



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 04:52 AM UTC

PDB ID : 4V8U / pdb_00004v8u
Title : Crystal Structure of 70S Ribosome with Both Cognate tRNAs in the E and P Sites Representing an Authentic Elongation Complex.
Authors : Gao, Y.G.; Feng, S.; Chen, Y.
Deposited on : 2012-08-28
Resolution : 3.70 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.48.1

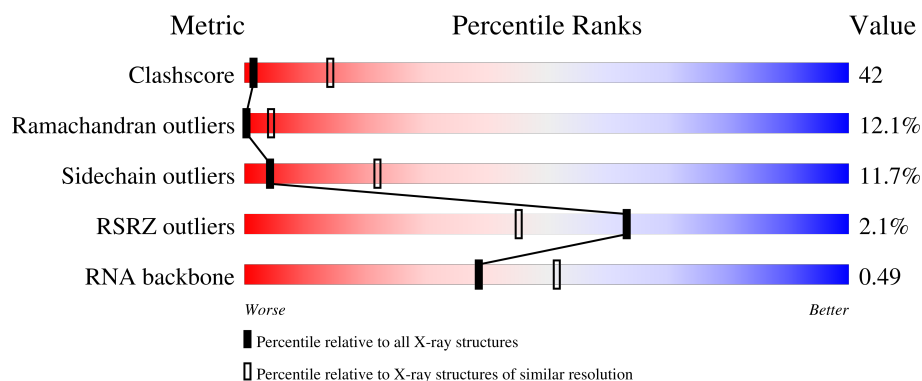
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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))
Clashscore	180529	1074 (3.80-3.60)
Ramachandran outliers	177936	1055 (3.80-3.60)
Sidechain outliers	177891	1052 (3.80-3.60)
RSRZ outliers	164620	1017 (3.80-3.60)
RNA backbone	3690	1122 (4.40-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1522	3% 29% 56% 12% ..
1	CA	1522	2% 28% 57% 12% ..
2	AB	256	20% 52% 19% 8%
2	CB	256	% 19% 53% 19% 8%
3	AC	239	18% 51% 15% 13%

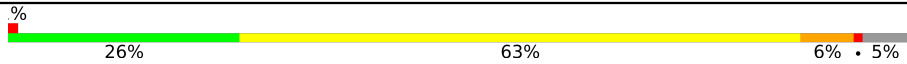
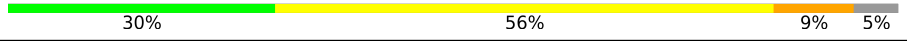
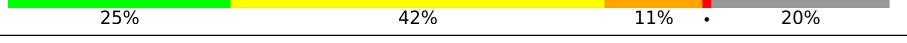
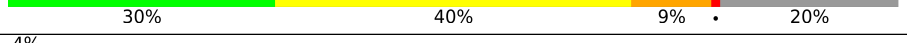
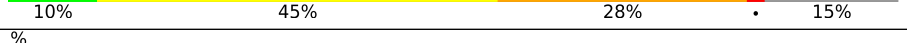
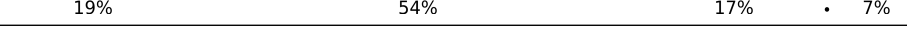
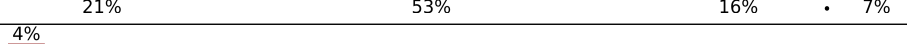
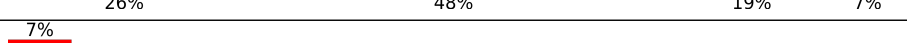
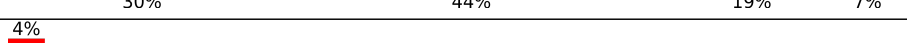
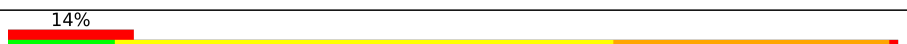
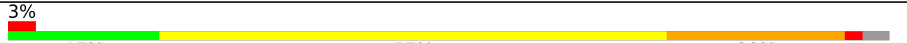
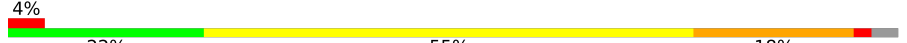
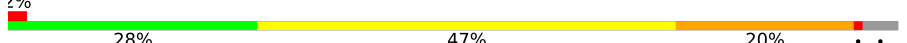
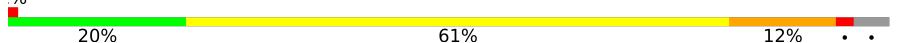
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	CC	239	% 18% 51% 16% • 13%
4	AD	209	% 28% 53% 16% •
4	CD	209	% 29% 55% 14% •
5	AE	162	% 32% 49% 12% 7%
5	CE	162	% 35% 47% 12% 7%
6	AF	101	30% 62% 7% •
6	CF	101	32% 60% 8%
7	AG	156	% 34% 50% 13% ••
7	CG	156	4% 36% 49% 13% ••
8	AH	138	% 38% 49% 12%
8	CH	138	39% 49% 12%
9	AI	128	28% 60% 10% ••
9	CI	128	% 27% 61% 10% ••
10	AJ	105	% 16% 57% 20% • 6%
10	CJ	105	3% 16% 55% 22% • 6%
11	AK	129	% 41% 39% 12% • 8%
11	CK	129	2% 39% 42% 11% • 8%
12	AL	132	25% 52% 14% • 5%
12	CL	132	% 23% 54% 15% • 5%
13	AM	126	5% 13% 64% 19% ••
13	CM	126	6% 15% 63% 19% ••
14	AN	61	2% 34% 51% 8% 5% •
14	CN	61	2% 36% 51% 7% 5% •
15	AO	89	30% 57% 11% •
15	CO	89	% 29% 57% 12% •

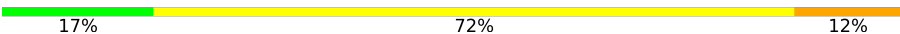
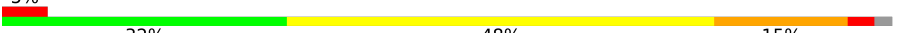
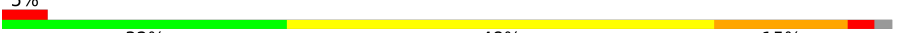
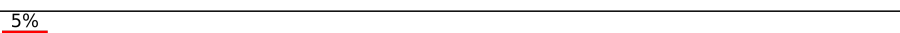
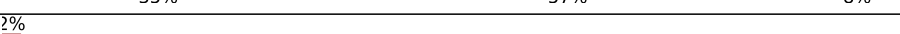
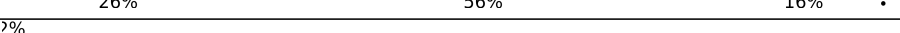
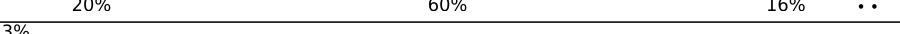
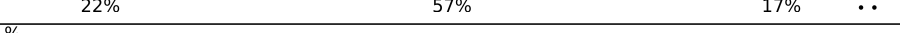
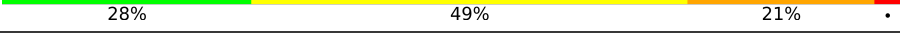
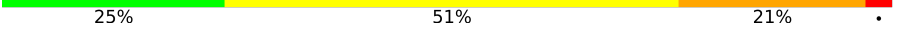
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	CV	76	
23	AW	77	
23	CW	77	
24	AX	25	
24	CX	25	
25	AY	691	
25	CY	691	
26	B0	85	
26	D0	85	
27	B1	98	
27	D1	98	
28	B2	72	

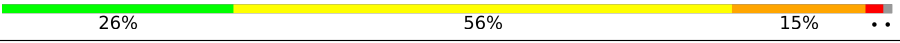
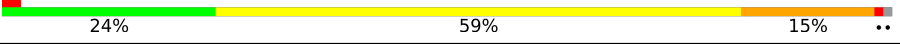
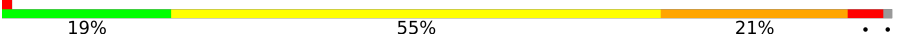
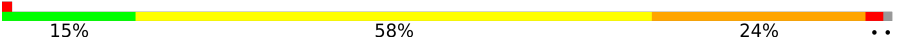
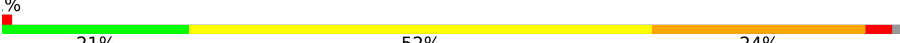
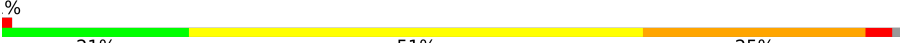
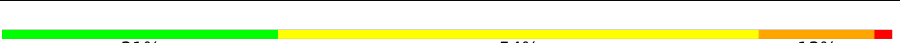
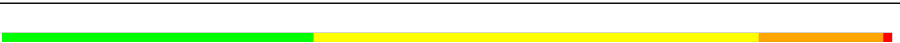
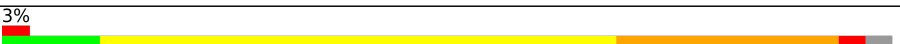
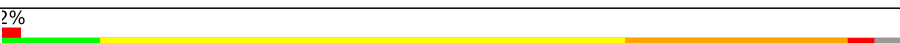
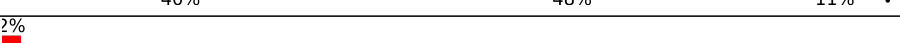
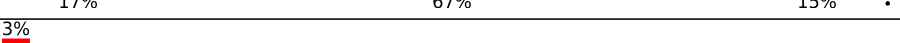
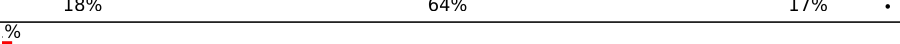
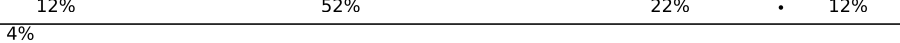
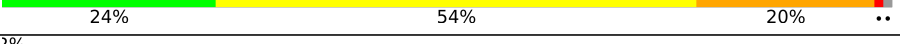
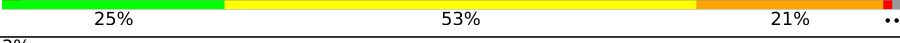
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229	
39	BD	276	
39	DD	276	
40	BE	206	
40	DE	206	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	BF	210	
41	DF	210	
42	BG	182	
42	DG	182	
43	BH	180	
43	DH	180	
44	BJ	173	
44	DJ	173	
45	BN	140	
45	DN	140	
46	BO	122	
46	DO	122	
47	BP	150	
47	DP	150	
48	BQ	141	
48	DQ	141	
49	BR	118	
49	DR	118	
50	BS	112	
50	DS	112	
51	BT	146	
51	DT	146	
52	BU	118	
52	DU	118	
53	BV	101	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	DV	101	
54	BW	113	
54	DW	113	
55	BX	96	
55	DX	96	
56	BY	110	
56	DY	110	
57	BZ	206	
57	DZ	206	

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
59	FUA	CY	701	-	-	X	-
60	GDP	AY	702	-	-	X	-
60	GDP	CY	702	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 307606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	CI	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 23 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			
23	CW	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			

- Molecule 24 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	12	Total	C	N	O	P	0	0	0
			257	116	49	80	12			
24	CX	12	Total	C	N	O	P	0	0	0
			257	116	49	80	12			

- Molecule 25 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	667	Total	C	N	O	S	0	0	1
			5215	3316	893	988	18			
25	CY	667	Total	C	N	O	S	0	0	1
			5215	3316	893	988	18			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
27	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
28	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
29	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			
30	D4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
31	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
32	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
33	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
34	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
35	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 36 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			
36	DA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			

- Molecule 37 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
37	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			
38	DC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
39	DD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
40	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
41	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	167	Total	C	N	O	S	0	0	1
			1269	803	238	227	1			
43	DH	167	Total	C	N	O	S	0	0	1
			1269	803	238	227	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BJ	170	Total	C	N	O	S	0	0	0
			851	510	170	171				
44	DJ	170	Total	C	N	O	S	0	0	0
			851	510	170	171				

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
45	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
46	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
47	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BR	117	Total	C	N	O		0	0	0
			960	599	202	159				
49	DR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				
50	DS	99	Total	C	N	O		0	0	1
			771	486	155	130				

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
51	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
52	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
53	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
54	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
55	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BY	107	Total	C	N	O	S	0	0	1
			811	520	155	131	5			
56	DY	107	Total	C	N	O	S	0	0	1
			811	520	155	131	5			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			
57	DZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

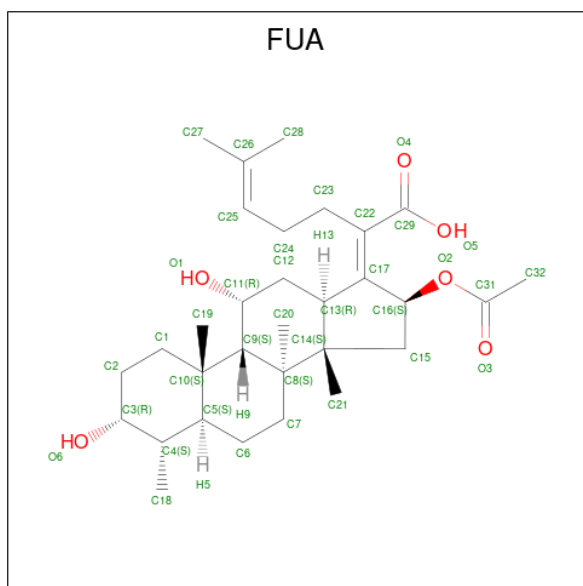
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AD	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

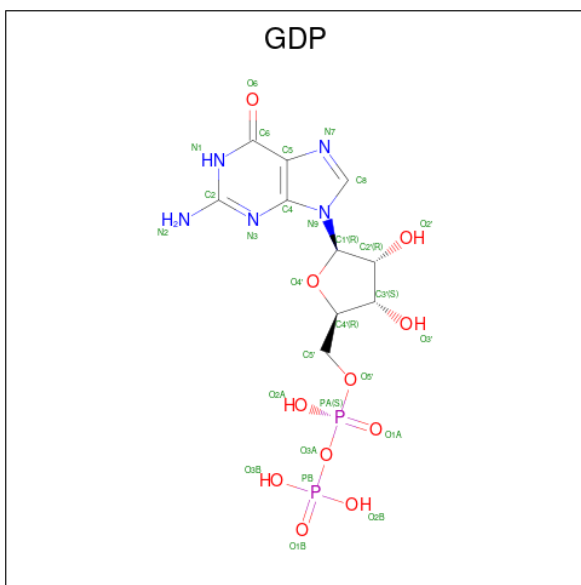
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AN	1	Total	Zn	0	0
			1	1		
58	B4	1	Total	Zn	0	0
			1	1		
58	B9	1	Total	Zn	0	0
			1	1		
58	CD	1	Total	Zn	0	0
			1	1		
58	CN	1	Total	Zn	0	0
			1	1		
58	D4	1	Total	Zn	0	0
			1	1		
58	D9	1	Total	Zn	0	0
			1	1		

- Molecule 59 is FUSIDIC ACID (CCD ID: FUA) (formula: $C_{31}H_{48}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	AY	1	Total	C	O	0	0
			37	31	6		
59	CY	1	Total	C	O	0	0
			37	31	6		

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
60	AY	1	Total 28	C 10	N 5	O 11	P 2	0	0
60	CY	1	Total 28	C 10	N 5	O 11	P 2	0	0

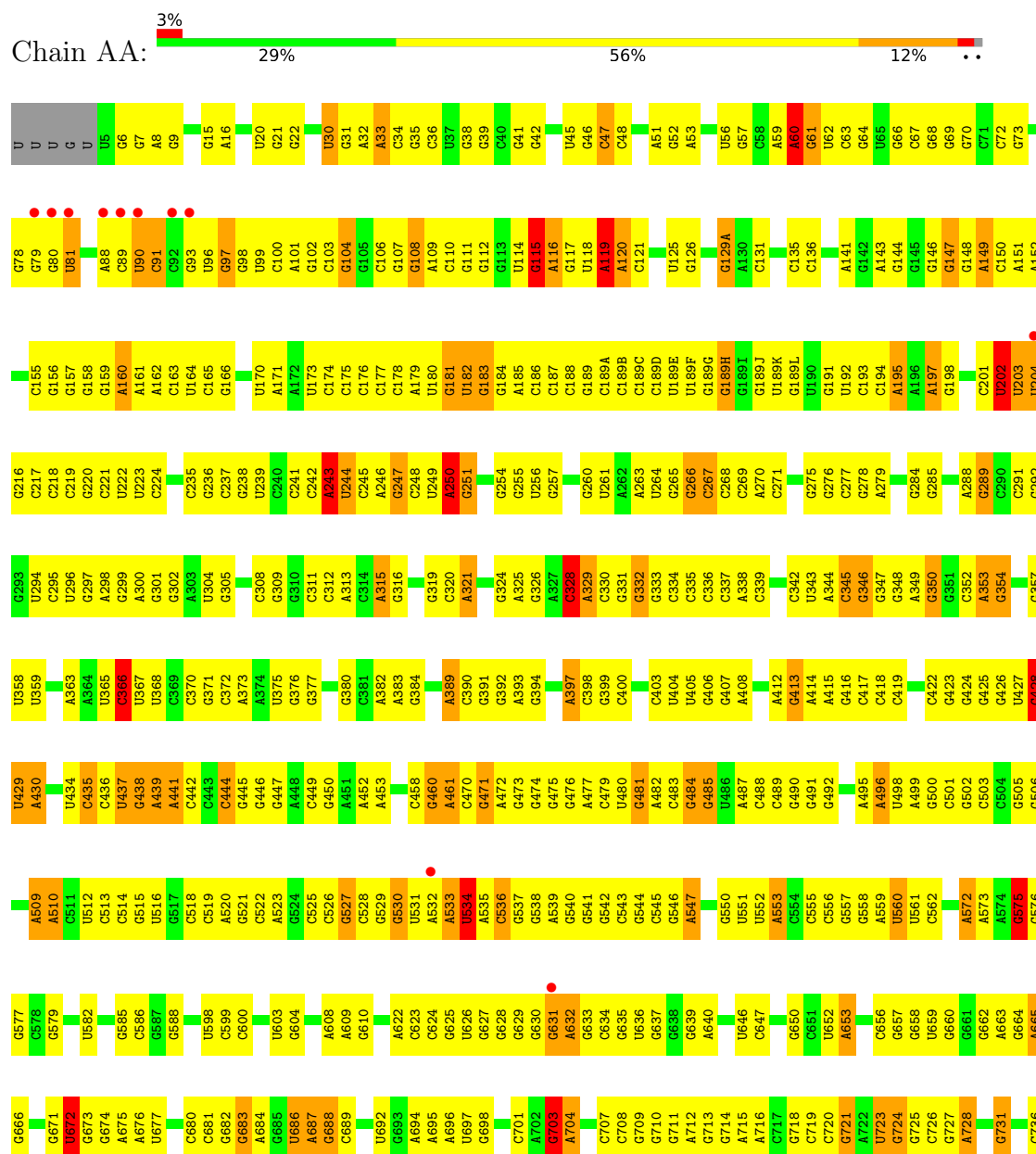
- Molecule 61 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

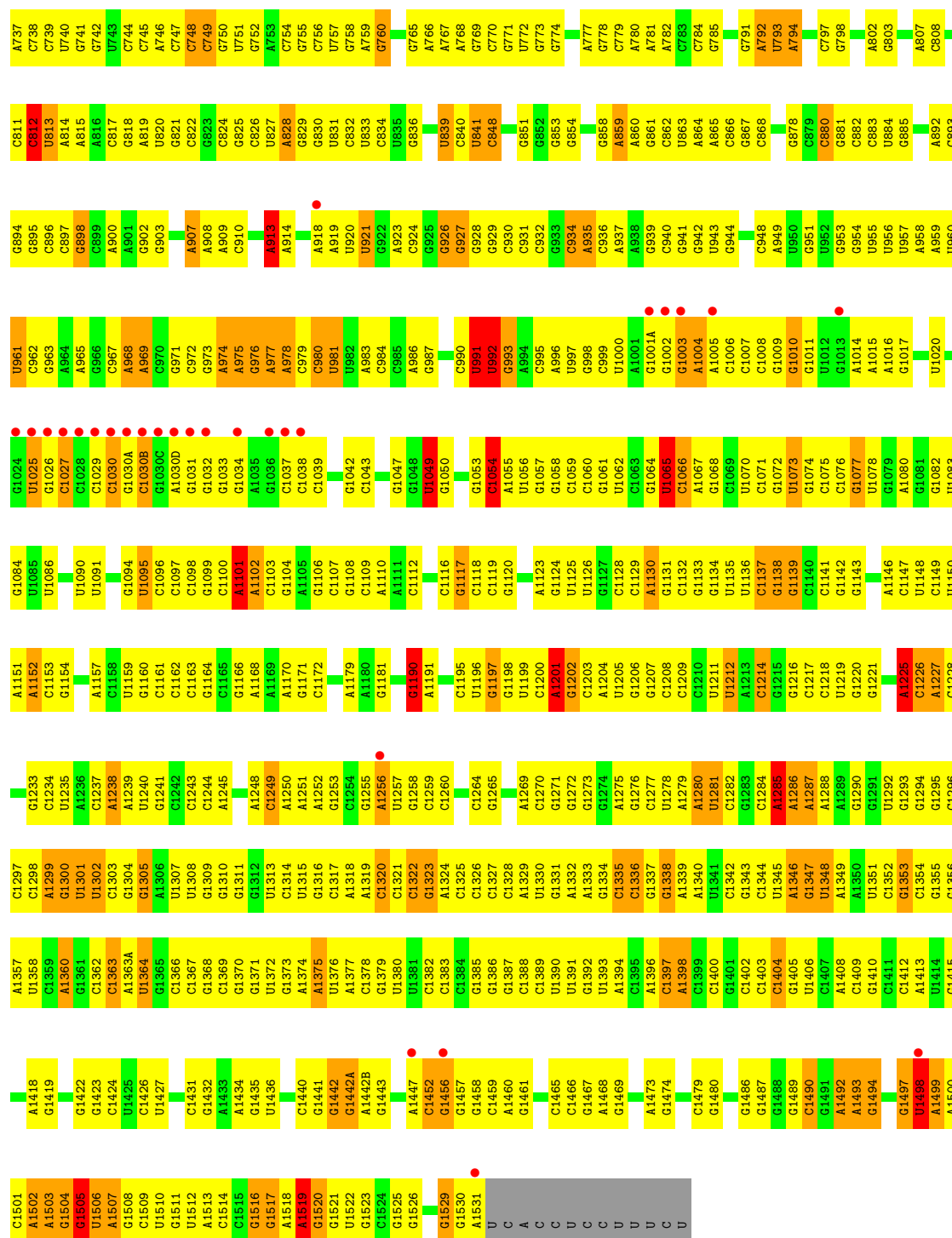
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AY	1	Total Mg 1 1	0	0
61	CY	1	Total Mg 1 1	0	0

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.

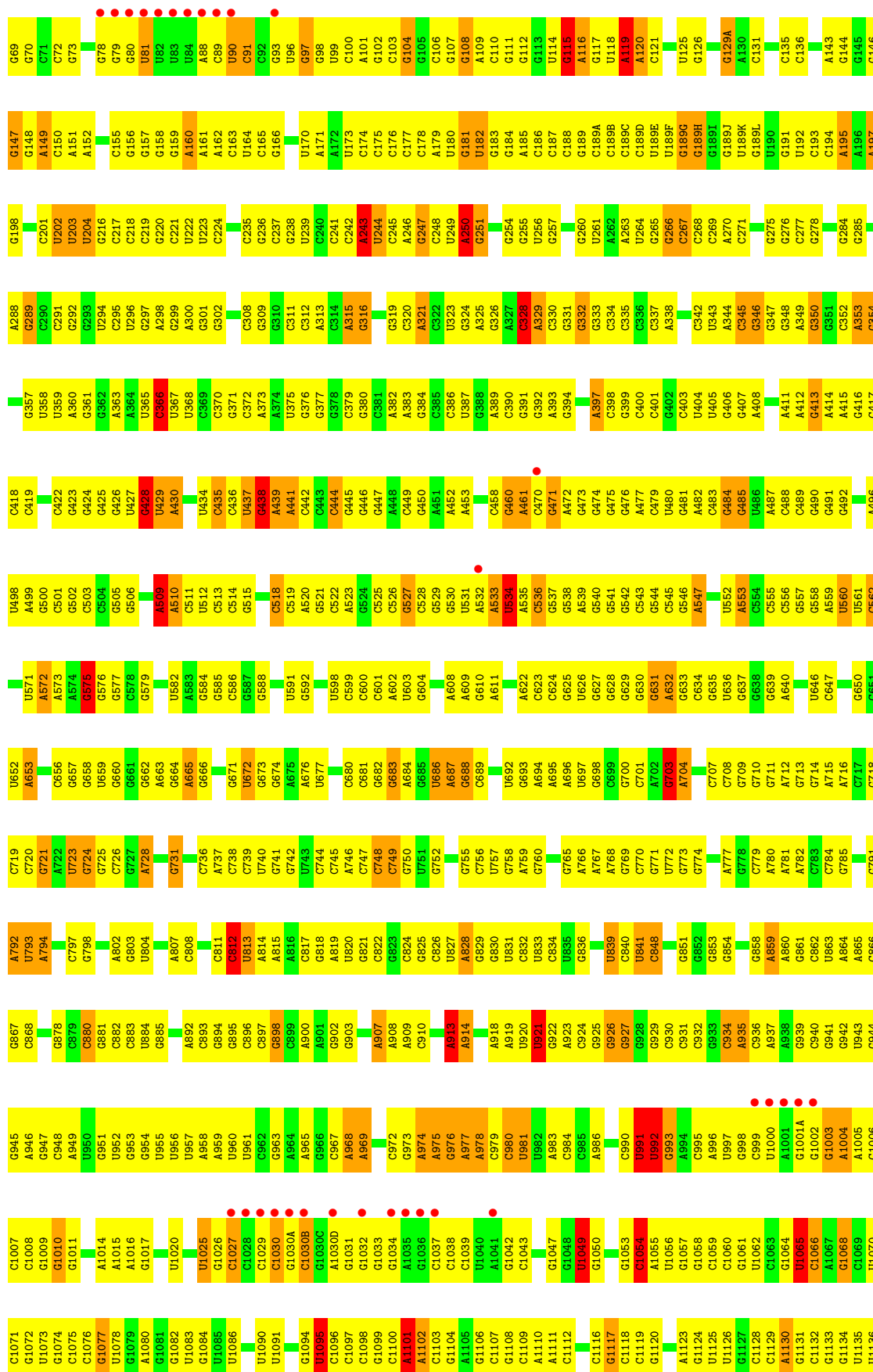
• Molecule 1: 16S RIBOSOMAL RNA

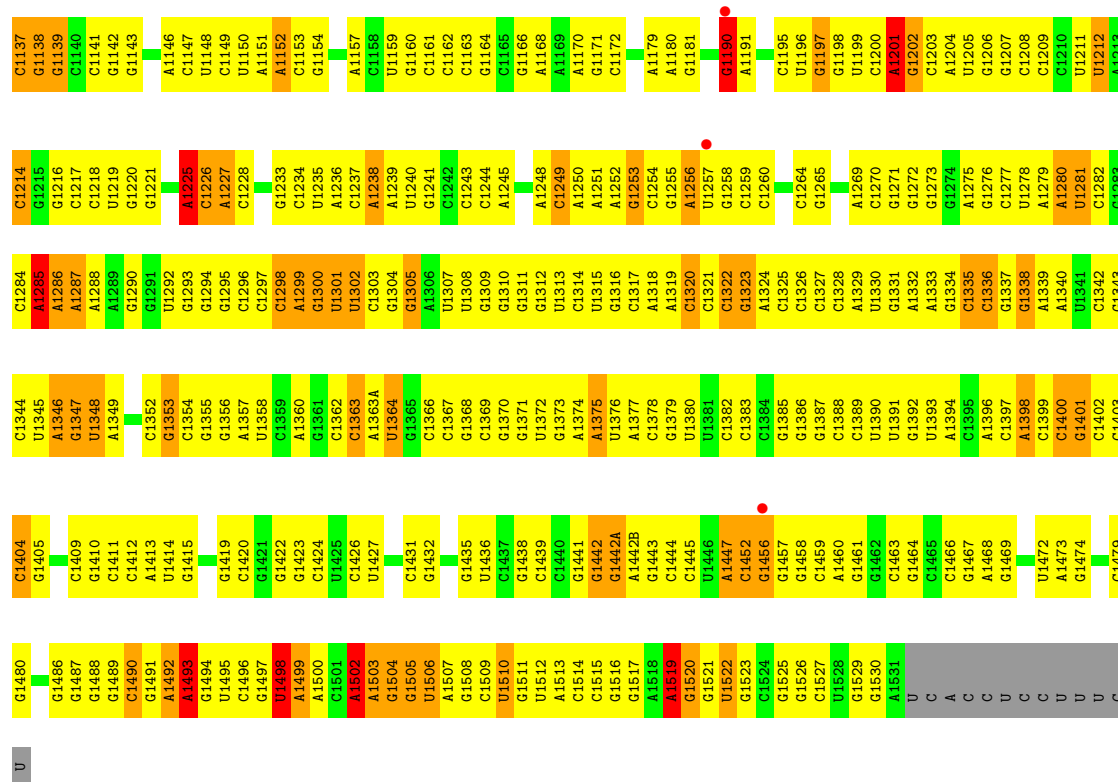




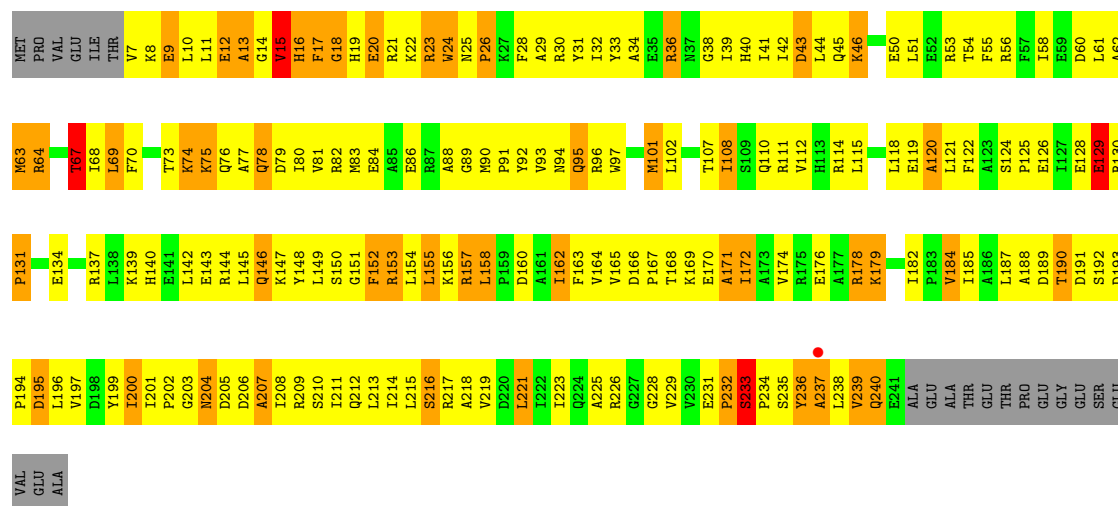
• Molecule 1: 16S RIBOSOMAL RNA





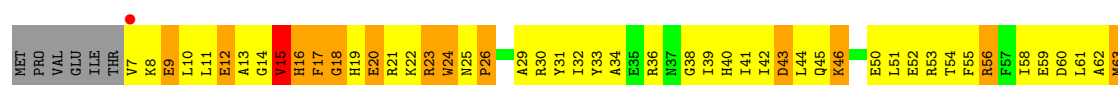


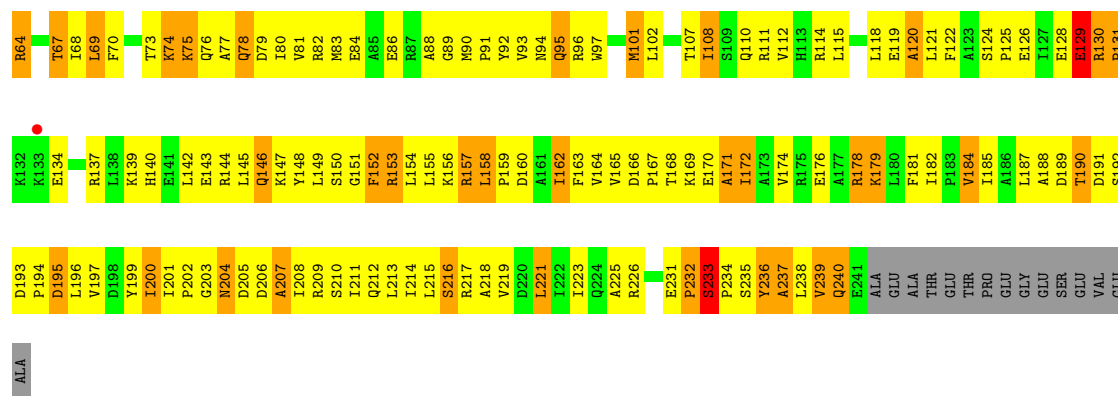
Chain AB:



• Molecule 2: 30S RIBOSOMAL PROTEIN S2

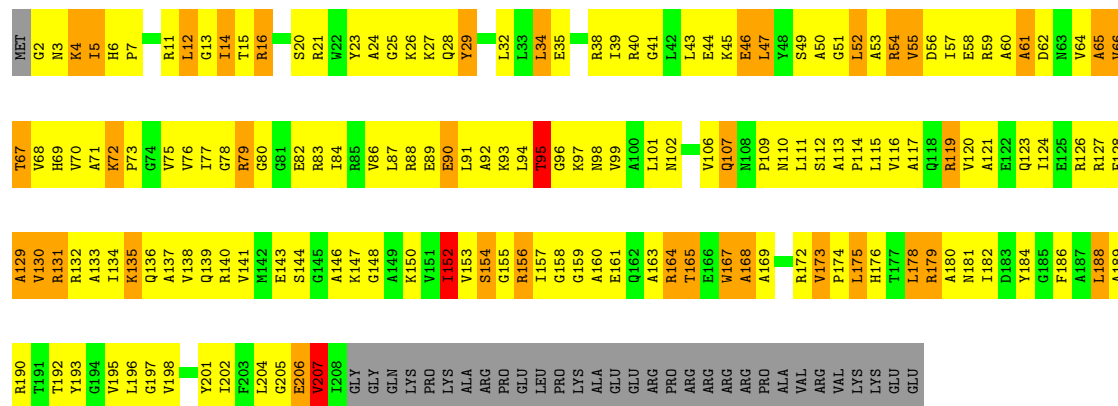
Chain CB:





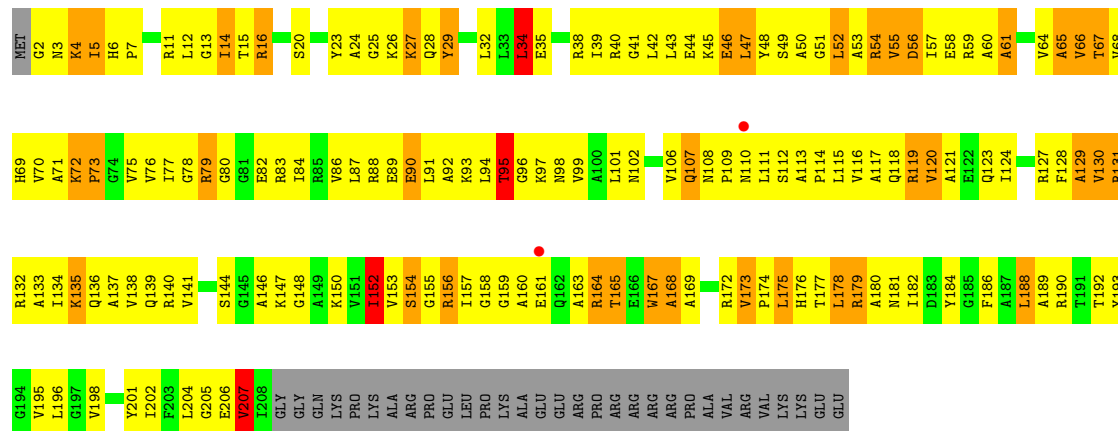
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC: 18% 51% 15% 13%



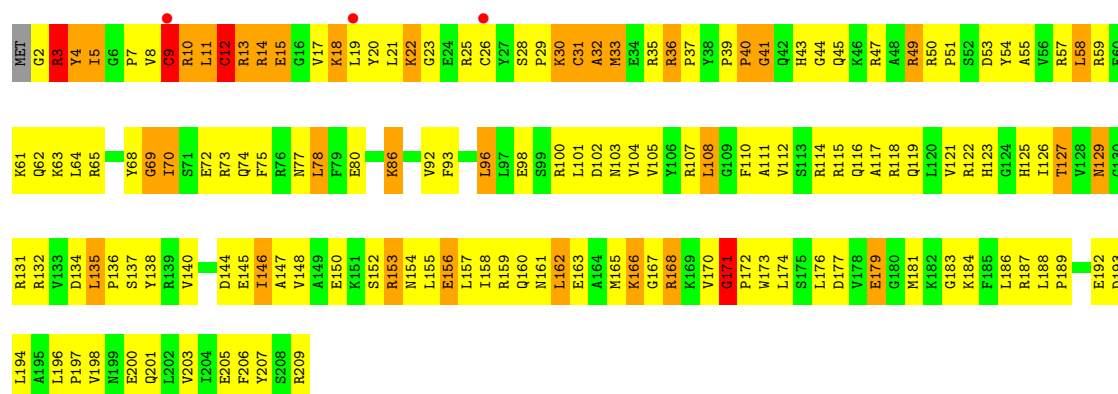
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC: 18% 51% 16% 13%

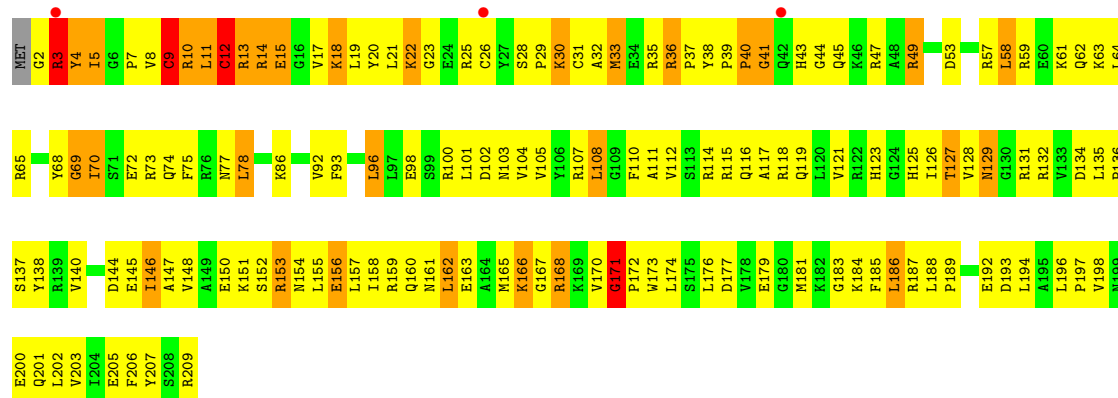


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD: 28% 53% 16%



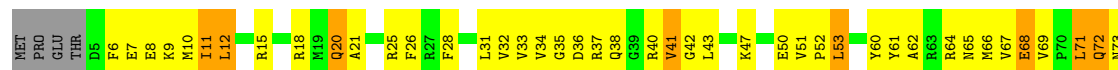
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

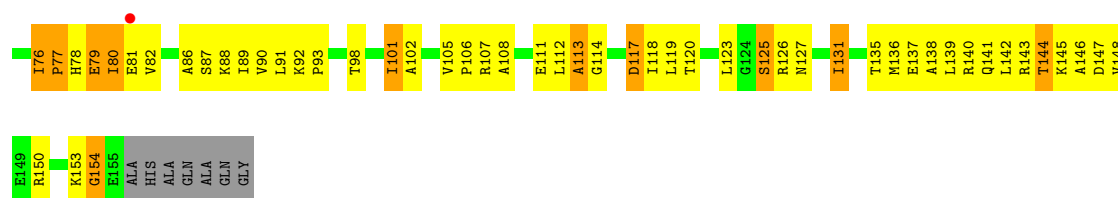


• Molecule 5: 30S RIBOSOMAL PROTEIN S5



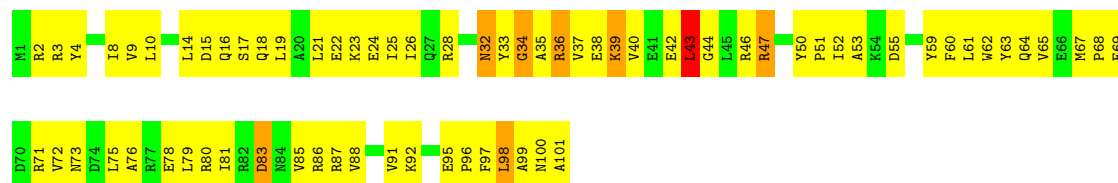
• Molecule 5: 30S RIBOSOMAL PROTEIN S5





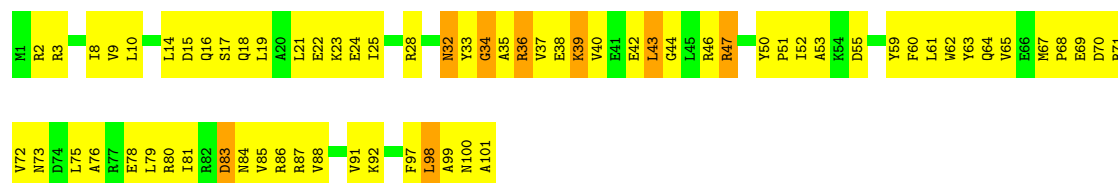
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF: 30% 62% 7%



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF: 32% 60% 8%



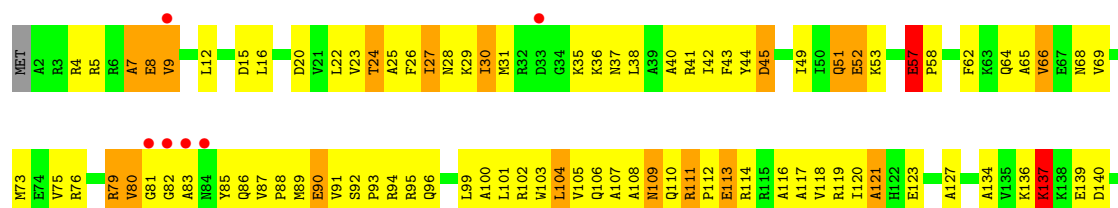
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG: 34% 50% 13%



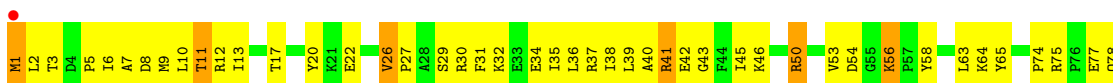
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG: 4% 36% 49% 13%

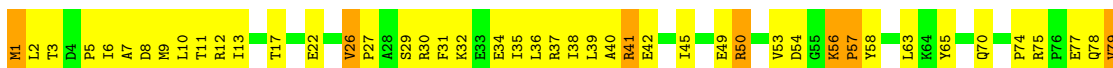




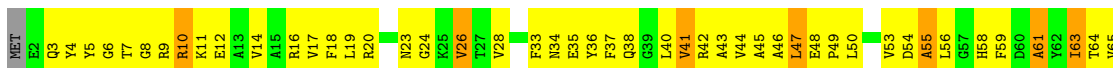
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



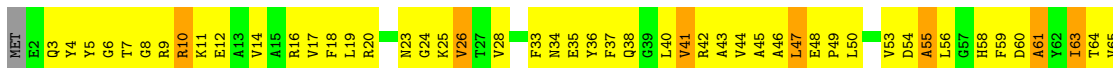
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



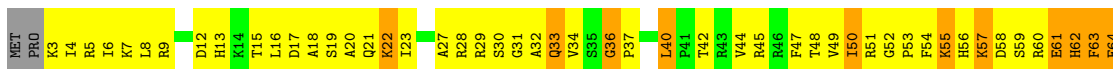
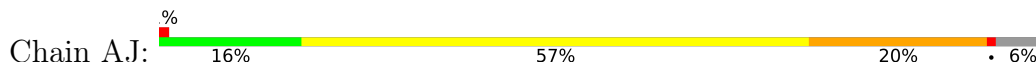
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

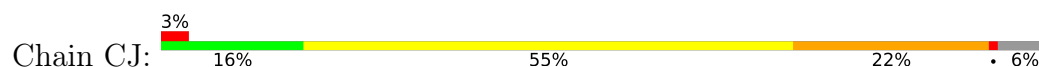


• Molecule 10: 30S RIBOSOMAL PROTEIN S10





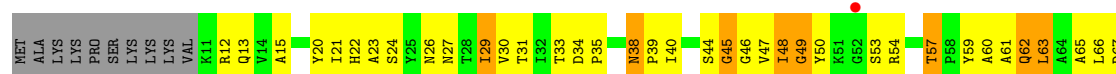
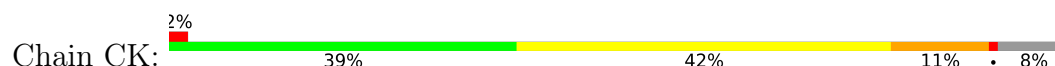
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



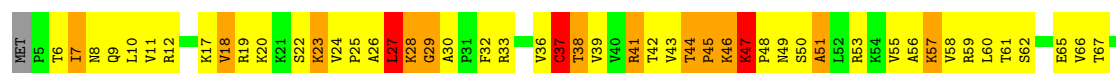
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

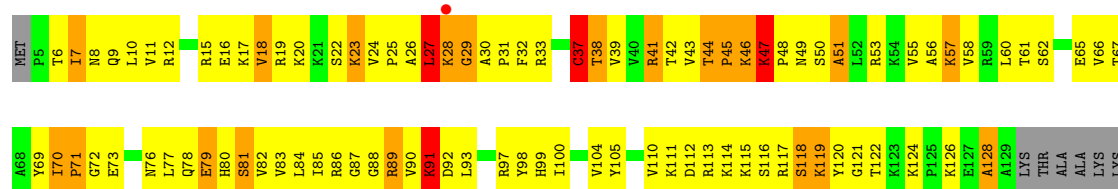


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

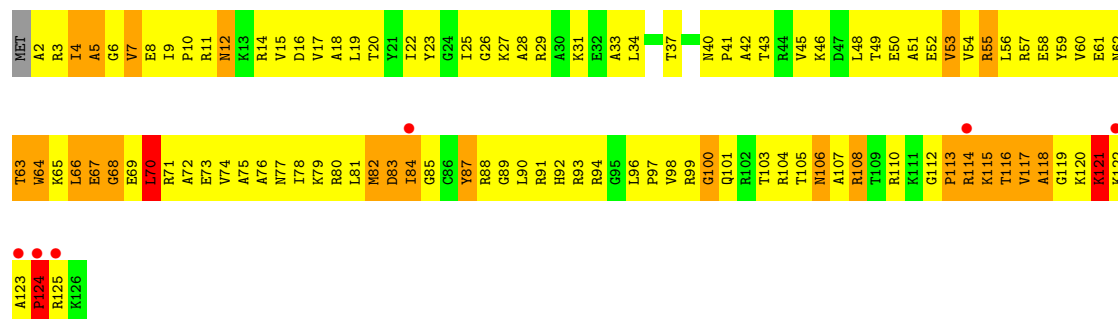


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

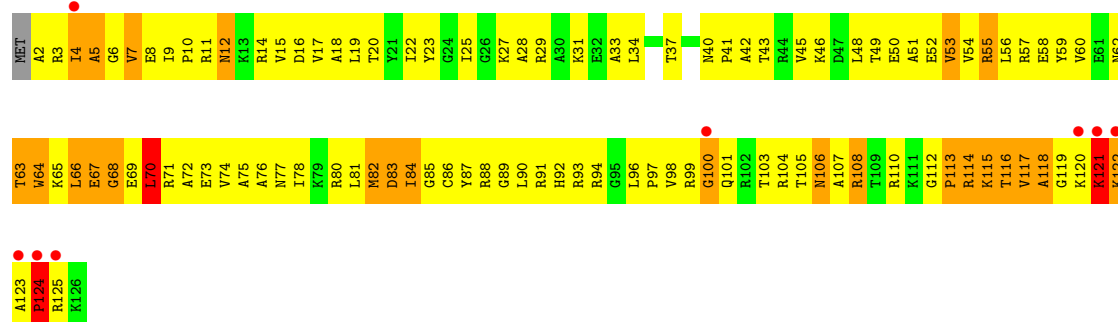




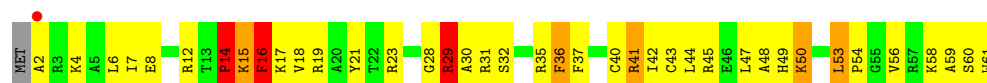
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



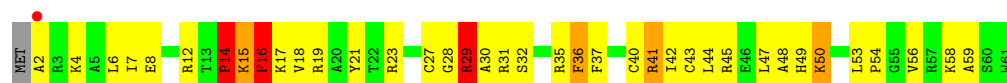
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



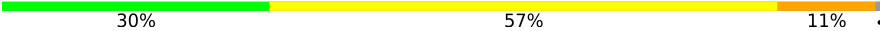
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

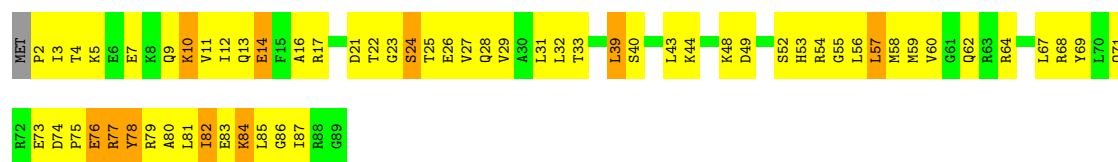


• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



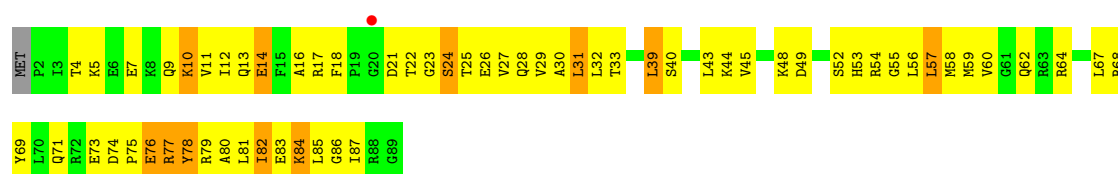
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:  30% 57% 11% .



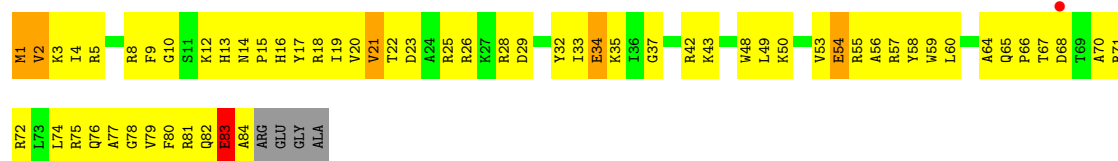
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:  29% 57% 12% .



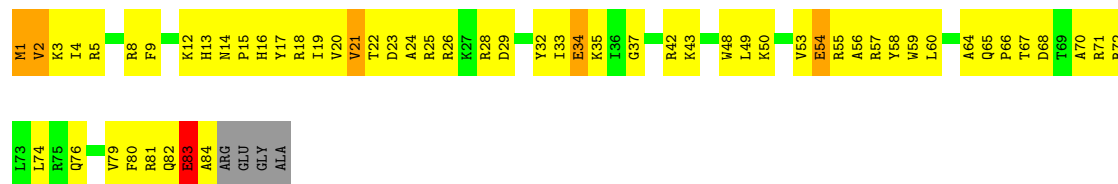
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:  26% 63% 6% • 5%



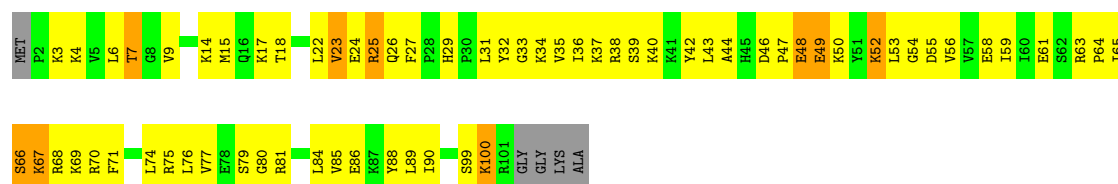
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:  30% 59% 6% • 5%

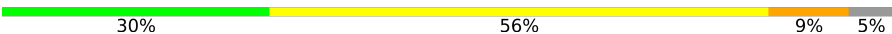


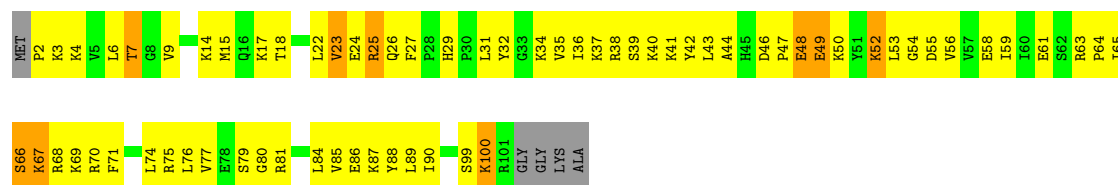
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:  32% 54% 9% 5%

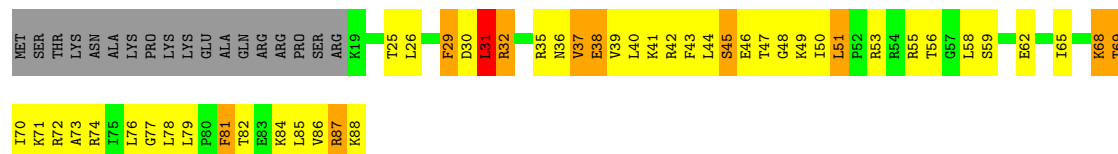


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

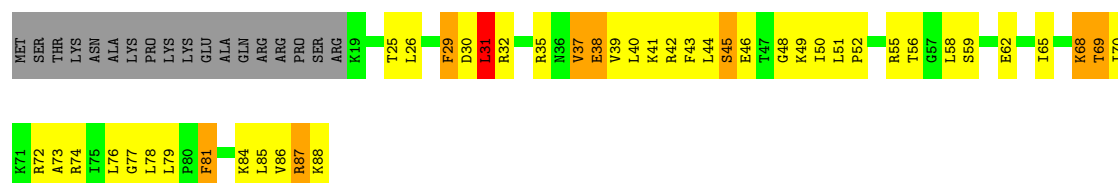
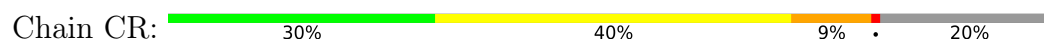
Chain CQ:  30% 56% 9% 5%



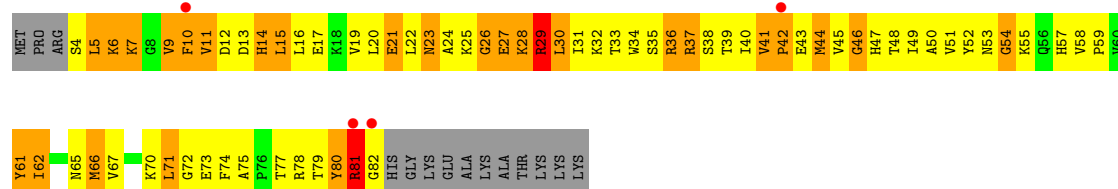
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



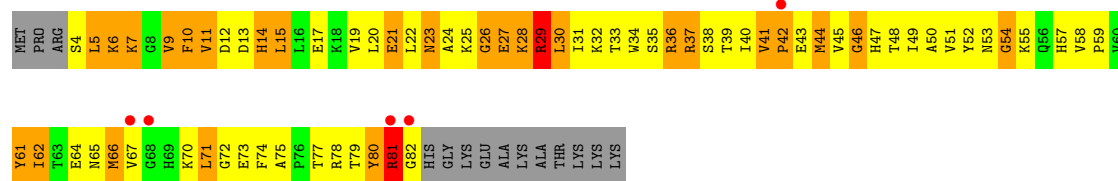
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

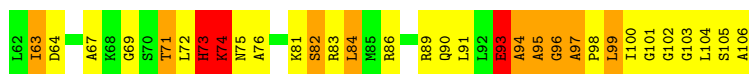
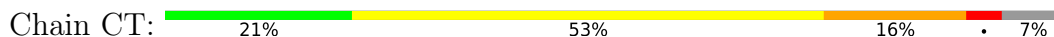


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

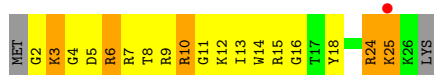




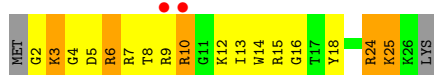
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



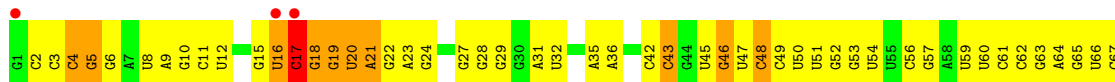
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



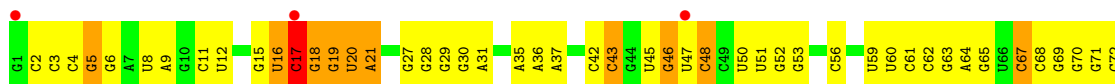
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



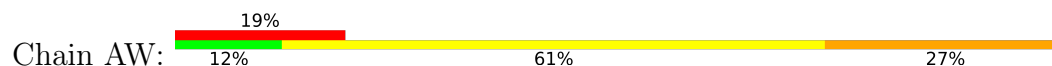
• Molecule 22: MRNA



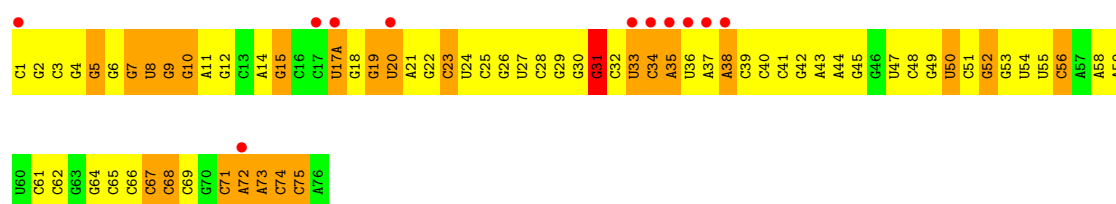
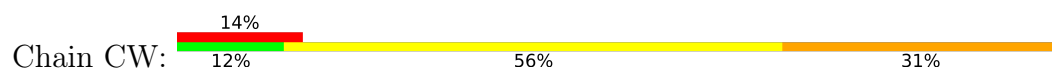
• Molecule 22: MRNA



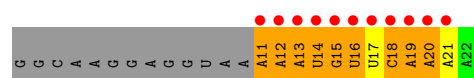
● Molecule 23: RNA



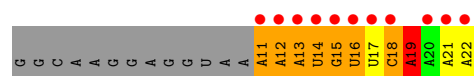
● Molecule 23: RNA



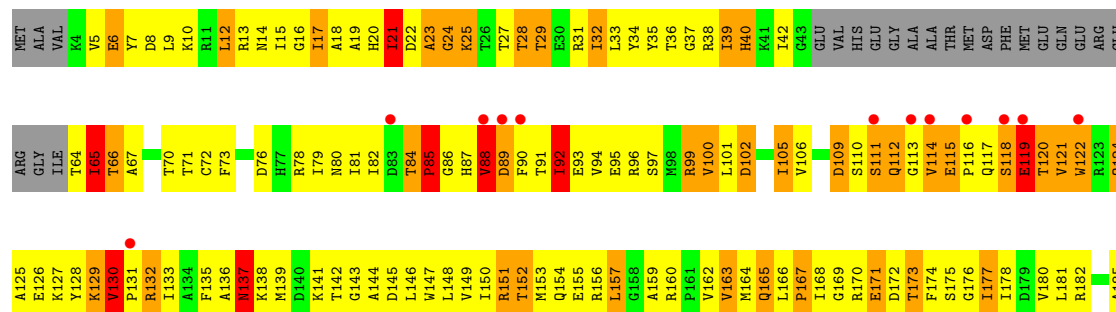
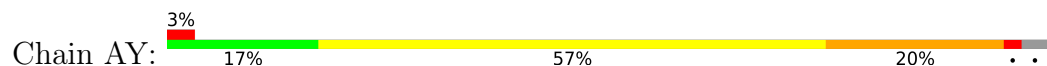
● Molecule 24: RNA

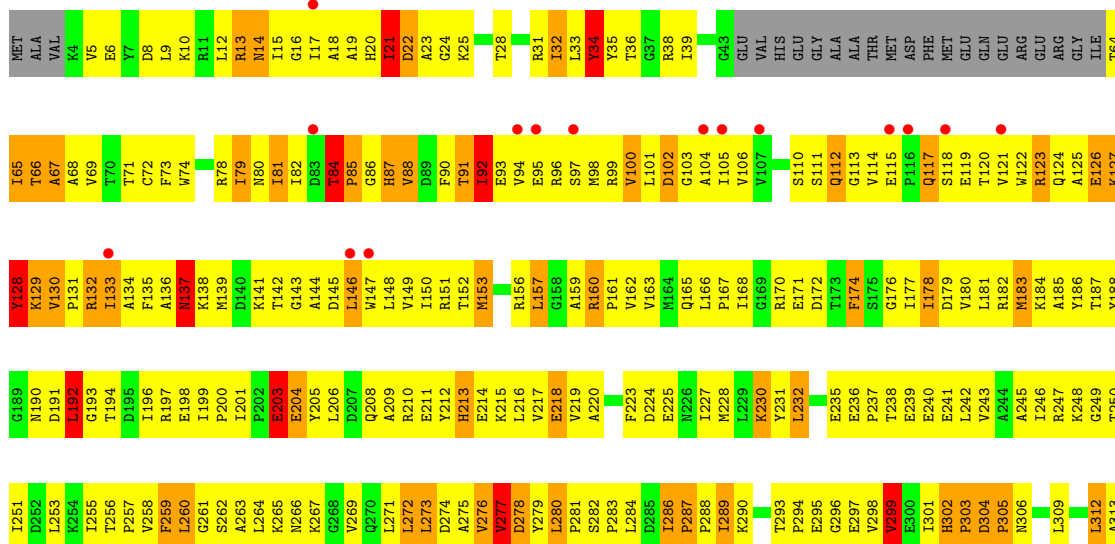


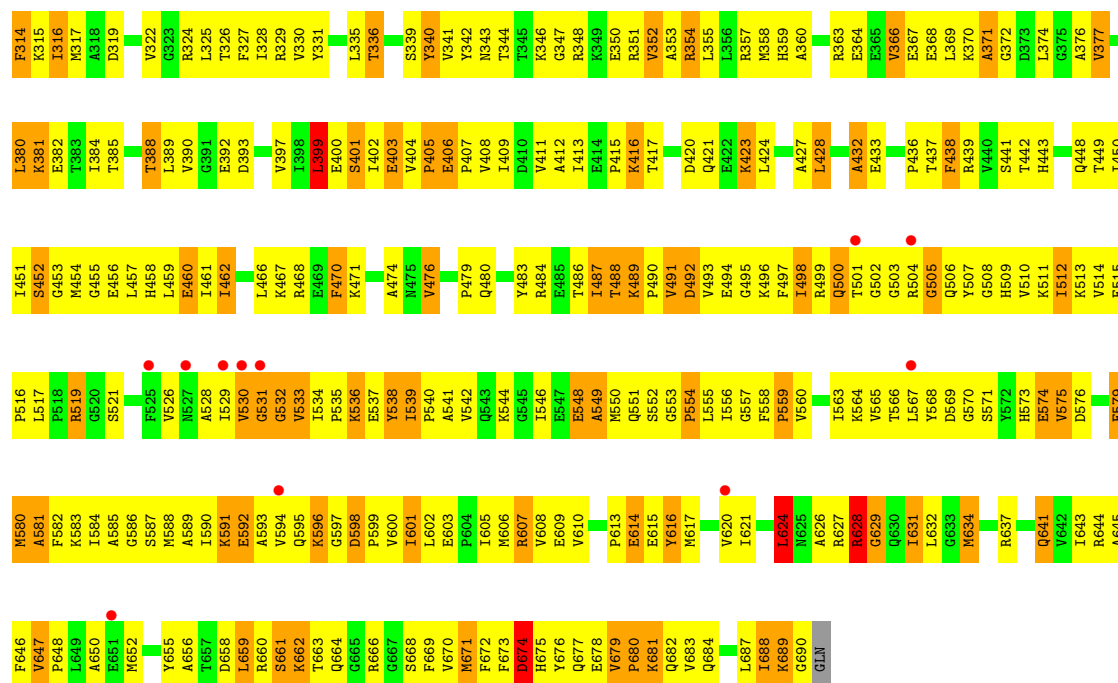
● Molecule 24: RNA



● Molecule 25: ELONGATION FACTOR G

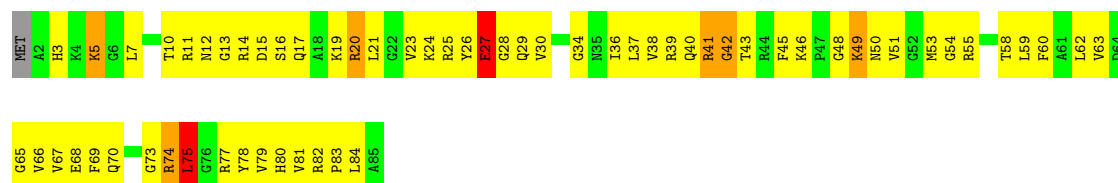






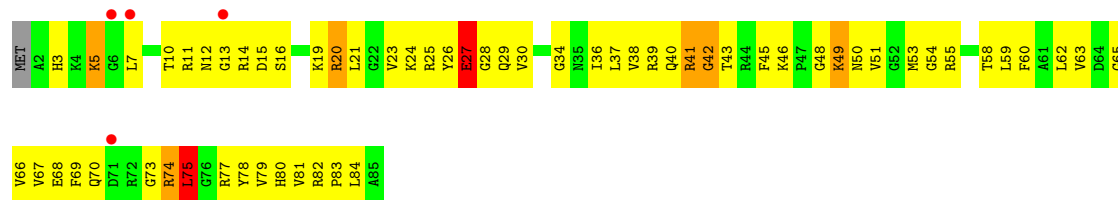
• Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain B0: 26% 64% 7% ..



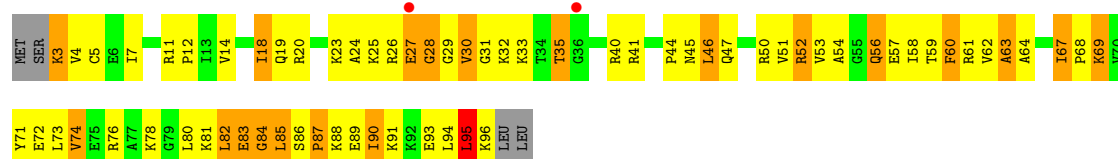
• Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain D0: 5% 27% 62% 7% ..

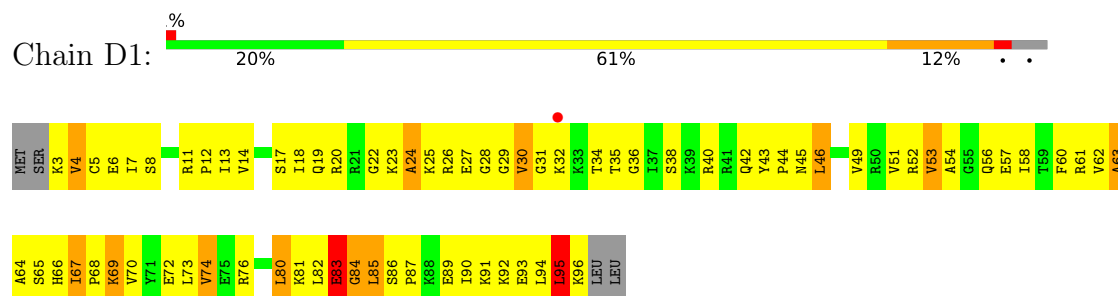


• Molecule 27: 50S RIBOSOMAL PROTEIN L28

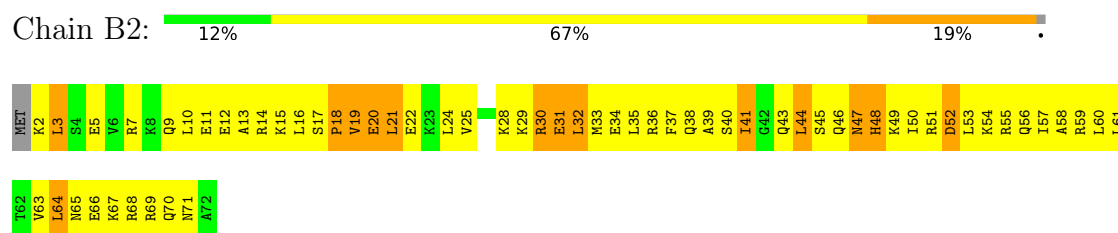
Chain B1: 2% 28% 47% 20% ..



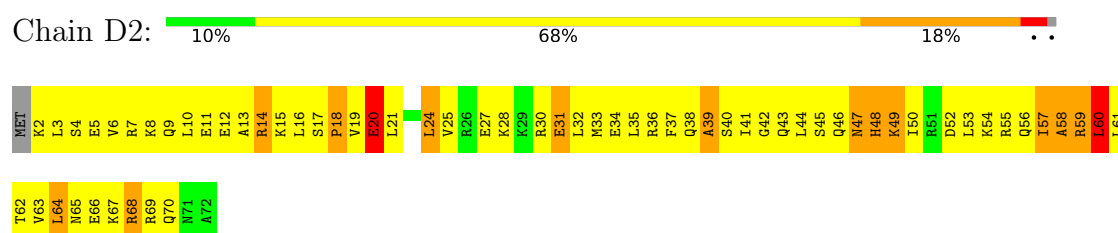
● Molecule 27: 50S RIBOSOMAL PROTEIN L28



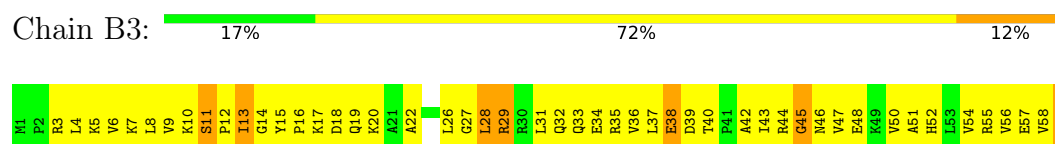
● Molecule 28: 50S RIBOSOMAL PROTEIN L29



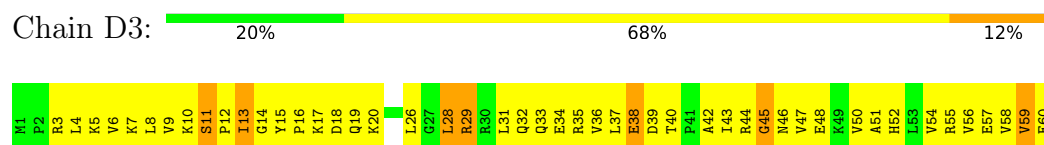
● Molecule 28: 50S RIBOSOMAL PROTEIN L29



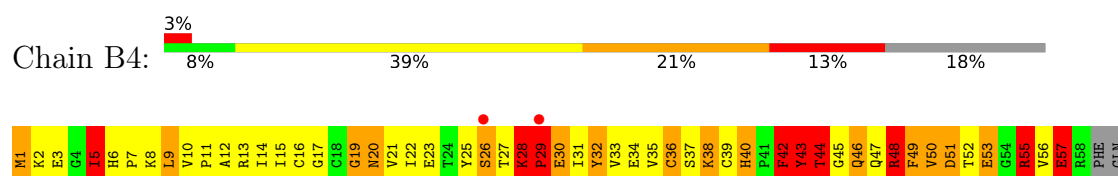
● Molecule 29: 50S RIBOSOMAL PROTEIN L30



● Molecule 29: 50S RIBOSOMAL PROTEIN L30



● Molecule 30: 50S RIBOSOMAL PROTEIN L31



ARG
ARG
TYR
GLY
ASP
SER
TYR
ARG
LYS
GLY
ARG

• Molecule 30: 50S RIBOSOMAL PROTEIN L31



M1 K2 E3 G4 I5 H6 P7 K8 L9 V10 P11 A12 A13 I14 I15 C16 C17 G18 G19 N20 V21 V22 E23 E24 Y25 Y26 S26 T27 K28 P29 E30 I31 Y32 Y33 V34 E35 C36 S37 K38 C39 H40 P41 F42 Y43 T44 G45 Q46 Q47 R48 F49 V50 D51 T52 E53 G54 R55 V56 E57 R58 PHE GLN

ARG
ARG
TYR
GLY
ASP
SER
TYR
ARG
LYS
GLY
ARG

• Molecule 31: 50S RIBOSOMAL PROTEIN L32



MET A2 K3 H4 P5 V6 P7 K10 T11 R16 R19 R20 H23 A24 L25 T26 T27 P28 T29 C33 P34 E35 C36 K37 A38 N39 K40 P41 P42 H43 T44 V45 C46 F47 E48 C49 G50 Y51 Y52 A53 G54 R55 K56 V57 L58 E59 V60

• Molecule 31: 50S RIBOSOMAL PROTEIN L32



MET A2 K3 H4 P5 V6 P7 K10 T11 R16 R19 R20 H23 A24 L25 T26 T27 P28 T29 C33 P34 E35 C36 K37 A38 N39 K40 P41 P42 H43 T44 V45 C46 F47 E48 C49 G50 Y51 Y52 A53 G54 R55 K56 V57 L58 E59 V60

• Molecule 32: 50S RIBOSOMAL PROTEIN L33



MET ALA SER GLU V5 R6 I7 K8 L9 L10 L11 E12 C13 T14 E15 C16 C17 R18 R19 N20 Y21 A22 T23 E24 K25 N26 R27 R28 N29 T30 P31 N32 K33 L34 E35 L36 R37 K38 T39 C40 P41 W42 C43 R44 K45 H46 T47 V48 H49 R50 E51 V52 K53 I54

• Molecule 32: 50S RIBOSOMAL PROTEIN L33



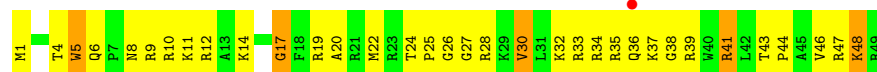
MET ALA SER GLU V5 R6 I7 K8 L9 L10 L11 E12 C13 T14 E15 C16 C17 R18 R19 N20 Y21 A22 T23 E24 K25 N26 R27 R28 N29 T30 P31 N32 K33 L34 E35 L36 R37 K38 T39 C40 P41 W42 C43 R44 K45 H46 T47 V48 H49 R50 E51 V52 K53 I54

• Molecule 33: 50S RIBOSOMAL PROTEIN L34

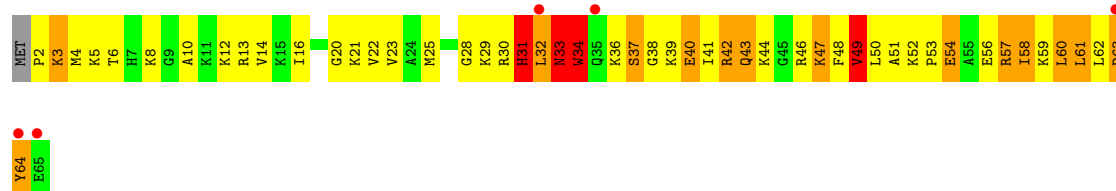


M1 T4 W5 Q6 P7 N8 R9 R10 K11 K12 A13 K14 G17 F18 R19 A20 R21 R22 R23 T24 G26 G27 R28 R29 V30 L31 K32 R33 R34 R35 Q36 K37 G38 R39 V40 L41 L42 T43 P44 A45 V46 R47 K48 R49

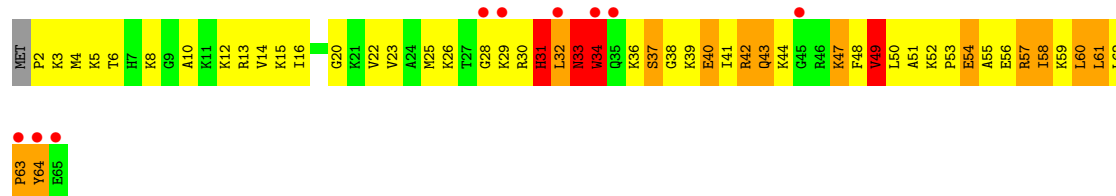
• Molecule 33: 50S RIBOSOMAL PROTEIN L34



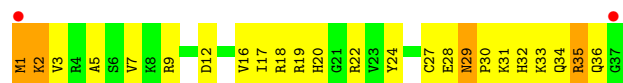
• Molecule 34: 50S RIBOSOMAL PROTEIN L35



• Molecule 34: 50S RIBOSOMAL PROTEIN L35



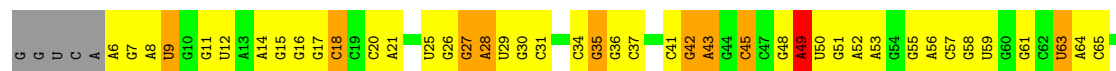
• Molecule 35: 50S RIBOSOMAL PROTEIN L36

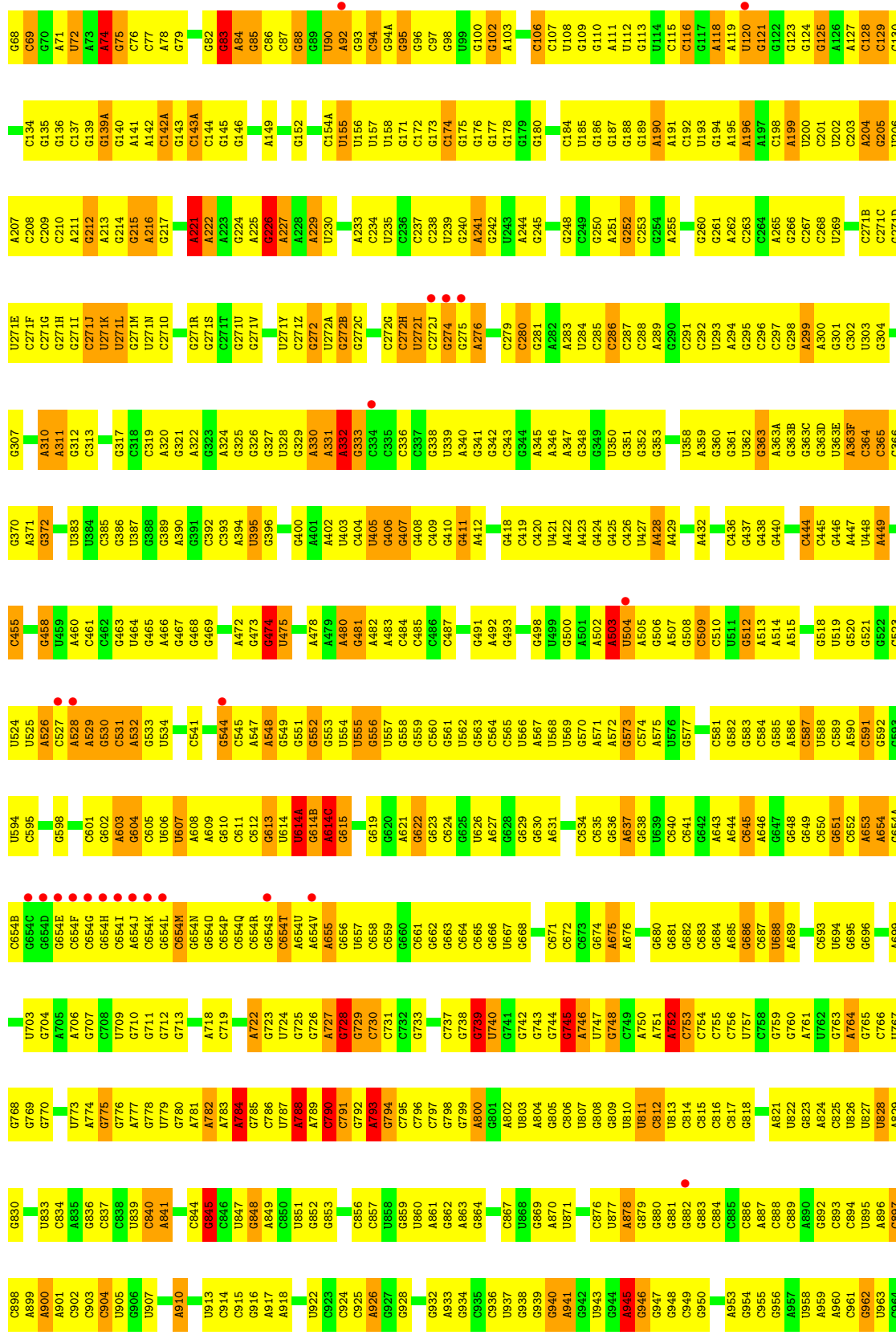


• Molecule 35: 50S RIBOSOMAL PROTEIN L36



• Molecule 36: 23S RIBOSOMAL RNA

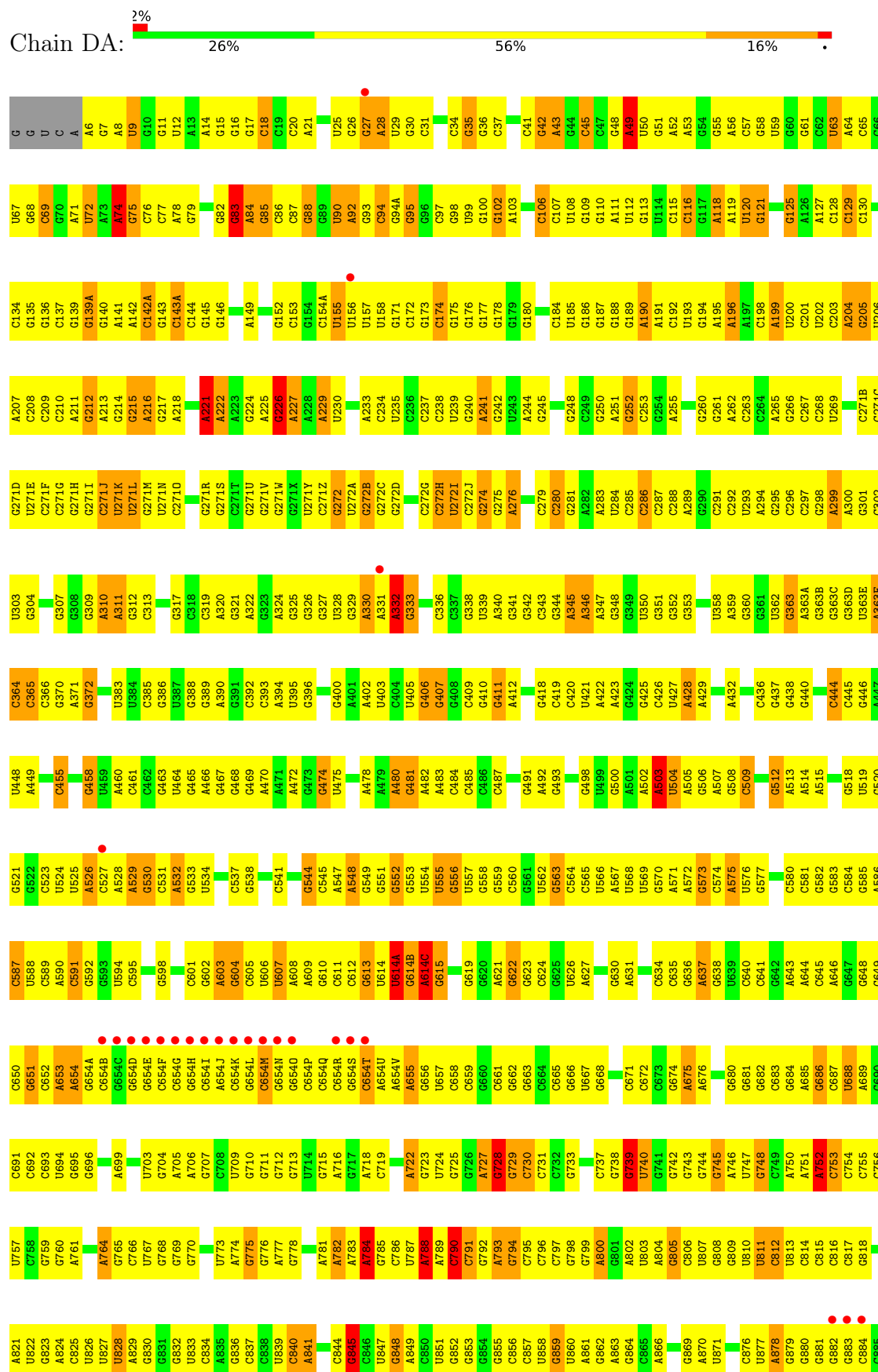




C1866	C1712	A1632	G1557	G1487	U1420	C1350	G1219	A1155	U1094	A1029	C965
A1876	U1713	G1633	A1558	G1488	G1421	C1351	A1220	A1156	A1095	G1030	G966
G1877	G1714	A1634	G1559	U1489	G1422	A1286	C1221	C1157	U1033		
	G1717	G1635	A1490	A1489	G1423	A1287	C1221A	C1158	U1097		U969
	G1718	C1636	C1565	G1491	G1424	U1288	C1222	A1098	A1034		C970
C1882	G1719	A1637	G1566	G1492	A1427	U1289	G1223	G1160	U1035		C971
G1883	U1720	C1638	C1493	C1493	C1428	C1290	C1224	C1161	G1036		G972
A1884	G1721	U1639	A1494	A1494	G1429	C1291		G1162	G1037		A973
A1885	A1722	U1640	A1495	A1496	A1430	U1292	G1227	G1163	G1038		G974
C1886	U1739	G1640	A1496	U1497	G1431	C1293	G1228	U1164	G1039		C975
C1887	G1740	C1644	U1497		U1432	U1294		U1165	G975A		G975
A1888	A1741				C1433	C1295	G1231	U1166	G1042		G976
A1889			U1503	U1503	U1434	G1296	G1232	U1167	C1043		G977
	C1744	C1648	C1504	C1504	A1434	C1297	C1233	G1106	C1044		G978
G1899	C1745	G1649	C1505	C1506	G1435	C1298	U1234	U1168	G1045		G979
A1900		G1650	U1506	U1507	G1436	C1299		G1169	A1046		A980
A1901	G1747A	G1651	A1507	U1508	C1437	U1300	G1236	G1170	G1047		C981
C1902	G1748	A1652	C1509	C1509	U1438	A1301	A1237	G1171	A1048		C982
G1903	A1749	G1653	A1509A	A1509A	A1439	A1302	G1238	A1174	C1049		A983
		A1654	A1509B	A1509B	G1440		G1239	U1175	A1050		A984
G1906	C1754	A1655	G1510	G1510	G1441	C1306	U1240	G1176	G1051		A985
G1907	A1755	C1656	C1511	C1511	G1442	A1307	A1241	A1177	C1052		C986
C1908	G1756	C1657	U1512	U1512		A1308	A1242	C1178	C1053		C987
C1909	U1757	C1658	C1513	C1513	A1445	G1309	G1243	C1179	A1054		A988
G1910	G1758	U1659	U1514	U1514	G1445A	G1310	G1244	G1180	G1055		C989
U1911	A1759	C1660	G1515	G1515	C1446	G1311	G1245		G1056		A990
A1912	A1760	G1661	C1516	C1516	G1447	U1312	A1246	G1183	A1057		C991
A1913	C1761	C1662	U1517	U1517	G1448	U1313	A1247	G1184	C1058		C992
C1914	A1762	C1663	U1518	U1518	A1449	C1314	G1248	C1185	U1059		G993
C1915	G1763	C1664	C1519	C1519	G1450	C1315	U1249	G1186	C1060		
A1916	G1764	G1666	G1520	G1520	C1450A	U1316	G1250	G1187	U1061		A996
U1917		G1667	U1523	U1523	C1451	A1317	C1251	U1188	G1062		C997
A1918	C1767	A1668	G1524	G1524	C1452	C1318	G1252	A1189	G1063		C999
A1919	U1768	A1669	C1525	C1525	U1453	C1387		G1190	C1064		A1001
C1920	G1769	C1670	G1526	G1526	G1455	A1322	A1254	G1191	A1067		G1002
G1921	C1770	C1671	G1527	G1527	G1459		U1255	G1192	G1068		C1005
C1922	G1771	G1674	A1528	A1528	A1460	G1325	C1257	G1193	A1069		C1006
	G1772	C1675	A1528A	A1528A	G1461	U1326	G1258		A1070		
C1925	A1773	A1676	C1531	C1531	C1462	C1327	C1259	C1196	G1071		A1009
U1926	C1774	G1677	C1532	C1532	C1463	G1328	G1260	G1197	C1072		A1010
	U1775	G1678	G1533	G1533	C1464	U1329	C1261	U1198	A1073		G1011
G1929	C1776	U1679	U1534	U1534	G1465	C1331	A1262	C1200	G1074		U1012
C1930	U1777	G1680	A1609	A1609	G1466	G1332	U1263		C1075		G1013
U1931	U1778	G1681	A1610	A1610	C1467	C1333	G1264		G1076		C1014
A1932	U1779	G1682	C1611	C1611		C1334	U1265		U1077		G1015
G1933	A1780	C1683	A1614	A1614	A1472	U1335	A1266				G1016
C1934	C1781	C1684	C1615	C1615	G1473	U1336	U1267	G1206	C1080		G1017
G1935	C1782	A1689	U1616	U1616	C1474	G1337	A1268	C1207	A1081		C1018
A1936	A1783	A1690	G1617	G1617	G1475	C1338	A1269	G1208	U1082		U1019
U1937	A1784	A1691	A1618	A1618	C1476	G1339	C1270	G1209	U1083		
A1938	A1785		A1542	A1542	A1477	U1340	G1271	A1210			A1020
	A1786	C1694	C1619	C1619	A1478	U1341	A1272	C1146	A1086		A1021
C1942	U1787	G1695	A1543	A1543	G1479	U1342	U1273	C1147	G1087		G1022
U1943	C1788	G1696	A1544	A1544	C1411	G1344	A1274	A1148	C1088		U1023
U1944	A1789	G1697	C1546	C1546	U1415	G1345	A1275	G1149	G1089		G1024
G1945	C1790	A1698			U1416	G1346	A1276	A1214	U1090		G1025
U1946	A1791	G1699	A1553	A1553	G1482	G1347	A1277	G1215	G1091		U1026
C1947	A1792		A1554	A1554	G1484	U1348	A1278	G1216	C1092		A1027
G1948			A1555	A1555	G1485	C1417	G1279	G1217	C1093		
U1949	C1795		C1556	C1556	A1486			G1154			A1028

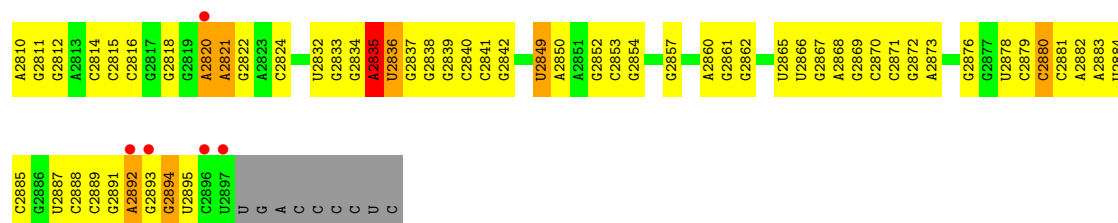
G1950	G1951	G1952	G1955	G1959	G1960	G1963	G1964	G1967	G1968	G1969	G1970	G1971	G1972	G1973	G1977	G1984	G1985	G1986	G1989	G1990	G1991	G1992	G1993	G1996	G1997	G1998	G2000	A2001	G2002	G2003	G2004	G2007	G2008	G2009	G2010	U2011	G2012	A2013	A2014	A2015	U2016	U2017	G2018	A2019	A2020	C2021	U2022	G2023									
C2026	C2027	U2028	G2029	A2030	G2031	G2032	G2033	G2034	G2035	G2036	G2037	G2038	C2039	C2040	A2041	A2042	C2043	G2046	G2049	C2050	A2051	G2052	G2053	A2054	G2055	G2056	A2057	A2060	G2061	A2062	C2065	U2068	G2069	G2070	A2071	G2072	G2073	U2074	U2075	U2076	U2079	G2080	C2081	A2082	G2083	C2084	U2085	G2086	G2087	G2088	G2089	G2090	U2091	U2092	G2093	G2097	
U2098	U2099	G2100	C2103	G2104	G2105	C2106	C2107	G2110	G2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	G2125	A2126	G2127	U2130	U2131	U2132	G2133	A2134	C2137	C2138	C2139	C2143	U2144	G2145	G2146	G2147	G2148	G2149	U2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	A2158	U2159	G2160	C2161	G2162	C2163			
C2164	G2165	G2166	U2167	G2168	A2169	A2170	A2171	U2172	A2173	C2174	C2175	C2178	G2182	G2183	G2184	C2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	G2193	C2194	C2195	G2196	U2197	A2198	A2199	C2200	C2201	C2202	C2203	C2205	G2206	G2207	A2208	U2218	G2219	G2220	G2221	G2222	G2223	G2224	A2225	C2226	C2229	G2230	U2231	U2232	U2233	G2234	G2235	G2237		
G2238	G2239	C2240	A2241	G2242	U2243	U2244	U2245	U2246	C2247	C2248	U2249	G2256	U2257	G2258	G2259	G2260	C2261	U2262	C2263	A2266	A2267	U2272	A2273	G2274	C2275	G2276	G2277	A2278	G2279	G2282	C2283	G2284	C2285	A2286	A2287	A2288	G2289	G2290	U2291	C2292	C2293	U2296	C2297	A2298	G2299	G2300	C2301	G2304	A2305	C2306	G2307	G2308	A2309				
A2310	A2311	U2312	C2313	G2314	G2315	G2316	G2317	G2318	G2319	A2320	G2321	A2322	G2323	C2324	G2325	C2326	A2327	A2328	G2329	G2330	G2331	U2332	A2333	G2334	A2335	A2336	G2337	G2338	U2344	G2345	A2346	C2347	U2348	G2349	G2350	G2351	A2352	G2353	G2358	C2359	A2360	C2364	G2365	A2366	G2367	C2368	A2369	G2370	G2371	G2372	G2373	C2374	G2375	A2376	A2377	A2378	
C2381	G2382	G2383	G2384	G2385	G2386	U2387	A2388	G2389	U2390	G2391	A2392	A2393	C2394	G2395	G2396	G2397	U2398	U2401	C2402	U2405	U2406	G2407	U2408	G2409	G2410	A2411	A2412	G2413	G2414	G2415	A2416	C2417	A2418	U2419	C2420	G2421	A2422	U2423	C2424	A2425	A2426	C2427	G2428	G2429	A2430	U2431	A2432	C2433	A2434	A2435	U2438	A2439	C2440	C2441	C2442		
C2443	G2444	G2445	G2446	G2447	A2448	U2449	A2450	A2451	G2454	G2455	C2456	U2457	G2458	U2461	U2462	G2463	C2464	G2465	C2466	G2467	G2468	A2469	G2470	G2471	G2472	U2473	G2474	A2475	A2476	G2477	A2478	G2481	G2482	C2483	G2484	G2485	G2486	G2487	A2488	G2489	U2492	U2493	G2494	G2495	C2496	A2497	C2498	C2499	U2500	G2501	G2502	A2503	U2504	G2505	U2506		
C2507	G2508	G2509	C2510	U2511	G2512	G2513	U2514	C2515	G2516	A2518	U2519	C2520	G2523	G2524	G2525	G2526	G2529	A2530	A2531	G2532	A2533	U2537	C2538	G2539	C2540	A2541	A2542	U2543	G2544	G2545	U2546	U2547	G2548	G2549	G2550	C2551	U2552	G2553	U2554	U2555	C2556	G2557	A2558	C2559	G2560	A2561	U2562	A2565	A2566	G2567	G2568	G2569	C2570	U2571			
A2572	C2573	G2574	G2575	G2576	A2577	G2578	C2579	U2580	G2581	G2582	G2583	U2584	U2585	U2586	A2587	A2590	C2591	G2592	U2593	C2594	G2597	A2600	C2601	G2602	G2603	G2606	G2607	G2608	U2609	C2610	U2611	C2612	U2613	A2614	U2615	C2616	U2617	G2618	C2626	G2627	G2628	A2629	G2630	G2631	A2632	U2636	U2639	G2640	G2645	G2646	U2647						
C2648	U2649	U2650	C2651	C2652	G2655	U2656	U2657	A2658	G2659	A2660	G2661	A2662	G2663	G2664	G2665	C2666	C2667	G2668	G2669	A2670	G2671	G2672	G2673	G2677	G2678	G2679	C2680	C2681	U2682	G2685	G2686	U2688	U2689	C2690	C2691	G2692	A2693	G2694	C2695	U2696	G2697	U2698	C2701	U2702	C2703	C2704	A2705	G2706	G2707	G2708	G2709	G2710	A2711	G2712			
A2712A	A2713	G2714	C2715	U2716	G2717	U2720	A2721	G2722	C2723	C2724	A2725	U2726	G2727	U2728	G2729	C2730	G2731	G2732	A2733	A2734	G2735	G2736	A2740	A2741	C2742	A2743	G2744	C2745	U2746	G2747	A2748	A2749	G2750	G2751	C2752	A2753	U2754	C2755	U2756	A2757	G2758	G2759	C2760	G2761	G2762	C2763	A2764	A2765	G2766	C2767	G2768	G2769	G2770	C2771	G2772	C2773	C2774
A2775	A2776	A2777	A2778	U2779	G2780	A2781	G2782	G2783	C2784	G2787	G2788	C2789	A2790	C2791	G2792	C2793	C2794	G2795	U2796	C2799	A2801	A2801A	G2802	C2803	C2804	G2805	G2807	U2808	A2809	A2810	G2811	A2812	C2814	C2815	C2816	U2817	G2818	C2819	A2820	A2821	C2822	U2823	C2824	U2832	G2833	G2834	U2835	U2836	G2837	G2838	G2839	C2840	C2841	G2845	G2846		
U2849	U2850	A2851	G2852	G2853	G2854	A2860	G2861	G2862	U2865	U2866	G2867	A2868	G2869	C2870	C2871	G2872	A2873	G2876	U2877	U2878	C2879	C2880	C2881	A2882	A2883	U2884	C2885	U2886	U2887	C2888	C2889	G2891	A2892	G2893	G2894	U2895	U2896	U2897	U	G	A	C	C	C	C	U	C										

- Molecule 36: 23S RIBOSOMAL RNA



A1780	C1883	G1538	A1472	G1403	G1334	C1269	C1146	A1086	A1020	G957	C886
C1781	C1884	G1539	G1473	C1404	U1335	A1210	C1147	A1087	A1021	U958	A857
A1782	A1689	U1540	G1474	U1405	G1336	G1271	A1148	A1088	G1022	A959	C888
A1783	C1615	G1541	G1475	U1406	G1337	G1212	G1149	A1089	U1023	A960	C889
A1784	A1616	A1542	C1476	C1407	G1338	G1213	C1150	U1090	G1024	C961	A890
A1785	C1617	C1543	A1477	C1408	G1339	A1214	C1151	U1091	G1025	G962	G892
A1786	A1618	A1544	G1478	C1409	U1340	G1215	C1152	G1091	U1026	U963	C893
A1787	G1619	C1545	G1479	G1410	U1341	G1216	C1153	C1092	A1027	C964	C894
C1788	G1695	C1546	G1480	C1411	U1342	G1217	C1154	G1093	A1028	C965	U895
A1789	G1697	C1547	U1481	U1415	C1344	G1218	A1155	U1094	A1029	U896	C897
C1790	G1698	C1548	G1482	G1416	C1345	C1219	A1156	U1095	A1030	C966	C898
A1791	C1625	C1549	G1485	C1417	G1346	A1220	G1157	A1096	G1033	U969	C899
U1709	U1629	A1553	A1486	U1420	G1347	C1221	C1158	U1097	U1033	C970	A899
C1710	G1630	A1554	G1487	U1421	A1349	C1222	U1159	A1098	G1034	C971	A900
C1711	U1796	C1555	G1488	G1421	C1350	G1223	G1160	G1099	U1035	G972	A901
C1712	A1632	C1556	U1489	G1422	C1351	C1224	G1161	C1100	A1036	A973	C902
U1713	G1633	A1557	U1490	C1423	U1352	U1287	G1162	U1101	G1037	G974	C903
U1714	A1634	G1558	A1491	G1424	C1353	U1288	G1163	C1102	C1038	C975	C904
G1717	G1635	G1559	G1492	U1431	A1354	C1289	G1164	A1103	G1039	G975A	U905
C1718	C1636	C1565	C1493	A1427	U1354	C1290	U1165	G1104	A1045	C976	G966
U1719	A1637	A1566	A1494	C1428	U1355	C1291	C1166	U1105	G1042	C977	U907
U1720	C1638	A1567	A1495	G1429	A1359	U1292	U1167	G1106	C1043	G978	C915
C1804	U1639	G1568	A1496	C1430	A1360	C1293	G1168	G1107	G1044	G979	G916
U1805	C1640	A1569	U1497	U1431	G1361	U1294	G1169	U1108	A1045	A980	A917
U1739	U1644	C1573	U1503	C1432	C1362	C1295	G1170	C1109	A1046	A981	C914
G1740	C1644	G1574	C1504	U1433	C1363	G1296	G1171	G1110	G1047	C982	C915
A1741	C1647	C1575	A1505	A1434	G1364	C1297	A1173	A1111	A1048	A983	C916
C1744	C1648	U1576	C1506	G1435	A1365	G1298	U1174	G1112	A1049	A984	A918
C1745	G1649	C1577	C1506	G1436	A1366	G1299	U1175	U1113	A1050	C985	C918
U1814	G1650	U1578	C1509	C1437	G1367	U1300	G1176	G1114	G1051	C986	C924
A1815	G1651	A1579	U1509	U1438	C1368	A1301	A1177	G1115	C1052	G987	C925
G1747A	A1652	C1582	A1509A	A1439	G1369	A1302	C1178	C1116	C1053	A988	C926
G1748	C1653	C1583	U1509B	G1440	U1370	C1306	C1179	G1117	A1054	G989	A926
C1754	A1654	A1583	G1510	G1441	C1375	A1307	C1180	C1118	G1055	A990	G927
A1755	A1655	C1584	U1511	G1442	C1376	A1308	C1181	C1119	A1056	C991	G928
G1756	C1656	A1586	U1512	U1445	G1377	G1309	A1182	G1120	G1057	C992	G932
U1820	U1757	C1587	C1445A	A1445	C1378	G1310	G1183	C1121	G1058	G993	A933
G1822	C1657	C1588	C1446	C1446A	A1379	G1311	G1184	G1122	G1059	A996	G934
A1759	C1658	C1589	G1447	G1447	U1378	U1312	C1185	C1123	U1060	C997	C935
G1823	U1659	U1590	G1448	G1448	G1380	U1313	G1186	C1124	U1061	C998	C936
A1760	C1660	G1516	C1449	C1449	G1381	C1314	G1187	G1125	G1062	C999	U937
G1761	G1661	U1518	G1450	G1450	C1382	G1315	U1188	A1126	G1063	U999	G938
A1825	C1662	C1592	G1451	G1451A	C1383	C1316	A1189	A1127	C1064	A1000	G939
G1826	C1663	G1593	C1452	C1452A	A1384	U1317	G1191	A1128	A1067	A1001	G940
C1827	G1666	G1594	U1523	C1453	G1385	A1318	G1192	G1131	G1068	G1002	A941
A1828	G1667	G1595	G1524	A1452	C1386	G1319	G1193	C1005	A1069	C1006	G942
C1830	A1668	A1596	G1525	U1453	C1387	G1320	C1196	U1133	A1070	C1006	U943
U1768	A1669	G1526	G1455	G1455	G1388	A1321	C1197	C1135	G1071	C1006	G944
G1769	C1670	U1527	U1456	G1456	U1389	A1322	G1197	G1136	C1072	A1009	A945
C1770	U1674	A1528	G1459	G1459	U1390	G1325	U1198	G1137	A1073	A1010	G946
G1771	C1675	A1529A	A1460	A1460	U1391	U1326	G1199	G1138	G1074	G1011	G947
G1772	A1676	C1531	G1461	C1462	U1392	C1327	C1200	G1139	C1075	U1012	G948
A1773	C1677	G1532	C1462	C1462	A1395	G1328	C1199	C1140	C1076	C1013	C949
C1774	A1677	G1533	C1463	C1463	U1396	U1329	C1200	C1141	A1077	U1014	G950
U1775	U1678	G1534	C1464	C1464	U1397	G1329	C1200	U1142	C1080	G1015	A953
G1776	U1679	U1534	G1465	G1465	U1398	C1330	C1200	A1142A	G1016	G1016	G954
C1843	U1777	A1535	G1466	G1466	U1399	C1331	C1200	A1143	U1081	G1017	C955
U1778	G1681	C1536	C1467	C1467	G1400	G1332	C1200	A1144	U1082	C1018	G956
U1779	U1682	A1610	G1537	C1467	C1402	C1333	C1200	C1145	U1083	U1019	

G2747	G2685	U2611	U2547	G2417	G2350	C2283	U2203		U2074	C2008	G1933	G1846
A2748	G2686	C2612	G2548	A2418	G2351	C2284	C2205		U2075	G2009	G1934	A1847
A2749	U2687	U2613	G2549	U2419	G2352	C2285	G2206		U2076	G2010	G1935	A1848
A2750	U2688	A2614	G2550	G2420	G2353	A2286	G2207			U2011	A1936	G1849
G2751	U2689	U2615	G2551	G2421	G2484	A2287	G2208		U2079	G2012	A1937	U1850
G2752	G2690	G2616	U2552	G2422	G2485	A2288	U2218		G2080	A2013	U1938	U1851
A2753	G2691	G2617	G2553	U2423	G2486	G2289	G2219		C2081	A2014		C1852
U2754	C2692	G2618	U2554	G2424	G2487	G2290	G2220		C2082	A2015		
U2755	A2693		U2555	A2425	A2488	G2291	G2221		U2082	U2016		G1856
U2756	G2694	G2624	G2556	A2426	G2489	C2292	G2222		G2083	U2017		G1857
A2757	G2695	G2625	G2557	G2427	G2490	C2293	G2223		C2084	G2018		G1858
A2758	U2696	G2626	U2492	G2428	U2493	U2286	G2224		U2085	G2019		A1859
G2759	U2697	G2627	G2493	G2429	G2494	C2287	G2225		U2086	A2020		U1946
G2760	U2698	G2628	G2494	A2430	G2495	C2287	G2226		G2087	U2021		U1947
G2761		A2629	U2561	U2431	G2496	C2287				C2021		G1862
G2762	C2701	G2630	U2562	A2432	A2639	C2287			G2090	U2022		G1865
G2763	U2702	G2631	A2563	A2433	A2640	G2289			U2091	G2023		G1866
A2764	C2703	A2632	A2565	A2434		G2300			U2092	U1951		A1876
A2765	C2704		A2566	A2435	G2301	G2302			G2094	A1952		G1877
A2766	A2705	U2636	A2567		G2302	G2303			G2095	G1953		G1878
G2767	G2706		G2568	U2438	G2303	G2304			U2096	U2028		
G2768	G2707		G2569	A2439	G2305	G2306			G2097	G2029		C1882
G2769	G2708		A2570	G2440	G2307	G2308			U2098	A2030		G1883
G2770	C2709		U2504	C2441	G2308	G2309			U2099	A2031		A1884
G2771	G2710	G2645	G2505	G2442	G2309				G2100	G2032		A1885
G2772	A2711	C2646	U2506	G2443	A2310					A2033		A1886
G2773	U2712	U2647	C2507	G2444	A2311					U2034		C1887
G2774	A2712A	G2648	G2508	G2445	G2312				G2103	G2037		G1888
A2775	A2713	U2649	G2509	G2446	U2313				G2104	G1963		A1889
A2776	G2714	U2650	G2510	G2447	G2314				G2105	G1964		
A2777	G2715	G2651	U2511	G2448	G2315				G2106	C2039		
G2778	G2716	C2652	C2512	U2449	G2316				C2107	U2041		G1899
U2779	G2717		U2513	A2450	G2317					G2042		A1900
G2780	G2718	U2655	U2514	A2451	G2318				G2110	A2043		A1901
A2781	G2719	U2656	G2515	G2452	G2319				G2111	G2044		G1902
G2782	U2720	A2657	G2516	A2453	G2320				G2112	C2045		G1903
A2783	G2721	G2658	G2517	G2454	G2321				U2113	A1972		
G2784	G2722	G2659	U2518	G2455	G2322				A2114	G2046		G1906
G2785	C2723	A2660	U2519	G2456	G2323				G2115	G1907		G1907
U2786	G2724	G2661	G2520	U2457	G2324				G2116	C1908		C1908
G2787	U2725	A2662	G2521	G2458	G2325				A2117	G1909		G1909
G2788	G2726	G2663			G2326				U2118	A2051		G1910
G2789	U2727	G2664	G2523		G2327				A2119	G2052		U1911
A2790	G2728	A2665	G2524	C2461	A2328				G2120	G2053		A1912
G2791	G2729	G2666	G2525	U2462	A2329				G2121	A2054		A1913
G2792	U2730	G2667	G2526	G2463	G2330				U2122	C2055		C1914
G2793	G2731	G2668		C2464	G2331				G2123	G2056		U1915
G2794	A2732	G2669	A2530	C2465	G2332				G2124	A2057		A1916
G2795	U2733	A2670	A2531	C2466	U2333				G2125	U1993		U1917
U2796	G2734			G2467	A2334				A2126	A1918		A1918
U2797	A2735	G2671	U2537	G2468	U2406				G2127			
U2798	G2736	G2672	C2538	A2469	G2407					G2061		G1921
A2801	A2801A	G2673	U2539	G2470	U2408					A2062		G1922
G2802	G2802		C2539	C2471	G2409				U2130	G1998		
G2803	A2740	G2677	C2540	G2472	G2410				G2065	G1999		C1925
G2804	A2741	A2678	A2541	U2473	A2411					G2000		U1926
G2805	G2742	A2679	A2542	U2474	A2412				U2068	A2001		
G2806	C2743	G2680	G2543	C2475	G2413				U2069	G2002		G1929
G2807	G2744	G2681	G2544	A2476	G2414					A2071		G1930
U2808	C2745	U2682	G2545	A2477	U2347					G2070		G1931
A2809	U2746		U2546	A2478	G2349					G2071		A1932
										C2073		



• Molecule 37: 5S RIBOSOMAL RNA



• Molecule 37: 5S RIBOSOMAL RNA

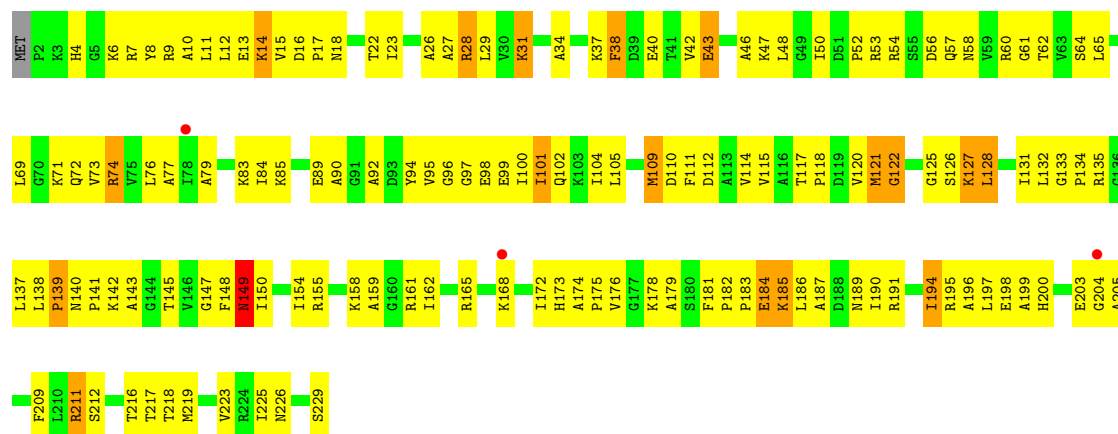


• Molecule 38: 50S RIBOSOMAL PROTEIN L1



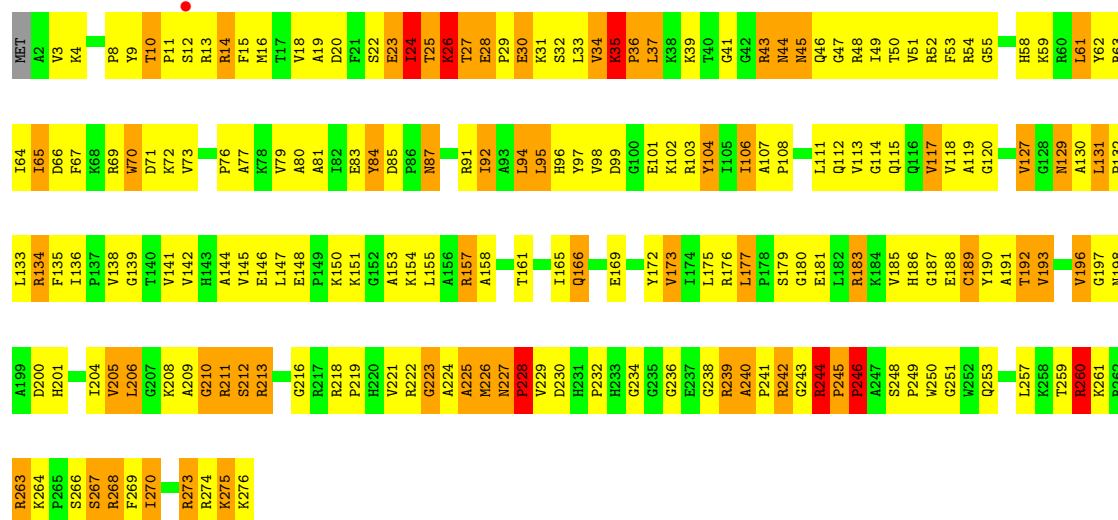
• Molecule 38: 50S RIBOSOMAL PROTEIN L1





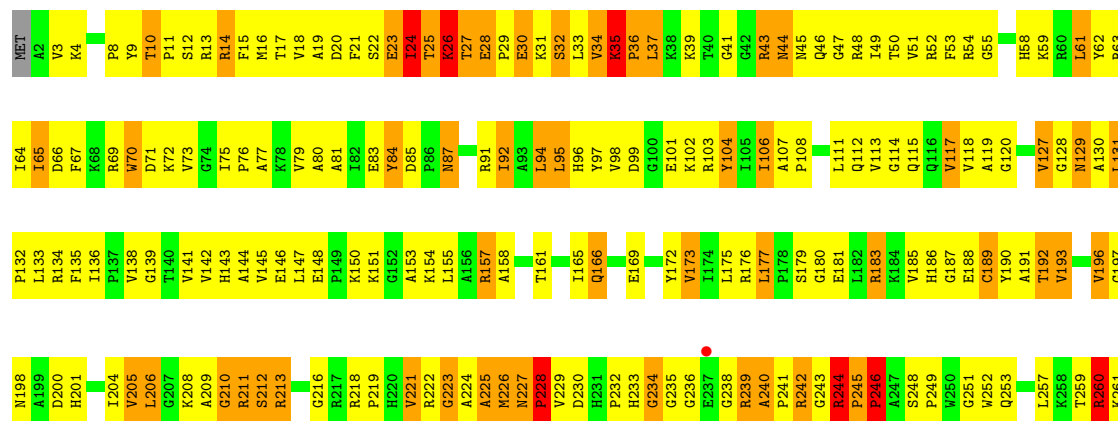
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

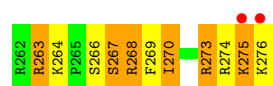
Chain BD: 28% 49% 21%



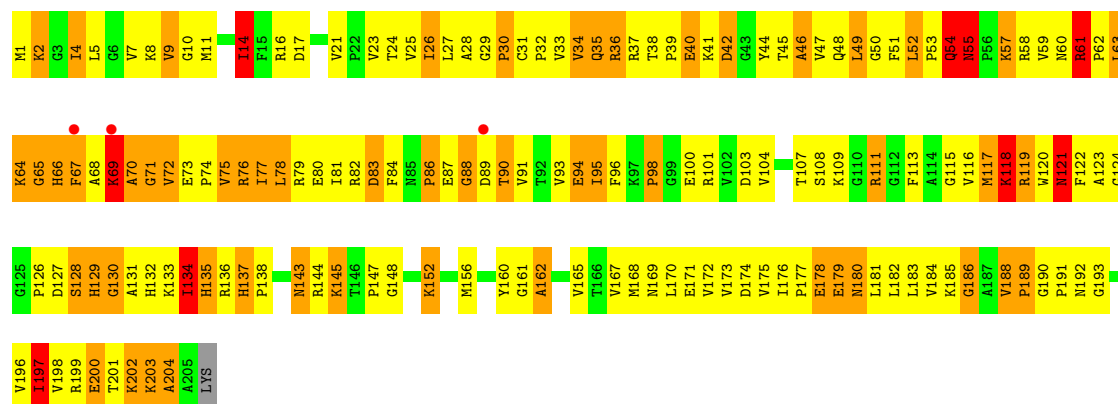
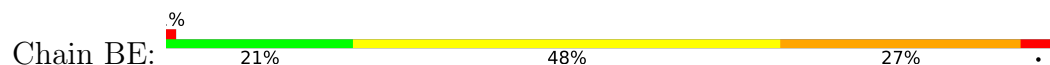
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

Chain DD: 25% 51% 21%

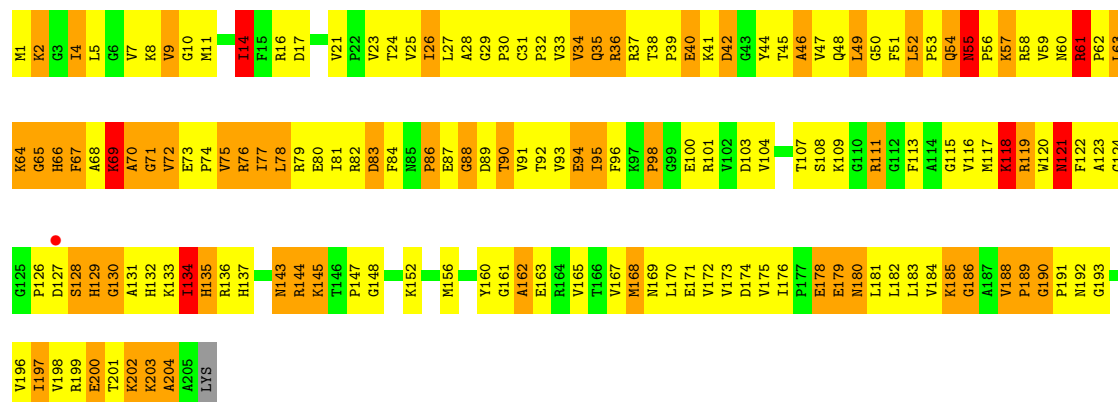
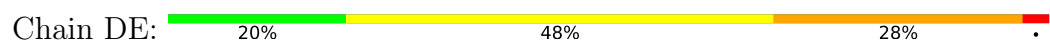




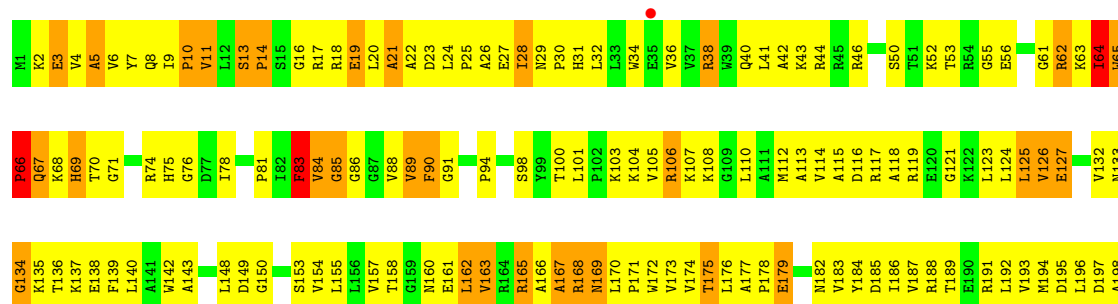
• Molecule 40: 50S RIBOSOMAL PROTEIN L3



• Molecule 40: 50S RIBOSOMAL PROTEIN L3

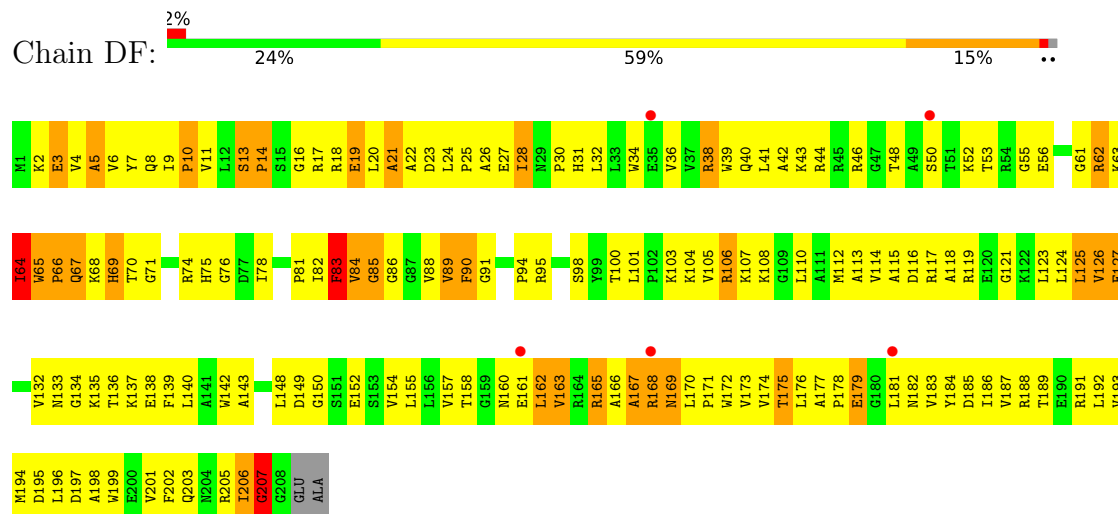


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

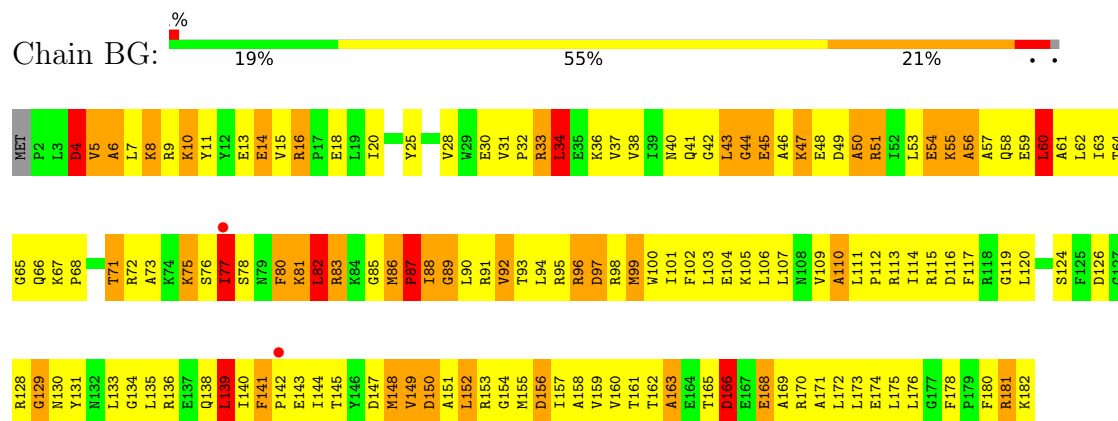




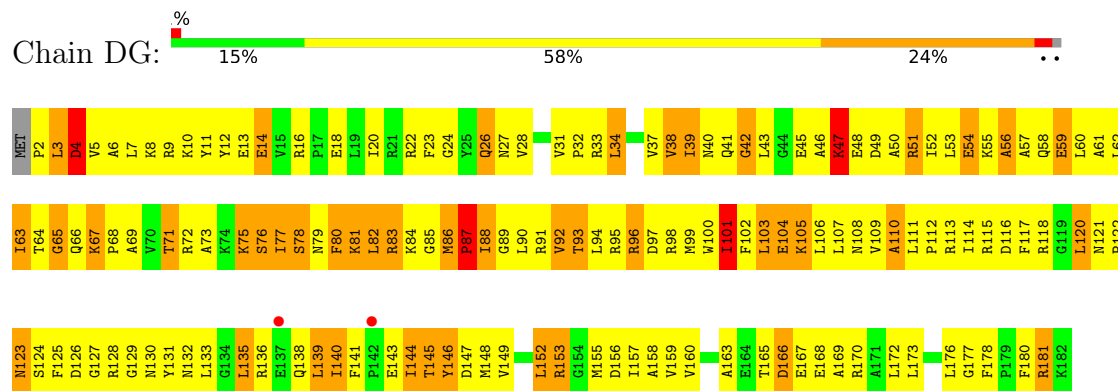
• Molecule 41: 50S RIBOSOMAL PROTEIN L4



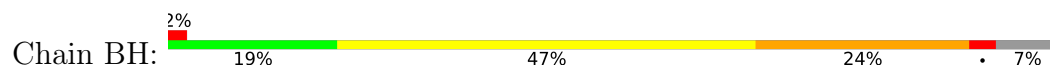
• Molecule 42: 50S RIBOSOMAL PROTEIN L5

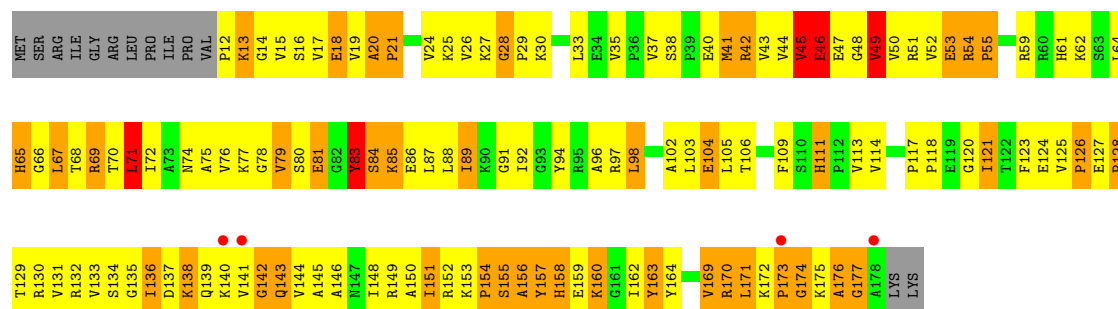


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

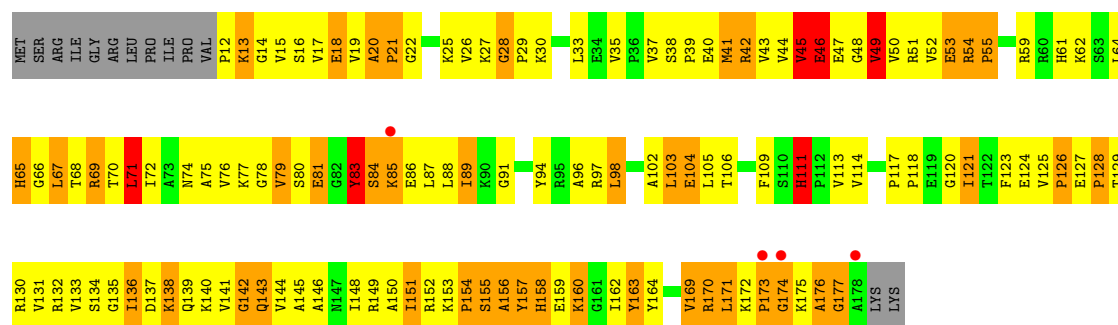
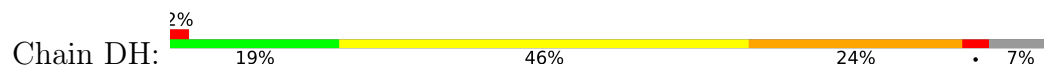


• Molecule 43: 50S RIBOSOMAL PROTEIN L6

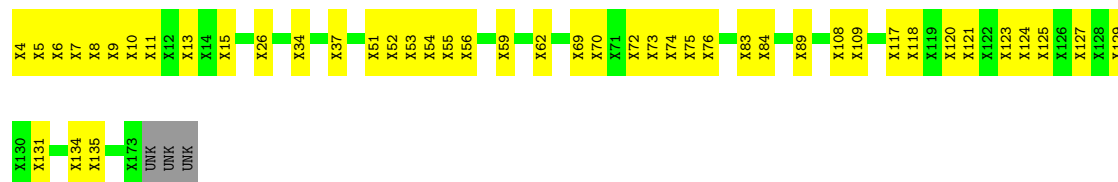




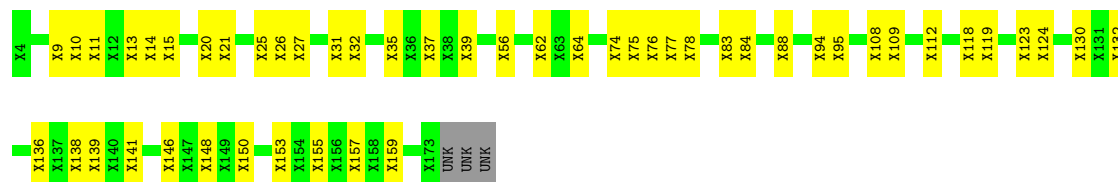
• Molecule 43: 50S RIBOSOMAL PROTEIN L6



• Molecule 44: 50S RIBOSOMAL PROTEIN L10

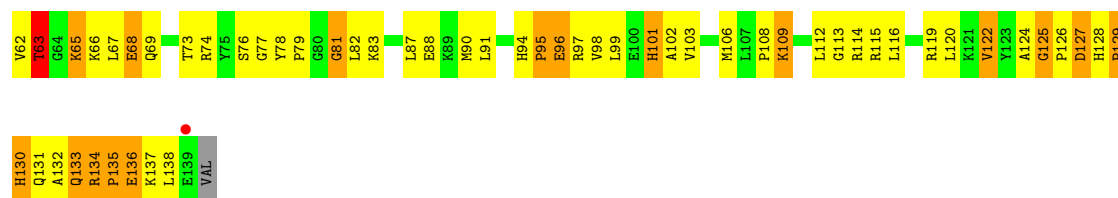


• Molecule 44: 50S RIBOSOMAL PROTEIN L10

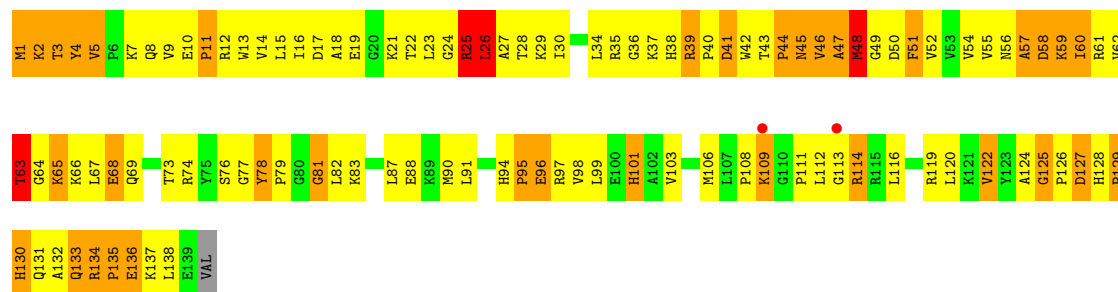


• Molecule 45: 50S RIBOSOMAL PROTEIN L13

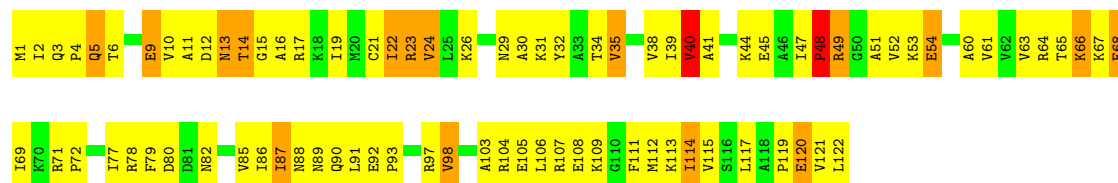
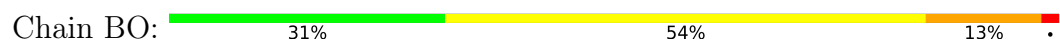




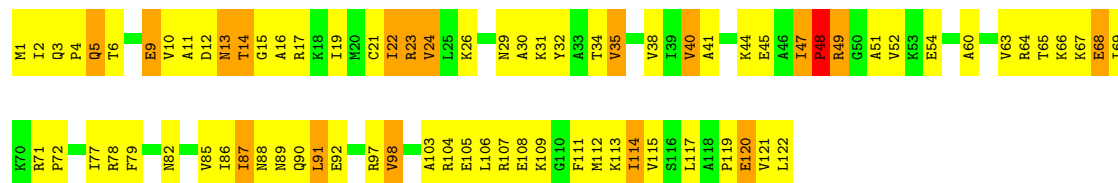
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



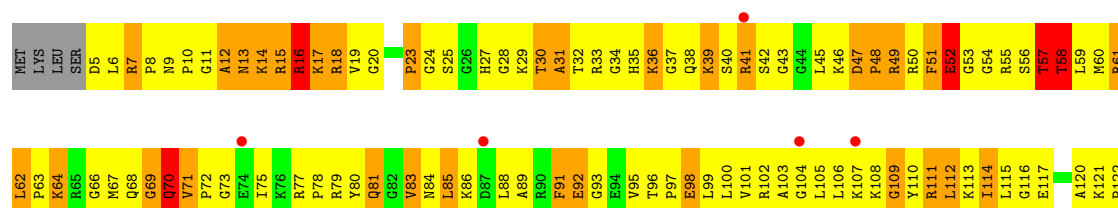
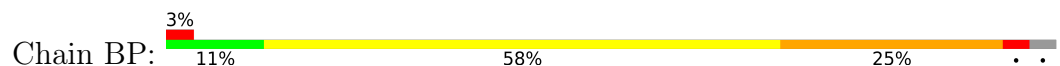
• Molecule 46: 50S RIBOSOMAL PROTEIN L14

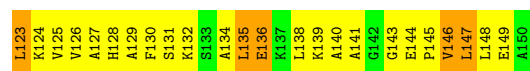


• Molecule 46: 50S RIBOSOMAL PROTEIN L14

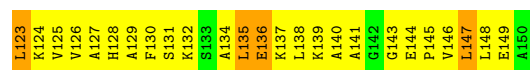
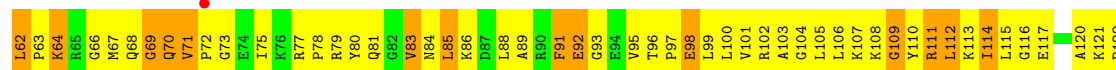
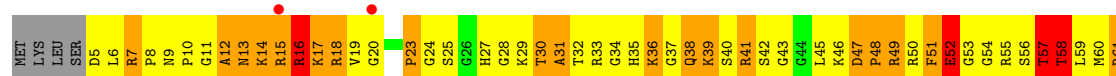
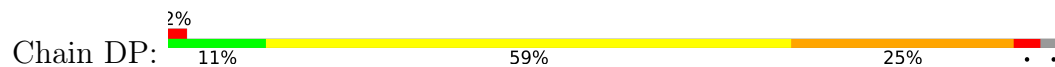


• Molecule 47: 50S RIBOSOMAL PROTEIN L15

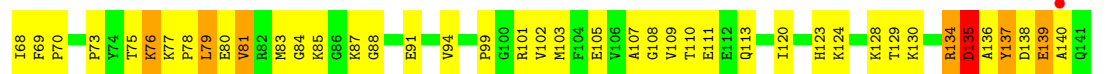
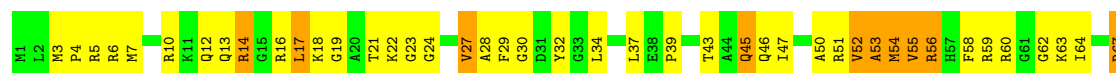




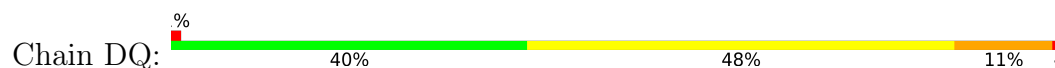
• Molecule 47: 50S RIBOSOMAL PROTEIN L15



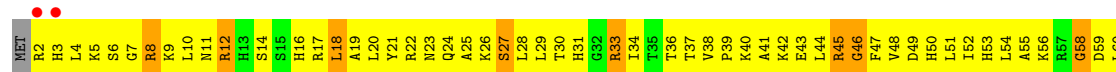
• Molecule 48: 50S RIBOSOMAL PROTEIN L16



• Molecule 48: 50S RIBOSOMAL PROTEIN L16

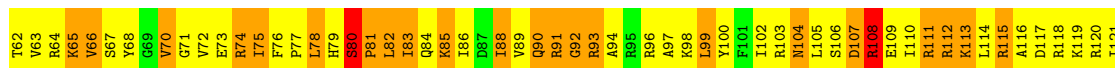


• Molecule 49: 50S RIBOSOMAL PROTEIN L17



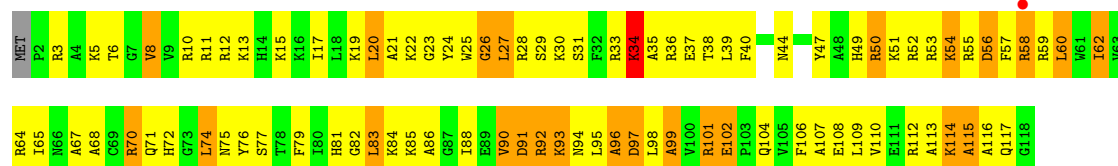
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



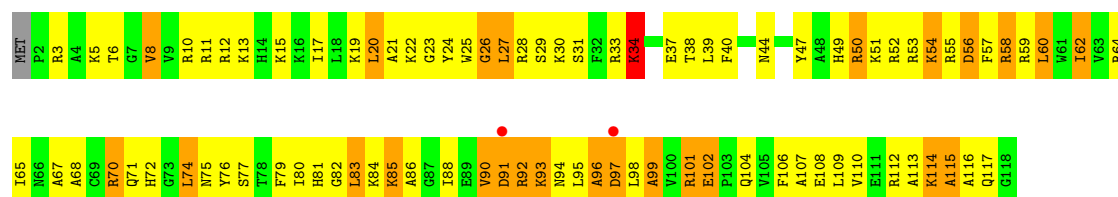




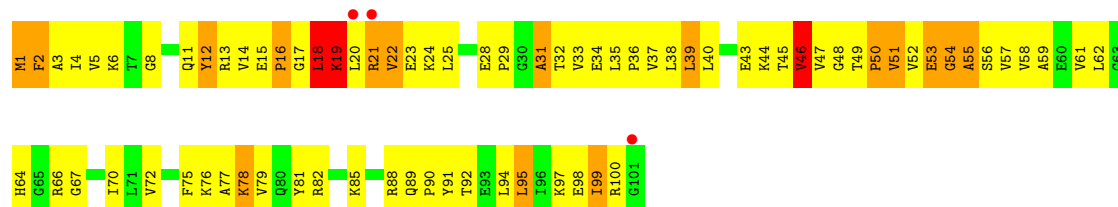
• Molecule 52: 50S RIBOSOMAL PROTEIN L20



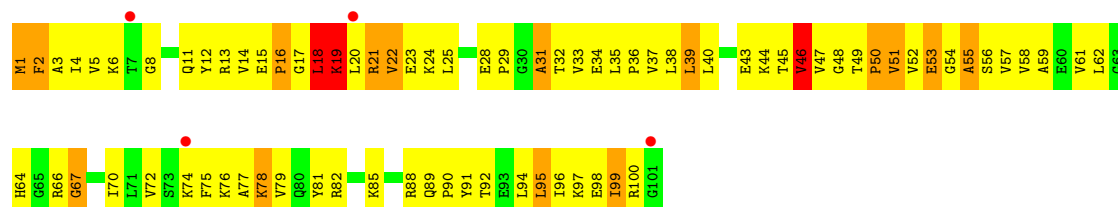
• Molecule 52: 50S RIBOSOMAL PROTEIN L20



• Molecule 53: 50S RIBOSOMAL PROTEIN L21

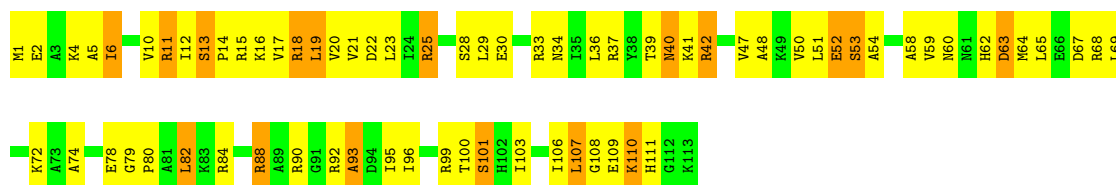


• Molecule 53: 50S RIBOSOMAL PROTEIN L21

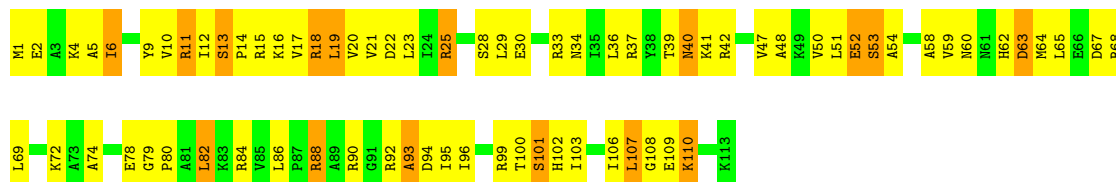


• Molecule 54: 50S RIBOSOMAL PROTEIN L22

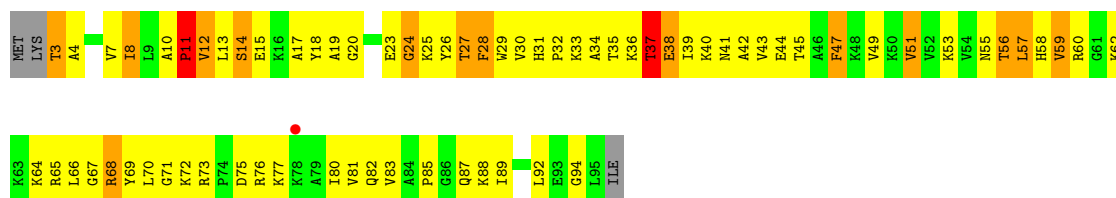




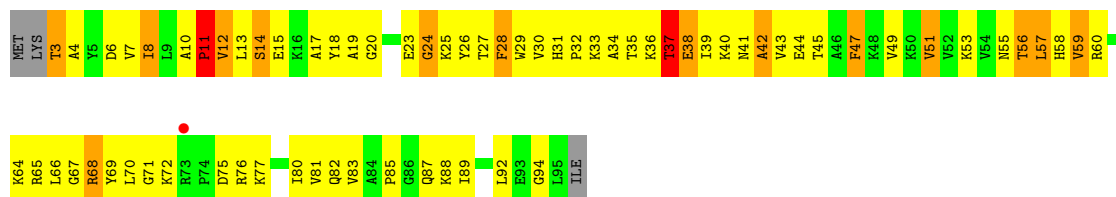
• Molecule 54: 50S RIBOSOMAL PROTEIN L22



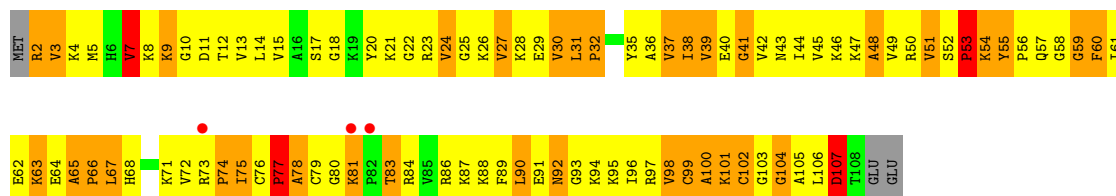
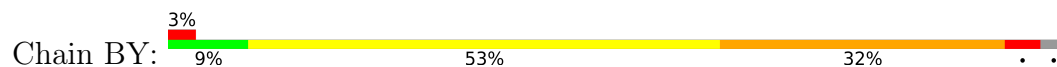
• Molecule 55: 50S RIBOSOMAL PROTEIN L23



• Molecule 55: 50S RIBOSOMAL PROTEIN L23

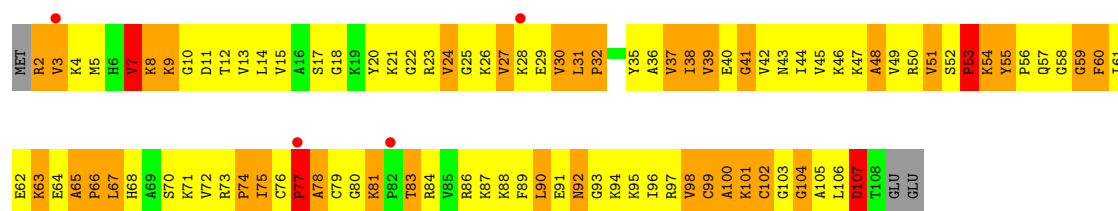


• Molecule 56: 50S RIBOSOMAL PROTEIN L24



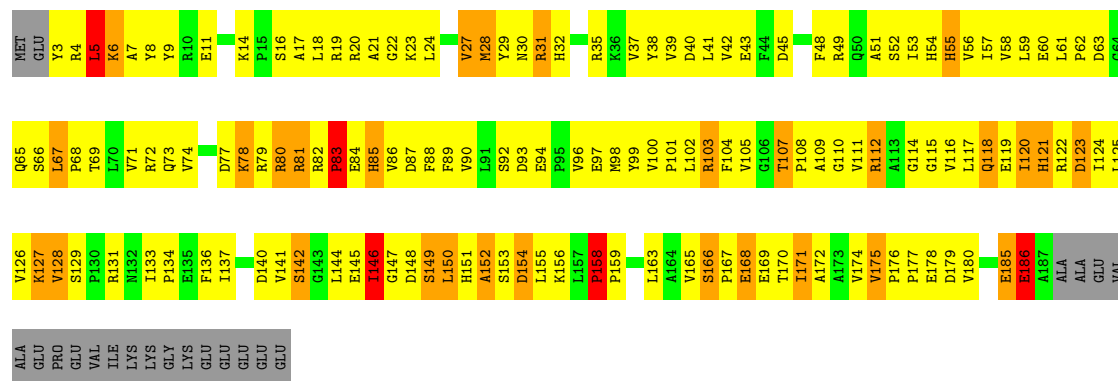
• Molecule 56: 50S RIBOSOMAL PROTEIN L24





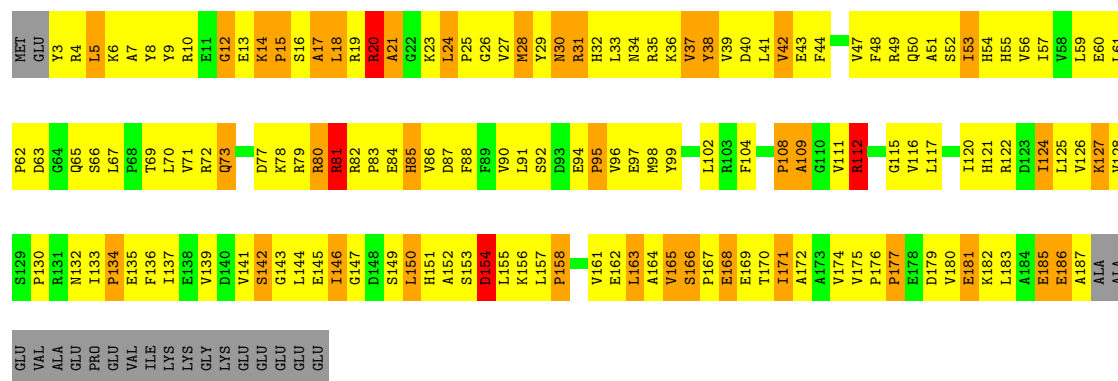
• Molecule 57: 50S RIBOSOMAL PROTEIN L25

Chain BZ: 18% 55% 14% 10%



• Molecule 57: 50S RIBOSOMAL PROTEIN L25

Chain DZ: 17% 53% 18% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	291.36Å 269.43Å 401.95Å 90.00° 91.78° 90.00°	Depositor
Resolution (Å)	49.75 – 3.70 49.75 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.75-3.70) 99.8 (49.75-3.70)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.214 , 0.249 0.213 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	84.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 98.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	307606	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 5MU, ZN, FUA, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.46	0/36190	0.70	46/56486 (0.1%)
1	CA	0.45	0/36190	0.70	42/56486 (0.1%)
2	AB	0.59	1/1936 (0.1%)	1.04	15/2611 (0.6%)
2	CB	0.52	1/1936 (0.1%)	1.04	14/2611 (0.5%)
3	AC	0.66	1/1637 (0.1%)	1.01	7/2207 (0.3%)
3	CC	0.56	1/1637 (0.1%)	1.00	8/2207 (0.4%)
4	AD	0.49	0/1733	1.02	7/2318 (0.3%)
4	CD	0.47	0/1733	1.00	6/2318 (0.3%)
5	AE	0.64	1/1163 (0.1%)	1.05	7/1566 (0.4%)
5	CE	0.61	1/1163 (0.1%)	1.06	8/1566 (0.5%)
6	AF	0.52	0/856	0.95	1/1154 (0.1%)
6	CF	0.46	0/856	0.95	0/1154
7	AG	0.54	0/1276	0.97	7/1709 (0.4%)
7	CG	0.47	0/1276	0.97	6/1709 (0.4%)
8	AH	0.58	0/1136	1.07	7/1527 (0.5%)
8	CH	0.52	0/1136	1.05	5/1527 (0.3%)
9	AI	0.52	0/1027	0.98	6/1373 (0.4%)
9	CI	0.43	0/1027	0.96	5/1373 (0.4%)
10	AJ	0.59	1/808 (0.1%)	1.01	2/1087 (0.2%)
10	CJ	0.52	1/808 (0.1%)	1.00	2/1087 (0.2%)
11	AK	0.60	0/900	1.11	6/1213 (0.5%)
11	CK	0.53	0/900	1.07	4/1213 (0.3%)
12	AL	0.59	1/987 (0.1%)	1.05	8/1322 (0.6%)
12	CL	0.56	1/987 (0.1%)	1.04	4/1322 (0.3%)
13	AM	0.55	1/999 (0.1%)	1.02	8/1338 (0.6%)
13	CM	0.51	1/999 (0.1%)	1.03	7/1338 (0.5%)
14	AN	0.61	0/501	1.02	4/664 (0.6%)
14	CN	0.53	0/501	0.99	2/664 (0.3%)
15	AO	0.54	0/745	0.88	2/992 (0.2%)
15	CO	0.50	0/745	0.87	2/992 (0.2%)
16	AP	0.53	1/717 (0.1%)	0.92	0/965
16	CP	0.52	1/717 (0.1%)	0.92	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.59	1/837 (0.1%)	0.98	1/1119 (0.1%)
17	CQ	0.56	1/837 (0.1%)	0.97	1/1119 (0.1%)
18	AR	0.55	0/579	1.03	4/768 (0.5%)
18	CR	0.50	0/579	0.98	1/768 (0.1%)
19	AS	0.52	1/643 (0.2%)	1.01	4/867 (0.5%)
19	CS	0.49	1/643 (0.2%)	1.00	4/867 (0.5%)
20	AT	0.50	0/765	1.05	8/1007 (0.8%)
20	CT	0.47	0/765	1.04	8/1007 (0.8%)
21	AU	0.63	1/213 (0.5%)	0.98	1/279 (0.4%)
21	CU	0.57	1/213 (0.5%)	0.98	1/279 (0.4%)
22	AV	0.41	0/1809	0.62	2/2819 (0.1%)
22	CV	0.39	0/1809	0.61	2/2819 (0.1%)
23	AW	0.37	0/1810	0.63	0/2821
23	CW	0.80	2/1810 (0.1%)	0.60	1/2821 (0.0%)
24	AX	0.34	0/288	0.68	0/446
24	CX	0.57	1/288 (0.3%)	0.77	1/446 (0.2%)
25	AY	0.64	2/5313 (0.0%)	1.14	54/7195 (0.8%)
25	CY	0.62	3/5313 (0.1%)	1.10	50/7195 (0.7%)
26	B0	0.51	0/671	0.95	2/892 (0.2%)
26	D0	0.46	0/671	0.95	2/892 (0.2%)
27	B1	0.54	1/739 (0.1%)	1.08	6/983 (0.6%)
27	D1	0.54	1/739 (0.1%)	1.08	5/983 (0.5%)
28	B2	0.40	0/600	0.98	2/793 (0.3%)
28	D2	0.38	0/600	0.95	2/793 (0.3%)
29	B3	0.56	1/473 (0.2%)	0.96	3/636 (0.5%)
29	D3	0.51	1/473 (0.2%)	0.95	2/636 (0.3%)
30	B4	0.63	1/461 (0.2%)	1.27	9/623 (1.4%)
30	D4	0.63	1/461 (0.2%)	1.28	10/623 (1.6%)
31	B5	0.52	0/473	1.08	2/639 (0.3%)
31	D5	0.53	0/473	1.06	2/639 (0.3%)
32	B6	0.70	0/440	1.33	7/586 (1.2%)
32	D6	0.66	0/440	1.29	6/586 (1.0%)
33	B7	0.56	1/427 (0.2%)	1.10	6/563 (1.1%)
33	D7	0.54	1/427 (0.2%)	1.09	3/563 (0.5%)
34	B8	0.67	1/516 (0.2%)	1.13	4/681 (0.6%)
34	D8	0.61	1/516 (0.2%)	1.13	4/681 (0.6%)
35	B9	0.51	0/310	0.88	1/407 (0.2%)
35	D9	0.51	0/310	0.89	1/407 (0.2%)
36	BA	0.45	0/69972	0.70	84/109237 (0.1%)
36	DA	0.45	0/69972	0.70	75/109237 (0.1%)
37	BB	0.40	0/2853	0.67	2/4451 (0.0%)
37	DB	0.42	0/2853	0.66	2/4451 (0.0%)
38	BC	0.90	4/1774 (0.2%)	0.96	7/2391 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DC	0.56	3/1774 (0.2%)	0.96	4/2391 (0.2%)
39	BD	0.60	0/2195	1.14	16/2955 (0.5%)
39	DD	0.55	0/2195	1.13	16/2955 (0.5%)
40	BE	0.56	1/1597 (0.1%)	1.06	12/2155 (0.6%)
40	DE	0.54	1/1597 (0.1%)	1.06	11/2155 (0.5%)
41	BF	0.47	1/1659 (0.1%)	1.02	10/2246 (0.4%)
41	DF	0.43	1/1659 (0.1%)	1.01	10/2246 (0.4%)
42	BG	0.54	1/1498 (0.1%)	1.12	15/2013 (0.7%)
42	DG	0.49	0/1498	1.08	13/2013 (0.6%)
43	BH	0.48	1/1293 (0.1%)	1.07	12/1746 (0.7%)
43	DH	0.47	1/1293 (0.1%)	1.07	13/1746 (0.7%)
45	BN	0.45	1/1132 (0.1%)	1.06	9/1527 (0.6%)
45	DN	0.44	1/1132 (0.1%)	1.06	9/1527 (0.6%)
46	BO	0.58	0/943	1.01	5/1269 (0.4%)
46	DO	0.55	0/943	1.03	5/1269 (0.4%)
47	BP	0.53	0/1131	1.30	14/1504 (0.9%)
47	DP	0.51	1/1131 (0.1%)	1.28	15/1504 (1.0%)
48	BQ	0.55	0/1143	0.91	0/1527
48	DQ	0.51	0/1143	0.90	0/1527
49	BR	0.47	0/974	0.91	2/1302 (0.2%)
49	DR	0.46	0/974	0.91	2/1302 (0.2%)
50	BS	0.51	1/779 (0.1%)	1.01	5/1038 (0.5%)
50	DS	0.47	1/779 (0.1%)	1.00	5/1038 (0.5%)
51	BT	0.60	1/1156 (0.1%)	1.19	16/1544 (1.0%)
51	DT	0.59	2/1156 (0.2%)	1.19	16/1544 (1.0%)
52	BU	0.46	0/975	1.07	10/1297 (0.8%)
52	DU	0.45	0/975	1.06	10/1297 (0.8%)
53	BV	0.48	0/790	0.93	1/1057 (0.1%)
53	DV	0.45	0/790	0.92	0/1057
54	BW	0.48	0/907	0.95	6/1216 (0.5%)
54	DW	0.45	0/907	0.94	5/1216 (0.4%)
55	BX	0.50	1/740 (0.1%)	1.00	5/995 (0.5%)
55	DX	0.49	1/740 (0.1%)	1.00	4/995 (0.4%)
56	BY	0.50	1/824 (0.1%)	1.01	5/1100 (0.5%)
56	DY	0.51	1/824 (0.1%)	1.00	7/1100 (0.6%)
57	BZ	0.56	1/1500 (0.1%)	1.00	6/2037 (0.3%)
57	DZ	0.51	1/1500 (0.1%)	1.01	5/2037 (0.2%)
All	All	0.49	66/331626 (0.0%)	0.81	939/494526 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	1	26
1	CA	1	21
22	AV	0	1
36	BA	2	39
36	DA	2	37
All	All	6	124

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CW	38	A	O3'-P	29.88	2.06	1.61
38	BC	54	ARG	C-N	-29.12	0.98	1.33
38	DC	109	MET	SD-CE	9.74	2.03	1.79
38	DC	121	MET	SD-CE	9.32	2.02	1.79
38	BC	121	MET	SD-CE	8.96	2.02	1.79

The worst 5 of 939 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BA	1992	G	C2'-C3'-O3'	15.34	132.51	109.50
36	DA	1992	G	C2'-C3'-O3'	15.25	132.37	109.50
1	AA	1498	U	C2'-C3'-O3'	14.28	130.91	109.50
1	CA	1498	U	C2'-C3'-O3'	14.08	130.62	109.50
36	BA	1799	G	C2'-C3'-O3'	13.71	130.07	109.50

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1498	U	C3'
36	BA	1799	G	C3'
36	BA	1992	G	C3'
1	CA	1498	U	C3'
36	DA	1799	G	C3'

5 of 124 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	108	G	Sidechain
1	AA	118	U	Sidechain
1	AA	202	U	Sidechain
1	AA	250	A	Sidechain
1	AA	436	C	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1167	0
1	CA	32329	0	16318	1207	0
2	AB	1901	0	1951	243	0
2	CB	1901	0	1951	241	0
3	AC	1613	0	1677	199	0
3	CC	1613	0	1677	207	0
4	AD	1703	0	1763	182	0
4	CD	1703	0	1763	191	0
5	AE	1147	0	1207	122	0
5	CE	1147	0	1207	119	0
6	AF	843	0	857	81	0
6	CF	843	0	857	83	0
7	AG	1257	0	1296	98	0
7	CG	1257	0	1296	101	0
8	AH	1116	0	1177	95	0
8	CH	1116	0	1177	92	0
9	AI	1010	0	1035	145	0
9	CI	1010	0	1035	145	0
10	AJ	795	0	840	161	0
10	CJ	795	0	840	159	0
11	AK	885	0	904	64	0
11	CK	885	0	904	69	0
12	AL	971	0	1057	143	0
12	CL	971	0	1057	150	0
13	AM	988	0	1059	169	0
13	CM	988	0	1059	164	0
14	AN	492	0	529	64	0
14	CN	492	0	529	64	0
15	AO	734	0	771	75	0
15	CO	734	0	771	79	0
16	AP	701	0	720	72	0
16	CP	701	0	720	72	0
17	AQ	824	0	891	63	0
17	CQ	824	0	891	69	0
18	AR	574	0	644	84	0
18	CR	574	0	644	83	0
19	AS	630	0	652	109	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	630	0	652	115	0
20	AT	763	0	861	109	0
20	CT	763	0	861	106	0
21	AU	209	0	221	20	0
21	CU	209	0	221	19	0
22	AV	1619	0	822	62	0
22	CV	1619	0	822	60	0
23	AW	1641	0	839	125	0
23	CW	1641	0	840	115	0
24	AX	257	0	130	45	0
24	CX	257	0	130	51	0
25	AY	5215	0	5288	897	0
25	CY	5215	0	5287	839	0
26	B0	662	0	688	99	0
26	D0	662	0	688	100	0
27	B1	732	0	808	130	0
27	D1	732	0	808	117	0
28	B2	598	0	653	93	0
28	D2	598	0	653	124	0
29	B3	468	0	523	63	0
29	D3	468	0	523	63	0
30	B4	451	0	449	95	0
30	D4	451	0	449	93	0
31	B5	459	0	480	102	0
31	D5	459	0	480	100	0
32	B6	433	0	461	151	0
32	D6	433	0	461	153	0
33	B7	419	0	467	40	0
33	D7	419	0	467	38	0
34	B8	508	0	576	102	0
34	D8	508	0	576	102	0
35	B9	307	0	335	30	0
35	D9	307	0	335	28	0
36	BA	62474	0	31497	2608	0
36	DA	62474	0	31497	2646	0
37	BB	2551	0	1295	132	0
37	DB	2551	0	1295	140	0
38	BC	1742	0	1797	171	0
38	DC	1742	0	1798	170	0
39	BD	2145	0	2234	311	0
39	DD	2145	0	2234	326	0
40	BE	1564	0	1629	261	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DE	1564	0	1629	257	0
41	BF	1624	0	1677	251	0
41	DF	1624	0	1677	240	0
42	BG	1474	0	1534	251	0
42	DG	1474	0	1534	276	0
43	BH	1269	0	1337	184	0
43	DH	1269	0	1337	184	0
44	BJ	851	0	194	31	0
44	DJ	851	0	195	32	0
45	BN	1105	0	1180	195	0
45	DN	1105	0	1180	201	0
46	BO	933	0	996	114	0
46	DO	933	0	996	108	0
47	BP	1114	0	1187	302	0
47	DP	1114	0	1187	303	0
48	BQ	1122	0	1179	137	0
48	DQ	1122	0	1179	127	0
49	BR	960	0	1021	157	0
49	DR	960	0	1021	160	0
50	BS	771	0	832	162	0
50	DS	771	0	832	154	0
51	BT	1142	0	1202	249	0
51	DT	1142	0	1202	247	0
52	BU	958	0	1015	142	0
52	DU	958	0	1015	150	0
53	BV	779	0	852	143	0
53	DV	779	0	852	145	0
54	BW	896	0	953	101	0
54	DW	896	0	953	104	0
55	BX	726	0	778	82	0
55	DX	726	0	778	86	0
56	BY	811	0	901	184	0
56	DY	811	0	901	189	0
57	BZ	1468	0	1492	207	0
57	DZ	1468	0	1492	232	0
58	AD	1	0	0	0	0
58	AN	1	0	0	0	0
58	B4	1	0	0	0	0
58	B9	1	0	0	0	0
58	CD	1	0	0	0	0
58	CN	1	0	0	0	0
58	D4	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	D9	1	0	0	0	0
59	AY	37	0	47	15	0
59	CY	37	0	47	26	0
60	AY	28	0	12	14	0
60	CY	28	0	12	10	0
61	AY	1	0	0	0	0
61	CY	1	0	0	0	0
All	All	307606	0	211582	21971	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

The worst 5 of 21971 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)
38:BC:121:MET:CE	38:BC:121:MET:SD	2.02	1.48
1:CA:1503:A:N1	24:CX:11:A:C2	1.82	1.47
23:CW:34:C:C3'	23:CW:35:A:H5''	1.42	1.47
38:DC:121:MET:SD	38:DC:121:MET:CE	2.02	1.46
38:DC:109:MET:SD	38:DC:109:MET:CE	2.03	1.44

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	148 (64%)	52 (22%)	33 (14%)	0	3
2	CB	233/256 (91%)	148 (64%)	52 (22%)	33 (14%)	0	3
3	AC	205/239 (86%)	146 (71%)	32 (16%)	27 (13%)	0	3
3	CC	205/239 (86%)	148 (72%)	31 (15%)	26 (13%)	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AD	206/209 (99%)	138 (67%)	47 (23%)	21 (10%)	0	6
4	CD	206/209 (99%)	138 (67%)	49 (24%)	19 (9%)	0	8
5	AE	149/162 (92%)	117 (78%)	26 (17%)	6 (4%)	2	22
5	CE	149/162 (92%)	118 (79%)	26 (17%)	5 (3%)	3	26
6	AF	99/101 (98%)	69 (70%)	26 (26%)	4 (4%)	2	22
6	CF	99/101 (98%)	69 (70%)	26 (26%)	4 (4%)	2	22
7	AG	153/156 (98%)	112 (73%)	27 (18%)	14 (9%)	0	8
7	CG	153/156 (98%)	112 (73%)	29 (19%)	12 (8%)	1	11
8	AH	136/138 (99%)	106 (78%)	26 (19%)	4 (3%)	3	28
8	CH	136/138 (99%)	105 (77%)	27 (20%)	4 (3%)	3	28
9	AI	121/128 (94%)	85 (70%)	27 (22%)	9 (7%)	1	12
9	CI	121/128 (94%)	87 (72%)	25 (21%)	9 (7%)	1	12
10	AJ	97/105 (92%)	67 (69%)	19 (20%)	11 (11%)	0	5
10	CJ	97/105 (92%)	68 (70%)	18 (19%)	11 (11%)	0	5
11	AK	117/129 (91%)	85 (73%)	23 (20%)	9 (8%)	1	11
11	CK	117/129 (91%)	85 (73%)	23 (20%)	9 (8%)	1	11
12	AL	123/132 (93%)	84 (68%)	19 (15%)	20 (16%)	0	2
12	CL	123/132 (93%)	84 (68%)	19 (15%)	20 (16%)	0	2
13	AM	123/126 (98%)	75 (61%)	30 (24%)	18 (15%)	0	3
13	CM	123/126 (98%)	75 (61%)	30 (24%)	18 (15%)	0	3
14	AN	58/61 (95%)	43 (74%)	10 (17%)	5 (9%)	0	9
14	CN	58/61 (95%)	42 (72%)	11 (19%)	5 (9%)	0	9
15	AO	86/89 (97%)	55 (64%)	24 (28%)	7 (8%)	1	10
15	CO	86/89 (97%)	54 (63%)	25 (29%)	7 (8%)	1	10
16	AP	82/88 (93%)	62 (76%)	15 (18%)	5 (6%)	1	15
16	CP	82/88 (93%)	63 (77%)	14 (17%)	5 (6%)	1	15
17	AQ	98/105 (93%)	80 (82%)	15 (15%)	3 (3%)	3	27
17	CQ	98/105 (93%)	80 (82%)	15 (15%)	3 (3%)	3	27
18	AR	68/88 (77%)	47 (69%)	13 (19%)	8 (12%)	0	4
18	CR	68/88 (77%)	48 (71%)	12 (18%)	8 (12%)	0	4
19	AS	77/93 (83%)	42 (54%)	17 (22%)	18 (23%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	CS	77/93 (83%)	40 (52%)	19 (25%)	18 (23%)	0	0
20	AT	97/106 (92%)	57 (59%)	28 (29%)	12 (12%)	0	4
20	CT	97/106 (92%)	57 (59%)	27 (28%)	13 (13%)	0	3
21	AU	23/27 (85%)	13 (56%)	7 (30%)	3 (13%)	0	4
21	CU	23/27 (85%)	13 (56%)	7 (30%)	3 (13%)	0	4
25	AY	663/691 (96%)	458 (69%)	126 (19%)	79 (12%)	0	4
25	CY	663/691 (96%)	482 (73%)	125 (19%)	56 (8%)	0	9
26	B0	82/85 (96%)	63 (77%)	15 (18%)	4 (5%)	2	18
26	D0	82/85 (96%)	63 (77%)	15 (18%)	4 (5%)	2	18
27	B1	92/98 (94%)	74 (80%)	8 (9%)	10 (11%)	0	5
27	D1	92/98 (94%)	71 (77%)	12 (13%)	9 (10%)	0	7
28	B2	69/72 (96%)	40 (58%)	21 (30%)	8 (12%)	0	4
28	D2	69/72 (96%)	34 (49%)	26 (38%)	9 (13%)	0	4
29	B3	58/60 (97%)	35 (60%)	19 (33%)	4 (7%)	1	13
29	D3	58/60 (97%)	35 (60%)	19 (33%)	4 (7%)	1	13
30	B4	56/71 (79%)	27 (48%)	14 (25%)	15 (27%)	0	0
30	D4	56/71 (79%)	27 (48%)	14 (25%)	15 (27%)	0	0
31	B5	57/60 (95%)	37 (65%)	10 (18%)	10 (18%)	0	2
31	D5	57/60 (95%)	37 (65%)	10 (18%)	10 (18%)	0	2
32	B6	48/54 (89%)	21 (44%)	13 (27%)	14 (29%)	0	0
32	D6	48/54 (89%)	21 (44%)	13 (27%)	14 (29%)	0	0
33	B7	47/49 (96%)	38 (81%)	8 (17%)	1 (2%)	5	33
33	D7	47/49 (96%)	38 (81%)	8 (17%)	1 (2%)	5	33
34	B8	62/65 (95%)	30 (48%)	18 (29%)	14 (23%)	0	0
34	D8	62/65 (95%)	30 (48%)	18 (29%)	14 (23%)	0	0
35	B9	35/37 (95%)	25 (71%)	6 (17%)	4 (11%)	0	5
35	D9	35/37 (95%)	25 (71%)	6 (17%)	4 (11%)	0	5
38	BC	226/229 (99%)	175 (77%)	42 (19%)	9 (4%)	2	22
38	DC	226/229 (99%)	176 (78%)	40 (18%)	10 (4%)	2	20
39	BD	273/276 (99%)	184 (67%)	54 (20%)	35 (13%)	0	4
39	DD	273/276 (99%)	185 (68%)	53 (19%)	35 (13%)	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BE	203/206 (98%)	123 (61%)	39 (19%)	41 (20%)	0	1
40	DE	203/206 (98%)	122 (60%)	39 (19%)	42 (21%)	0	1
41	BF	206/210 (98%)	138 (67%)	45 (22%)	23 (11%)	0	5
41	DF	206/210 (98%)	138 (67%)	44 (21%)	24 (12%)	0	4
42	BG	177/182 (97%)	116 (66%)	39 (22%)	22 (12%)	0	4
42	DG	177/182 (97%)	112 (63%)	44 (25%)	21 (12%)	0	4
43	BH	165/180 (92%)	89 (54%)	40 (24%)	36 (22%)	0	1
43	DH	165/180 (92%)	90 (54%)	40 (24%)	35 (21%)	0	1
45	BN	137/140 (98%)	87 (64%)	26 (19%)	24 (18%)	0	2
45	DN	137/140 (98%)	88 (64%)	25 (18%)	24 (18%)	0	2
46	BO	120/122 (98%)	97 (81%)	13 (11%)	10 (8%)	0	9
46	DO	120/122 (98%)	97 (81%)	13 (11%)	10 (8%)	0	9
47	BP	144/150 (96%)	79 (55%)	38 (26%)	27 (19%)	0	1
47	DP	144/150 (96%)	79 (55%)	39 (27%)	26 (18%)	0	1
48	BQ	139/141 (99%)	106 (76%)	25 (18%)	8 (6%)	1	16
48	DQ	139/141 (99%)	107 (77%)	25 (18%)	7 (5%)	1	18
49	BR	115/118 (98%)	81 (70%)	23 (20%)	11 (10%)	0	7
49	DR	115/118 (98%)	81 (70%)	22 (19%)	12 (10%)	0	6
50	BS	97/112 (87%)	42 (43%)	32 (33%)	23 (24%)	0	0
50	DS	97/112 (87%)	41 (42%)	34 (35%)	22 (23%)	0	0
51	BT	136/146 (93%)	77 (57%)	32 (24%)	27 (20%)	0	1
51	DT	136/146 (93%)	78 (57%)	31 (23%)	27 (20%)	0	1
52	BU	115/118 (98%)	78 (68%)	30 (26%)	7 (6%)	1	15
52	DU	115/118 (98%)	76 (66%)	31 (27%)	8 (7%)	1	13
53	BV	99/101 (98%)	69 (70%)	17 (17%)	13 (13%)	0	3
53	DV	99/101 (98%)	68 (69%)	18 (18%)	13 (13%)	0	3
54	BW	111/113 (98%)	78 (70%)	23 (21%)	10 (9%)	0	8
54	DW	111/113 (98%)	76 (68%)	25 (22%)	10 (9%)	0	8
55	BX	91/96 (95%)	55 (60%)	27 (30%)	9 (10%)	0	7
55	DX	91/96 (95%)	55 (60%)	26 (29%)	10 (11%)	0	5
56	BY	105/110 (96%)	44 (42%)	32 (30%)	29 (28%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	DY	105/110 (96%)	44 (42%)	32 (30%)	29 (28%)	0	0
57	BZ	183/206 (89%)	116 (63%)	39 (21%)	28 (15%)	0	3
57	DZ	183/206 (89%)	118 (64%)	34 (19%)	31 (17%)	0	2
All	All	12924/13672 (94%)	8641 (67%)	2723 (21%)	1560 (12%)	0	4

5 of 1560 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	12	GLU
2	AB	13	ALA
2	AB	15	VAL
2	AB	74	LYS
2	AB	75	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	182 (90%)	20 (10%)	6	27
2	CB	202/220 (92%)	183 (91%)	19 (9%)	7	29
3	AC	160/188 (85%)	137 (86%)	23 (14%)	2	16
3	CC	160/188 (85%)	137 (86%)	23 (14%)	2	16
4	AD	180/181 (99%)	158 (88%)	22 (12%)	4	20
4	CD	180/181 (99%)	158 (88%)	22 (12%)	4	20
5	AE	115/123 (94%)	103 (90%)	12 (10%)	5	25
5	CE	115/123 (94%)	103 (90%)	12 (10%)	5	25
6	AF	90/90 (100%)	84 (93%)	6 (7%)	13	40
6	CF	90/90 (100%)	85 (94%)	5 (6%)	17	45
7	AG	126/127 (99%)	114 (90%)	12 (10%)	7	29
7	CG	126/127 (99%)	114 (90%)	12 (10%)	7	29
8	AH	119/119 (100%)	107 (90%)	12 (10%)	6	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	119/119 (100%)	108 (91%)	11 (9%)	7	30
9	AI	98/99 (99%)	91 (93%)	7 (7%)	12	39
9	CI	98/99 (99%)	91 (93%)	7 (7%)	12	39
10	AJ	88/92 (96%)	75 (85%)	13 (15%)	2	15
10	CJ	88/92 (96%)	74 (84%)	14 (16%)	2	13
11	AK	90/99 (91%)	84 (93%)	6 (7%)	13	40
11	CK	90/99 (91%)	84 (93%)	6 (7%)	13	40
12	AL	104/109 (95%)	94 (90%)	10 (10%)	7	28
12	CL	104/109 (95%)	94 (90%)	10 (10%)	7	28
13	AM	99/101 (98%)	90 (91%)	9 (9%)	7	30
13	CM	99/101 (98%)	90 (91%)	9 (9%)	7	30
14	AN	49/50 (98%)	45 (92%)	4 (8%)	9	34
14	CN	49/50 (98%)	45 (92%)	4 (8%)	9	34
15	AO	79/80 (99%)	74 (94%)	5 (6%)	15	42
15	CO	79/80 (99%)	74 (94%)	5 (6%)	15	42
16	AP	72/74 (97%)	68 (94%)	4 (6%)	17	45
16	CP	72/74 (97%)	68 (94%)	4 (6%)	17	45
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	14	42
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	11	37
18	AR	61/77 (79%)	59 (97%)	2 (3%)	33	57
18	CR	61/77 (79%)	59 (97%)	2 (3%)	33	57
19	AS	69/80 (86%)	60 (87%)	9 (13%)	3	19
19	CS	69/80 (86%)	60 (87%)	9 (13%)	3	19
20	AT	76/82 (93%)	67 (88%)	9 (12%)	4	21
20	CT	76/82 (93%)	67 (88%)	9 (12%)	4	21
21	AU	19/22 (86%)	18 (95%)	1 (5%)	19	46
21	CU	19/22 (86%)	18 (95%)	1 (5%)	19	46
25	AY	563/582 (97%)	486 (86%)	77 (14%)	3	17
25	CY	563/582 (97%)	494 (88%)	69 (12%)	4	20
26	B0	66/67 (98%)	59 (89%)	7 (11%)	5	25
26	D0	66/67 (98%)	59 (89%)	7 (11%)	5	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	B1	78/83 (94%)	68 (87%)	10 (13%)	3	19
27	D1	78/83 (94%)	73 (94%)	5 (6%)	14	42
28	B2	66/67 (98%)	59 (89%)	7 (11%)	5	25
28	D2	66/67 (98%)	59 (89%)	7 (11%)	5	25
29	B3	51/52 (98%)	47 (92%)	4 (8%)	10	36
29	D3	51/52 (98%)	47 (92%)	4 (8%)	10	36
30	B4	51/63 (81%)	38 (74%)	13 (26%)	0	4
30	D4	51/63 (81%)	38 (74%)	13 (26%)	0	4
31	B5	51/52 (98%)	48 (94%)	3 (6%)	16	44
31	D5	51/52 (98%)	48 (94%)	3 (6%)	16	44
32	B6	49/52 (94%)	37 (76%)	12 (24%)	0	4
32	D6	49/52 (94%)	37 (76%)	12 (24%)	0	4
33	B7	41/42 (98%)	38 (93%)	3 (7%)	11	38
33	D7	41/42 (98%)	38 (93%)	3 (7%)	11	38
34	B8	53/55 (96%)	46 (87%)	7 (13%)	3	18
34	D8	53/55 (96%)	46 (87%)	7 (13%)	3	18
35	B9	34/34 (100%)	31 (91%)	3 (9%)	8	32
35	D9	34/34 (100%)	31 (91%)	3 (9%)	8	32
38	BC	180/181 (99%)	169 (94%)	11 (6%)	15	43
38	DC	180/181 (99%)	167 (93%)	13 (7%)	12	38
39	BD	217/218 (100%)	176 (81%)	41 (19%)	1	8
39	DD	217/218 (100%)	176 (81%)	41 (19%)	1	8
40	BE	165/166 (99%)	136 (82%)	29 (18%)	1	10
40	DE	165/166 (99%)	136 (82%)	29 (18%)	1	10
41	BF	165/166 (99%)	153 (93%)	12 (7%)	11	38
41	DF	165/166 (99%)	153 (93%)	12 (7%)	11	38
42	BG	155/156 (99%)	131 (84%)	24 (16%)	2	14
42	DG	155/156 (99%)	128 (83%)	27 (17%)	1	10
43	BH	136/148 (92%)	122 (90%)	14 (10%)	6	25
43	DH	136/148 (92%)	122 (90%)	14 (10%)	6	25
45	BN	117/119 (98%)	104 (89%)	13 (11%)	5	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DN	117/119 (98%)	104 (89%)	13 (11%)	5	24
46	BO	100/100 (100%)	90 (90%)	10 (10%)	6	26
46	DO	100/100 (100%)	89 (89%)	11 (11%)	5	24
47	BP	112/116 (97%)	94 (84%)	18 (16%)	2	13
47	DP	112/116 (97%)	95 (85%)	17 (15%)	2	14
48	BQ	111/111 (100%)	99 (89%)	12 (11%)	5	24
48	DQ	111/111 (100%)	99 (89%)	12 (11%)	5	24
49	BR	100/101 (99%)	88 (88%)	12 (12%)	4	20
49	DR	100/101 (99%)	88 (88%)	12 (12%)	4	20
50	BS	77/88 (88%)	69 (90%)	8 (10%)	5	25
50	DS	77/88 (88%)	69 (90%)	8 (10%)	5	25
51	BT	120/127 (94%)	93 (78%)	27 (22%)	1	5
51	DT	120/127 (94%)	93 (78%)	27 (22%)	1	5
52	BU	92/94 (98%)	81 (88%)	11 (12%)	4	20
52	DU	92/94 (98%)	81 (88%)	11 (12%)	4	20
53	BV	82/82 (100%)	71 (87%)	11 (13%)	3	18
53	DV	82/82 (100%)	71 (87%)	11 (13%)	3	18
54	BW	91/92 (99%)	83 (91%)	8 (9%)	8	32
54	DW	91/92 (99%)	83 (91%)	8 (9%)	8	32
55	BX	74/78 (95%)	64 (86%)	10 (14%)	3	18
55	DX	74/78 (95%)	64 (86%)	10 (14%)	3	18
56	BY	87/91 (96%)	74 (85%)	13 (15%)	2	15
56	DY	87/91 (96%)	74 (85%)	13 (15%)	2	15
57	BZ	162/179 (90%)	140 (86%)	22 (14%)	3	18
57	DZ	162/179 (90%)	147 (91%)	15 (9%)	7	30
All	All	10872/11344 (96%)	9600 (88%)	1272 (12%)	4	22

5 of 1272 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	D3	48	GLU
48	DQ	17	LEU
32	D6	39	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	D3	38	GLU
40	DE	119	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 384 such sidechains are listed below:

Mol	Chain	Res	Type
11	CK	13	GLN
27	D1	56	GLN
13	CM	40	ASN
25	CY	117	GLN
33	D7	36	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	256 (17%)	36 (2%)
1	CA	1503/1522 (98%)	253 (16%)	34 (2%)
22	AV	75/76 (98%)	13 (17%)	1 (1%)
22	CV	75/76 (98%)	15 (20%)	1 (1%)
23	AW	76/77 (98%)	27 (35%)	1 (1%)
23	CW	76/77 (98%)	27 (35%)	1 (1%)
24	AX	12/25 (48%)	8 (66%)	2 (16%)
24	CX	12/25 (48%)	7 (58%)	2 (16%)
36	BA	2900/2915 (99%)	590 (20%)	61 (2%)
36	DA	2900/2915 (99%)	587 (20%)	63 (2%)
37	BB	118/122 (96%)	25 (21%)	0
37	DB	118/122 (96%)	25 (21%)	0
All	All	9368/9474 (98%)	1833 (19%)	202 (2%)

5 of 1833 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	33	A

5 of 202 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	533	A
36	DA	221	A
36	DA	2799	C
1	CA	748	C
1	CA	1285	A

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
23	5MU	CW	54	23	19,22,23	0.21	0	27,32,35	0.38	0
23	5MU	AW	54	23	19,22,23	0.25	0	27,32,35	0.30	0

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
23	5MU	CW	54	23	-	0/7/25/26	0/2/2/2
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	CW	54	5MU	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	54	5MU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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
60	GDP	AY	702	61	25,30,30	1.28	2 (8%)	30,47,47	1.39	4 (13%)
59	FUA	CY	701	-	39,40,40	1.71	7 (17%)	50,64,64	1.56	10 (20%)
60	GDP	CY	702	61	25,30,30	1.42	3 (12%)	30,47,47	1.61	7 (23%)
59	FUA	AY	701	-	39,40,40	1.70	7 (17%)	50,64,64	1.70	8 (16%)

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
60	GDP	AY	702	61	-	2/12/32/32	0/3/3/3
59	FUA	CY	701	-	-	8/16/92/92	0/4/4/4
60	GDP	CY	702	61	-	0/12/32/32	0/3/3/3
59	FUA	AY	701	-	-	7/16/92/92	0/4/4/4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CY	701	FUA	C23-C22	-4.55	1.39	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AY	701	FUA	C23-C22	-4.43	1.39	1.51
59	AY	701	FUA	C23-C24	-4.35	1.39	1.53
59	CY	701	FUA	C23-C24	-4.35	1.39	1.53
59	AY	701	FUA	C29-C22	4.24	1.53	1.47

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AY	701	FUA	C24-C23-C22	5.35	124.11	112.72
60	CY	702	GDP	C4'-O4'-C1'	-4.40	105.89	109.92
59	CY	701	FUA	C16-O2-C31	-4.26	110.67	117.00
59	AY	701	FUA	C13-C12-C11	-4.18	105.84	111.90
59	CY	701	FUA	C24-C23-C22	4.09	121.43	112.72

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AY	701	FUA	C13-C17-C22-C23
59	AY	701	FUA	C13-C17-C22-C29
59	CY	701	FUA	C13-C17-C22-C23
59	CY	701	FUA	C13-C17-C22-C29
60	AY	702	GDP	C5'-O5'-PA-O1A

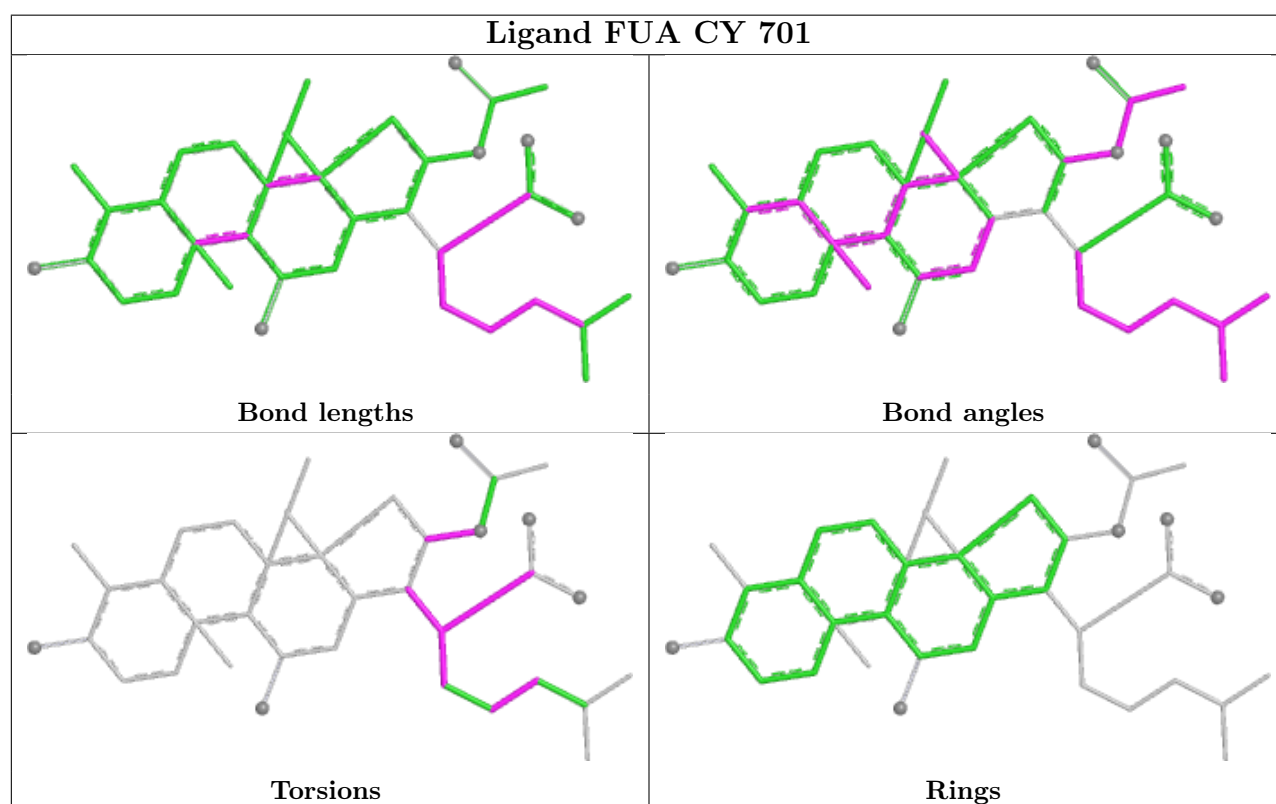
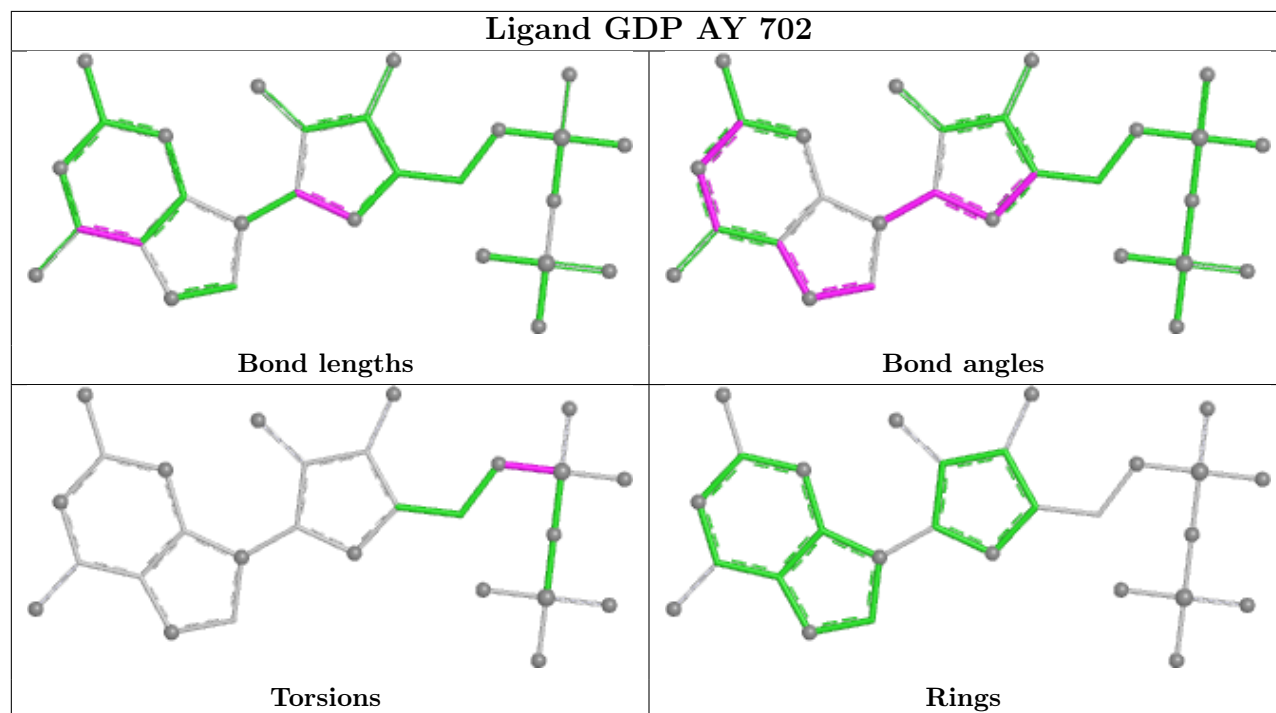
There are no ring outliers.

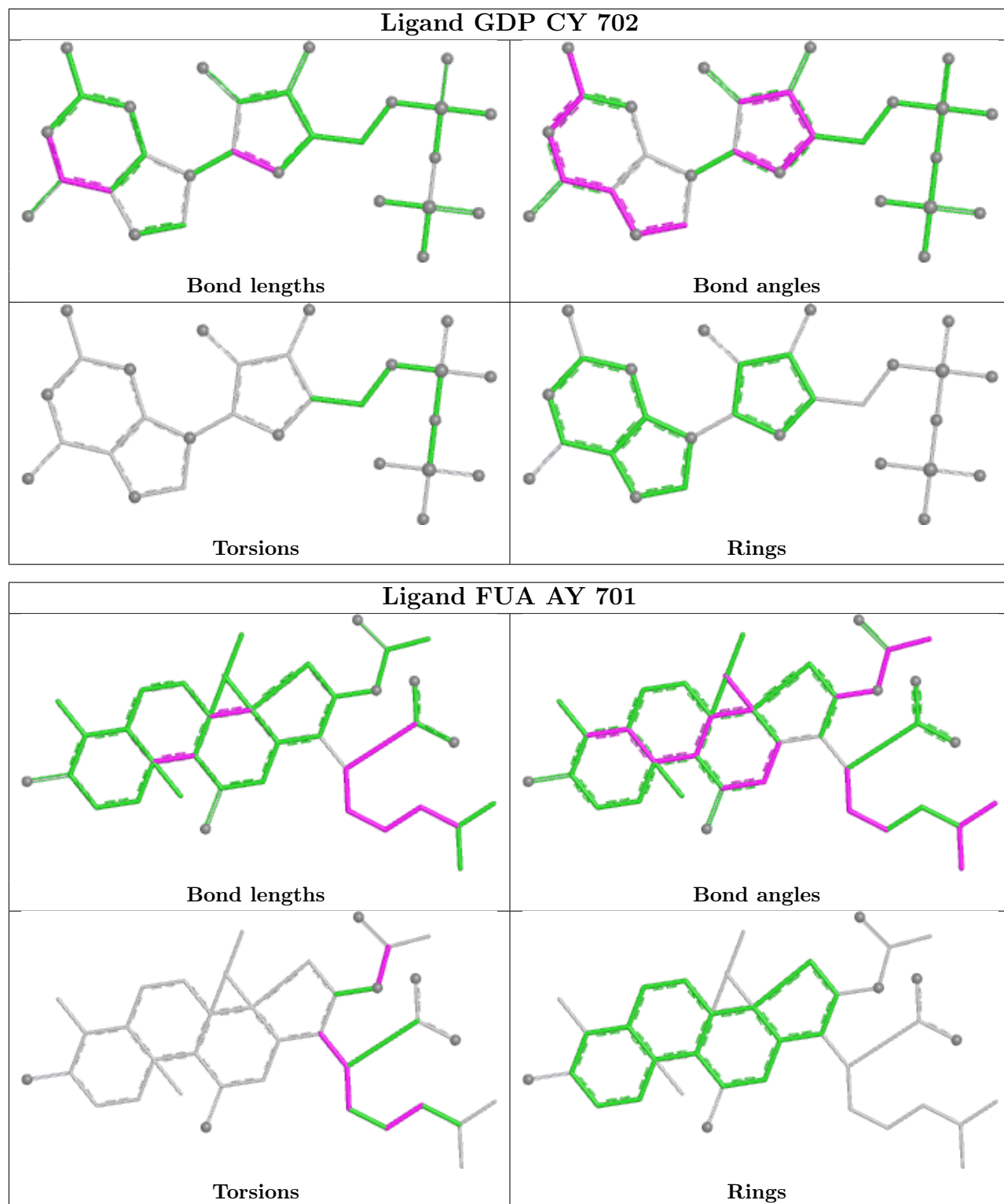
4 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	AY	702	GDP	14	0
59	CY	701	FUA	26	0
60	CY	702	GDP	10	0
59	AY	701	FUA	15	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	CI	2
9	AI	2
42	BG	1
42	DG	1
23	CW	1
38	BC	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BG	112:PRO	C	113:ARG	N	3.28
1	DG	112:PRO	C	113:ARG	N	3.21
1	CI	53:VAL	C	54:ASP	N	3.01
1	AI	53:VAL	C	54:ASP	N	3.00
1	CI	104:ARG	C	105:ASP	N	2.58

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	-0.04	39 (2%) 57 41	34, 72, 165, 200	0
1	CA	1504/1522 (98%)	0.05	34 (2%) 61 43	43, 89, 174, 200	0
2	AB	235/256 (91%)	-0.14	1 (0%) 89 76	40, 82, 172, 190	0
2	CB	235/256 (91%)	-0.02	2 (0%) 81 64	53, 102, 164, 194	0
3	AC	207/239 (86%)	-0.21	0 100 100	23, 69, 122, 174	0
3	CC	207/239 (86%)	-0.15	2 (0%) 79 61	45, 93, 143, 190	0
4	AD	208/209 (99%)	0.01	3 (1%) 73 54	46, 95, 144, 166	0
4	CD	208/209 (99%)	0.03	3 (1%) 73 54	48, 107, 157, 188	0
5	AE	151/162 (93%)	-0.44	1 (0%) 84 68	27, 62, 107, 187	0
5	CE	151/162 (93%)	-0.25	1 (0%) 84 68	45, 76, 117, 200	0
6	AF	101/101 (100%)	-0.31	0 100 100	44, 85, 125, 174	0
6	CF	101/101 (100%)	0.04	0 100 100	72, 115, 152, 183	0
7	AG	155/156 (99%)	-0.23	2 (1%) 74 55	36, 80, 126, 182	0
7	CG	155/156 (99%)	-0.02	6 (3%) 44 32	63, 108, 150, 193	0
8	AH	138/138 (100%)	-0.32	1 (0%) 84 68	35, 65, 111, 136	0
8	CH	138/138 (100%)	-0.24	0 100 100	44, 79, 117, 147	0
9	AI	127/128 (99%)	-0.05	0 100 100	41, 79, 135, 157	0
9	CI	127/128 (99%)	0.01	1 (0%) 82 66	68, 111, 151, 175	0
10	AJ	99/105 (94%)	0.35	1 (1%) 79 61	33, 87, 180, 193	0
10	CJ	99/105 (94%)	0.41	3 (3%) 52 37	60, 127, 179, 190	0
11	AK	119/129 (92%)	-0.34	1 (0%) 82 66	27, 62, 109, 171	0
11	CK	119/129 (92%)	-0.17	2 (1%) 69 50	48, 89, 126, 181	0
12	AL	125/132 (94%)	-0.19	0 100 100	37, 76, 118, 180	0
12	CL	125/132 (94%)	-0.06	1 (0%) 82 66	42, 82, 124, 200	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.24	6 (4%) 36 27	52, 98, 165, 200	0
13	CM	125/126 (99%)	0.33	8 (6%) 27 21	63, 126, 171, 200	0
14	AN	60/61 (98%)	-0.08	1 (1%) 69 50	35, 62, 103, 131	0
14	CN	60/61 (98%)	0.05	1 (1%) 69 50	58, 91, 127, 146	0
15	AO	88/89 (98%)	-0.32	0 100 100	27, 71, 116, 144	0
15	CO	88/89 (98%)	-0.21	1 (1%) 77 59	31, 82, 119, 141	0
16	AP	84/88 (95%)	0.07	1 (1%) 76 57	36, 85, 130, 160	0
16	CP	84/88 (95%)	-0.13	0 100 100	58, 95, 126, 166	0
17	AQ	100/105 (95%)	-0.21	0 100 100	40, 78, 112, 139	0
17	CQ	100/105 (95%)	-0.20	0 100 100	60, 84, 120, 147	0
18	AR	70/88 (79%)	-0.29	0 100 100	38, 72, 119, 167	0
18	CR	70/88 (79%)	-0.09	0 100 100	60, 95, 142, 167	0
19	AS	79/93 (84%)	0.12	4 (5%) 34 26	63, 95, 174, 182	0
19	CS	79/93 (84%)	0.32	5 (6%) 27 22	74, 117, 181, 199	0
20	AT	99/106 (93%)	0.01	1 (1%) 79 61	55, 95, 147, 176	0
20	CT	99/106 (93%)	0.09	0 100 100	72, 103, 153, 173	0
21	AU	25/27 (92%)	0.48	1 (4%) 43 31	33, 84, 132, 167	0
21	CU	25/27 (92%)	0.71	2 (8%) 20 16	77, 115, 145, 164	0
22	AV	76/76 (100%)	0.36	3 (3%) 44 32	51, 94, 154, 200	0
22	CV	76/76 (100%)	0.38	3 (3%) 44 32	67, 107, 165, 200	0
23	AW	76/77 (98%)	1.45	15 (19%) 3 5	97, 182, 200, 200	0
23	CW	76/77 (98%)	1.29	11 (14%) 7 10	97, 190, 200, 200	0
24	AX	12/25 (48%)	4.94	11 (91%) 0 0	52, 114, 167, 193	0
24	CX	12/25 (48%)	4.36	11 (91%) 0 0	52, 114, 172, 193	0
25	AY	667/691 (96%)	0.20	24 (3%) 46 34	71, 142, 179, 200	0
25	CY	667/691 (96%)	0.33	26 (3%) 44 32	84, 151, 186, 200	0
26	B0	84/85 (98%)	0.07	0 100 100	61, 87, 134, 191	0
26	D0	84/85 (98%)	0.36	4 (4%) 36 27	78, 109, 144, 172	0
27	B1	94/98 (95%)	-0.06	2 (2%) 63 45	50, 88, 142, 151	0
27	D1	94/98 (95%)	0.06	1 (1%) 77 59	59, 99, 153, 181	0
28	B2	71/72 (98%)	-0.03	0 100 100	79, 127, 176, 194	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	D2	71/72 (98%)	-0.15	0	100	100	82, 134, 172, 186	0
29	B3	60/60 (100%)	-0.11	0	100	100	55, 95, 148, 180	0
29	D3	60/60 (100%)	0.07	0	100	100	61, 105, 145, 174	0
30	B4	58/71 (81%)	0.59	2 (3%)	48	34	90, 141, 200, 200	0
30	D4	58/71 (81%)	0.38	1 (1%)	69	50	106, 166, 200, 200	0
31	B5	59/60 (98%)	0.29	3 (5%)	34	26	46, 96, 175, 192	0
31	D5	59/60 (98%)	0.35	3 (5%)	34	26	50, 104, 167, 200	0
32	B6	50/54 (92%)	0.53	7 (14%)	7	10	55, 97, 142, 173	0
32	D6	50/54 (92%)	0.22	2 (4%)	43	31	71, 111, 153, 178	0
33	B7	49/49 (100%)	0.28	3 (6%)	28	22	51, 79, 117, 200	0
33	D7	49/49 (100%)	0.19	1 (2%)	64	47	64, 91, 127, 166	0
34	B8	64/65 (98%)	0.51	5 (7%)	20	17	51, 81, 124, 148	0
34	D8	64/65 (98%)	0.81	9 (14%)	7	10	67, 104, 137, 168	0
35	B9	37/37 (100%)	0.07	2 (5%)	32	24	66, 89, 127, 141	0
35	D9	37/37 (100%)	0.20	2 (5%)	32	24	65, 91, 151, 187	0
36	BA	2901/2915 (99%)	0.15	55 (1%)	66	47	36, 88, 184, 200	0
36	DA	2901/2915 (99%)	0.19	45 (1%)	70	51	42, 102, 186, 200	0
37	BB	119/122 (97%)	0.19	3 (2%)	58	42	68, 101, 129, 160	0
37	DB	119/122 (97%)	0.38	4 (3%)	48	34	83, 126, 154, 189	0
38	BC	228/229 (99%)	-0.09	2 (0%)	81	64	44, 101, 163, 195	0
38	DC	228/229 (99%)	0.01	3 (1%)	74	55	66, 125, 187, 199	0
39	BD	275/276 (99%)	-0.27	1 (0%)	89	76	31, 64, 106, 155	0
39	DD	275/276 (99%)	-0.16	3 (1%)	77	59	40, 74, 115, 163	0
40	BE	205/206 (99%)	0.08	3 (1%)	71	53	37, 88, 146, 184	0
40	DE	205/206 (99%)	0.04	1 (0%)	87	72	50, 97, 157, 200	0
41	BF	208/210 (99%)	0.04	1 (0%)	87	72	53, 111, 183, 200	0
41	DF	208/210 (99%)	0.18	5 (2%)	59	43	58, 131, 186, 200	0
42	BG	181/182 (99%)	-0.05	2 (1%)	77	59	51, 99, 144, 194	0
42	DG	181/182 (99%)	0.01	2 (1%)	77	59	67, 122, 168, 192	0
43	BH	167/180 (92%)	0.14	4 (2%)	59	43	87, 131, 174, 185	0
43	DH	167/180 (92%)	0.18	4 (2%)	59	43	76, 133, 175, 185	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BN	139/140 (99%)	-0.07	1 (0%) 84 68	60, 99, 148, 177	0
45	DN	139/140 (99%)	0.09	2 (1%) 73 54	64, 108, 162, 176	0
46	BO	122/122 (100%)	-0.37	0 100 100	34, 72, 107, 128	0
46	DO	122/122 (100%)	-0.29	0 100 100	40, 79, 108, 156	0
47	BP	146/150 (97%)	0.37	5 (3%) 48 34	48, 104, 158, 195	0
47	DP	146/150 (97%)	0.41	3 (2%) 63 45	52, 127, 173, 195	0
48	BQ	141/141 (100%)	-0.20	1 (0%) 84 68	39, 77, 122, 173	0
48	DQ	141/141 (100%)	-0.09	1 (0%) 84 68	52, 86, 127, 185	0
49	BR	117/118 (99%)	-0.10	2 (1%) 69 50	36, 89, 128, 177	0
49	DR	117/118 (99%)	0.01	3 (2%) 57 41	46, 95, 135, 181	0
50	BS	99/112 (88%)	0.36	1 (1%) 79 61	53, 109, 156, 191	0
50	DS	99/112 (88%)	0.41	4 (4%) 43 31	51, 121, 164, 192	0
51	BT	138/146 (94%)	-0.02	2 (1%) 73 54	53, 95, 168, 200	0
51	DT	138/146 (94%)	0.14	1 (0%) 84 68	56, 103, 172, 200	0
52	BU	117/118 (99%)	0.04	1 (0%) 81 64	55, 91, 138, 200	0
52	DU	117/118 (99%)	0.17	2 (1%) 69 50	66, 104, 147, 191	0
53	BV	101/101 (100%)	0.10	3 (2%) 52 37	43, 112, 158, 177	0
53	DV	101/101 (100%)	0.25	4 (3%) 43 31	64, 126, 171, 193	0
54	BW	113/113 (100%)	-0.04	0 100 100	56, 95, 150, 195	0
54	DW	113/113 (100%)	-0.09	0 100 100	73, 106, 158, 194	0
55	BX	93/96 (96%)	0.17	1 (1%) 77 59	60, 101, 133, 176	0
55	DX	93/96 (96%)	0.17	1 (1%) 77 59	63, 111, 141, 154	0
56	BY	107/110 (97%)	0.52	3 (2%) 55 39	93, 138, 178, 187	0
56	DY	107/110 (97%)	0.46	4 (3%) 45 33	87, 147, 182, 200	0
57	BZ	185/206 (89%)	-0.06	0 100 100	50, 108, 163, 190	0
57	DZ	185/206 (89%)	0.15	0 100 100	54, 122, 170, 199	0
All	All	22516/23492 (95%)	0.09	469 (2%) 63 45	23, 98, 175, 200	0

The worst 5 of 469 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	CW	34	C	11.2
24	AX	12	A	8.5
24	AX	11	A	7.6
24	CX	14	U	7.1
24	AX	14	U	7.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
23	5MU	CW	54	21/22	0.58	0.12	200,200,200,200	0
23	5MU	AW	54	21/22	0.62	0.16	200,200,200,200	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
59	FUA	CY	701	37/37	0.19	0.29	102,104,107,109	0
59	FUA	AY	701	37/37	0.33	0.30	98,102,110,111	0
61	MG	AY	703	1/1	0.82	0.15	55,55,55,55	0
58	ZN	D4	1000	1/1	0.83	0.10	200,200,200,200	0
60	GDP	AY	702	28/28	0.90	0.10	93,97,99,99	0
58	ZN	B4	101	1/1	0.90	0.08	172,172,172,172	0
60	GDP	CY	702	28/28	0.94	0.07	96,102,109,110	0
61	MG	CY	703	1/1	0.94	0.11	46,46,46,46	0
58	ZN	CD	301	1/1	0.98	0.12	69,69,69,69	0
58	ZN	AD	301	1/1	0.98	0.18	78,78,78,78	0
58	ZN	AN	101	1/1	0.99	0.08	84,84,84,84	0
58	ZN	CN	101	1/1	0.99	0.03	86,86,86,86	0

Continued on next page...

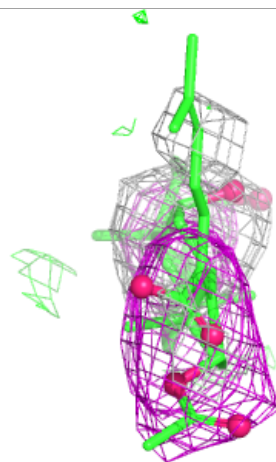
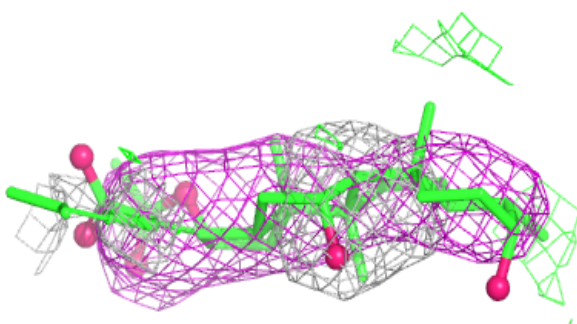
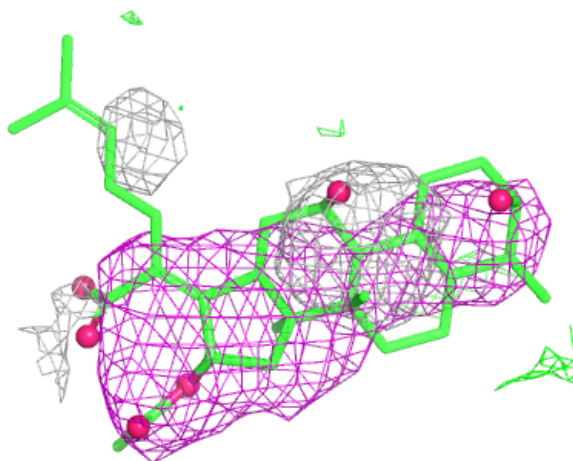
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	ZN	B9	101	1/1	0.99	0.03	93,93,93,93	0
58	ZN	D9	1000	1/1	1.00	0.02	123,123,123,123	0

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

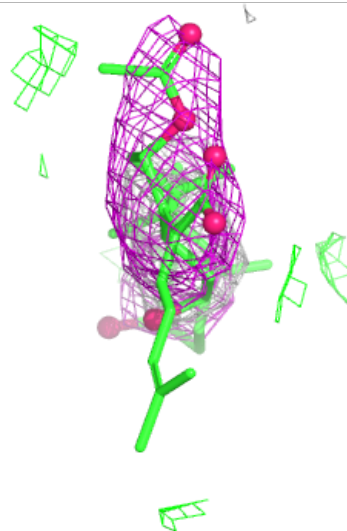
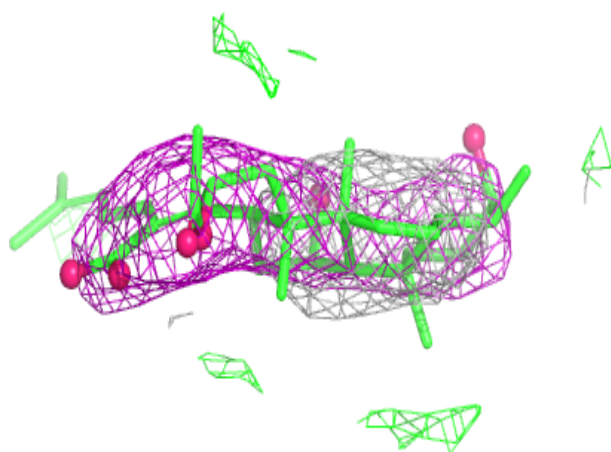
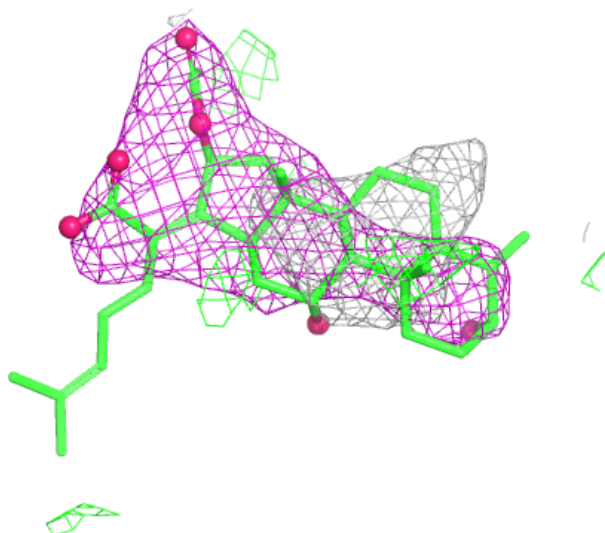
Electron density around FUA CY 701:

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



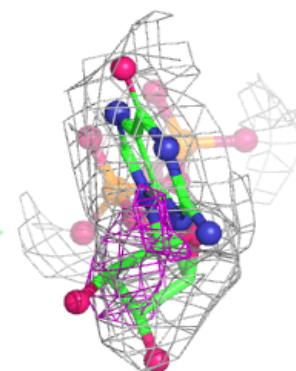
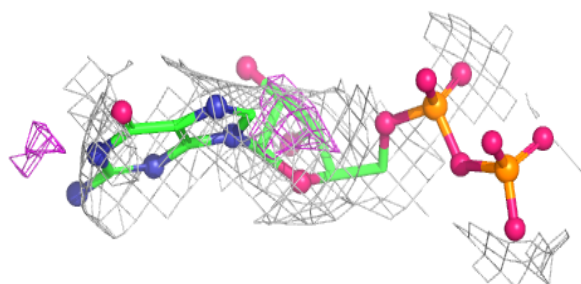
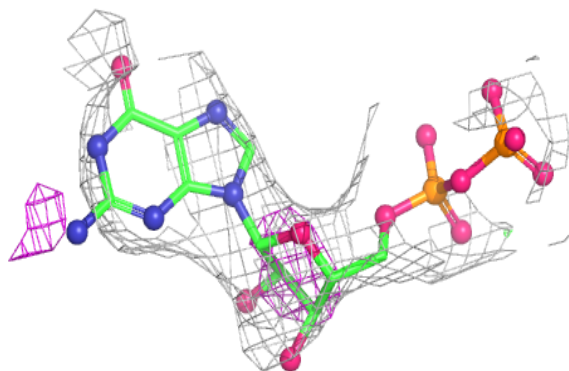
Electron density around FUA AY 701:

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

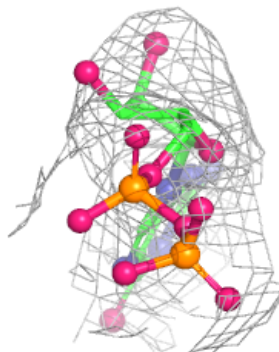
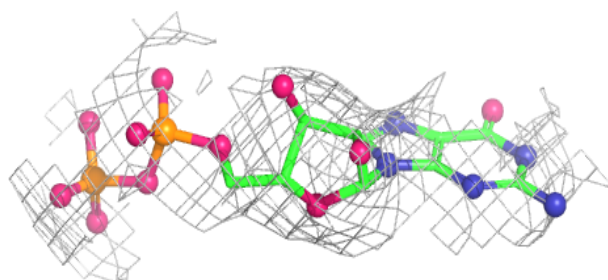
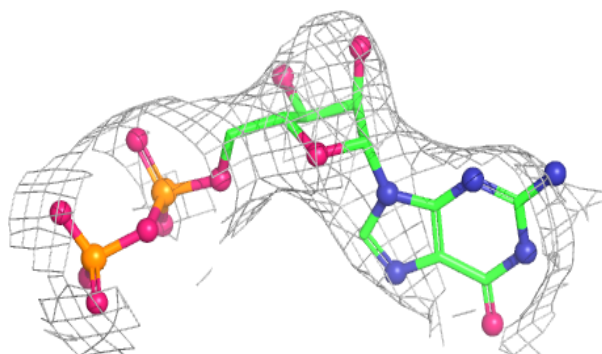


Electron density around GDP AY 702:

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

**Electron density around GDP CY 702:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.