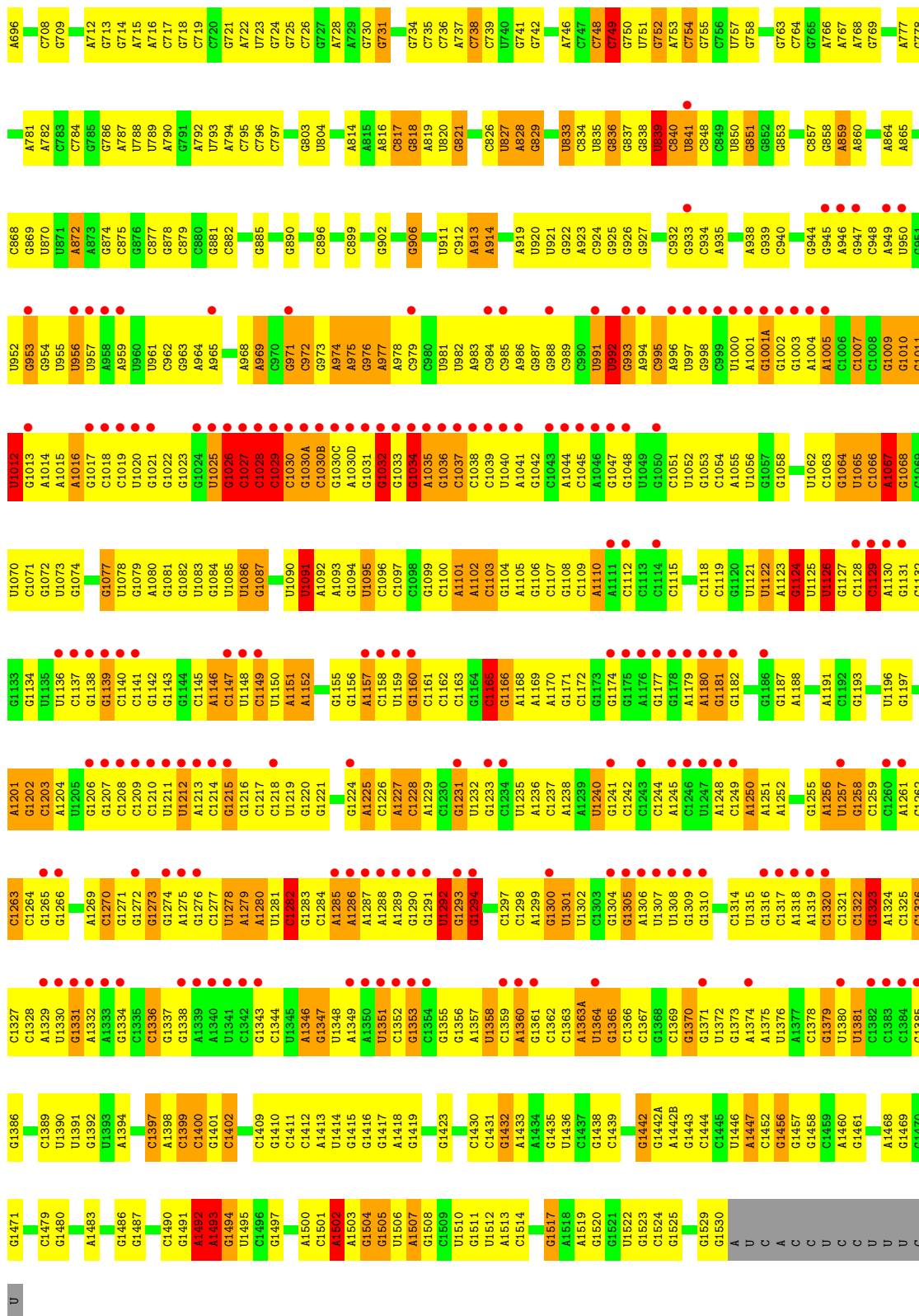


- Molecule 30: 50S ribosomal protein L35

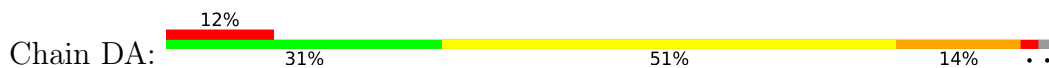


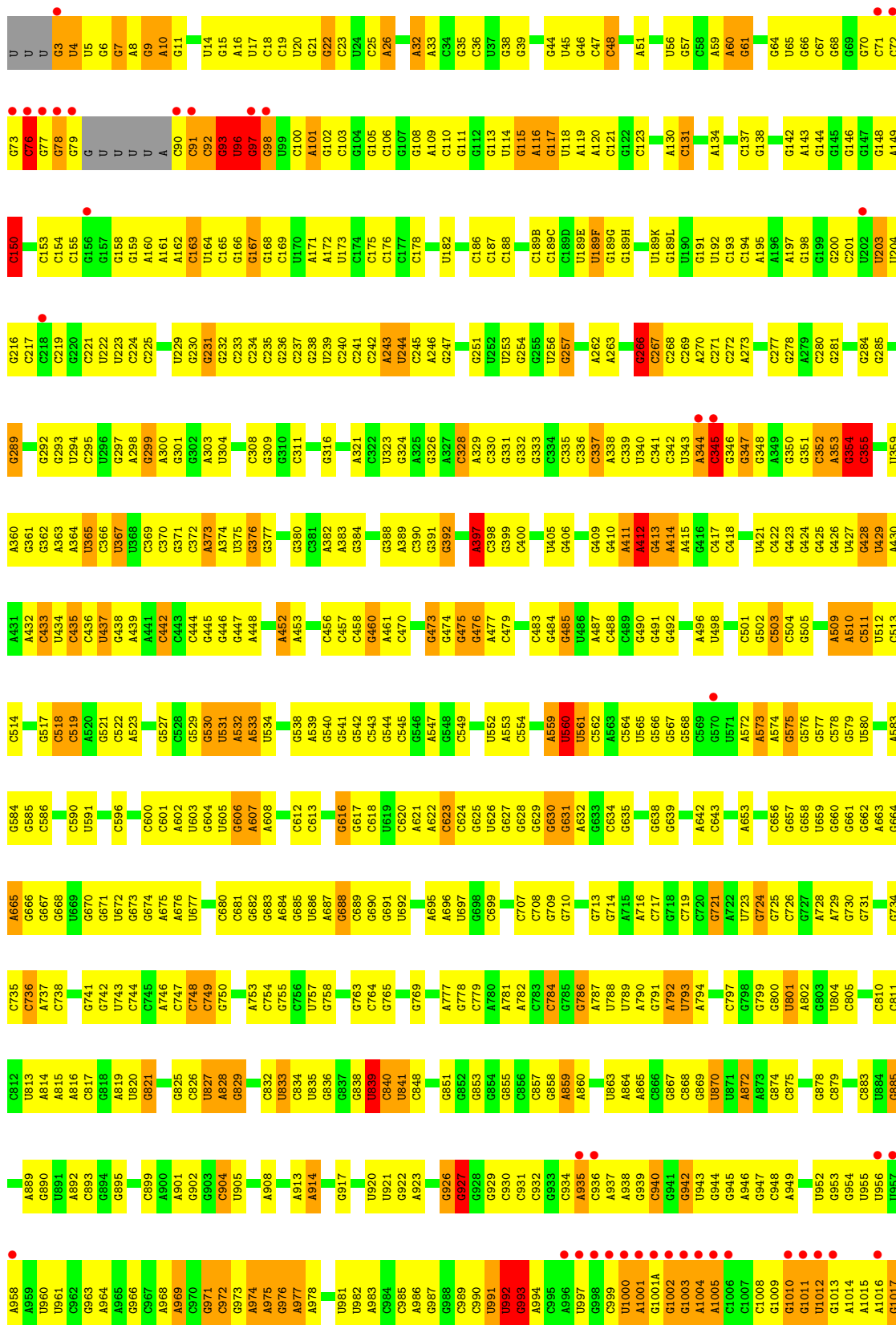
- Molecule 31: 16S ribosomal RNA

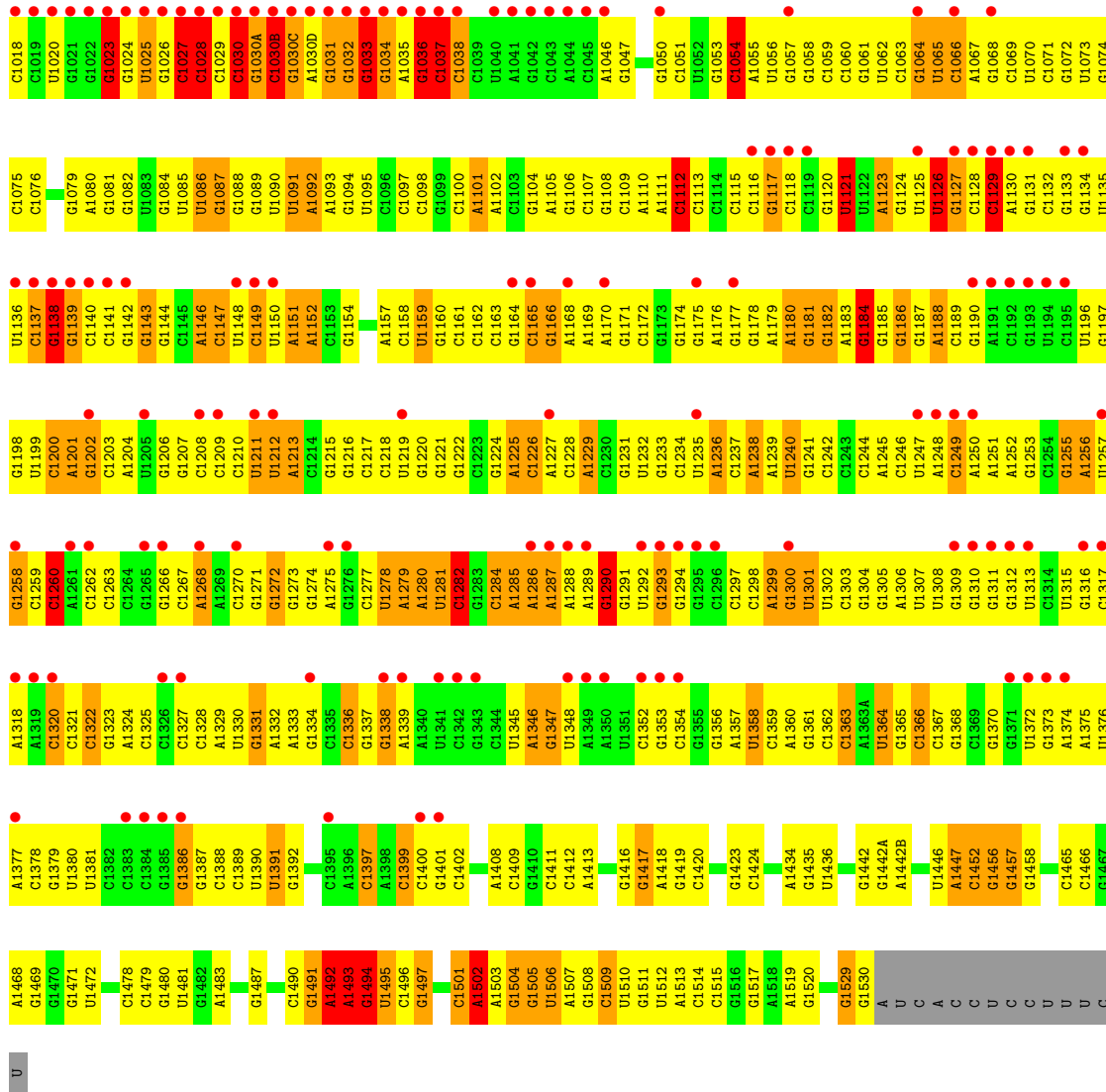




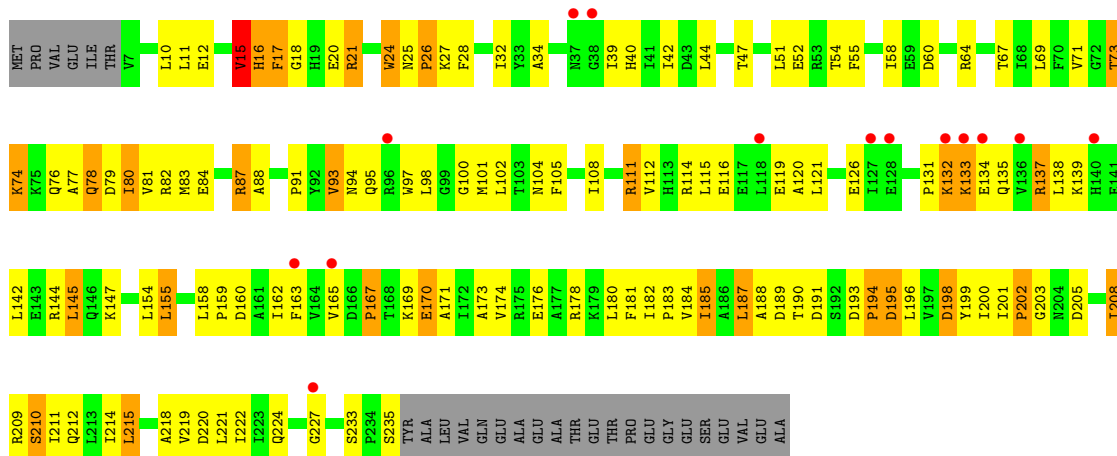
• Molecule 31: 16S ribosomal RNA



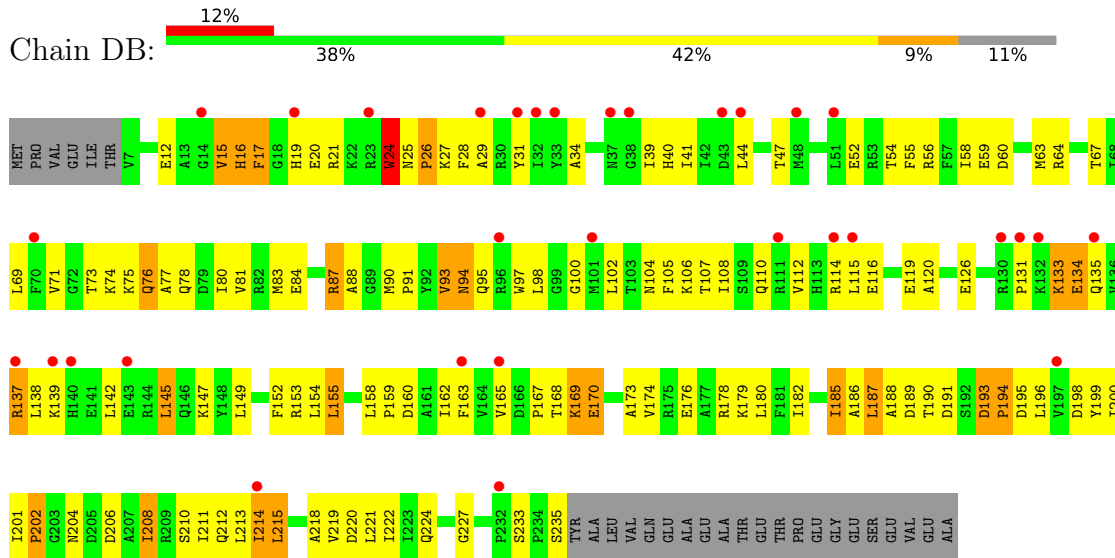




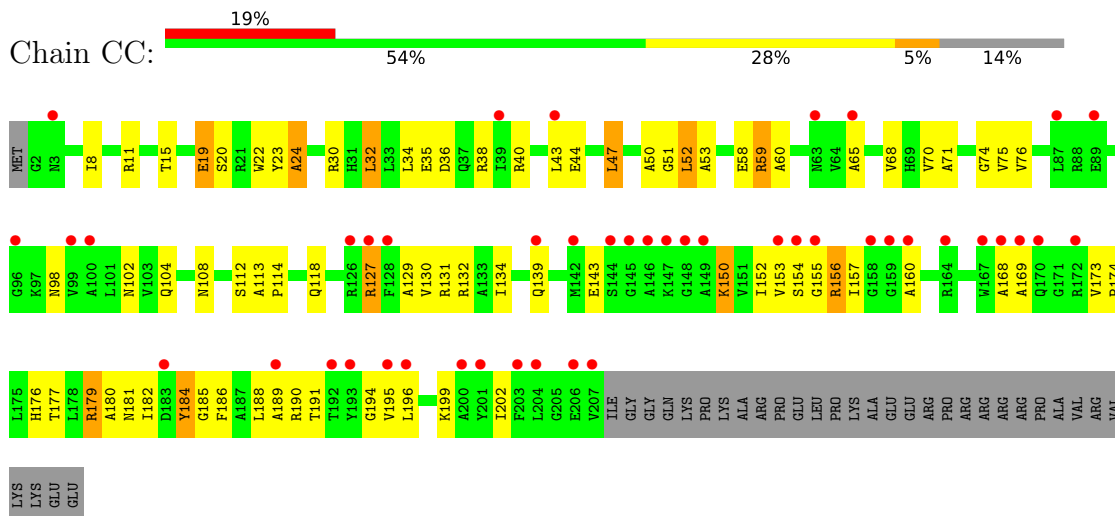
● Molecule 32: 30S ribosomal protein S2



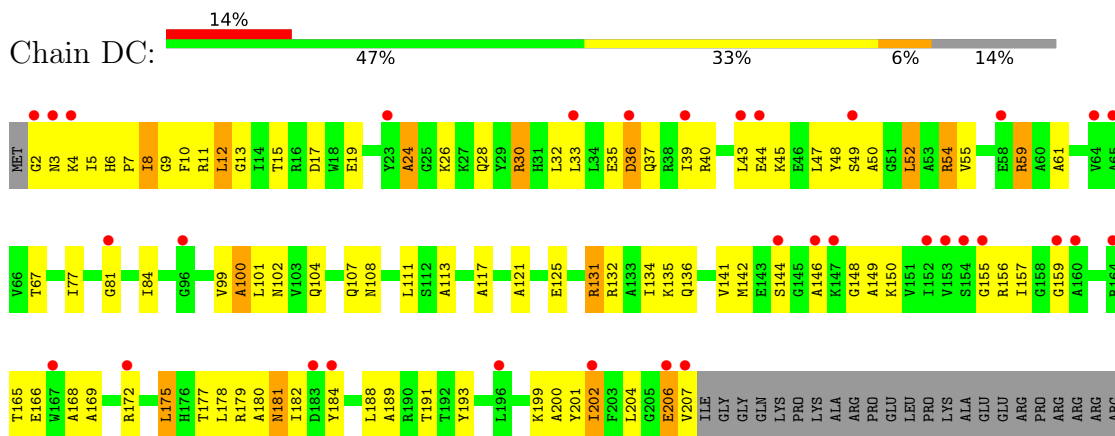
● Molecule 32: 30S ribosomal protein S2



● Molecule 33: 30S ribosomal protein S3

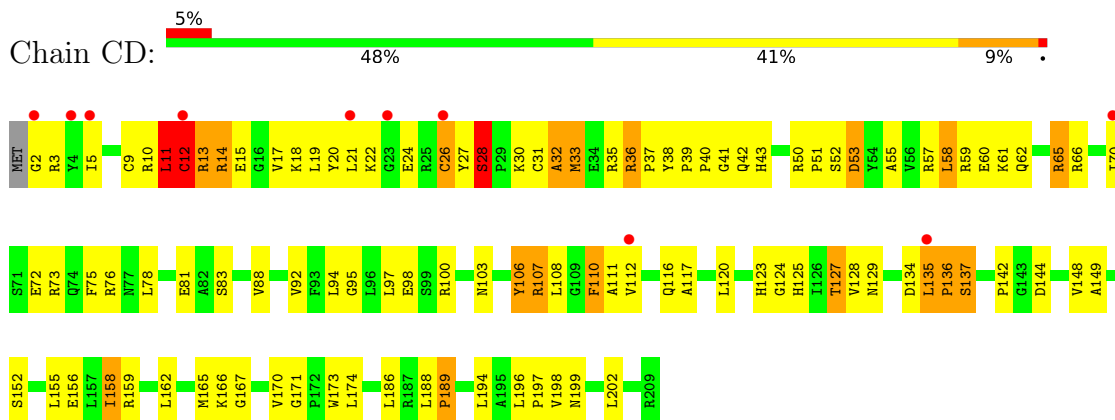


● Molecule 33: 30S ribosomal protein S3

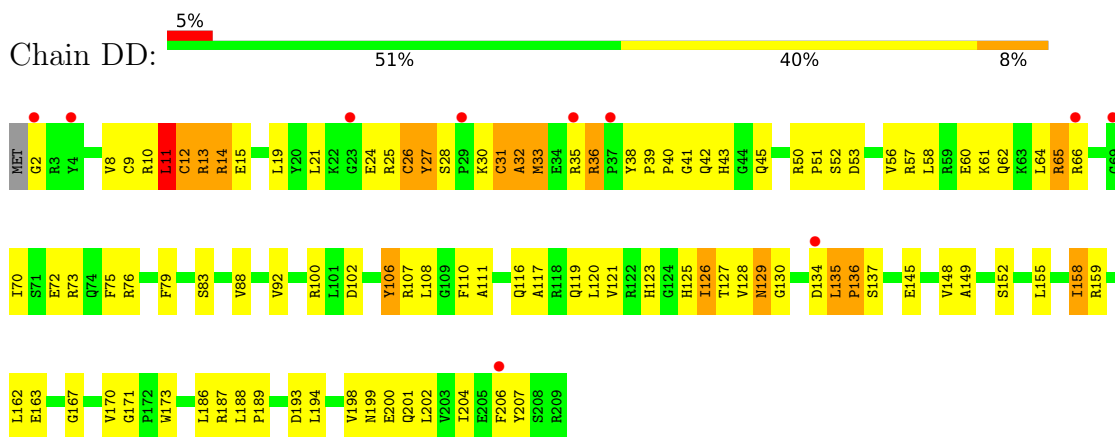


PRO
ALA
VAL
ARG
VAL
LVS
LVS
GLU
GLU

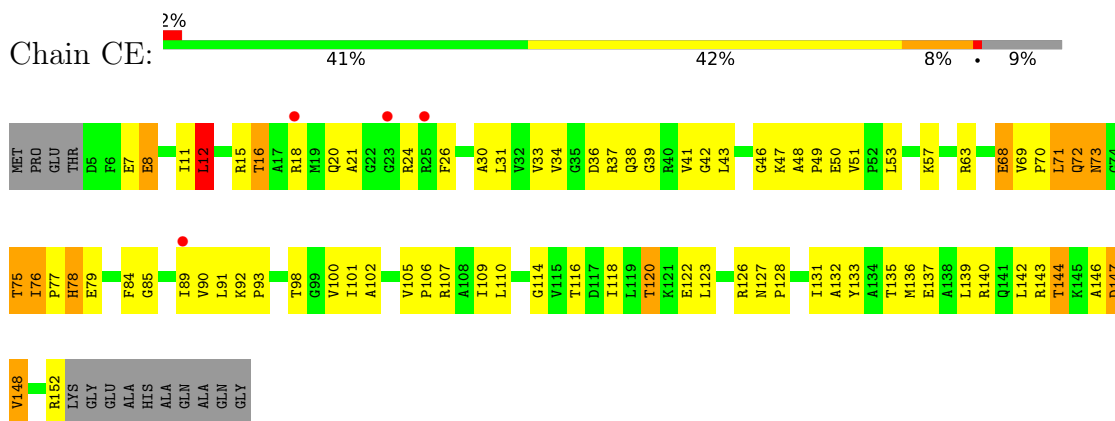
- Molecule 34: 30S ribosomal protein S4



- Molecule 34: 30S ribosomal protein S4

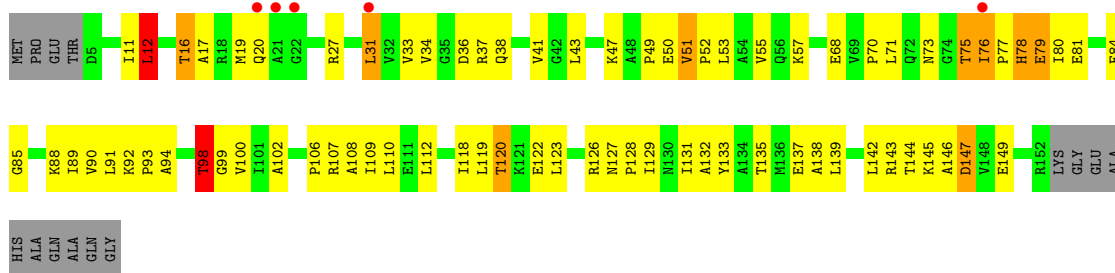


- Molecule 35: 30S ribosomal protein S5

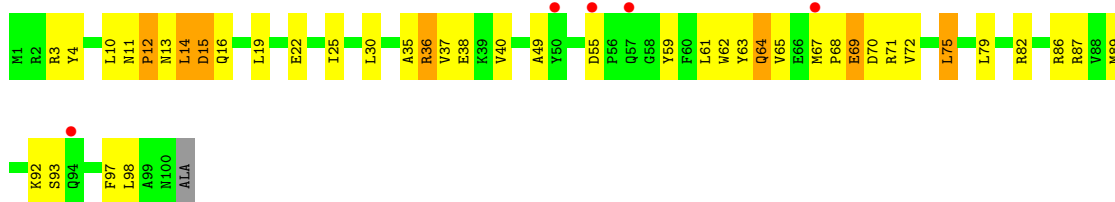


- Molecule 35: 30S ribosomal protein S5

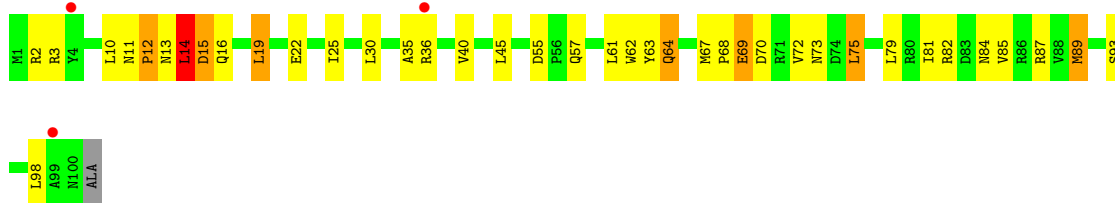




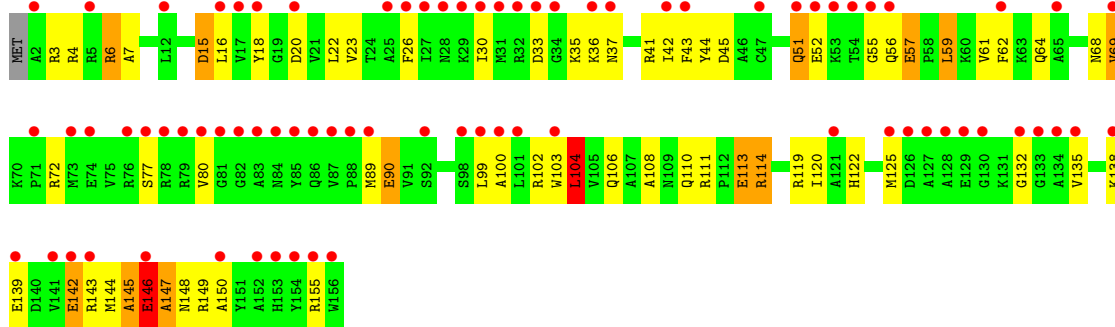
• Molecule 36: 30S ribosomal protein S6



• Molecule 36: 30S ribosomal protein S6

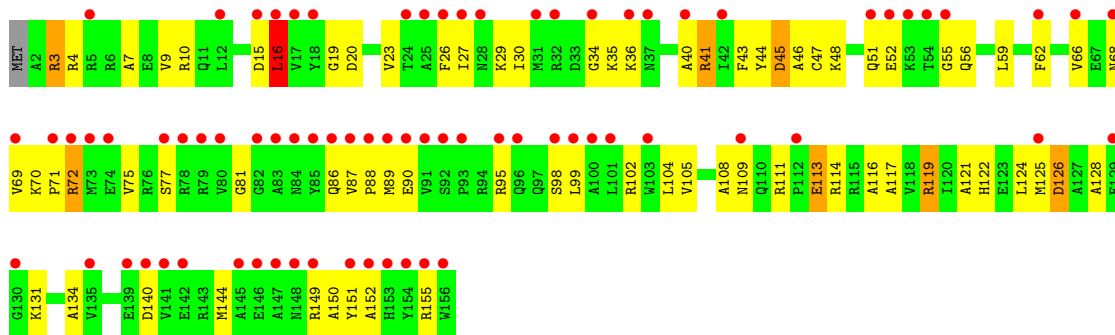


• Molecule 37: 30S ribosomal protein S7

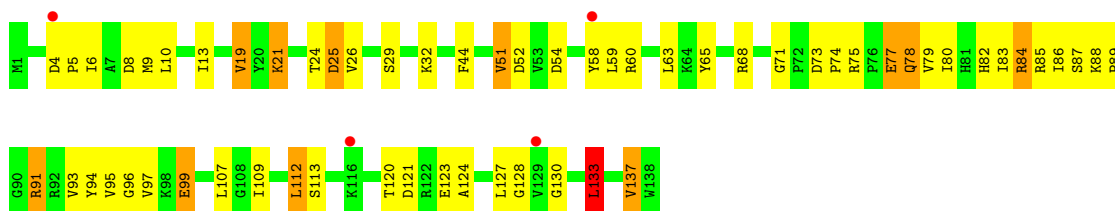


• Molecule 37: 30S ribosomal protein S7

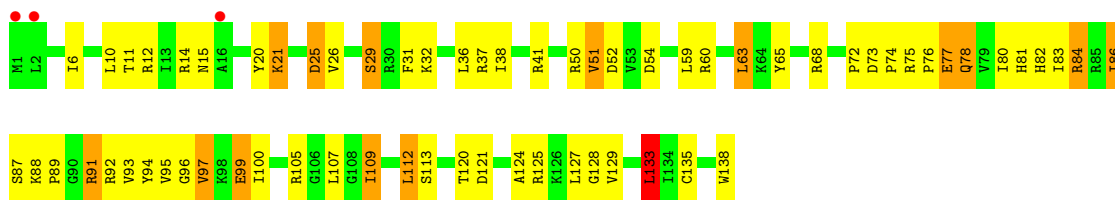




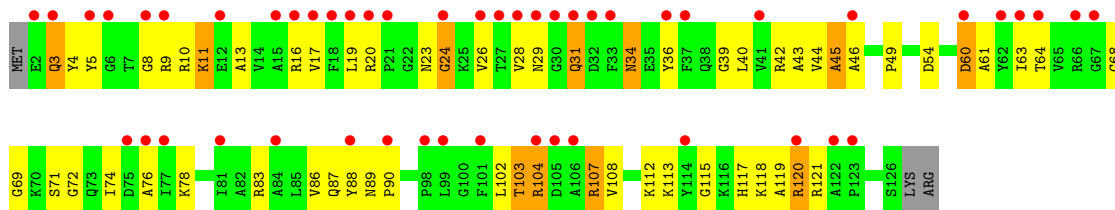
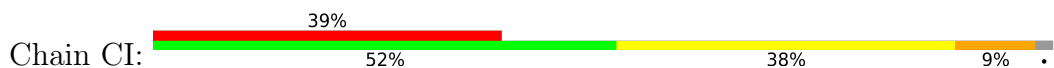
• Molecule 38: 30S ribosomal protein S8



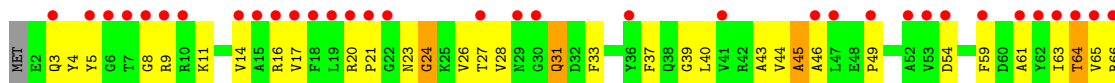
• Molecule 38: 30S ribosomal protein S8

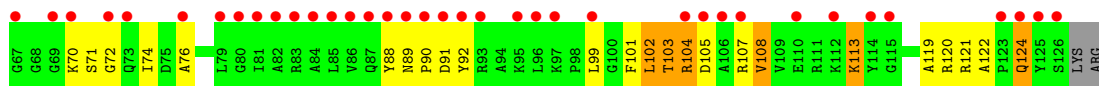


• Molecule 39: 30S ribosomal protein S9

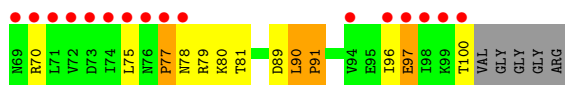
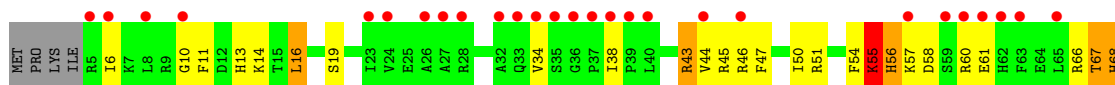
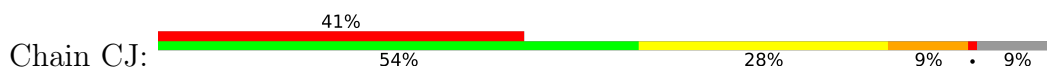


• Molecule 39: 30S ribosomal protein S9

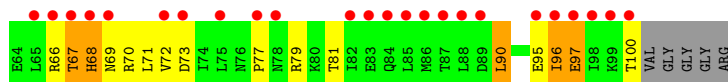
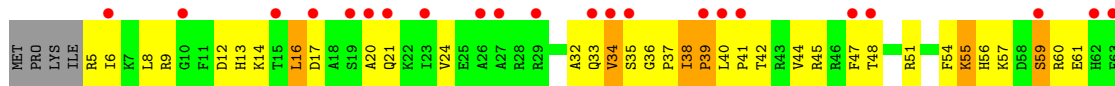
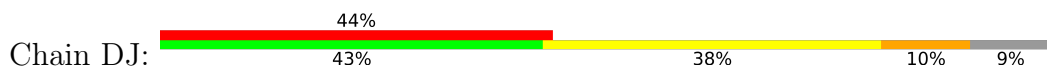




- Molecule 40: 30S ribosomal protein S10



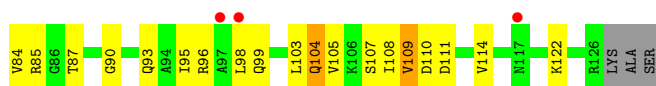
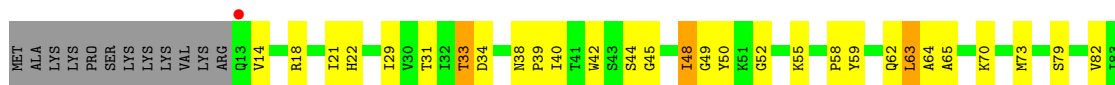
- Molecule 40: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S11



- Molecule 41: 30S ribosomal protein S11

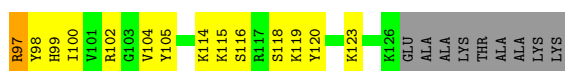
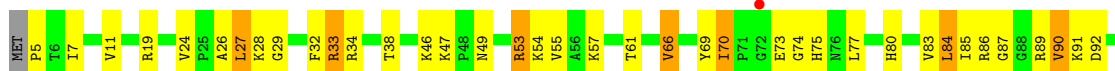


- Molecule 42: 30S ribosomal protein S12

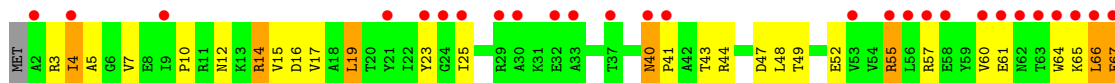
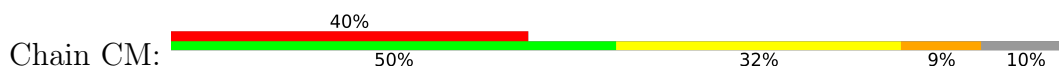




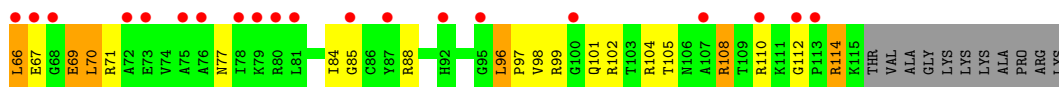
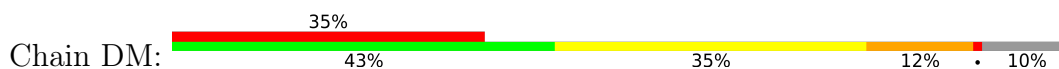
- Molecule 42: 30S ribosomal protein S12



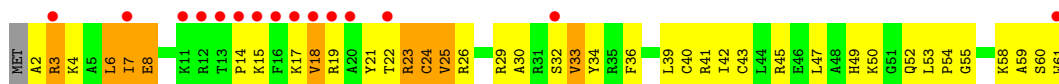
- Molecule 43: 30S ribosomal protein S13



- Molecule 43: 30S ribosomal protein S13

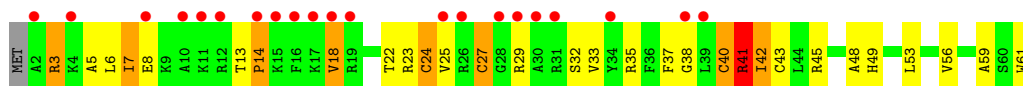


- Molecule 44: 30S ribosomal protein S14



- Molecule 44: 30S ribosomal protein S14





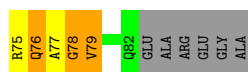
• Molecule 45: 30S ribosomal protein S15



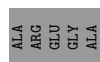
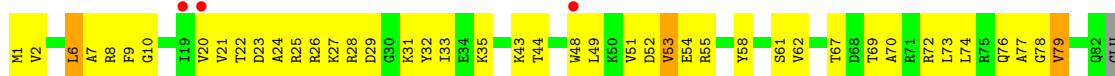
• Molecule 45: 30S ribosomal protein S15



• Molecule 46: 30S ribosomal protein S16

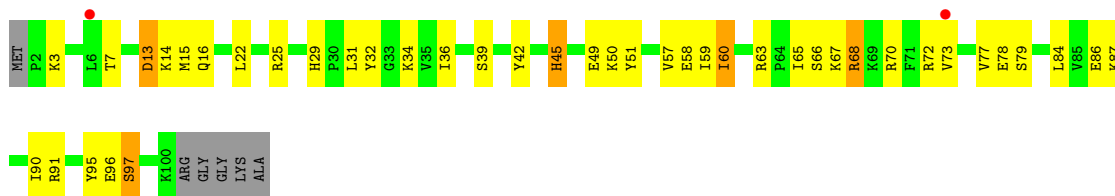


• Molecule 46: 30S ribosomal protein S16

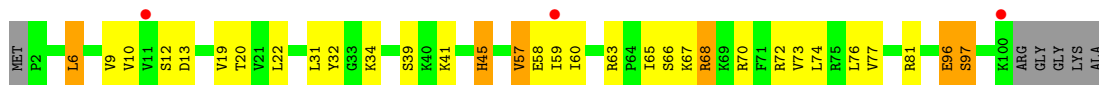


• Molecule 47: 30S ribosomal protein S17

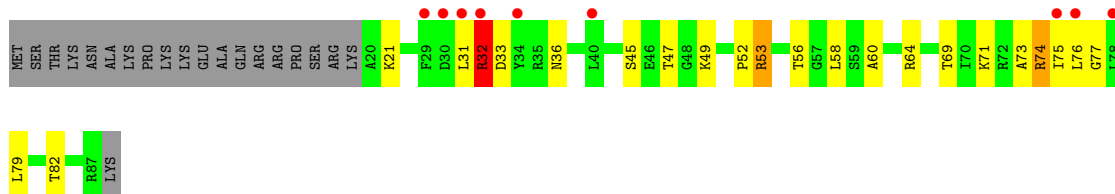




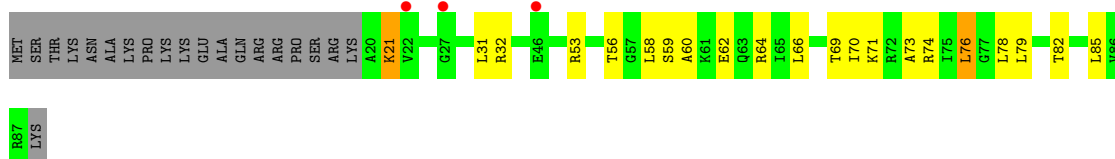
• Molecule 47: 30S ribosomal protein S17



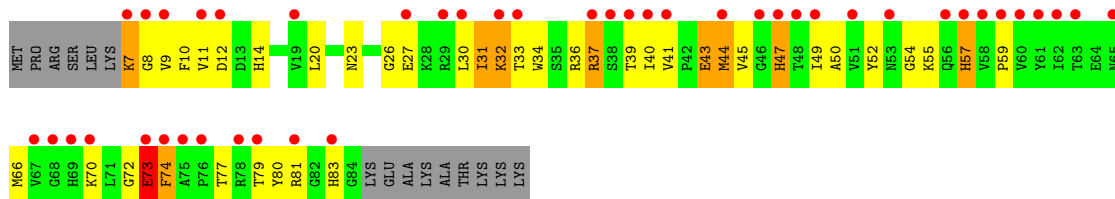
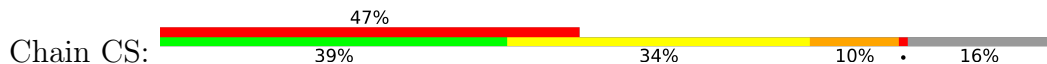
• Molecule 48: 30S ribosomal protein S18



• Molecule 48: 30S ribosomal protein S18

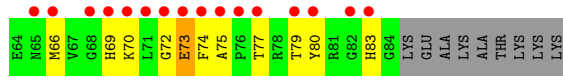
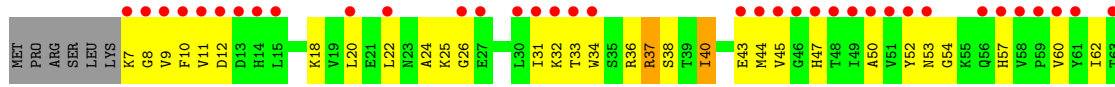


• Molecule 49: 30S ribosomal protein S19

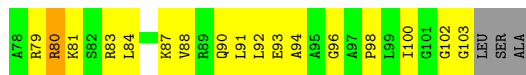


• Molecule 49: 30S ribosomal protein S19

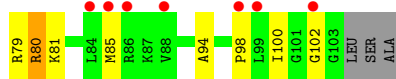




• Molecule 50: 30S ribosomal protein S20



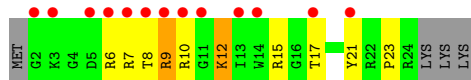
• Molecule 50: 30S ribosomal protein S20



• Molecule 51: 30S ribosomal protein THX



• Molecule 51: 30S ribosomal protein THX



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.37Å 445.46Å 619.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 3.20 49.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.29-3.20) 99.7 (49.43-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.91Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.273 0.228 , 0.273	Depositor DCC
R_{free} test set	63228 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtrriage
Anisotropy	0.180	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	279316	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, T8B

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	0.82	17/68203 (0.0%)	1.30	624/106459 (0.6%)
1	BA	1.20	70/68203 (0.1%)	1.37	800/106459 (0.8%)
2	AB	0.94	0/2879	1.25	21/4492 (0.5%)
2	BB	0.88	0/2879	1.26	21/4492 (0.5%)
3	AD	0.54	0/2186	0.75	2/2944 (0.1%)
3	BD	0.67	0/2186	0.81	4/2944 (0.1%)
4	AE	0.55	0/1588	0.76	0/2145
4	BE	0.72	0/1588	0.83	1/2145 (0.0%)
5	AF	0.51	0/1609	0.70	0/2177
5	BF	0.73	0/1609	0.77	0/2177
6	AG	0.61	0/1393	0.66	0/1892
6	BG	0.46	0/1393	0.64	0/1892
7	AH	0.58	0/1343	0.68	1/1820 (0.1%)
7	BH	0.59	0/1343	0.70	0/1820
8	AI	0.63	1/1061 (0.1%)	0.78	0/1451
8	BI	0.50	0/1061	0.74	0/1451
9	AN	0.52	0/1139	0.72	0/1538
9	BN	0.74	0/1139	0.78	0/1538
10	AO	0.50	0/933	0.72	1/1257 (0.1%)
10	BO	0.67	0/933	0.74	0/1257
11	AP	0.50	0/1135	0.75	1/1510 (0.1%)
11	BP	0.64	0/1135	0.81	2/1510 (0.1%)
12	AQ	0.53	0/1143	0.74	0/1527
12	BQ	0.64	0/1143	0.74	0/1527
13	AR	0.51	0/982	0.74	0/1312
13	BR	0.69	0/982	0.82	1/1312 (0.1%)
14	AS	0.64	0/875	0.79	0/1168
14	BS	0.53	0/875	0.79	1/1168 (0.1%)
15	AT	0.52	0/1077	0.73	0/1444
15	BT	0.61	0/1077	0.79	1/1444 (0.1%)
16	AU	0.56	0/977	0.69	0/1301
16	BU	0.88	1/977 (0.1%)	0.81	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AV	0.58	0/782	0.67	0/1049
17	BV	0.70	0/782	0.77	0/1049
18	AW	0.56	0/891	0.75	0/1197
18	BW	0.82	0/891	0.80	0/1197
19	AX	0.55	0/756	0.77	1/1016 (0.1%)
19	BX	0.66	0/756	0.76	1/1016 (0.1%)
20	AY	0.50	0/798	0.77	0/1073
20	BY	0.61	0/798	0.80	1/1073 (0.1%)
21	AZ	0.57	0/1555	0.68	0/2118
21	BZ	0.49	0/1555	0.71	0/2118
22	A0	0.50	0/602	0.69	0/804
22	B0	0.66	0/602	0.77	0/804
23	A1	0.51	0/752	0.72	0/1003
23	B1	0.62	0/752	0.76	0/1003
24	A2	0.59	0/590	0.68	0/781
24	B2	0.60	0/590	0.74	0/781
25	A3	0.45	0/463	0.69	0/623
25	B3	0.65	0/463	0.74	0/623
26	A4	0.65	0/358	0.74	0/487
26	B4	0.56	0/358	0.74	1/487 (0.2%)
27	A5	0.67	1/469 (0.2%)	0.83	2/634 (0.3%)
27	B5	0.79	0/469	0.88	0/634
28	A6	0.59	0/456	0.70	0/609
28	B6	0.68	0/456	0.74	0/609
29	A7	0.57	0/426	0.75	0/561
29	B7	0.78	0/426	0.84	0/561
30	A8	0.50	0/516	0.73	0/679
30	B8	0.70	0/516	0.82	0/679
31	CA	0.80	10/36054 (0.0%)	1.18	176/56272 (0.3%)
31	DA	0.77	7/36054 (0.0%)	1.19	211/56272 (0.4%)
32	CB	0.51	0/1811	0.69	0/2452
32	DB	0.56	0/1811	0.69	0/2452
33	CC	0.56	0/1474	0.65	0/2003
33	DC	0.58	0/1474	0.65	0/2003
34	CD	0.53	0/1550	0.72	3/2106 (0.1%)
34	DD	0.84	2/1550 (0.1%)	0.78	4/2106 (0.2%)
35	CE	0.49	0/1121	0.70	1/1517 (0.1%)
35	DE	0.52	0/1121	0.72	1/1517 (0.1%)
36	CF	0.49	0/794	0.64	0/1082
36	DF	0.49	0/794	0.67	1/1082 (0.1%)
37	CG	0.57	0/1186	0.65	0/1603
37	DG	0.56	0/1186	0.62	0/1603
38	CH	0.44	0/1065	0.67	0/1445

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DH	0.44	0/1065	0.64	0/1445
39	CI	0.62	0/867	0.71	0/1180
39	DI	0.62	0/867	0.69	0/1180
40	CJ	0.60	0/672	0.74	1/919 (0.1%)
40	DJ	0.60	0/672	0.70	1/919 (0.1%)
41	CK	0.47	0/843	0.71	0/1144
41	DK	0.47	0/843	0.67	0/1144
42	CL	0.44	0/925	0.67	0/1251
42	DL	0.46	0/925	0.69	0/1251
43	CM	0.67	0/811	0.72	0/1103
43	DM	0.63	0/811	0.73	1/1103 (0.1%)
44	CN	0.60	0/487	0.68	0/649
44	DN	0.59	0/487	0.74	0/649
45	CO	0.49	0/735	0.64	0/981
45	DO	0.47	0/735	0.61	0/981
46	CP	0.51	0/667	0.70	0/905
46	DP	0.43	0/667	0.65	0/905
47	CQ	0.46	0/836	0.68	0/1117
47	DQ	0.47	0/836	0.66	0/1117
48	CR	0.43	0/519	0.64	0/699
48	DR	0.50	0/519	0.67	0/699
49	CS	0.69	0/558	0.88	1/759 (0.1%)
49	DS	0.76	1/558 (0.2%)	0.87	3/759 (0.4%)
50	CT	0.47	0/710	0.72	0/940
50	DT	0.42	0/710	0.68	0/940
51	CU	0.64	0/203	0.67	0/266
51	DU	0.59	0/203	0.70	0/266
All	All	0.86	110/303650 (0.0%)	1.16	1892/454928 (0.4%)

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
26	A4	0	1
34	CD	0	1
34	DD	0	1
42	CL	0	1
42	DL	0	1
All	All	0	5

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	DD	12	CYS	CB-SG	19.94	2.16	1.82
34	DD	26	CYS	CB-SG	15.79	2.09	1.82
31	DA	1492	A	C6-N6	-12.21	1.24	1.33
31	CA	1492	A	C2-N3	12.12	1.44	1.33
31	CA	1493	A	N9-C4	-11.96	1.30	1.37

The worst 5 of 1892 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	DA	1492	A	C6-N1-C2	-28.45	101.53	118.60
31	DA	1492	A	C5-C6-N1	26.41	130.90	117.70
31	CA	1492	A	C8-N9-C4	-21.05	97.38	105.80
1	BA	1332	G	C2-N3-C4	-19.65	102.08	111.90
1	BA	1332	G	N3-C4-C5	17.99	137.59	128.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	A4	42	PHE	Peptide
34	CD	11	LEU	Peptide
42	CL	26	ALA	Peptide
34	DD	11	LEU	Peptide
42	DL	26	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	60900	0	30712	1406	0
1	BA	60900	0	30712	1060	0
2	AB	2574	0	1306	87	0
2	BB	2574	0	1306	35	0
3	AD	2136	0	2218	77	0
3	BD	2136	0	2218	81	0
4	AE	1555	0	1607	81	0
4	BE	1555	0	1607	54	0
5	AF	1576	0	1616	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	BF	1576	0	1616	59	0
6	AG	1368	0	1324	70	0
6	BG	1368	0	1324	61	0
7	AH	1317	0	1376	66	0
7	BH	1317	0	1376	33	0
8	AI	1046	0	1067	55	2
8	BI	1046	0	1067	47	0
9	AN	1112	0	1180	60	0
9	BN	1112	0	1180	34	0
10	AO	923	0	981	28	0
10	BO	923	0	981	23	0
11	AP	1119	0	1186	38	0
11	BP	1119	0	1186	40	0
12	AQ	1122	0	1179	43	0
12	BQ	1122	0	1179	47	0
13	AR	968	0	1033	43	0
13	BR	968	0	1033	33	0
14	AS	865	0	905	62	0
14	BS	865	0	905	54	0
15	AT	1063	0	1103	48	0
15	BT	1063	0	1103	37	0
16	AU	959	0	1019	31	0
16	BU	959	0	1019	20	0
17	AV	771	0	830	22	0
17	BV	771	0	830	15	0
18	AW	881	0	935	25	0
18	BW	881	0	935	24	0
19	AX	742	0	799	22	0
19	BX	742	0	799	23	0
20	AY	785	0	832	36	0
20	BY	785	0	832	30	0
21	AZ	1522	0	1511	56	0
21	BZ	1522	0	1511	47	0
22	A0	594	0	604	27	0
22	B0	594	0	604	21	0
23	A1	745	0	804	26	0
23	B1	745	0	804	26	0
24	A2	588	0	643	31	0
24	B2	588	0	643	18	0
25	A3	458	0	503	22	0
25	B3	458	0	503	6	0
26	A4	349	0	340	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B4	349	0	340	16	0
27	A5	455	0	476	25	0
27	B5	455	0	476	18	0
28	A6	449	0	464	19	0
28	B6	449	0	466	17	0
29	A7	418	0	467	18	0
29	B7	418	0	467	14	0
30	A8	509	0	565	23	0
30	B8	509	0	565	20	0
31	CA	32208	0	16256	921	2
31	DA	32208	0	16254	923	0
32	CB	1777	0	1747	100	0
32	DB	1777	0	1747	95	0
33	CC	1450	0	1314	45	0
33	DC	1450	0	1314	58	0
34	CD	1520	0	1407	73	0
34	DD	1520	0	1406	85	0
35	CE	1105	0	1130	48	0
35	DE	1105	0	1130	54	0
36	CF	781	0	741	25	0
36	DF	781	0	741	29	0
37	CG	1167	0	1108	39	0
37	DG	1167	0	1108	46	0
38	CH	1045	0	1033	45	0
38	DH	1045	0	1033	53	0
39	CI	852	0	742	43	0
39	DI	852	0	742	52	0
40	CJ	659	0	552	31	0
40	DJ	659	0	552	37	0
41	CK	828	0	822	24	0
41	DK	828	0	822	32	0
42	CL	909	0	927	43	0
42	DL	909	0	927	38	0
43	CM	801	0	743	33	0
43	DM	801	0	743	37	0
44	CN	478	0	498	33	0
44	DN	478	0	497	30	0
45	CO	724	0	749	32	0
45	DO	724	0	749	27	0
46	CP	651	0	638	33	0
46	DP	651	0	638	28	0
47	CQ	823	0	891	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	DQ	823	0	891	22	0
48	CR	514	0	530	19	0
48	DR	514	0	530	17	0
49	CS	544	0	457	21	0
49	DS	544	0	457	26	0
50	CT	708	0	764	37	0
50	DT	708	0	764	26	0
51	CU	199	0	208	8	0
51	DU	199	0	208	6	0
52	AA	44	0	20	31	0
52	BA	44	0	20	23	0
53	AA	2	0	0	0	0
53	BA	2	0	0	0	0
All	All	279316	0	185722	7170	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 7170 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AA:3001:T8B:C13	31:DA:1492:A:H5''	1.47	1.41
34:DD:26:CYS:SG	34:DD:26:CYS:CB	2.09	1.41
34:DD:12:CYS:SG	34:DD:12:CYS:CB	2.16	1.34
52:AA:3001:T8B:H13	52:AA:3001:T8B:C22	1.58	1.33
52:BA:3001:T8B:H13	52:BA:3001:T8B:C22	1.58	1.32

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AI:89:TYR:O	31:CA:357:G:O2'[2_654]	2.11	0.09
8:AI:91:SER:OG	31:CA:368:U:OP2[2_654]	2.12	0.08

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	
3	AD	273/276 (99%)	240 (88%)	27 (10%)	6 (2%)	6	35
3	BD	273/276 (99%)	246 (90%)	23 (8%)	4 (2%)	10	44
4	AE	202/206 (98%)	177 (88%)	18 (9%)	7 (4%)	3	24
4	BE	202/206 (98%)	174 (86%)	21 (10%)	7 (4%)	3	24
5	AF	198/205 (97%)	168 (85%)	25 (13%)	5 (2%)	5	32
5	BF	198/205 (97%)	170 (86%)	21 (11%)	7 (4%)	3	24
6	AG	179/182 (98%)	136 (76%)	33 (18%)	10 (6%)	2	14
6	BG	179/182 (98%)	135 (75%)	30 (17%)	14 (8%)	1	6
7	AH	172/180 (96%)	143 (83%)	21 (12%)	8 (5%)	2	17
7	BH	172/180 (96%)	144 (84%)	22 (13%)	6 (4%)	3	24
8	AI	143/148 (97%)	103 (72%)	28 (20%)	12 (8%)	1	5
8	BI	143/148 (97%)	109 (76%)	24 (17%)	10 (7%)	1	8
9	AN	138/140 (99%)	113 (82%)	16 (12%)	9 (6%)	1	10
9	BN	138/140 (99%)	119 (86%)	13 (9%)	6 (4%)	2	20
10	AO	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	4	25
10	BO	120/122 (98%)	109 (91%)	7 (6%)	4 (3%)	4	25
11	AP	143/150 (95%)	117 (82%)	18 (13%)	8 (6%)	2	14
11	BP	143/150 (95%)	126 (88%)	12 (8%)	5 (4%)	3	24
12	AQ	139/141 (99%)	126 (91%)	9 (6%)	4 (3%)	4	28
12	BQ	139/141 (99%)	126 (91%)	9 (6%)	4 (3%)	4	28
13	AR	116/118 (98%)	95 (82%)	16 (14%)	5 (4%)	2	20
13	BR	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	17	56
14	AS	108/112 (96%)	84 (78%)	21 (19%)	3 (3%)	5	29
14	BS	108/112 (96%)	93 (86%)	12 (11%)	3 (3%)	5	29
15	AT	129/146 (88%)	109 (84%)	16 (12%)	4 (3%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	BT	129/146 (88%)	116 (90%)	12 (9%)	1 (1%)	19	58
16	AU	114/118 (97%)	104 (91%)	10 (9%)	0	100	100
16	BU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	AV	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	7	38
17	BV	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	15	54
18	AW	110/113 (97%)	101 (92%)	8 (7%)	1 (1%)	17	56
18	BW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
19	AX	93/96 (97%)	82 (88%)	9 (10%)	2 (2%)	6	35
19	BX	93/96 (97%)	82 (88%)	9 (10%)	2 (2%)	6	35
20	AY	105/110 (96%)	90 (86%)	10 (10%)	5 (5%)	2	17
20	BY	105/110 (96%)	88 (84%)	13 (12%)	4 (4%)	3	22
21	AZ	196/206 (95%)	153 (78%)	32 (16%)	11 (6%)	2	14
21	BZ	196/206 (95%)	158 (81%)	31 (16%)	7 (4%)	3	23
22	A0	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	11	46
22	B0	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	11	46
23	A1	95/98 (97%)	88 (93%)	5 (5%)	2 (2%)	7	37
23	B1	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	4	26
24	A2	68/72 (94%)	59 (87%)	8 (12%)	1 (2%)	10	44
24	B2	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	A3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	B3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	8	41
26	A4	44/71 (62%)	30 (68%)	10 (23%)	4 (9%)	1	3
26	B4	44/71 (62%)	30 (68%)	10 (23%)	4 (9%)	1	3
27	A5	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	8	41
27	B5	57/60 (95%)	49 (86%)	6 (10%)	2 (4%)	3	24
28	A6	51/54 (94%)	46 (90%)	4 (8%)	1 (2%)	7	38
28	B6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	A7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	6	35
29	B7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	6	35
30	A8	62/65 (95%)	48 (77%)	13 (21%)	1 (2%)	9	43
30	B8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	CB	227/256 (89%)	171 (75%)	36 (16%)	20 (9%)	1	4
32	DB	227/256 (89%)	173 (76%)	39 (17%)	15 (7%)	1	9
33	CC	204/239 (85%)	163 (80%)	30 (15%)	11 (5%)	2	14
33	DC	204/239 (85%)	144 (71%)	42 (21%)	18 (9%)	1	4
34	CD	206/209 (99%)	154 (75%)	40 (19%)	12 (6%)	1	13
34	DD	206/209 (99%)	152 (74%)	47 (23%)	7 (3%)	3	24
35	CE	146/162 (90%)	112 (77%)	23 (16%)	11 (8%)	1	7
35	DE	146/162 (90%)	116 (80%)	25 (17%)	5 (3%)	3	24
36	CF	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	4	26
36	DF	98/101 (97%)	85 (87%)	9 (9%)	4 (4%)	3	21
37	CG	153/156 (98%)	127 (83%)	16 (10%)	10 (6%)	1	10
37	DG	153/156 (98%)	129 (84%)	18 (12%)	6 (4%)	3	22
38	CH	136/138 (99%)	116 (85%)	18 (13%)	2 (2%)	10	44
38	DH	136/138 (99%)	118 (87%)	13 (10%)	5 (4%)	3	22
39	CI	123/128 (96%)	93 (76%)	20 (16%)	10 (8%)	1	5
39	DI	123/128 (96%)	94 (76%)	21 (17%)	8 (6%)	1	10
40	CJ	94/105 (90%)	66 (70%)	19 (20%)	9 (10%)	0	3
40	DJ	94/105 (90%)	74 (79%)	14 (15%)	6 (6%)	1	10
41	CK	112/129 (87%)	96 (86%)	12 (11%)	4 (4%)	3	23
41	DK	112/129 (87%)	90 (80%)	19 (17%)	3 (3%)	5	30
42	CL	120/132 (91%)	98 (82%)	17 (14%)	5 (4%)	3	20
42	DL	120/132 (91%)	100 (83%)	15 (12%)	5 (4%)	3	20
43	CM	112/126 (89%)	84 (75%)	18 (16%)	10 (9%)	1	4
43	DM	112/126 (89%)	80 (71%)	20 (18%)	12 (11%)	0	2
44	CN	58/61 (95%)	43 (74%)	10 (17%)	5 (9%)	1	4
44	DN	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	15
45	CO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	3	24
45	DO	86/89 (97%)	68 (79%)	16 (19%)	2 (2%)	6	34
46	CP	80/88 (91%)	50 (62%)	23 (29%)	7 (9%)	1	4
46	DP	80/88 (91%)	52 (65%)	25 (31%)	3 (4%)	3	22
47	CQ	97/105 (92%)	84 (87%)	8 (8%)	5 (5%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DQ	97/105 (92%)	81 (84%)	13 (13%)	3 (3%)	4	26
48	CR	66/88 (75%)	55 (83%)	10 (15%)	1 (2%)	10	44
48	DR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	CS	76/93 (82%)	48 (63%)	17 (22%)	11 (14%)	0	1
49	DS	76/93 (82%)	54 (71%)	17 (22%)	5 (7%)	1	9
50	CT	94/106 (89%)	73 (78%)	13 (14%)	8 (8%)	1	4
50	DT	94/106 (89%)	72 (77%)	15 (16%)	7 (7%)	1	7
51	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
51	DU	21/27 (78%)	16 (76%)	3 (14%)	2 (10%)	0	3
All	All	11280/12044 (94%)	9338 (83%)	1460 (13%)	482 (4%)	2	20

5 of 482 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	239	ARG
3	AD	275	LYS
5	AF	60	SER
6	AG	14	GLU
6	AG	78	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AD	215/218 (99%)	185 (86%)	30 (14%)	3	16
3	BD	215/218 (99%)	189 (88%)	26 (12%)	5	22
4	AE	163/166 (98%)	139 (85%)	24 (15%)	3	14
4	BE	163/166 (98%)	134 (82%)	29 (18%)	2	9
5	AF	158/162 (98%)	133 (84%)	25 (16%)	2	12
5	BF	158/162 (98%)	138 (87%)	20 (13%)	4	20
6	AG	128/156 (82%)	110 (86%)	18 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BG	128/156 (82%)	114 (89%)	14 (11%)	6	26
7	AH	141/148 (95%)	125 (89%)	16 (11%)	6	25
7	BH	141/148 (95%)	124 (88%)	17 (12%)	5	22
8	AI	102/124 (82%)	76 (74%)	26 (26%)	0	2
8	BI	102/124 (82%)	76 (74%)	26 (26%)	0	2
9	AN	117/119 (98%)	94 (80%)	23 (20%)	1	7
9	BN	117/119 (98%)	91 (78%)	26 (22%)	1	4
10	AO	98/100 (98%)	89 (91%)	9 (9%)	9	33
10	BO	98/100 (98%)	89 (91%)	9 (9%)	9	33
11	AP	113/116 (97%)	96 (85%)	17 (15%)	3	14
11	BP	113/116 (97%)	97 (86%)	16 (14%)	3	15
12	AQ	111/111 (100%)	94 (85%)	17 (15%)	2	13
12	BQ	111/111 (100%)	94 (85%)	17 (15%)	2	13
13	AR	101/101 (100%)	80 (79%)	21 (21%)	1	6
13	BR	101/101 (100%)	79 (78%)	22 (22%)	1	5
14	AS	84/88 (96%)	67 (80%)	17 (20%)	1	6
14	BS	84/88 (96%)	72 (86%)	12 (14%)	3	15
15	AT	110/127 (87%)	99 (90%)	11 (10%)	7	30
15	BT	110/127 (87%)	100 (91%)	10 (9%)	9	34
16	AU	93/94 (99%)	83 (89%)	10 (11%)	6	27
16	BU	93/94 (99%)	77 (83%)	16 (17%)	2	10
17	AV	80/82 (98%)	63 (79%)	17 (21%)	1	5
17	BV	80/82 (98%)	63 (79%)	17 (21%)	1	5
18	AW	89/92 (97%)	75 (84%)	14 (16%)	2	12
18	BW	89/92 (97%)	78 (88%)	11 (12%)	4	21
19	AX	75/78 (96%)	67 (89%)	8 (11%)	6	27
19	BX	75/78 (96%)	66 (88%)	9 (12%)	5	22
20	AY	80/91 (88%)	70 (88%)	10 (12%)	4	21
20	BY	80/91 (88%)	72 (90%)	8 (10%)	7	30
21	AZ	159/179 (89%)	139 (87%)	20 (13%)	4	21
21	BZ	159/179 (89%)	137 (86%)	22 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	A0	59/67 (88%)	52 (88%)	7 (12%)	5	22
22	B0	59/67 (88%)	52 (88%)	7 (12%)	5	22
23	A1	78/83 (94%)	68 (87%)	10 (13%)	4	20
23	B1	78/83 (94%)	70 (90%)	8 (10%)	7	29
24	A2	65/67 (97%)	56 (86%)	9 (14%)	3	16
24	B2	65/67 (97%)	57 (88%)	8 (12%)	4	21
25	A3	49/52 (94%)	43 (88%)	6 (12%)	5	22
25	B3	49/52 (94%)	43 (88%)	6 (12%)	5	22
26	A4	39/63 (62%)	32 (82%)	7 (18%)	2	9
26	B4	39/63 (62%)	30 (77%)	9 (23%)	1	3
27	A5	50/52 (96%)	43 (86%)	7 (14%)	3	16
27	B5	50/52 (96%)	43 (86%)	7 (14%)	3	16
28	A6	50/52 (96%)	40 (80%)	10 (20%)	1	6
28	B6	50/52 (96%)	41 (82%)	9 (18%)	1	9
29	A7	41/42 (98%)	35 (85%)	6 (15%)	3	15
29	B7	41/42 (98%)	32 (78%)	9 (22%)	1	5
30	A8	52/55 (94%)	45 (86%)	7 (14%)	4	18
30	B8	52/55 (94%)	47 (90%)	5 (10%)	8	32
32	CB	177/220 (80%)	141 (80%)	36 (20%)	1	6
32	DB	177/220 (80%)	142 (80%)	35 (20%)	1	7
33	CC	114/188 (61%)	95 (83%)	19 (17%)	2	10
33	DC	114/188 (61%)	96 (84%)	18 (16%)	2	12
34	CD	139/181 (77%)	117 (84%)	22 (16%)	2	12
34	DD	139/181 (77%)	120 (86%)	19 (14%)	3	17
35	CE	108/123 (88%)	86 (80%)	22 (20%)	1	6
35	DE	108/123 (88%)	88 (82%)	20 (18%)	1	8
36	CF	77/90 (86%)	65 (84%)	12 (16%)	2	12
36	DF	77/90 (86%)	65 (84%)	12 (16%)	2	12
37	CG	104/127 (82%)	86 (83%)	18 (17%)	2	10
37	DG	104/127 (82%)	88 (85%)	16 (15%)	2	13
38	CH	103/119 (87%)	85 (82%)	18 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DH	103/119 (87%)	84 (82%)	19 (18%)	1	8
39	CI	62/99 (63%)	53 (86%)	9 (14%)	3	15
39	DI	62/99 (63%)	54 (87%)	8 (13%)	4	19
40	CJ	52/92 (56%)	42 (81%)	10 (19%)	1	8
40	DJ	52/92 (56%)	41 (79%)	11 (21%)	1	5
41	CK	81/99 (82%)	69 (85%)	12 (15%)	3	14
41	DK	81/99 (82%)	71 (88%)	10 (12%)	4	21
42	CL	92/109 (84%)	81 (88%)	11 (12%)	5	22
42	DL	92/109 (84%)	83 (90%)	9 (10%)	8	31
43	CM	63/101 (62%)	49 (78%)	14 (22%)	1	4
43	DM	63/101 (62%)	49 (78%)	14 (22%)	1	4
44	CN	46/50 (92%)	35 (76%)	11 (24%)	0	3
44	DN	46/50 (92%)	33 (72%)	13 (28%)	0	1
45	CO	77/80 (96%)	65 (84%)	12 (16%)	2	12
45	DO	77/80 (96%)	66 (86%)	11 (14%)	3	15
46	CP	63/74 (85%)	49 (78%)	14 (22%)	1	4
46	DP	63/74 (85%)	53 (84%)	10 (16%)	2	12
47	CQ	94/97 (97%)	90 (96%)	4 (4%)	29	64
47	DQ	94/97 (97%)	84 (89%)	10 (11%)	6	27
48	CR	49/77 (64%)	44 (90%)	5 (10%)	7	29
48	DR	49/77 (64%)	46 (94%)	3 (6%)	18	54
49	CS	42/80 (52%)	25 (60%)	17 (40%)	0	0
49	DS	42/80 (52%)	36 (86%)	6 (14%)	3	15
50	CT	65/82 (79%)	53 (82%)	12 (18%)	1	8
50	DT	65/82 (79%)	57 (88%)	8 (12%)	4	21
51	CU	18/22 (82%)	16 (89%)	2 (11%)	6	25
51	DU	18/22 (82%)	14 (78%)	4 (22%)	1	4
All	All	8652/9990 (87%)	7319 (85%)	1333 (15%)	2	13

5 of 1333 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	CH	19	VAL

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Mol	Chain	Res	Type
34	DD	158	ILE
40	CJ	16	LEU
37	CG	146	GLU
47	CQ	60	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
13	BR	13	HIS
40	DJ	13	HIS
35	CE	78	HIS
39	DI	124	GLN
45	DO	28	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2819/2915 (96%)	581 (20%)	59 (2%)
1	BA	2819/2915 (96%)	586 (20%)	60 (2%)
2	AB	119/122 (97%)	25 (21%)	0
2	BB	119/122 (97%)	21 (17%)	0
31	CA	1496/1521 (98%)	339 (22%)	31 (2%)
31	DA	1496/1521 (98%)	341 (22%)	27 (1%)
All	All	8868/9116 (97%)	1893 (21%)	177 (1%)

5 of 1893 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	G
1	AA	14	A
1	AA	15	G
1	AA	34	C
1	AA	45	C

5 of 177 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	BA	2689	U
31	CA	1165	C
31	CA	60	A

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Mol	Chain	Res	Type
31	CA	428	G
31	DA	60	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	T8B	BA	3001	53	48,48,48	0.99	2 (4%)	63,71,71	1.22	8 (12%)
52	T8B	AA	3001	53	48,48,48	0.99	2 (4%)	63,71,71	1.22	8 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	T8B	BA	3001	53	-	1/26/26/26	0/5/5/5
52	T8B	AA	3001	53	-	1/26/26/26	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	AA	3001	T8B	O11-C26	3.09	1.38	1.32
52	BA	3001	T8B	O11-C26	3.08	1.38	1.32
52	BA	3001	T8B	C25-C24	2.28	1.50	1.43
52	AA	3001	T8B	C25-C24	2.27	1.50	1.43

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	BA	3001	T8B	C21-C23-C24	-4.15	120.19	125.03
52	AA	3001	T8B	C21-C23-C24	-4.14	120.21	125.03
52	BA	3001	T8B	O5-C14-O6	3.13	120.29	116.44
52	AA	3001	T8B	O5-C14-O6	3.13	120.29	116.44
52	BA	3001	T8B	O11-C26-C25	2.76	124.96	121.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

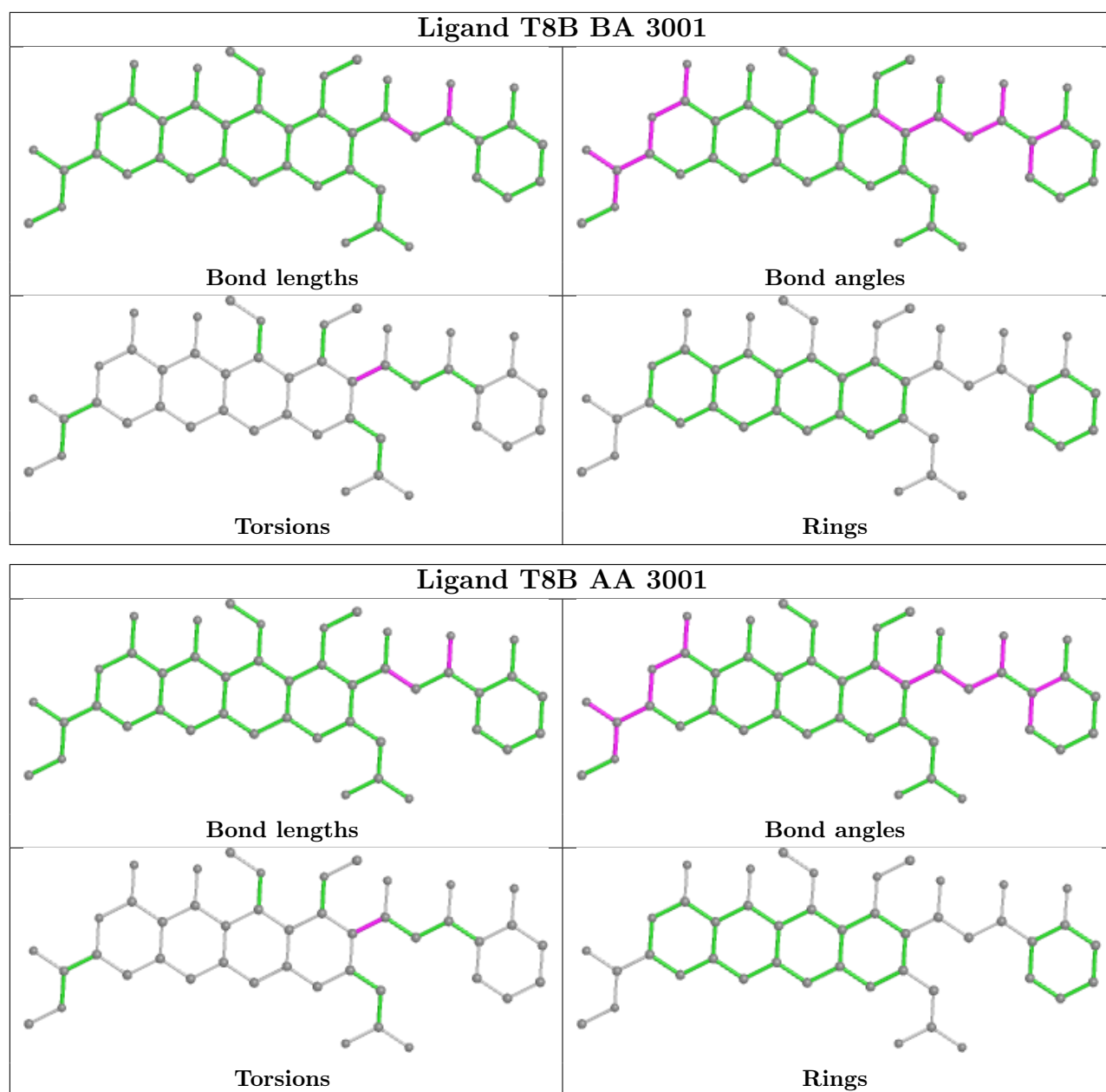
Mol	Chain	Res	Type	Atoms
52	AA	3001	T8B	C21-C23-C24-C25
52	BA	3001	T8B	C21-C23-C24-C25

There are no ring outliers.

2 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	BA	3001	T8B	23	0
52	AA	3001	T8B	31	0

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



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2827/2915 (96%)	0.03	117 (4%) 37 24	46, 70, 113, 128	0
1	BA	2827/2915 (96%)	0.08	73 (2%) 56 40	27, 56, 110, 126	0
2	AB	120/122 (98%)	0.03	4 (3%) 46 30	68, 95, 108, 111	0
2	BB	120/122 (98%)	-0.24	0 100 100	46, 80, 95, 103	0
3	AD	275/276 (99%)	-0.15	0 100 100	45, 67, 82, 103	0
3	BD	275/276 (99%)	-0.16	2 (0%) 87 81	36, 59, 78, 103	0
4	AE	204/206 (99%)	-0.10	1 (0%) 91 86	47, 72, 87, 98	0
4	BE	204/206 (99%)	-0.18	0 100 100	33, 60, 81, 96	0
5	AF	203/205 (99%)	-0.34	2 (0%) 82 72	44, 77, 95, 112	0
5	BF	203/205 (99%)	-0.23	0 100 100	26, 64, 90, 110	0
6	AG	181/182 (99%)	1.35	52 (28%) 0 0	89, 106, 114, 116	0
6	BG	181/182 (99%)	0.10	8 (4%) 34 21	81, 101, 110, 118	0
7	AH	174/180 (96%)	0.91	37 (21%) 0 1	80, 93, 101, 108	0
7	BH	174/180 (96%)	-0.16	0 100 100	63, 78, 91, 98	0
8	AI	145/148 (97%)	0.59	21 (14%) 2 1	72, 104, 116, 123	0
8	BI	145/148 (97%)	-0.10	1 (0%) 87 81	68, 90, 98, 100	0
9	AN	140/140 (100%)	-0.08	1 (0%) 87 81	58, 73, 90, 94	0
9	BN	140/140 (100%)	-0.19	0 100 100	38, 57, 82, 85	0
10	AO	122/122 (100%)	-0.33	0 100 100	56, 73, 85, 91	0
10	BO	122/122 (100%)	-0.22	0 100 100	43, 64, 82, 89	0
11	AP	147/150 (98%)	-0.01	4 (2%) 54 39	47, 81, 96, 105	0
11	BP	147/150 (98%)	-0.17	0 100 100	28, 68, 91, 100	0
12	AQ	141/141 (100%)	-0.04	1 (0%) 87 81	60, 78, 91, 97	0
12	BQ	141/141 (100%)	-0.09	0 100 100	44, 65, 78, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AR	118/118 (100%)	-0.18	0 100 100	47, 66, 78, 88	0
13	BR	118/118 (100%)	-0.19	0 100 100	35, 53, 69, 86	0
14	AS	110/112 (98%)	0.53	13 (11%) 4 2	74, 91, 102, 109	0
14	BS	110/112 (98%)	-0.13	0 100 100	58, 79, 93, 100	0
15	AT	131/146 (89%)	-0.22	1 (0%) 86 78	66, 76, 99, 109	0
15	BT	131/146 (89%)	-0.27	1 (0%) 86 78	55, 68, 91, 102	0
16	AU	116/118 (98%)	-0.05	0 100 100	53, 70, 84, 89	0
16	BU	116/118 (98%)	-0.15	0 100 100	34, 50, 70, 84	0
17	AV	101/101 (100%)	-0.19	1 (0%) 82 72	48, 79, 93, 103	0
17	BV	101/101 (100%)	-0.31	0 100 100	31, 61, 81, 95	0
18	AW	112/113 (99%)	-0.24	0 100 100	50, 59, 80, 104	0
18	BW	112/113 (99%)	-0.31	0 100 100	36, 45, 75, 106	0
19	AX	95/96 (98%)	-0.08	0 100 100	54, 71, 89, 93	0
19	BX	95/96 (98%)	-0.17	0 100 100	33, 59, 83, 91	0
20	AY	107/110 (97%)	0.15	7 (6%) 18 11	71, 81, 94, 105	0
20	BY	107/110 (97%)	-0.24	1 (0%) 84 75	56, 71, 89, 103	0
21	AZ	198/206 (96%)	0.01	7 (3%) 44 28	80, 92, 103, 108	0
21	BZ	198/206 (96%)	-0.35	0 100 100	64, 82, 97, 103	0
22	A0	76/85 (89%)	0.24	2 (2%) 56 40	59, 74, 84, 89	0
22	B0	76/85 (89%)	-0.24	0 100 100	46, 60, 74, 82	0
23	A1	97/98 (98%)	0.12	2 (2%) 63 49	54, 71, 94, 99	0
23	B1	97/98 (98%)	-0.08	1 (1%) 82 72	42, 65, 91, 95	0
24	A2	70/72 (97%)	-0.05	1 (1%) 75 63	65, 81, 92, 101	0
24	B2	70/72 (97%)	-0.13	0 100 100	52, 70, 85, 102	0
25	A3	59/60 (98%)	0.46	5 (8%) 10 6	63, 74, 92, 101	0
25	B3	59/60 (98%)	-0.16	0 100 100	43, 56, 84, 94	0
26	A4	46/71 (64%)	0.54	7 (15%) 2 1	101, 109, 113, 119	0
26	B4	46/71 (64%)	0.26	6 (13%) 3 2	98, 107, 113, 118	0
27	A5	59/60 (98%)	-0.35	0 100 100	46, 64, 78, 91	0
27	B5	59/60 (98%)	-0.19	0 100 100	28, 52, 71, 89	0
28	A6	53/54 (98%)	0.14	3 (5%) 23 13	62, 76, 87, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	B6	53/54 (98%)	-0.10	0 100 100	52, 66, 77, 85	0
29	A7	48/49 (97%)	0.14	4 (8%) 11 6	43, 54, 79, 99	0
29	B7	48/49 (97%)	-0.00	1 (2%) 63 49	29, 44, 73, 89	0
30	A8	64/65 (98%)	0.13	0 100 100	60, 68, 76, 85	0
30	B8	64/65 (98%)	0.13	0 100 100	45, 56, 65, 79	0
31	CA	1498/1521 (98%)	0.57	190 (12%) 3 2	59, 99, 120, 126	0
31	DA	1498/1521 (98%)	0.52	180 (12%) 4 2	65, 99, 120, 128	0
32	CB	229/256 (89%)	0.12	14 (6%) 21 12	93, 103, 111, 117	0
32	DB	229/256 (89%)	0.65	32 (13%) 2 1	95, 105, 112, 115	0
33	CC	206/239 (86%)	1.00	45 (21%) 0 0	92, 106, 112, 115	0
33	DC	206/239 (86%)	0.87	33 (16%) 1 1	97, 108, 115, 120	0
34	CD	208/209 (99%)	0.03	10 (4%) 30 18	85, 98, 108, 114	0
34	DD	208/209 (99%)	0.02	10 (4%) 30 18	87, 97, 107, 123	0
35	CE	148/162 (91%)	-0.14	4 (2%) 54 39	74, 93, 103, 110	0
35	DE	148/162 (91%)	0.10	5 (3%) 45 29	84, 96, 104, 110	0
36	CF	100/101 (99%)	-0.07	5 (5%) 28 16	80, 92, 101, 107	0
36	DF	100/101 (99%)	-0.14	3 (3%) 50 34	84, 93, 103, 110	0
37	CG	155/156 (99%)	2.14	77 (49%) 0 0	99, 109, 115, 120	0
37	DG	155/156 (99%)	2.07	75 (48%) 0 0	97, 109, 115, 119	0
38	CH	138/138 (100%)	0.05	4 (2%) 51 36	82, 94, 101, 104	0
38	DH	138/138 (100%)	-0.09	3 (2%) 62 48	86, 96, 102, 106	0
39	CI	125/128 (97%)	1.89	50 (40%) 0 0	97, 111, 117, 120	0
39	DI	125/128 (97%)	2.77	71 (56%) 0 0	100, 112, 118, 120	0
40	CJ	96/105 (91%)	2.13	43 (44%) 0 0	100, 109, 115, 117	0
40	DJ	96/105 (91%)	1.91	46 (47%) 0 0	97, 110, 115, 119	0
41	CK	114/129 (88%)	-0.12	1 (0%) 84 75	72, 93, 101, 105	0
41	DK	114/129 (88%)	0.22	4 (3%) 44 28	75, 95, 103, 107	0
42	CL	122/132 (92%)	-0.23	0 100 100	72, 85, 96, 100	0
42	DL	122/132 (92%)	-0.15	1 (0%) 86 78	77, 87, 96, 105	0
43	CM	114/126 (90%)	2.13	51 (44%) 0 0	102, 111, 118, 126	0
43	DM	114/126 (90%)	1.76	44 (38%) 0 0	101, 109, 115, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	CN	60/61 (98%)	1.19	15 (25%) 0 0	99, 108, 116, 118	0
44	DN	60/61 (98%)	1.59	21 (35%) 0 0	103, 111, 116, 122	0
45	CO	88/89 (98%)	0.02	2 (2%) 60 47	72, 91, 101, 107	0
45	DO	88/89 (98%)	0.18	5 (5%) 23 13	81, 93, 103, 107	0
46	CP	82/88 (93%)	0.62	6 (7%) 15 9	88, 96, 106, 112	0
46	DP	82/88 (93%)	0.43	3 (3%) 41 26	86, 94, 103, 111	0
47	CQ	99/105 (94%)	0.04	2 (2%) 65 51	78, 90, 98, 102	0
47	DQ	99/105 (94%)	0.17	3 (3%) 50 34	79, 92, 100, 103	0
48	CR	68/88 (77%)	0.15	9 (13%) 3 2	80, 91, 102, 103	0
48	DR	68/88 (77%)	0.21	3 (4%) 34 21	85, 93, 104, 106	0
49	CS	78/93 (83%)	2.61	44 (56%) 0 0	107, 111, 117, 123	0
49	DS	78/93 (83%)	2.84	52 (66%) 0 0	91, 112, 117, 119	0
50	CT	96/106 (90%)	0.18	3 (3%) 49 32	84, 93, 99, 102	0
50	DT	96/106 (90%)	0.69	10 (10%) 6 4	82, 92, 100, 101	0
51	CU	23/27 (85%)	2.89	12 (52%) 0 0	106, 112, 117, 119	0
51	DU	23/27 (85%)	2.65	13 (56%) 0 0	104, 109, 112, 113	0
All	All	20372/21160 (96%)	0.26	1591 (7%) 13 7	26, 84, 115, 128	0

The worst 5 of 1591 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
39	CI	30	GLY	12.5
49	CS	40	ILE	12.5
43	CM	85	GLY	12.2
31	CA	1353	G	11.0
31	CA	1286	A	10.7

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	T8B	AA	3001	44/44	0.85	0.28	20,20,20,20	0
53	MG	BA	3002	1/1	0.85	0.15	30,30,30,30	0
52	T8B	BA	3001	44/44	0.89	0.34	20,20,20,20	0
53	MG	BA	3003	1/1	0.94	0.16	30,30,30,30	0
53	MG	AA	3002	1/1	0.95	0.20	30,30,30,30	0
53	MG	AA	3003	1/1	0.98	0.17	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.