



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2024 – 12:45 am BST

PDB ID : 4V8U  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

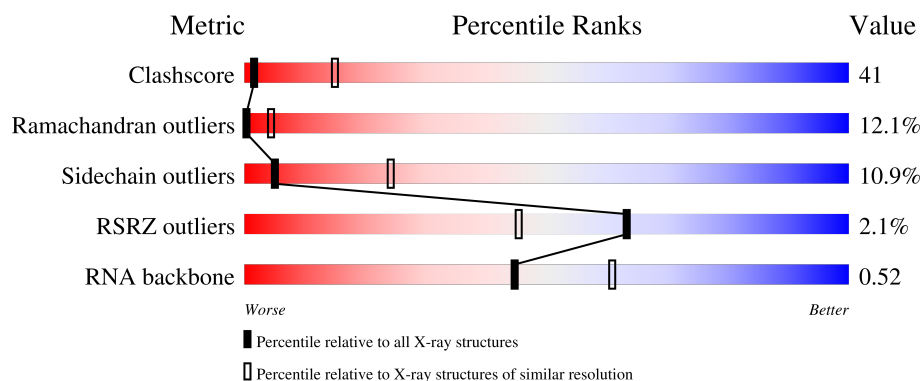
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

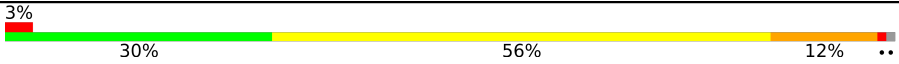
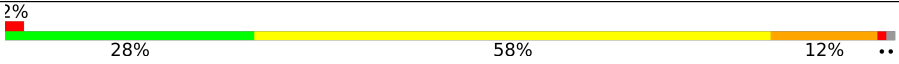
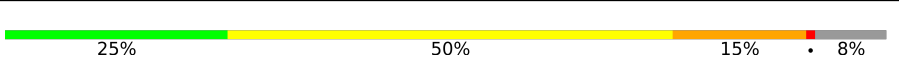
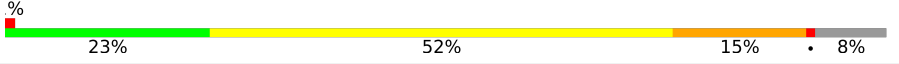
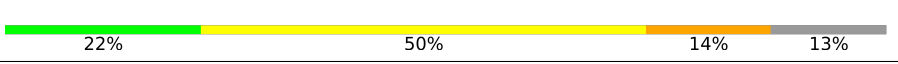
The reported resolution of this entry is 3.70 Å.

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	
1	CA	1522	
2	AB	256	
2	CB	256	
3	AC	239	

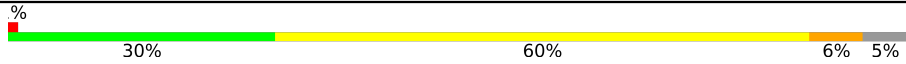
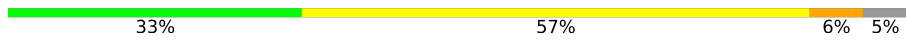


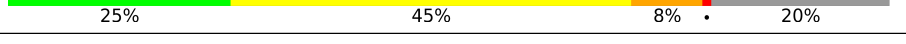
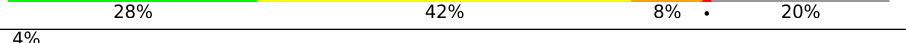
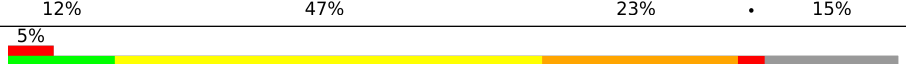
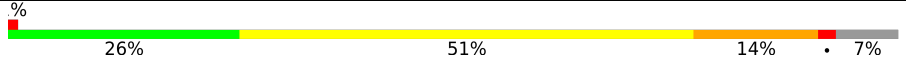
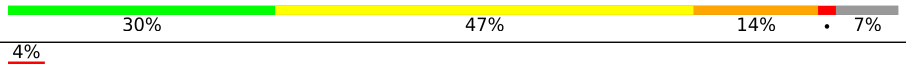
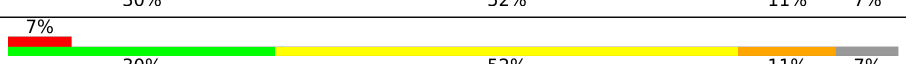
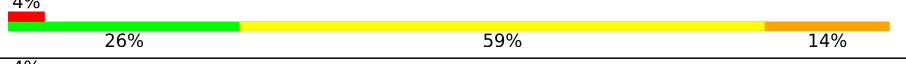

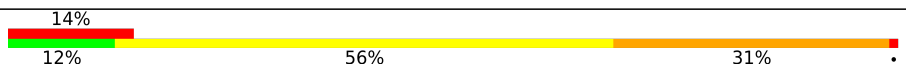


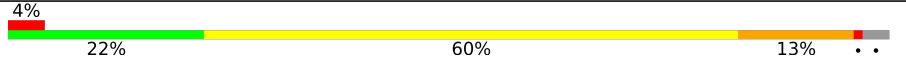

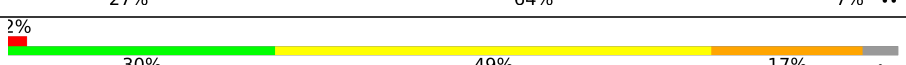
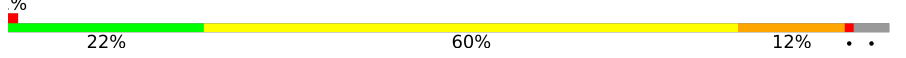
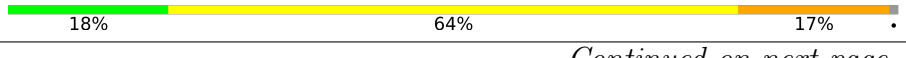


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Mol	Chain	Length	Quality of chain
3	CC	239	% 21% 51% 15% 13%
4	AD	209	% 32% 53% 14%
4	CD	209	% 31% 55% 13%
5	AE	162	% 36% 49% 9% 7%
5	CE	162	% 38% 46% 9% 7%
6	AF	101	33% 58% 9%
6	CF	101	34% 57% 9%
7	AG	156	% 42% 48% 9% ..
7	CG	156	4% 42% 49% 8% .
8	AH	138	% 41% 53% 7%
8	CH	138	41% 53% 7%
9	AI	128	30% 62% 8% .
9	CI	128	% 27% 64% 8% .
10	AJ	105	% 16% 62% 16% 6%
10	CJ	105	3% 15% 62% 17% 6%
11	AK	129	% 46% 42% 5% 8%
11	CK	129	2% 41% 46% 5% 8%
12	AL	132	27% 53% 12% . 5%
12	CL	132	% 26% 52% 14% . 5%
13	AM	126	5% 20% 62% 16% ..
13	CM	126	6% 20% 62% 16% ..
14	AN	61	2% 34% 54% 5% 5% .
14	CN	61	2% 34% 54% 5% 5% .
15	AO	89	34% 55% 10% .
15	CO	89	% 33% 55% 11% .

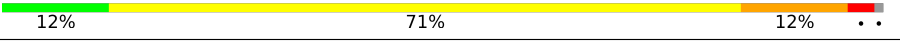

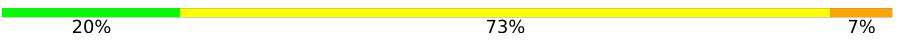



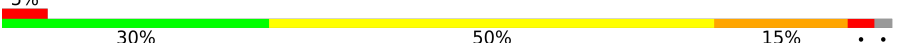
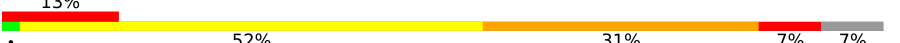
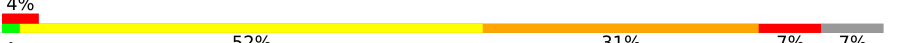

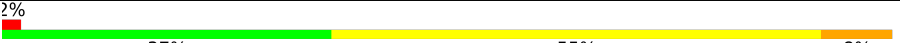
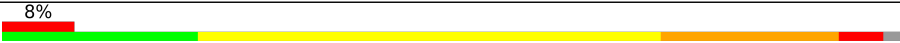
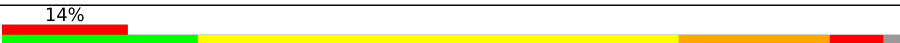
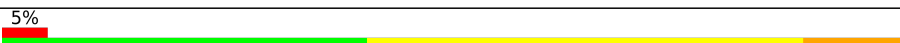
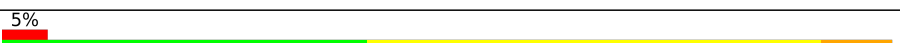

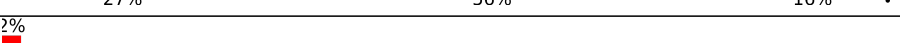
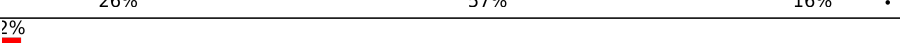
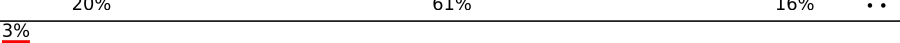
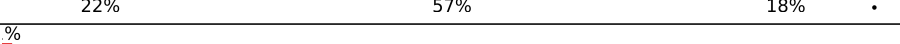



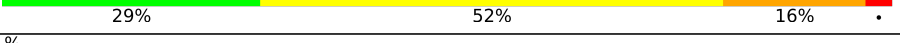
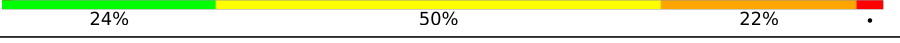
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Mol	Chain	Length	Quality of chain
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	CV	76	
23	AW	77	
23	CW	77	
24	AX	25	
24	CX	25	
25	AY	691	
25	CY	691	
26	B0	85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


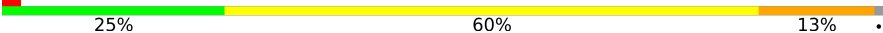
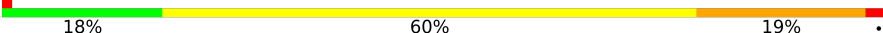
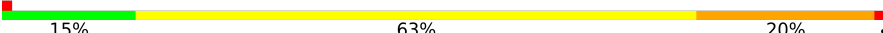
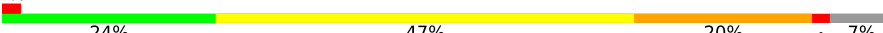
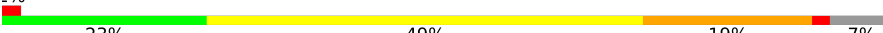





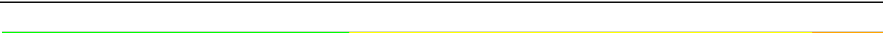





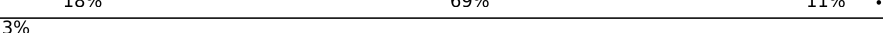
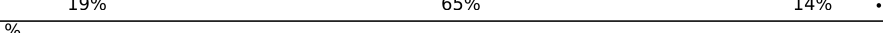






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Mol	Chain	Length	Quality of chain
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229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

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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	

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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			

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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			

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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			

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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 (three-letter code: ZN) (formula: Zn).

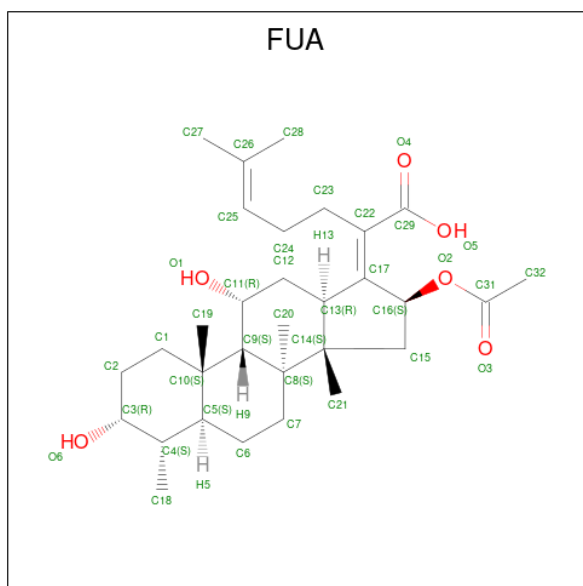
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AD	1	Total	Zn	0	0
			1	1		

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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 (three-letter code: 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 (three-letter code: 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

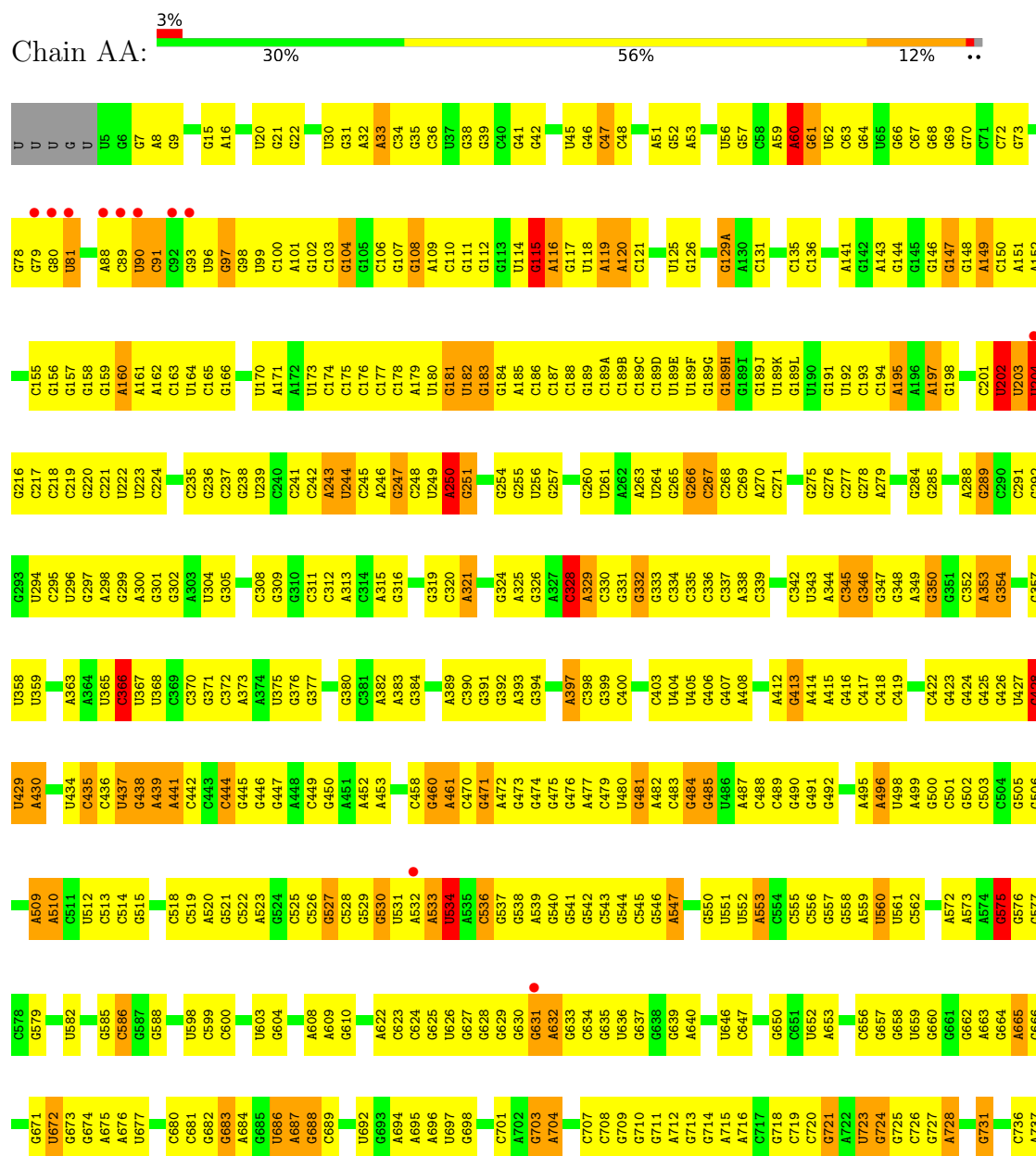
- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

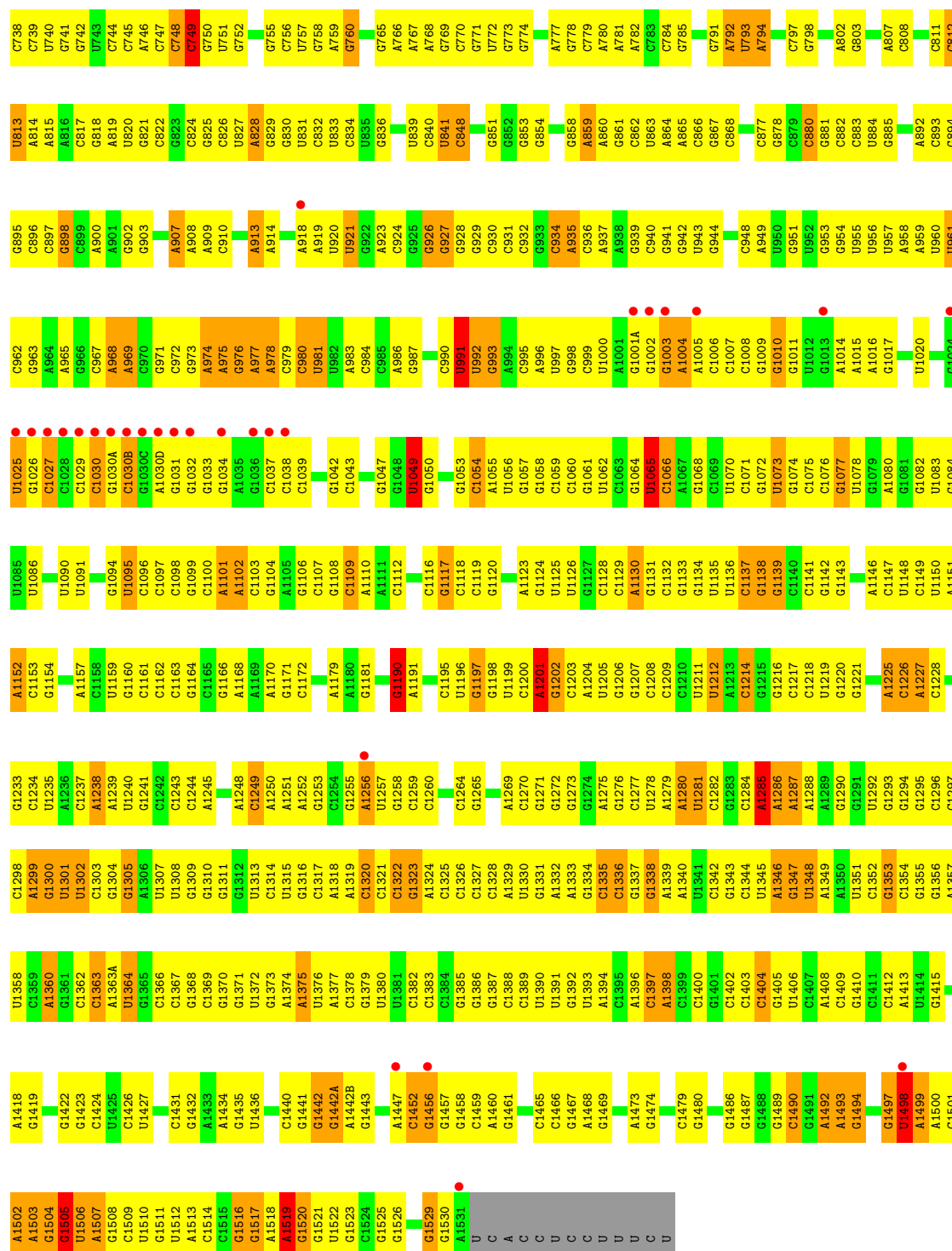
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AY	1	Total Mg 1 1	0	0
61	CY	1	Total Mg 1 1	0	0

### 3 Residue-property plots [i](#)

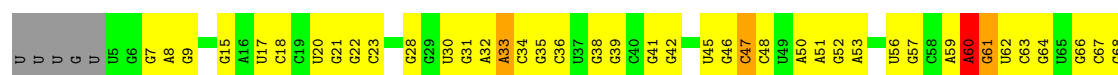
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

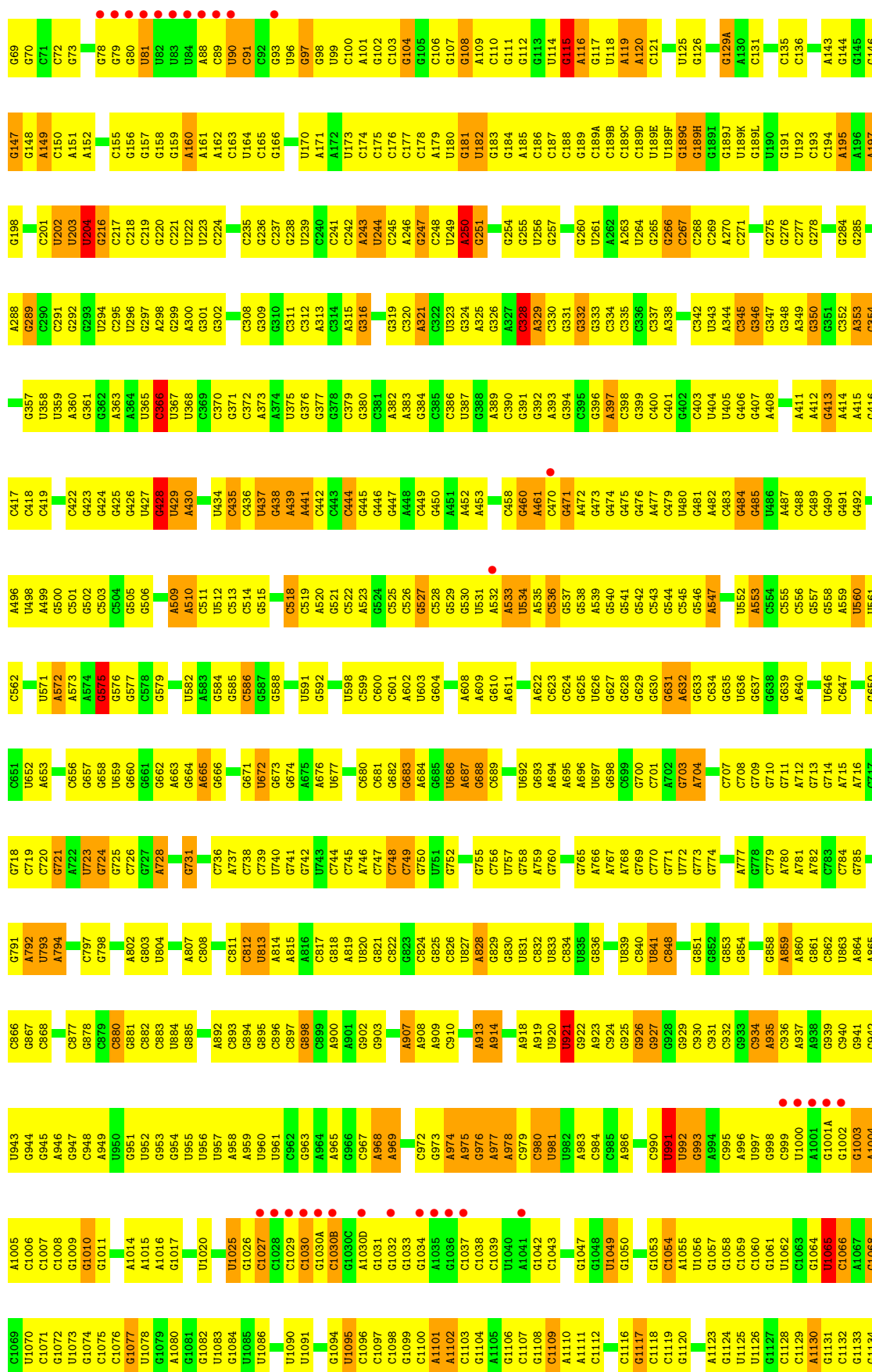
#### • Molecule 1: 16S RIBOSOMAL RNA

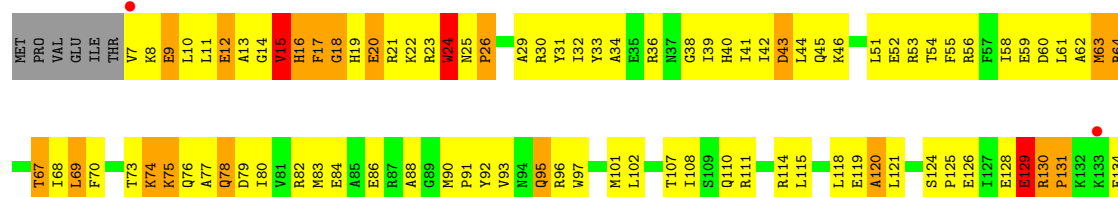




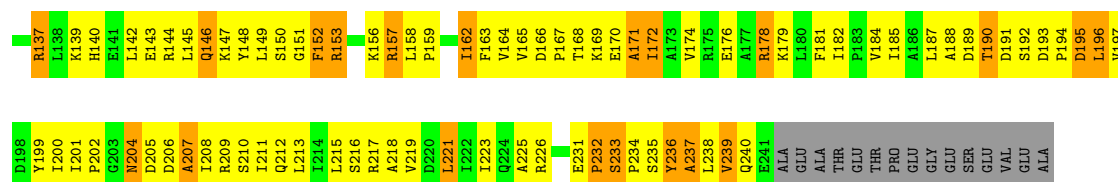
- Molecule 1: 16S RIBOSOMAL RNA





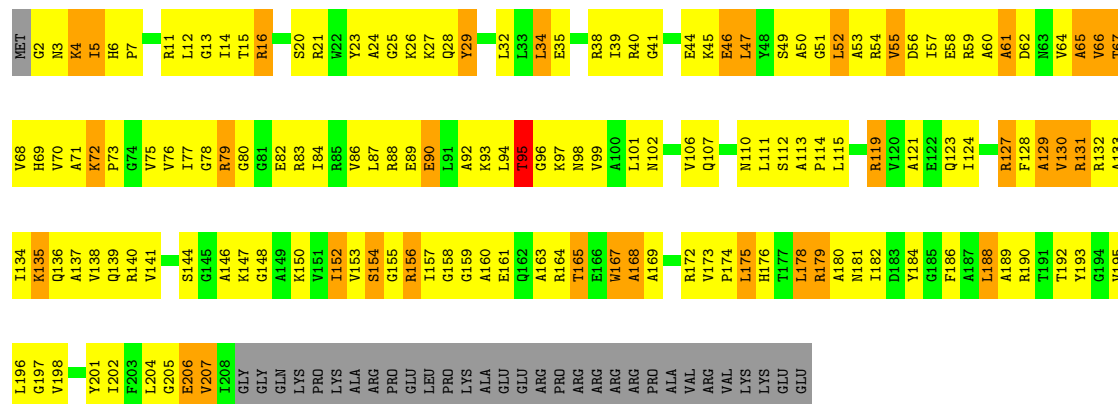






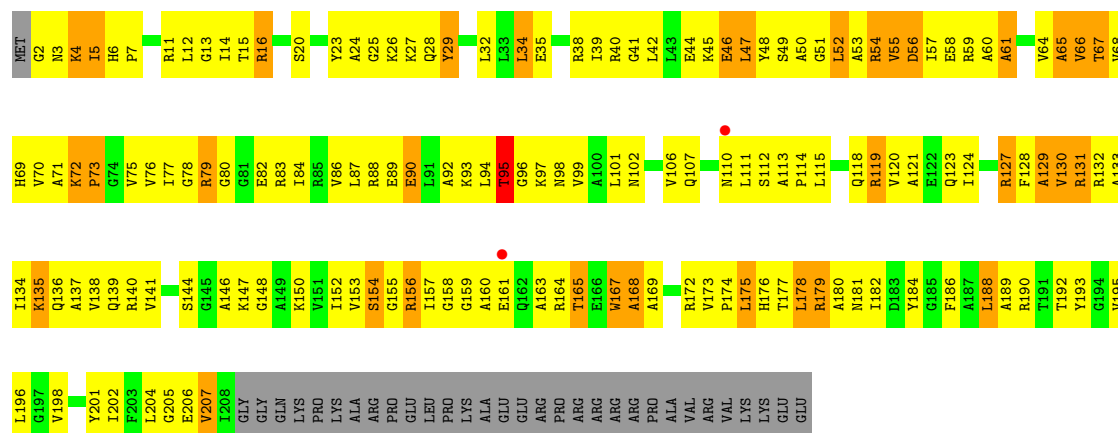
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:



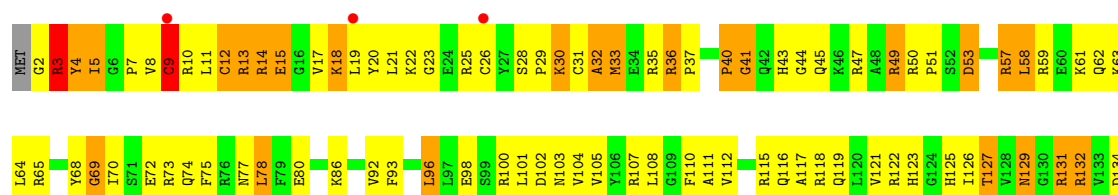
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3

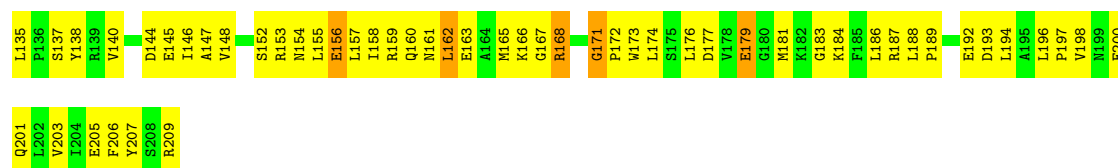
Chain CC:



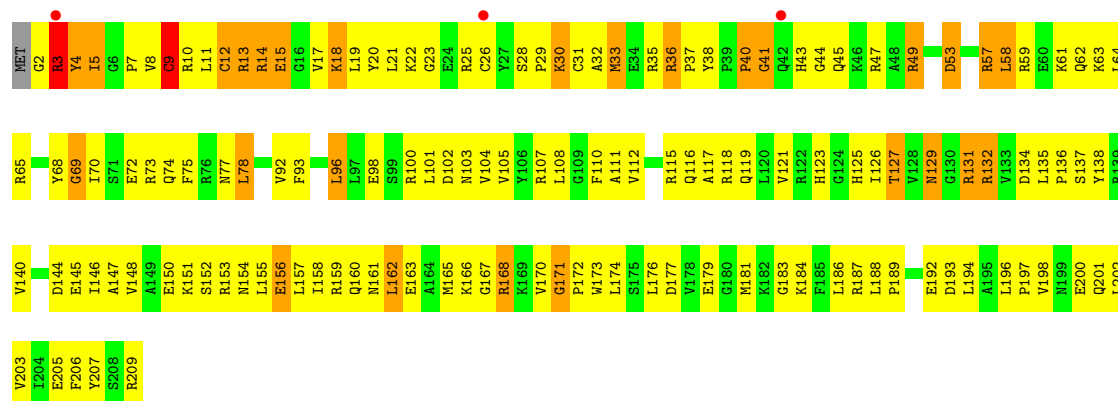
### • Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:

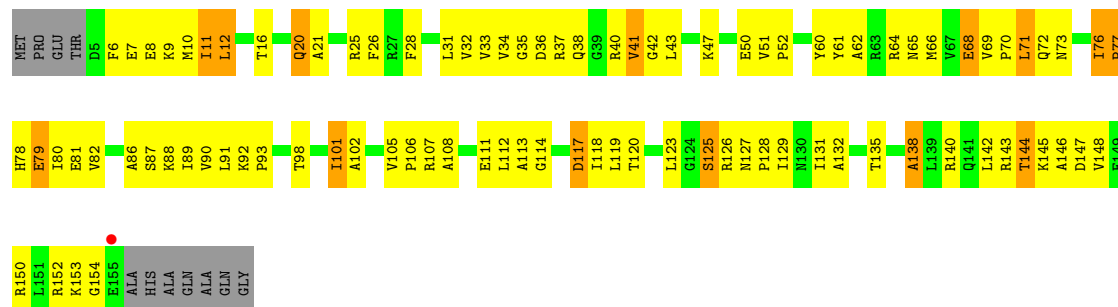




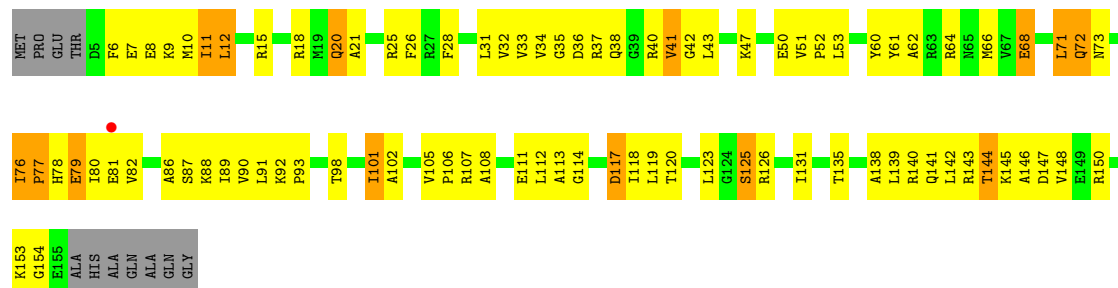
### • Molecule 4: 30S RIBOSOMAL PROTEIN S4



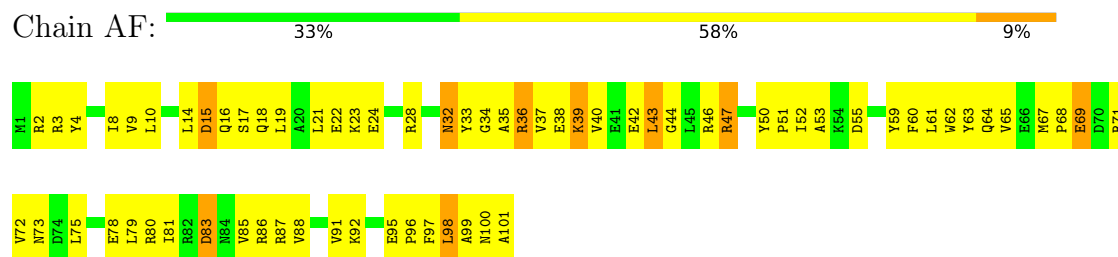
### • Molecule 5: 30S RIBOSOMAL PROTEIN S5



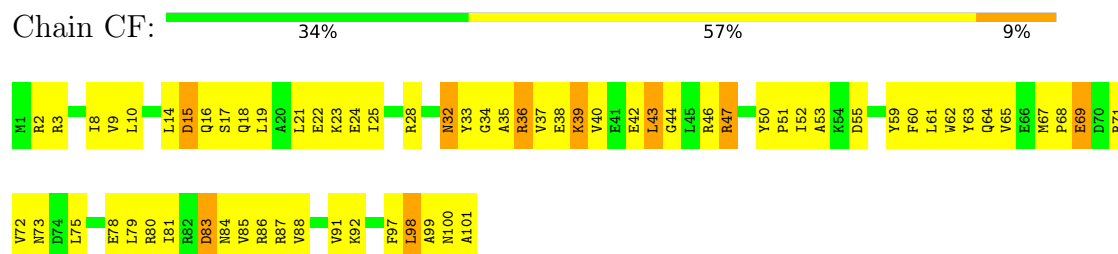
### • Molecule 5: 30S RIBOSOMAL PROTEIN S5



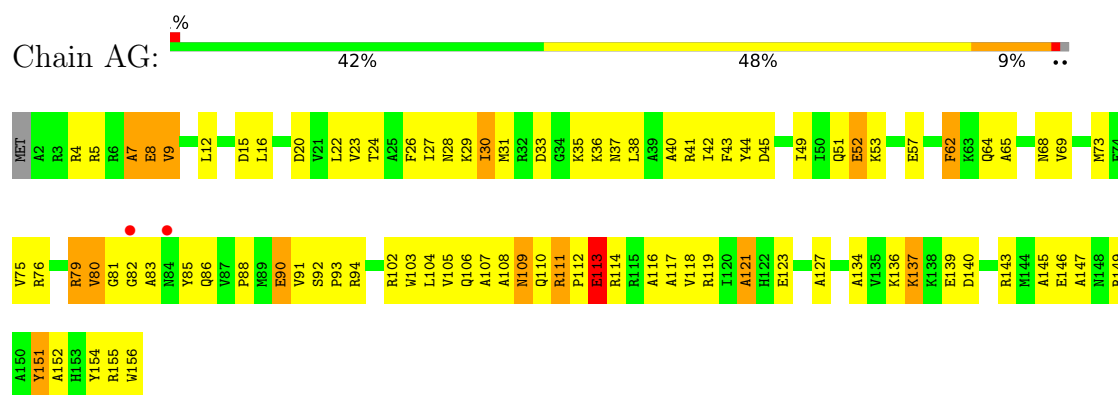
### • Molecule 6: 30S RIBOSOMAL PROTEIN S6



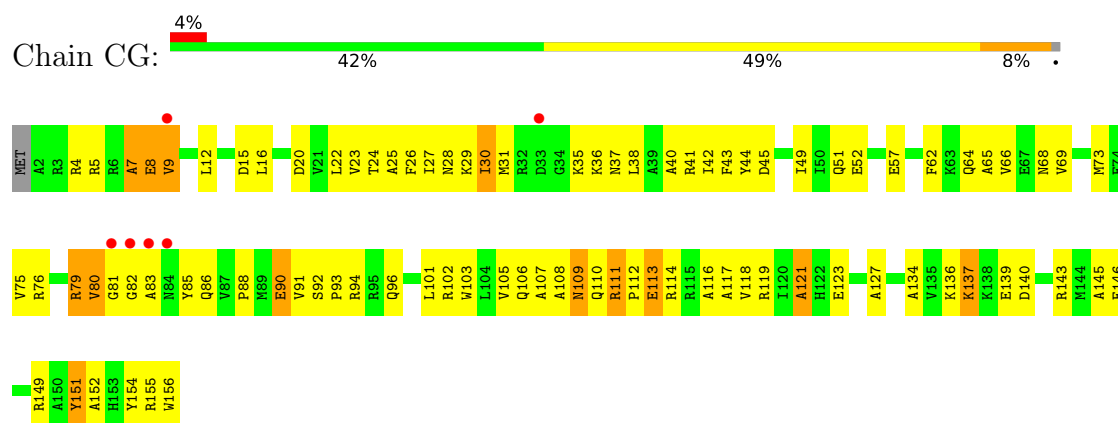
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



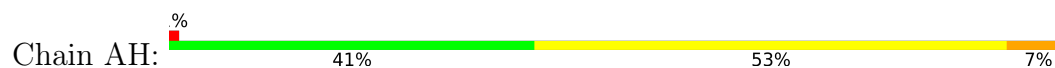
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

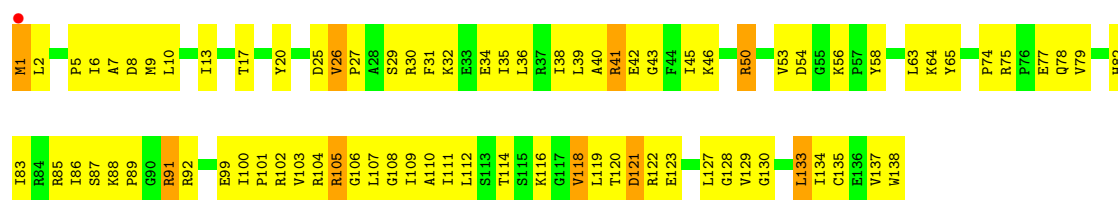


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

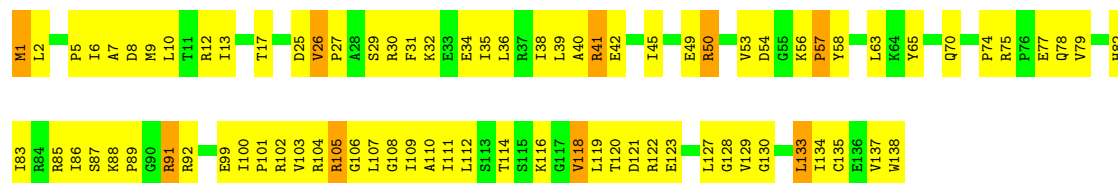


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

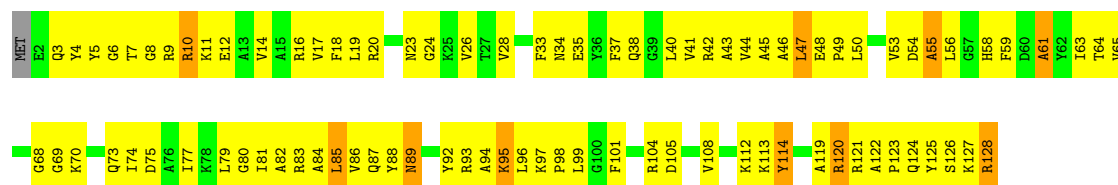
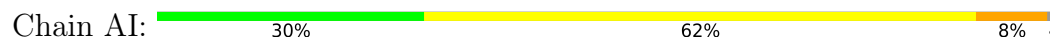




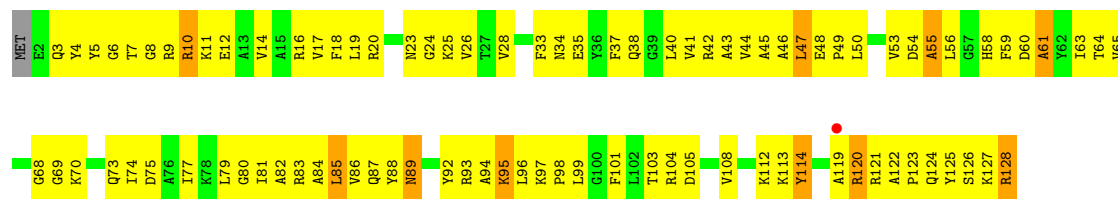
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



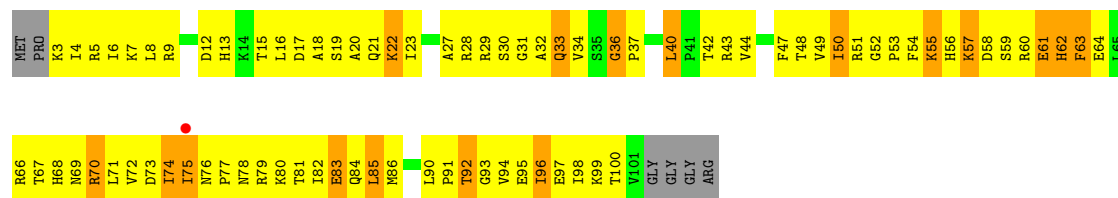
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



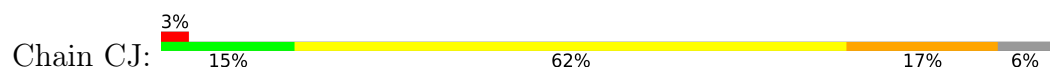
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

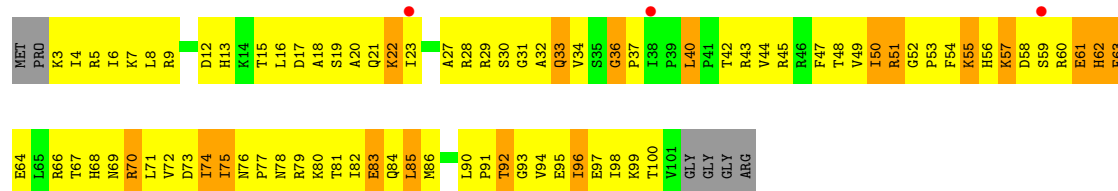


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

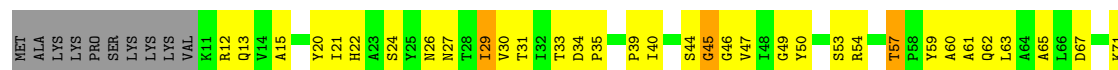


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

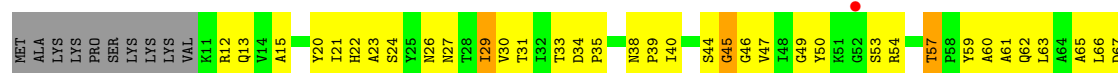
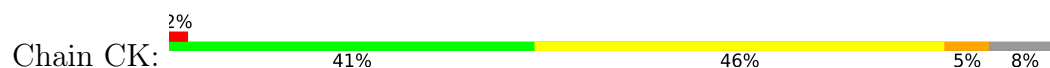




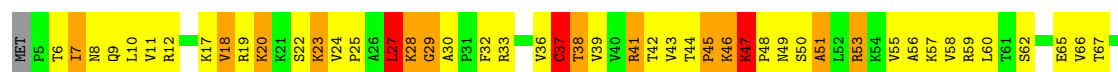
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



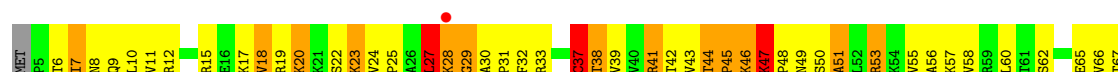
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



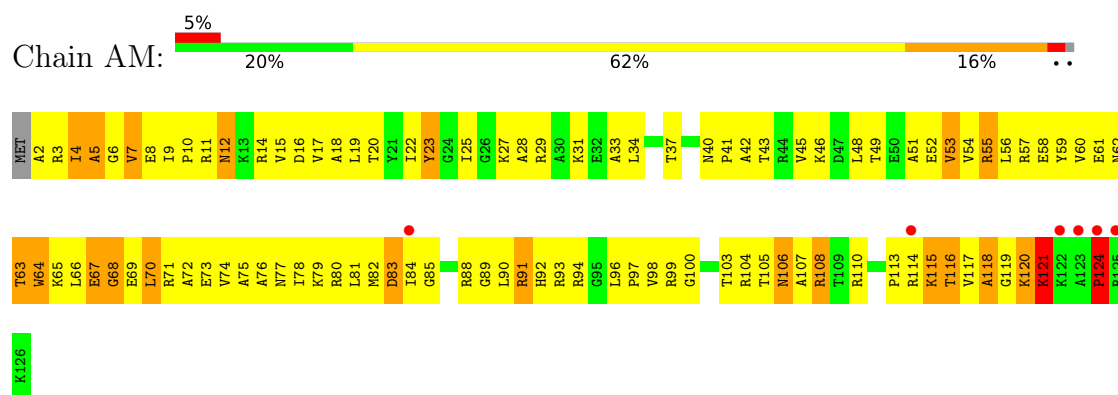
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



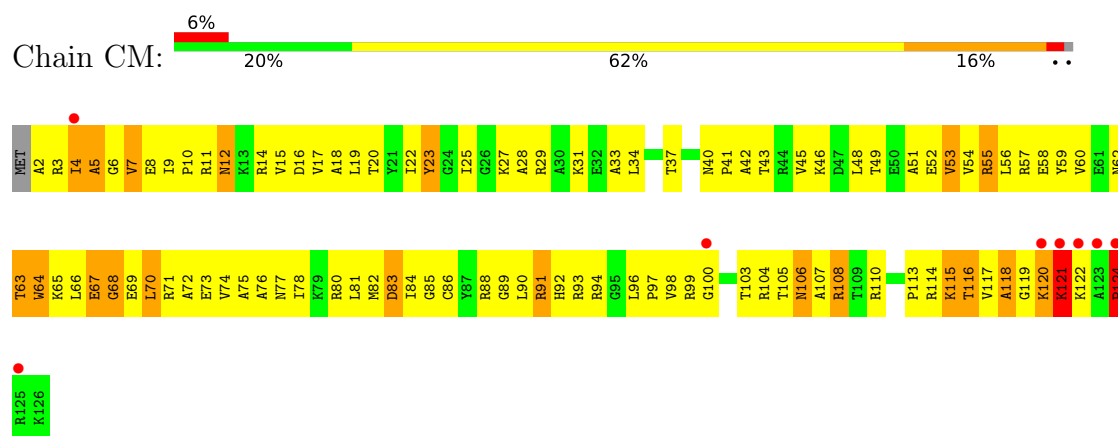
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



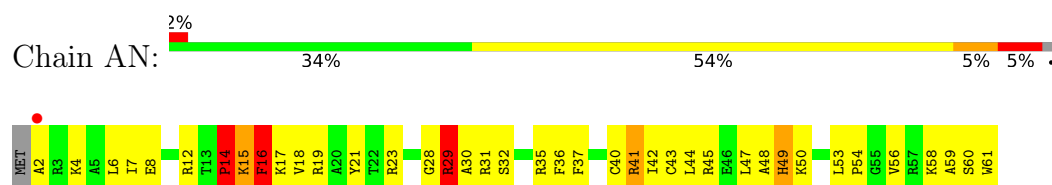
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



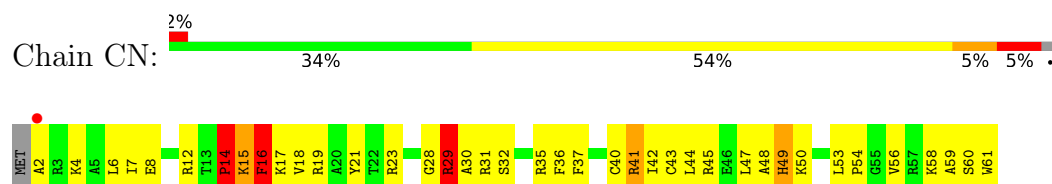
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



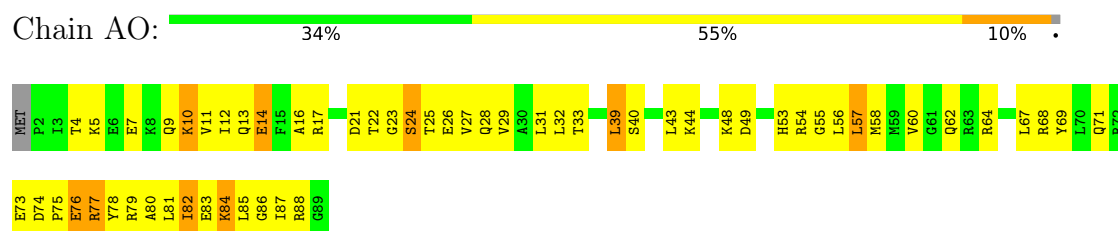
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



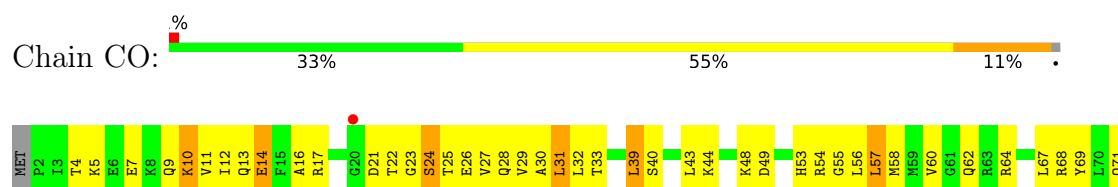
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



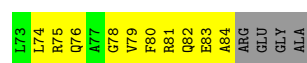
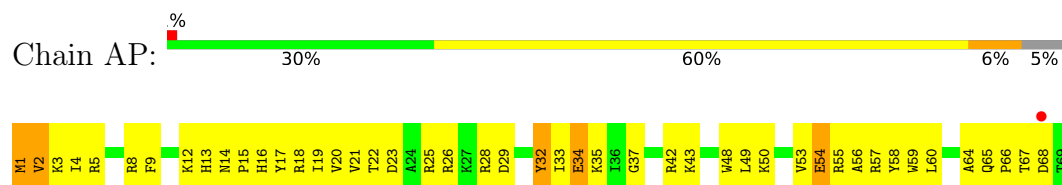
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



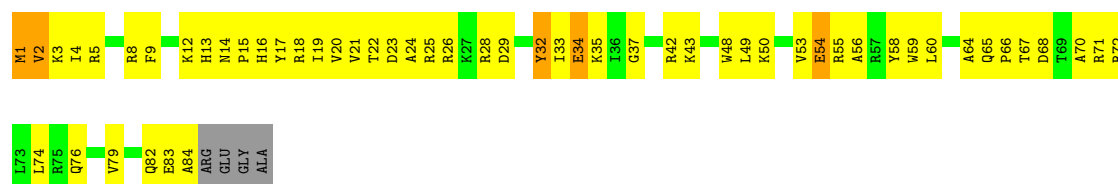
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



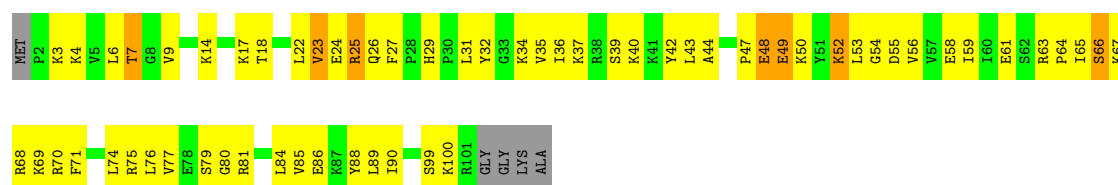
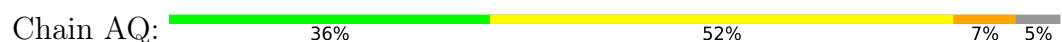
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



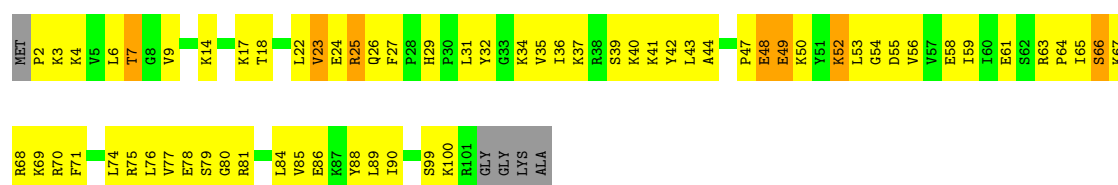
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



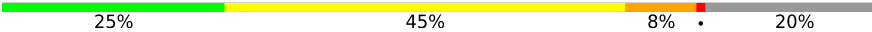
● Molecule 17: 30S RIBOSOMAL PROTEIN S17

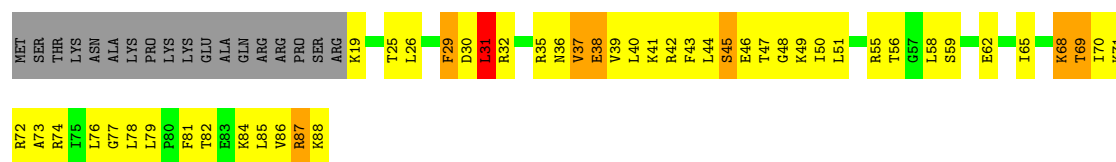


● Molecule 17: 30S RIBOSOMAL PROTEIN S17



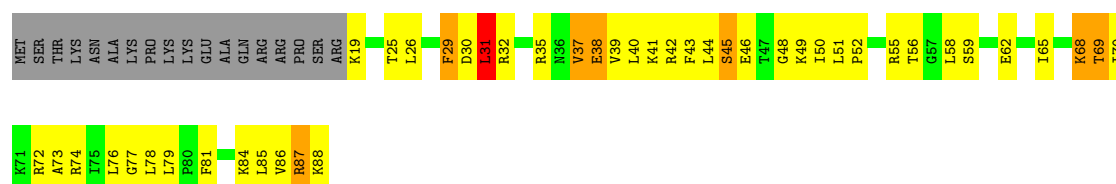
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR: 




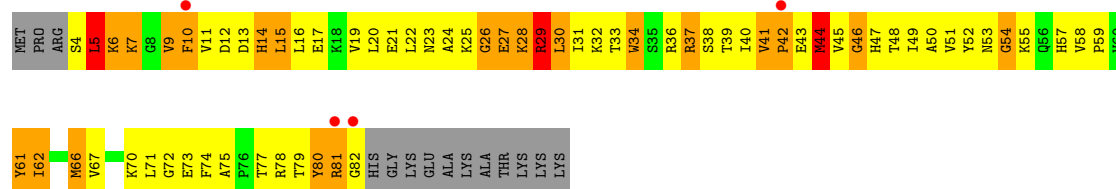
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR: 

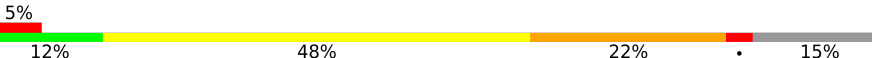


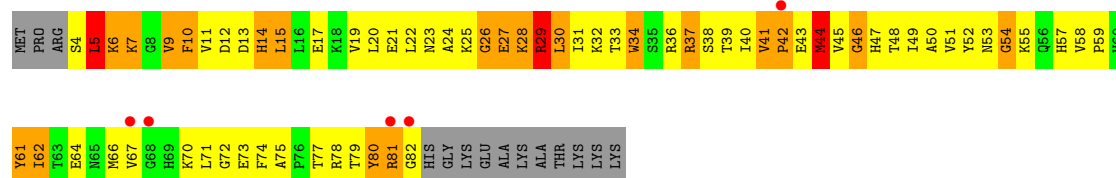
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS: 



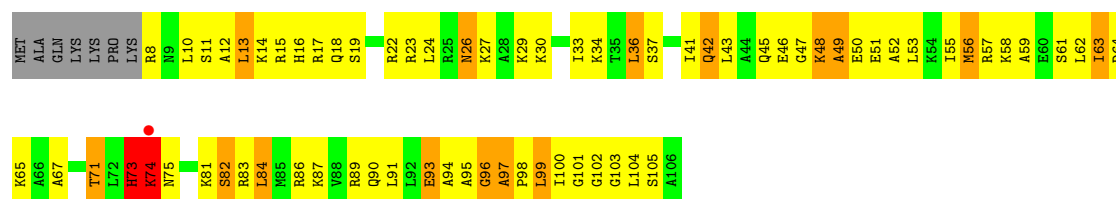
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS: 



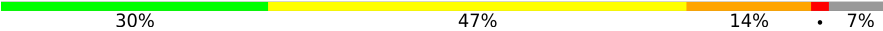
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

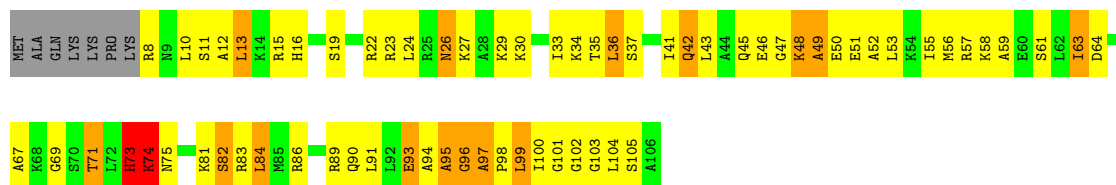
Chain AT: 



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

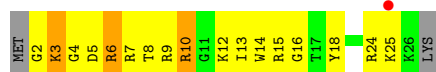


Chain CT:  30% 47% 14% 7%



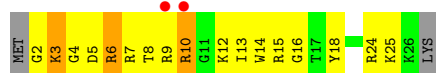
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:  4% 30% 52% 11% 7%



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:  7% 30% 52% 11% 7%




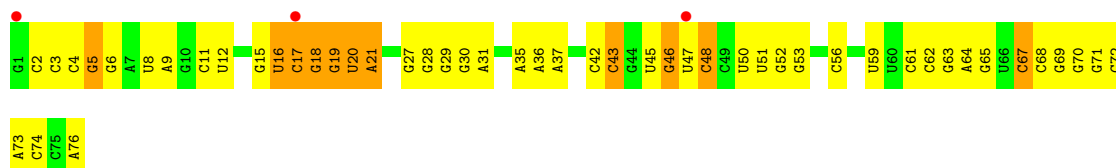
• Molecule 22: MRNA

Chain AV:  4% 26% 59% 14%




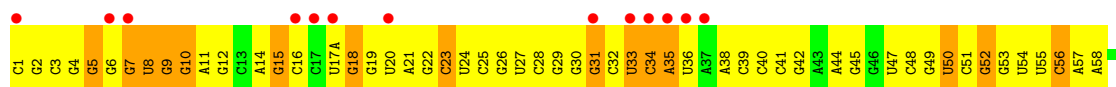
• Molecule 22: MRNA

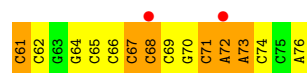
Chain CV:  4% 34% 51% 14%



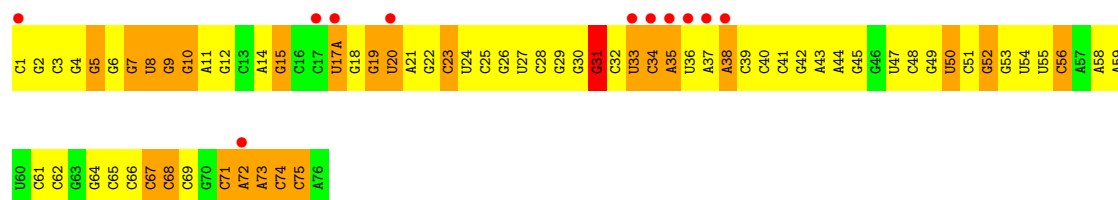
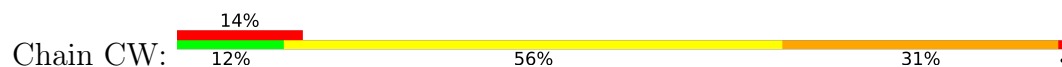
• Molecule 23: RNA

Chain AW:  19% 12% 61% 27%

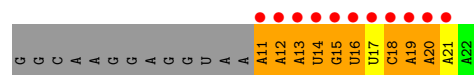




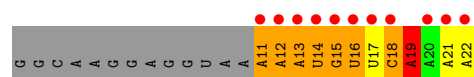
• Molecule 23: RNA



• Molecule 24: RNA

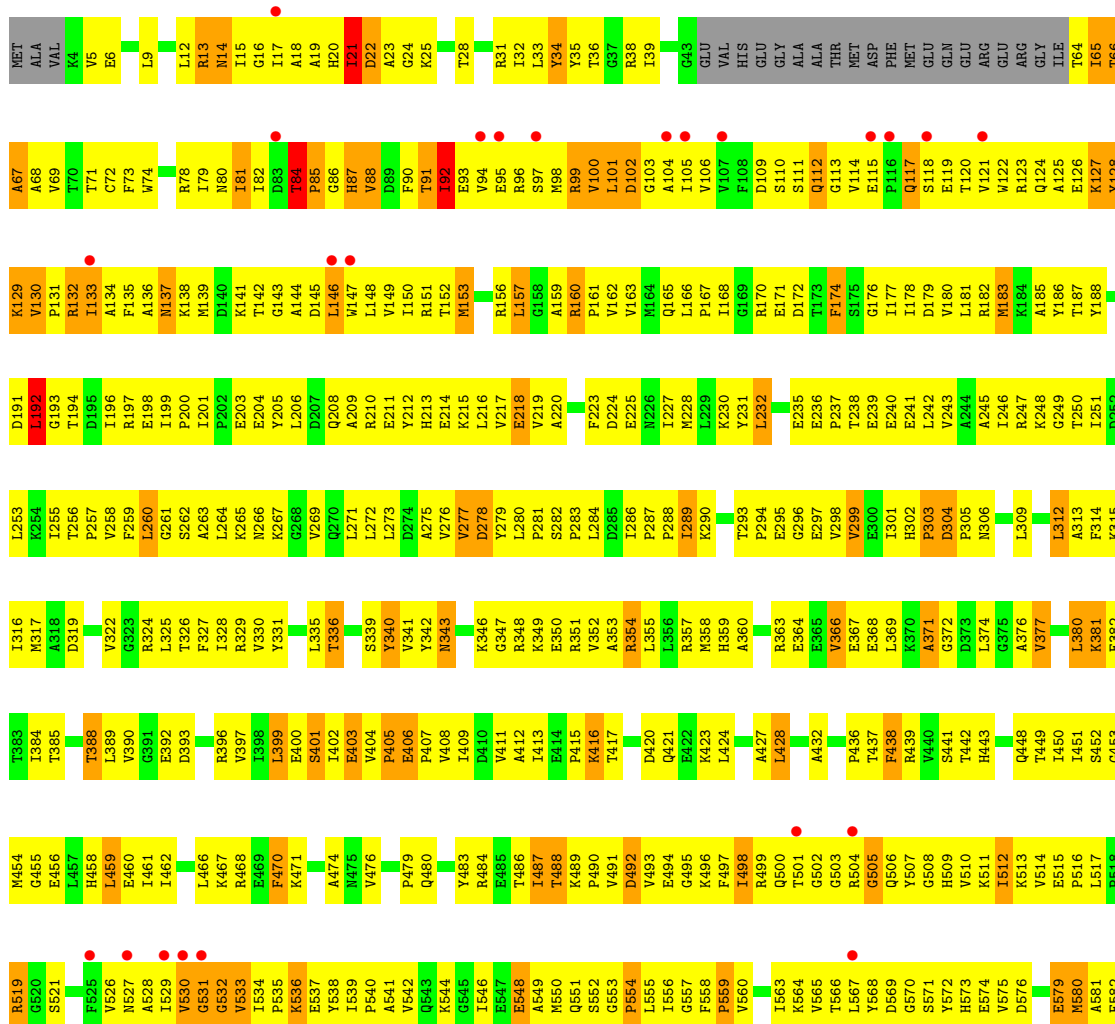


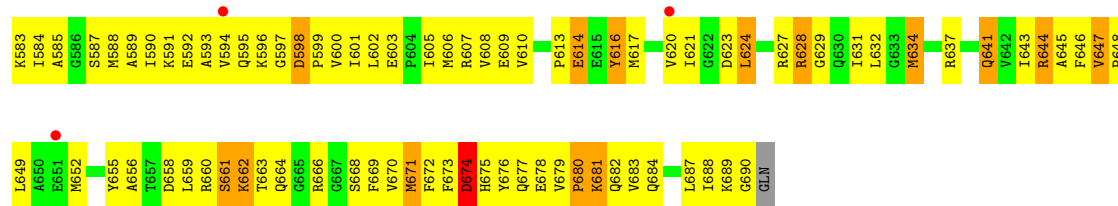
• Molecule 24: RNA



• Molecule 25: ELONGATION FACTOR G

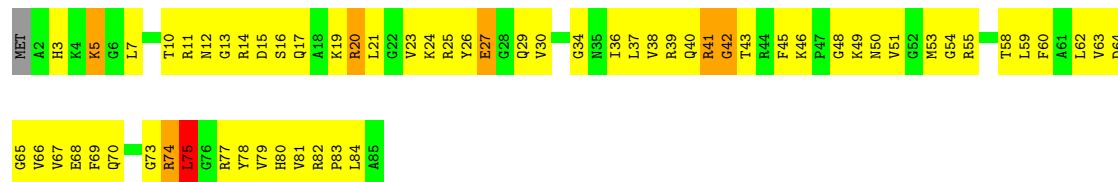






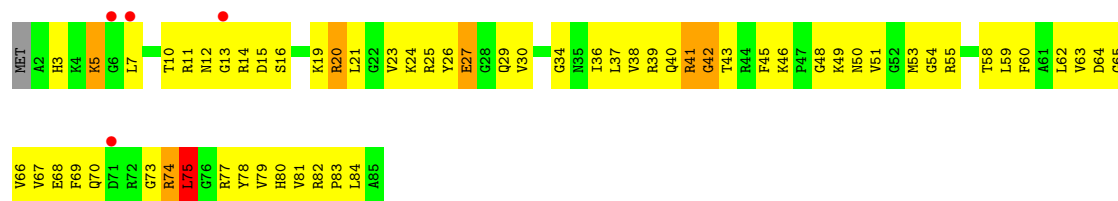
● Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain B0: 26% 65% 7% ..



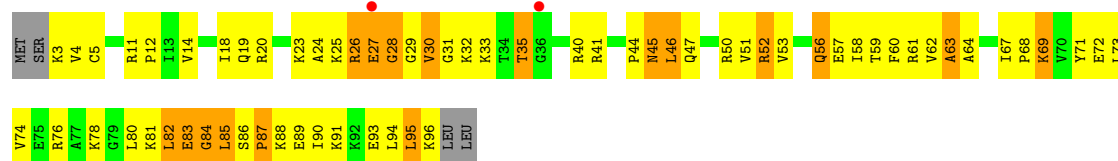
● Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain D0: 5% 27% 64% 7% ..



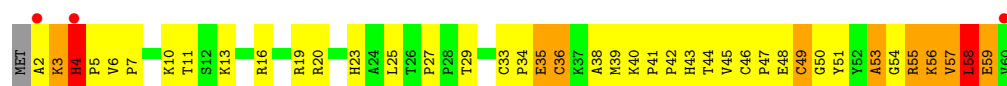
● Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain B1: 2% 30% 49% 17% .

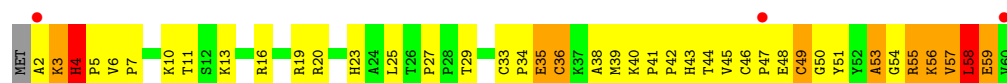




- Molecule 31: 50S RIBOSOMAL PROTEIN L32



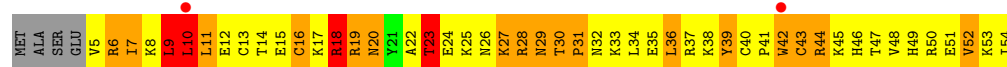
- Molecule 31: 50S RIBOSOMAL PROTEIN L32



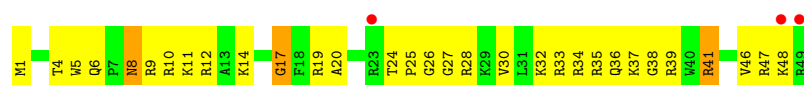
- Molecule 32: 50S RIBOSOMAL PROTEIN L33



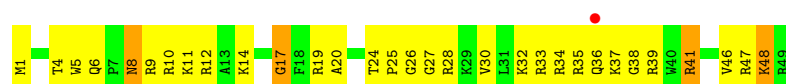
- Molecule 32: 50S RIBOSOMAL PROTEIN L33



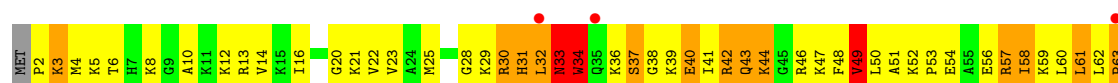
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



- Molecule 33: 50S RIBOSOMAL PROTEIN L34

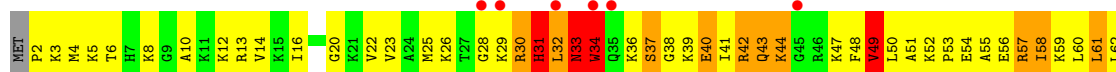


- Molecule 34: 50S RIBOSOMAL PROTEIN L35





• Molecule 34: 50S RIBOSOMAL PROTEIN L35



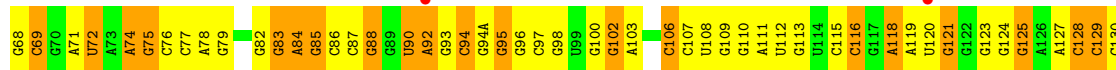
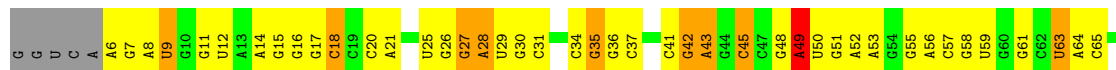
• Molecule 35: 50S RIBOSOMAL PROTEIN L36



• Molecule 35: 50S RIBOSOMAL PROTEIN L36



• Molecule 36: 23S RIBOSOMAL RNA

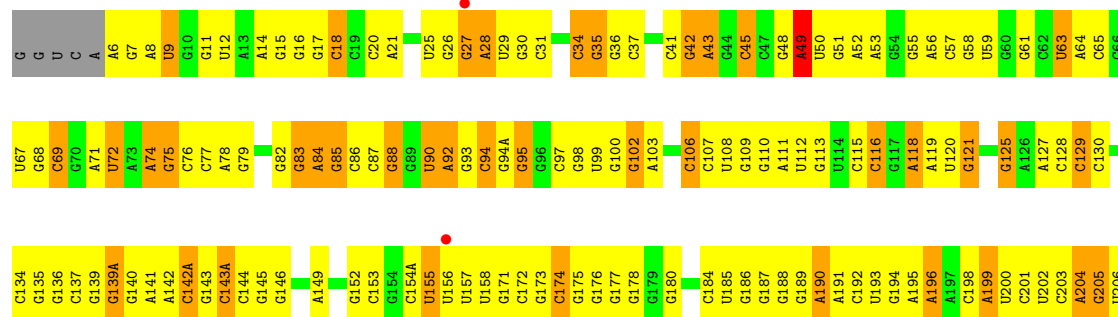






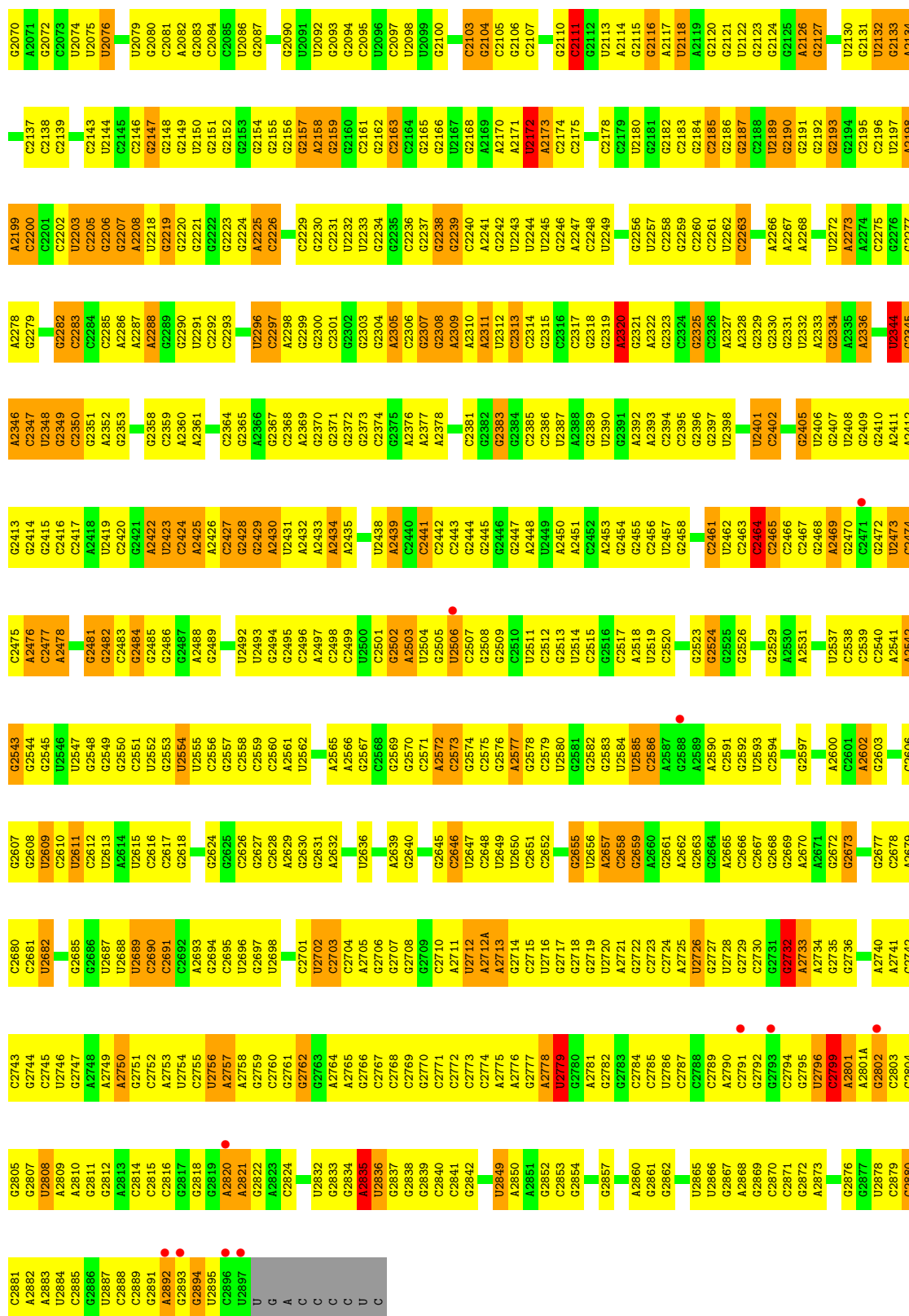
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G2168	A2169	G2029	U1955	G1876	U1798	G1714	A1634	G1859	U1469	G1422	U1552	A1286	C1221
A2170	G2105	A2030	U1955	C1882	G1799	G1717	G1635	G1565	A1490	G1423	A1353	A1287	C1221A
A2171	G2106	A2031	G1959	A1883	G1800	G1718	G1636	G1566	G1491	G1424	A1354	U1288	C1222
U2172	A2032	A2032	A1960	A1884	G1801	G1719	A1637	A1567	G1492	A1427	G1289	G1289	G1223
A2173	U2034	U2034	A1885	A1885	A1802	U1720	G1638	G1568	C1493	C1428	C1290	C1291	C1224
C2174	G2035	G2035	C1886	C1887	A1803	G1721	U1639	G1569	A1494	G1429	G1358	C1291	G1227
C2175	U1963	U1964	C1887	A1888	G1804	A1722	C1640	A1569	A1495	G1430	A1359	U1292	G1228
C2178	G1967	G1967	A1889	A1889	U1905	G1740	C1644	G1573	U1497	U1431	A1360	C1293	G1231
G2182	U1968	U1968	G1899	G1899	A1809	A1741	G1647	U1575	U1503	G1432	A1362	G1296	G1232
C2183	A1969	A1969	G1811	G1811	G1810	C1744	C1647	C1576	C1504	U1433	G1363	C1297	G1233
G2184	A1970	A1970	A1812	C1745	A1812	C1745	G1649	C1577	G1505	U1434	G1364	G1297	U1234
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G2187	G1973	G1903	A1815	A1652	A1652	A1652	A1652	G1579	U1438	U1438	A1301	G1300	A1237
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U2189	A1977	G1907	G1817	A1654	A1655	C1754	C1655	C1583	A1509B	G1441	G1374	C1306	U1240
G2190	G1984	C1908	U1818	A1655	C1656	A1755	C1656	C1584	G1510	G1442	C1375	A1307	A1241
G2191	G1985	C1909	A1819	C1657	C1657	A1756	C1657	A1586	C1511	G1443	C1376	A1308	A1242
G2192	A1986	G1910	U1820	C1657	C1657	U1757	C1658	A1587	U1512	G1444	G1377	G1309	G1243
G2193	G1989	G1911	A1821	C1658	C1658	U1757	C1658	C1588	C1513	A1445	G1378	G1310	G1244
G2194	C1990	U1911	G1822	U1659	U1659	G1758	U1659	C1589	U1514	C1445A	A1378	G1311	G1245
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C2201	G1998	A1918	A1829	A1667	A1667	C1767	A1667	U1523	U1523	C1451	C1385	A1317	G1252
C2202	C1999	C1920	C1836	A1668	A1668	U1768	A1668	G1524	G1524	A1452	C1386	C1318	G1253
U2203	G2000	G1921	C1837	A1669	A1669	G1769	A1669	G1525	U1463	U1463	C1387	G1322	A1254
G2206	A2001	G1922	C1838	C1670	C1670	C1770	C1670	G1526	G1389	G1455	G1388	G1326	A1255
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G2218	G2004	U1929	U1841	A1676	A1676	A1773	A1677	C1531	G1461	C1462	G1328	G1329	G1259
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G2220	C2008	U1931	C1843	G1678	G1678	U1775	U1679	U1533	U1397	C1464	C1332	A1262	U1263
G2221	G2009	A1932	C1844	U1680	U1680	G1776	U1680	U1534	G1400	G1465	U1332	G1264	A1265
G2222	G2010	G1933	G1845	G1681	G1681	U1777	G1681	A1535	G1401	G1466	G1333	A1266	A1266
G2223	G2011	G1934	U1846	G1682	C1682	U1779	G1682	C1537	C1402	C1467	G1334	G1267	G1268
G2224	G2012	C1935	A1848	C1683	C1683	A1780	C1683	G1538	C1403	G1472	U1335	A1269	C1270
A2225	A2013	A1936	G1849	C1684	C1684	C1781	C1684	G1539	C1404	A1472	G1336	G1271	A1272
G2226	A1937	A1937	G1850	A1689	A1689	C1782	A1690	U1540	C1403	G1473	A1337	U1273	U1273
G2229	A1938	C1938	U1851	C1690	C1690	A1783	A1690	G1541	U1406	C1474	G1338	A1274	A1274
C2230	C1942	U1943	C1852	C1694	C1694	A1784	C1694	A1542	U1407	C1475	G1339	A1275	A1275
C2231	U1944	U1944	G1856	G1695	G1695	A1785	G1695	C1543	A1477	C1476	U1340	G1346	G1276
U2232	U1945	U1945	G1857	G1696	G1696	A1786	G1696	C1544	A1478	A1477	U1341	G1347	G1277
U2233	A2020	G1946	C1788	G1697	G1697	A1787	G1697	A1545	C1408	G1479	U1342	G1348	A1278
G2234	C2021	U1946	A1789	G1698	G1698	C1790	G1698	C1546	C1409	G1479	G1344	A1349	G1279
G2235	C1947	G1699	C1625	G1699	G1699	A1791	G1699	A1553	U1415	U1481	G1345	G1347	G1277
C2236	G1948	G1948	G1662	G1710	G1710	C1791	G1710	A1554	U1416	G1482	G1346	G1347	G1277
G2237	G1949	G1949	G1865	C1711	C1711	U1794	C1711	A1555	G1484	G1484	G1347	G1348	A1278
G2238	U1951	U1951	C1866	G1712	G1712	G1796	G1712	C1556	G1485	A1486	A1349	A1349	G1279
G2239	G2027	G2027	A1876	A1632	A1632	U1796	A1632	A1557	U1420	G1487	C1350	C1350	G1279

- Molecule 36: 23S RIBOSOMAL RNA



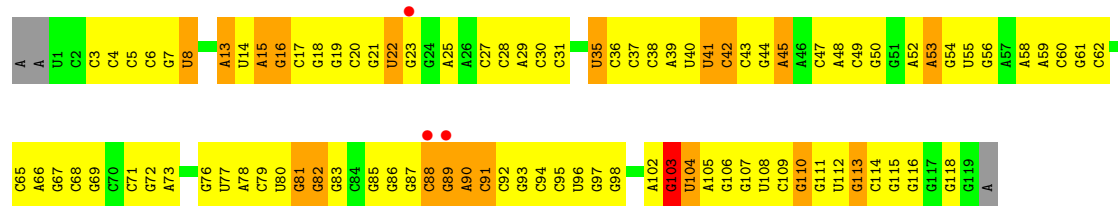
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U448	A449	A454	C455	G458	U459	A460	C461	C462	G463	U464	G465	A466	G467	G468	C469	A470	A471	A472	G473	G474	U475	A478	A479	A480	G481	A482	A483	C484	G485	C486	C487	G491	A492	G493	G498	U499	G500	A501	A502	U503	A504	A505	G506	A507	G508	C509	G512	A513	A514	A515	C516	G518																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
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U303	G304	G307	G308	G309	A310	A311	G312	C313	G317	C318	C319	A320	G321	A322	A323	C324	G325	G326	U327	U328	G329	A330	A331	G332	G333	C336	G337	G338	U339	G340	G341	G342	C343	G344	A345	A346	A347	G348	G349	U350	G351	G352	G353	U358	A359	G360	G361	G362	G363	G364	G365	G366	G367	G368	U369																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G271D	U271E	C271F	G271G	G271H	G271I	C271J	U271K	U271L	U271M	U271N	C271O	G271R	C271S	C271T	G271U	G271V	G271W	G271X	U271Y	C271Z	G272	U272A	G272B	G272C	G272D	C272E	C272F	G272G	U272H	U272I	C272J	G272K	G272L	G272M	G272N	G272O	G272P	G272Q	G272R	G272S	G272T	G272U	G272V	G272W	G272X	G272Y	G272Z	C273	C273H	U273I	U273J	G273K	G273L	G273M	G273N	G273O	G273P	G273Q	G273R	G273S	G273T	G273U	G273V	G273W	G273X	G273Y	G273Z	C274	G274A	G274B	G274C	G274D	G274E	G274F	G274G	G274H	G274I	G274J	G274K	G274L	G274M	G274N	G274O	G274P	G274Q	G274R	G274S	G274T	G274U	G274V	G274W	G274X	G274Y	G274Z	C275	G275A	G275B	G275C	G275D	G275E	G275F	G275G	G275H	G275I	G275J	G275K	G275L	G275M	G275N	G275O	G275P	G275Q	G275R	G275S	G275T	G275U	G275V	G275W	G275X	G275Y	G275Z	C276	C276A	C276B	C276C	C276D	C276E	C276F	C276G	C276H	C276I	C276J	C276K	C276L	C276M	C276N	C276O	C276P	C276Q	C276R	C276S	C276T	C276U	C276V	C276W	C276X	C276Y	C276Z	C277	C277A	C277B	C277C	C277D	C277E	C277F	C277G	C277H	C277I	C277J	C277K	C277L	C277M	C277N	C277O	C277P	C277Q	C277R	C277S	C277T	C277U	C277V	C277W	C277X	C277Y	C277Z	C278	C278A	C278B	C278C	C278D	C278E	C278F	C278G	C278H	C278I	C278J	C278K	C278L	C278M	C278N	C278O	C278P	C278Q	C278R	C278S	C278T	C278U	C278V	C278W	C278X	C278Y	C278Z	C279	C279A	C279B	C279C	C279D	C279E	C279F	C279G	C279H	C279I	C279J	C279K	C279L	C279M	C279N	C279O	C279P	C279Q	C279R	C279S	C279T	C279U	C279V	C279W	C279X	C279Y	C279Z	C280	C280A	C280B	C280C	C280D	C280E	C280F	C280G	C280H	C280I	C280J	C280K	C280L	C280M	C280N	C280O	C280P	C280Q	C280R	C280S	C280T	C280U	C280V	C280W	C280X	C280Y	C280Z	C281	C281A	C281B	C281C	C281D	C281E	C281F	C281G	C281H	C281I	C281J	C281K	C281L	C281M	C281N	C281O	C281P	C281Q	C281R	C281S	C281T	C281U	C281V	C281W	C281X	C281Y	C281Z	C282	C282A	C282B	C282C	C282D	C282E	C282F	C282G	C282H	C282I	C282J	C282K	C282L	C282M	C282N	C282O	C282P	C282Q	C282R	C282S	C282T	C282U	C282V	C282W	C282X	C282Y	C282Z	C283	C283A	C283B	C283C	C283D	C283E	C283F	C283G	C283H	C283I	C283J	C283K	C283L	C283M	C283N	C283O	C283P	C283Q	C283R	C283S	C283T	C283U	C283V	C283W	C283X	C283Y	C283Z	C284	C284A	C284B	C284C	C284D	C284E	C284F	C284G	C284H	C284I	C284J	C284K	C284L	C284M	C284N	C284O	C284P	C284Q	C284R	C284S	C284T	C284U	C284V	C284W	C284X	C284Y	C284Z	C285	C285A	C285B	C285C	C285D	C285E	C285F	C285G	C285H	C285I	C285J	C285K	C285L	C285M	C285N	C285O	C285P	C285Q	C285R	C285S	C285T	C285U	C285V	C285W	C285X	C285Y	C285Z	C286	C286A	C286B	C286C	C286D	C286E	C286F	C286G	C286H	C286I	C286J	C286K	C286L	C286M	C286N	C286O	C286P	C286Q	C286R	C286S	C286T	C286U	C286V	C286W	C286X	C286Y	C286Z	C287	C287A	C287B	C287C	C287D	C287E	C287F	C287G	C287H	C287I	C287J	C287K	C287L	C287M	C287N	C287O	C287P	C287Q	C287R	C287S	C287T	C287U	C287V	C287W	C287X	C287Y	C287Z	C288	C288A	C288B	C288C	C288D	C288E	C288F	C288G	C288H	C288I	C288J	C288K	C288L	C288M	C288N	C288O	C288P	C288Q	C288R	C288S	C288T	C288U	C288V	C288W	C288X	C288Y	C288Z	C289	C289A	C289B	C289C	C289D	C289E	C289F	C289G	C289H	C289I	C289J	C289K	C289L	C289M	C289N	C289O	C289P	C289Q	C289R	C289S	C289T	C289U	C289V	C289W	C289X	C289Y	C289Z	C290	C290A	C290B	C290C	C290D	C290E	C290F	C290G	C290H	C290I	C290J	C290K	C290L	C290M	C290N	C290O	C290P	C290Q	C290R	C290S	C290T	C290U	C290V	C290W	C290X	C290Y	C290Z	C291	C291A	C291B	C291C	C291D	C291E	C291F	C291G	C291H	C291I	C291J	C291K	C291L	C291M	C291N	C291O	C291P	C291Q	C291R	C291S	C291T	C291U	C291V	C291W	C291X	C291Y	C291Z	C292	C292A	C292B	C292C	C292D	C292E	C292F	C292G	C292H	C292I	C292J	C292K	C292L	C292M	C292N	C292O	C292P	C292Q	C292R	C292S	C292T	C292U	C292V	C292W	C292X	C292Y	C292Z	C293	C293A	C293B	C293C	C293D	C293E	C293F	C293G	C293H	C293I	C293J	C293K	C293L	C293M	C293N	C293O	C293P	C293Q	C293R	C293S	C293T	C293U	C293V	C293W	C293X	C293Y	C293Z	C294	C294A	C294B	C294C	C294D	C294E	C294F	C294G	C294H	C294I	C294J	C294K	C294L	C294M	C294N	C294O	C294P	C294Q	C294R	C294S	C294T	C294U	C294V	C294W	C294X	C294Y	C294Z	C295	C295A	C295B	C295C	C295D	C295E	C295F	C295G	C295H	C295I	C295J	C295K	C295L	C295M	C295N	C295O	C295P	C295Q	C295R	C295S	C295T	C295U	C295V	C295W	C295X	C295Y	C295Z	C296	C296A	C296B	C296C	C296D	C296E	C296F	C296G	C296H	C296I	C296J	C296K	C296L	C296M	C296N	C296O	C296P	C296Q	C296R	C296S	C296T	C296U	C296V	C296W	C296X	C296Y	C296Z	C297	C297A	C297B	C297C	C297D	C297E	C297F	C297G	C297H	C297I	C297J	C297K	C297L	C297M	C297N	C297O	C297P	C297Q	C297R	C297S	C297T	C297U	C297V	C297W	C297X	C297Y	C297Z	C298	C298A	C298B	C298C	C298D	C298E	C298F	C298G	C298H	C298I	C298J	C298K	C298L	C298M	C298N	C298O	C298P	C298Q	C298R	C298S	C298T	C298U	C298V	C298W	C298X	C298Y	C298Z	C299	C299A	C299B	C299C	C299D	C299E	C299F	C299G	C299H	C299I	C299J	C299K	C299L	C299M	C299N	C299O	C299P	C299Q	C299R	C299S	C299T	C299U	C299V	C299W	C299X	C299Y	C299Z	C300	C300A	C300B	C300C	C300D	C300E	C300F	C300G	C300H	C300I	C300J	C300K	C300L	C300M	C300N	C300O	C300P	C30

G2004	G1930	C1843	U1777	U1680	A1608	A1535	G1466	G1400	A1331	G1266	G1206	U1081
C2007	U1931	C1844	U1778	G1681	A1609	C1536	C1467	G1401	G1332	U1267	C1207	U1082
C2008	A1932	G1845	U1779	G1682	A1610	G1537	A1472	C1402	C1333	A1268	G1208	U1083
G2009	G1933	G1846	A1780	C1683	C1611	G1538	G1473	C1403	G1334	A1269	G1209	A1086
G2010	A1934	A1847	C1781	C1684	A1614	U1540	C1474	C1404	U1335	C1270	A1210	A1087
G2011	G1935	A1848	C1782	A1689	C1615	G1541	G1475	U1405	A1336	A1271	A1211	A1088
G2012	A1936	G1849	A1783	A1690	C1616	G1542	G1476	C1407	G1337	A1272	G1212	A1089
A2013	A1938	G1850	A1784	A1691	C1617	C1543	A1477	C1408	G1338	U1273	A1213	A1090
A2014	C1942	C1852	A1785	C1694	C1618	A1544	G1478	C1409	G1339	A1274	G1214	U1091
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A2016	A1944	G1857	A1787	G1697	G1620	C1546	G1480	C1411	U1341	A1276	G1216	G1093
A2017	G1945	G1858	A1789	A1698	G1621	C1549	G1481	U1415	G1344	G1277	G1217	A1094
A2018	U1946	G1859	C1790	A1699	G1622	C1549	G1482	U1416	C1345	A1278	C1218	A1095
A2019	A1947	A1859	A1791	G1699	C1625	A1553	G1483	U1417	G1346	G1279	G1219	A1096
C2021	U1794	G1862	U1709	U1709	U1629	A1554	G1484	U1418	G1347	G1280	A1220	A1097
C2022	G1948	G1865	C1710	C1710	U1630	A1555	A1486	C1417	G1348	C1221	G1157	U1098
C2023	G1950	C1866	C1711	C1711	U1631	C1556	G1487	U1420	A1349	G1222	G1159	A1098
C2026	U1951	A1867	C1712	C1712	A1632	C1557	U1488	G1421	C1350	A1287	G1223	C1100
G2027	A1952	G1868	C1713	G1713	G1633	A1558	U1489	G1422	C1351	U1288	G1224	U1101
U2028	G1953	A1868	G1714	G1714	A1634	A1559	G1490	G1423	U1352	C1289	G1227	C1102
G2029	G1954	G1878	G1717	G1717	G1635	G1560	G1492	G1424	A1353	C1290	G1228	A1103
A2030	U1955	C1882	G1718	G1718	G1636	C1565	C1493	A1427	G1354	C1291	G1229	C1104
A2031	A1956	G1883	G1719	A1802	A1637	A1566	A1494	C1428	G1358	U1292	G1230	G1105
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G2035	A1960	C1887	U1723	C1640	A1569	U1578	U1497	C1432	C1362	G1296	U1234	G1110
G2036	U1963	G1888	G1740	C1644	G1573	C1579	U1503	U1433	C1363	C1297	G1235	G1111
G2037	G1964	A1889	A1741	C1647	C1574	C1576	C1504	A1434	G1364	C1298	G1236	G1112
G2038	C1967	G1890	C1744	C1648	C1575	U1576	C1506	G1435	A1365	U1299	A1237	U1113
C2039	A1968	G1891	C1745	G1649	U1577	C1577	C1506	G1436	A1366	G1239	G1238	G1114
C2040	G1969	G1892	C1746	G1650	U1578	C1578	C1509	C1437	A1367	A1301	G1239	G1115
A2041	A1970	A1815	G1747A	G1651	G1581	A1579	A1509A	U1438	G1368	A1302	G1240	C1116
C2042	A1971	G1816	G1748	G1652	A1582	A1579	A1509B	A1439	G1369	G1306	A1241	G1117
C2043	A1972	G1817	C1754	G1653	C1582	C1582	G1510	G1440	G1374	C1307	A1242	G1118
C2044	G1973	G1818	A1755	A1684	A1583	C1583	G1511	G1441	C1375	A1308	G1243	C1119
G2046	A1977	G1819	G1756	A1685	C1584	C1584	U1512	G1442	C1376	G1309	G1244	C1120
G2049	G1984	U1820	U1757	C1656	A1586	A1586	C1513	A1445	G1377	G1310	G1245	C1121
C2050	G1985	G1822	G1758	C1657	A1587	A1587	U1514	C1445A	G1378	G1311	A1246	C1122
G2051	A1986	G1823	A1759	C1658	C1588	C1588	G1515	C1446	A1379	G1312	G1247	C1123
G2052	G1989	U1911	G1760	U1659	C1589	C1589	G1516	G1447	G1380	U1313	U1248	C1124
A2053	G1990	G1824	G1761	C1660	U1590	U1590	G1517	G1448	G1381	C1314	G1250	G1125
A2054	C1991	G1825	G1762	G1661	G1591	G1591	U1518	A1449	G1382	C1251	G1251	A1126
A2055	G1992	C1826	G1763	C1662	C1592	C1592	G1519	G1450	C1383	G1315	G1252	A1127
G2056	U1915	G1827	G1764	G1666	G1593	G1593	U1520	A1384	A1391	U1316	A1253	G1190
A2057	A1916	G1828	G1765	G1667	G1594	G1594	G1523	C1451	G1385	A1317	A1254	G1191
A2060	U1917	A1829	C1767	A1668	A1596	A1596	G1526	C1452	C1386	G1319	U1255	G1192
A2061	A1918	A1830	U1768	A1669	C1597	C1597	G1527	U1453	G1387	C1320	G1257	G1193
A2062	G1835	G1836	G1769	C1670	C1598	C1598	A1528A	G1455	G1388	A1322	C1258	C1196
A2063	C1837	G1838	G1770	G1671	C1599	C1599	U1528	G1459	U1390	G1325	C1259	G1197
A2064	G1839	G1839	G1771	G1672	C1600	C1600	A1528A	G1461	U1391	G1326	G1260	U1198
A2065	A1773	A1773	A1772	A1676	G1601	G1601	C1531	C1462	A1395	C1327	C1261	U1199
A2066	G1774	G1774	U1775	A1677	C1605	C1605	C1532	C1463	U1396	G1328	U1263	G1136
A2067	U1776	U1776	G1776	G1678	G1606	G1606	U1534	C1464	U1397	G1329	U1264	G1137
G2069	G1842	G1842	G1776	U1679	C1607	C1607	U1534	G1465	G1398	C1330	A1285	G1138
												G1139
												C1140
												U1141
												A1204
												A1142A

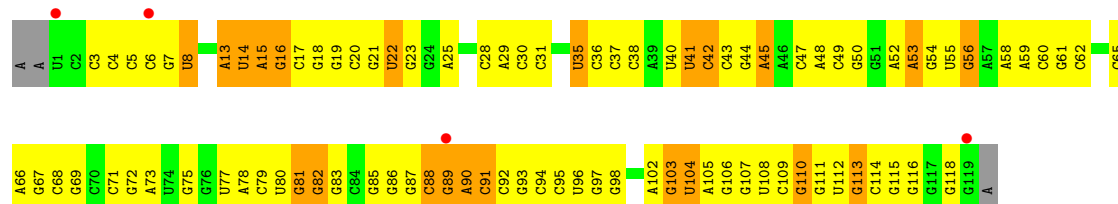


• Molecule 37: 5S RIBOSOMAL RNA

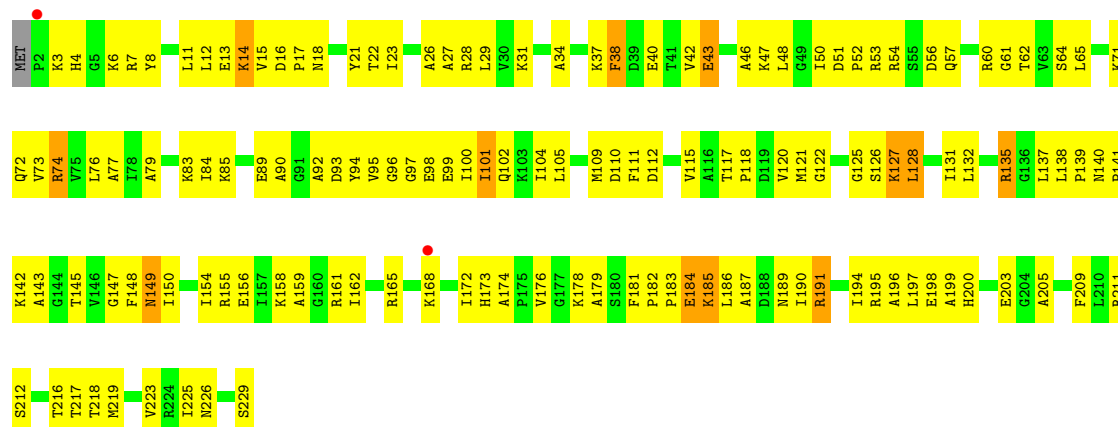




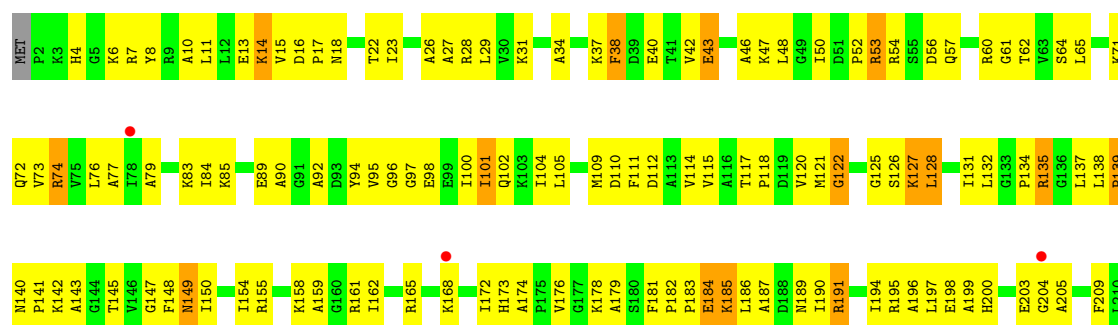
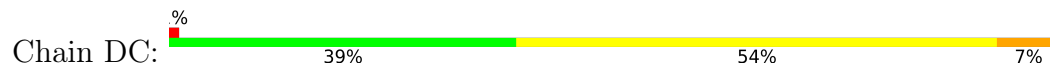
• Molecule 37: 5S RIBOSOMAL RNA



• Molecule 38: 50S RIBOSOMAL PROTEIN L1



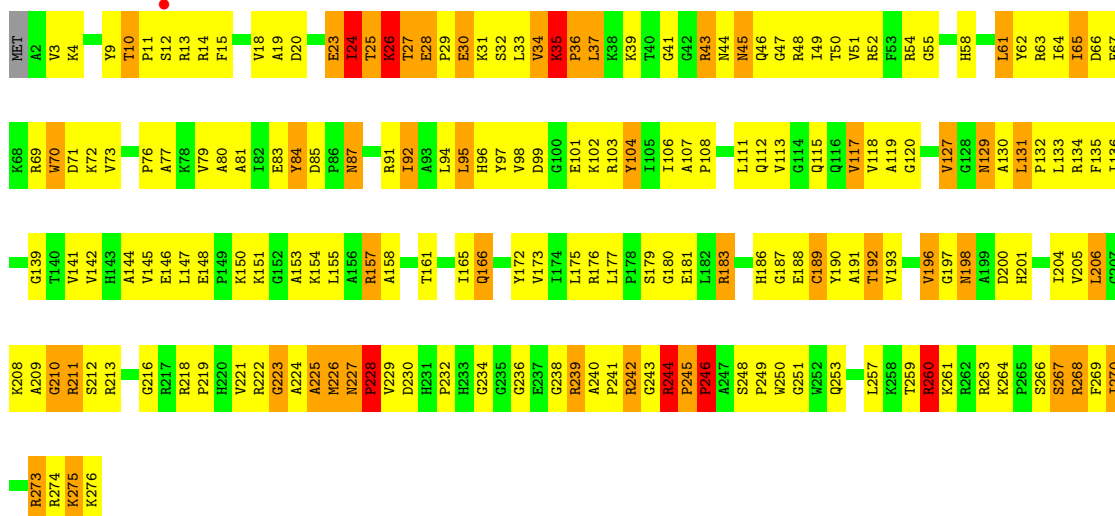
• Molecule 38: 50S RIBOSOMAL PROTEIN L1





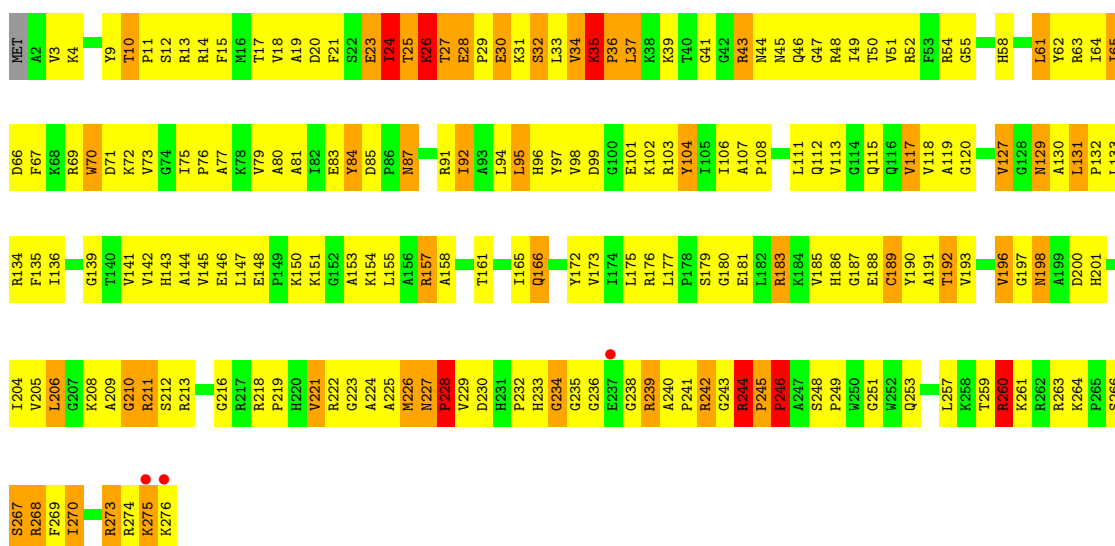
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

Chain BD: 31% 50% 16%



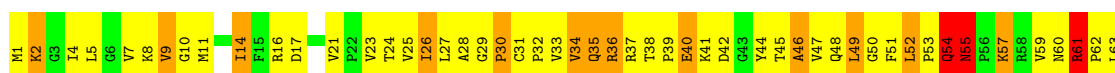
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

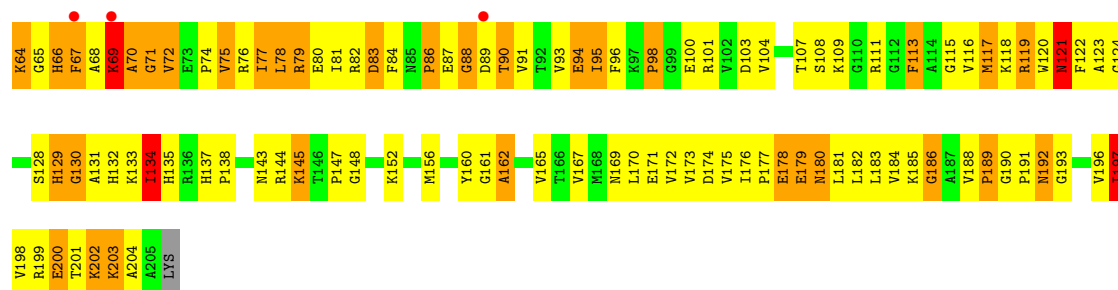
Chain DD: 29% 52% 16%



• Molecule 40: 50S RIBOSOMAL PROTEIN L3

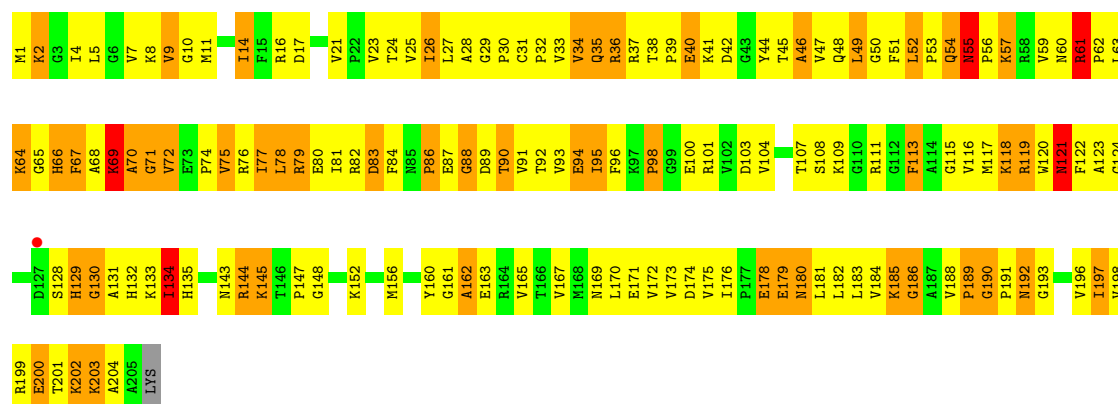
Chain BE: 24% 50% 22%





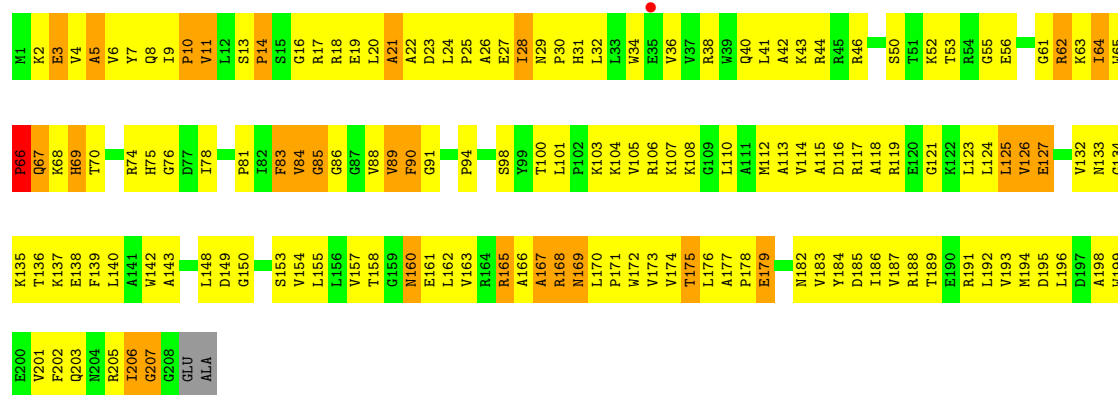
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain DE: 24% 49% 24%



• Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain BF: 27% 58% 13%

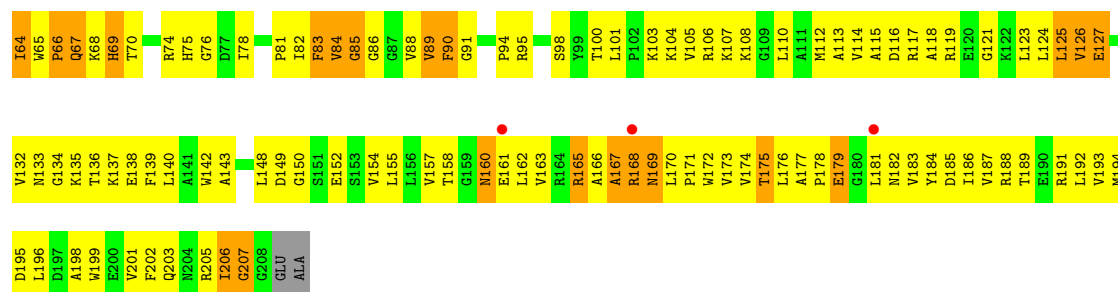


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

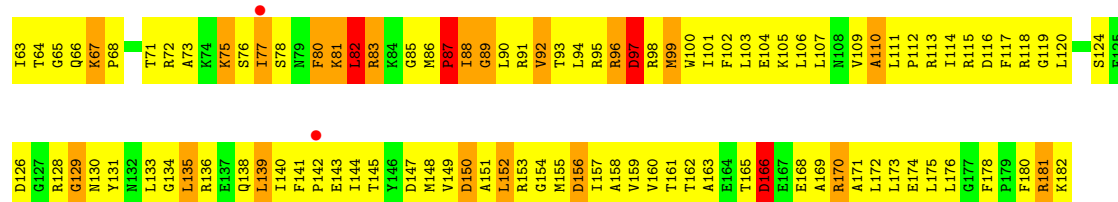
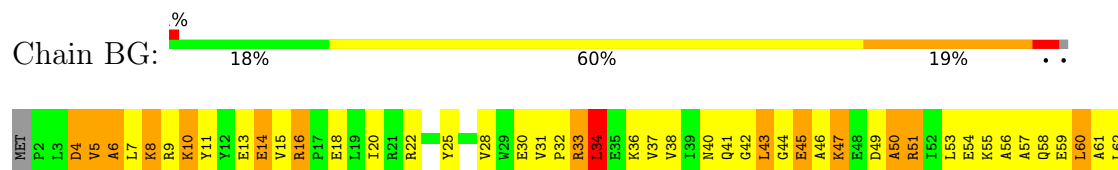
Chain DF: 2% 25% 60% 13%



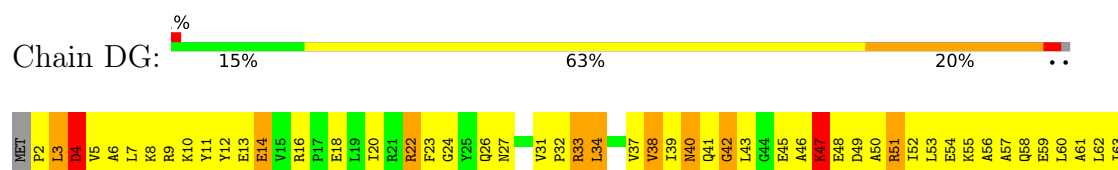




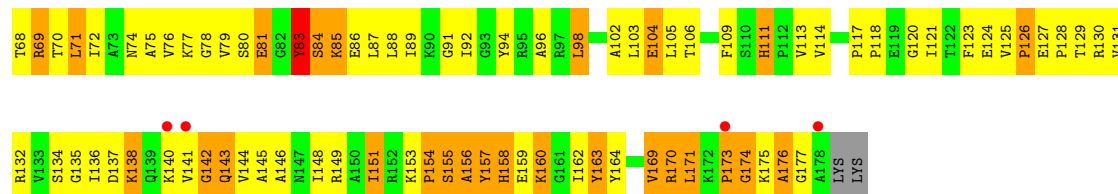
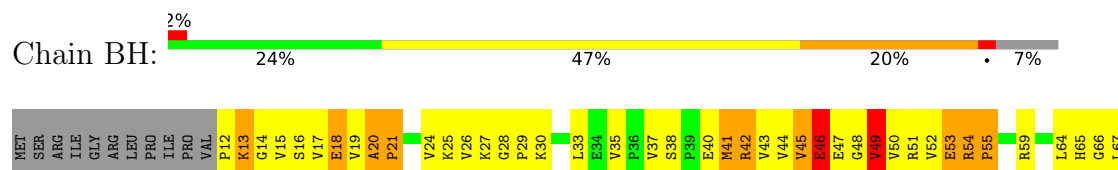
### • Molecule 42: 50S RIBOSOMAL PROTEIN L5



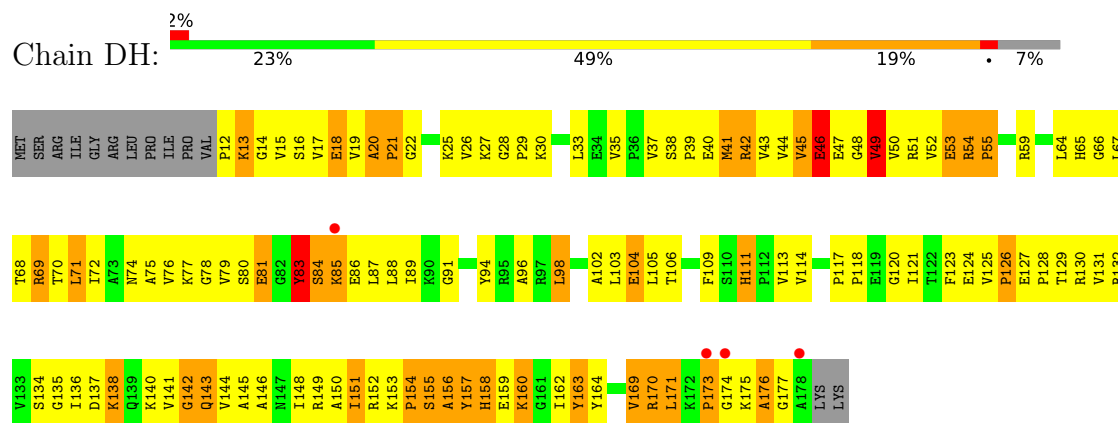
### • Molecule 42: 50S RIBOSOMAL PROTEIN L5



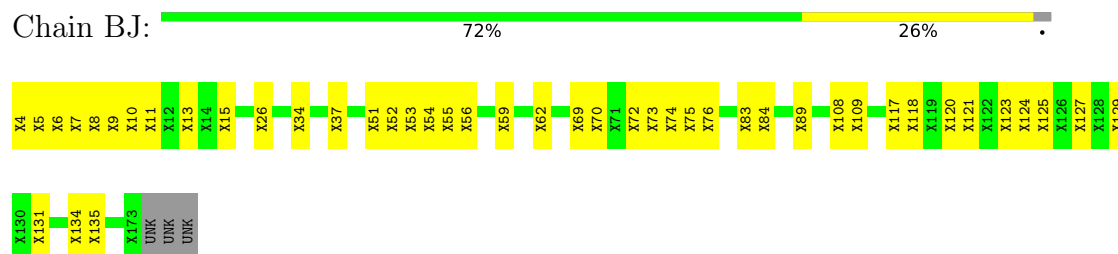
### • Molecule 43: 50S RIBOSOMAL PROTEIN L6



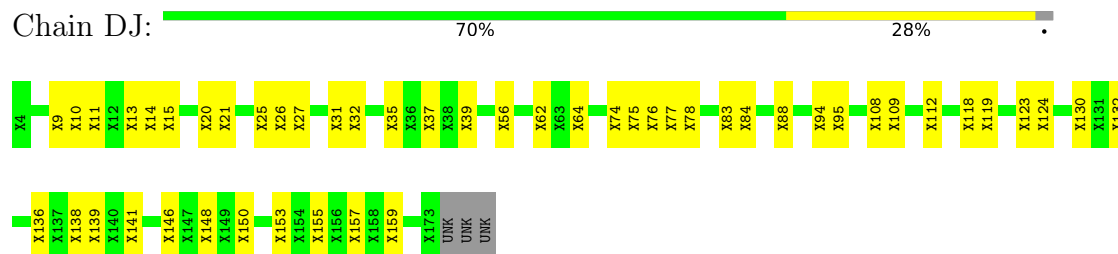
## • Molecule 43: 50S RIBOSOMAL PROTEIN L6



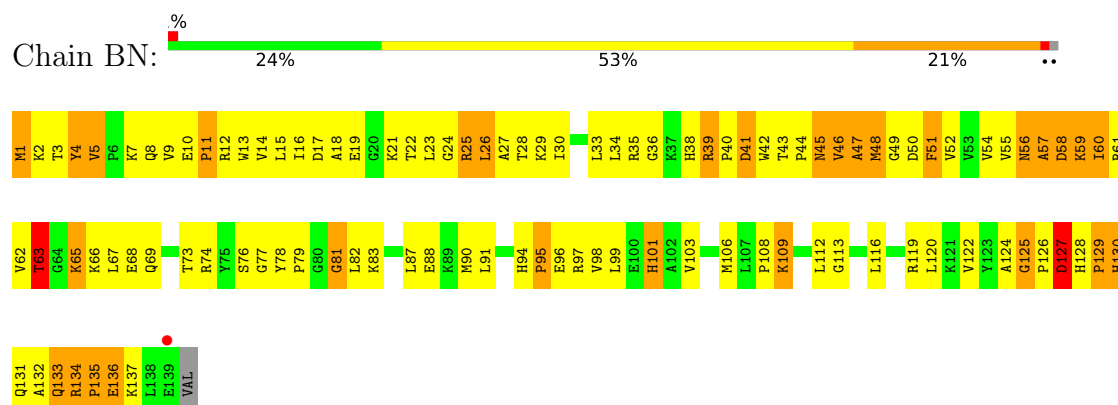
## • Molecule 44: 50S RIBOSOMAL PROTEIN L10



## • Molecule 44: 50S RIBOSOMAL PROTEIN L10

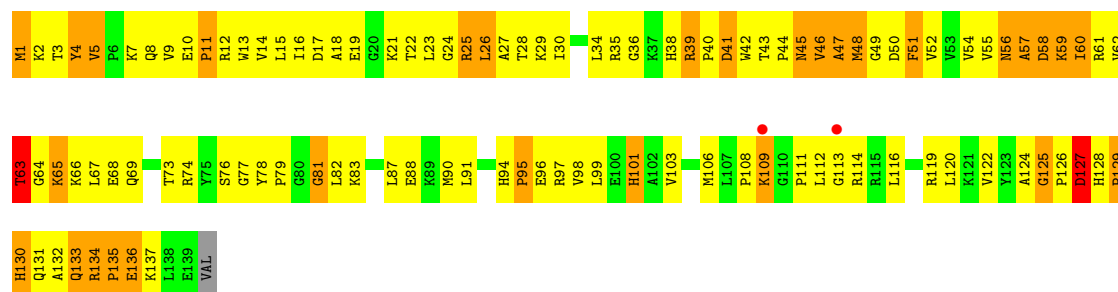


## • Molecule 45: 50S RIBOSOMAL PROTEIN L13



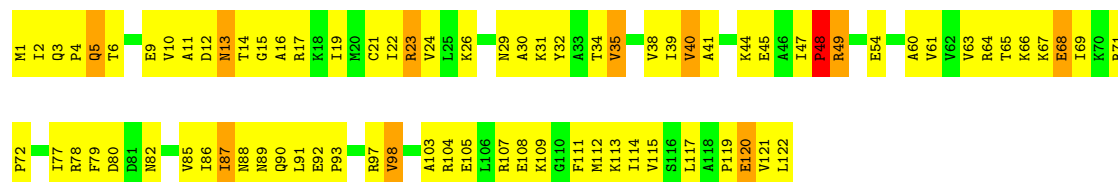
## • Molecule 45: 50S RIBOSOMAL PROTEIN L13





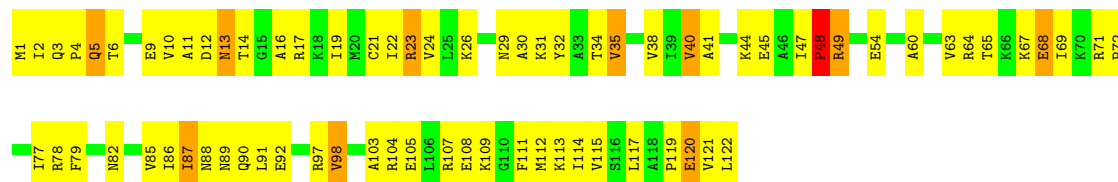
• Molecule 46: 50S RIBOSOMAL PROTEIN L14

Chain BO: 34% 57% 8%



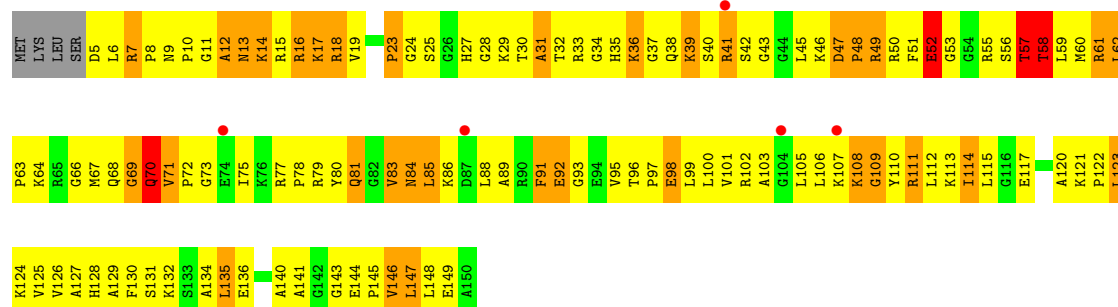
• Molecule 46: 50S RIBOSOMAL PROTEIN L14

Chain DO: 39% 52% 8%



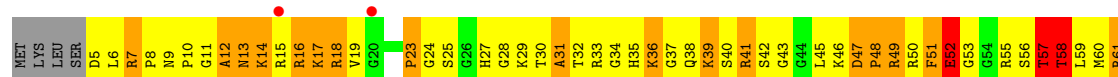
• Molecule 47: 50S RIBOSOMAL PROTEIN L15

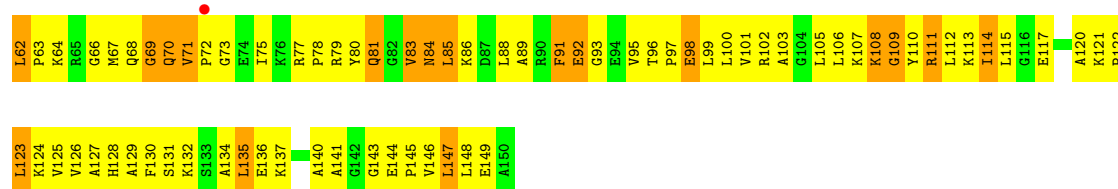
Chain BP: 3% 15% 57% 23%



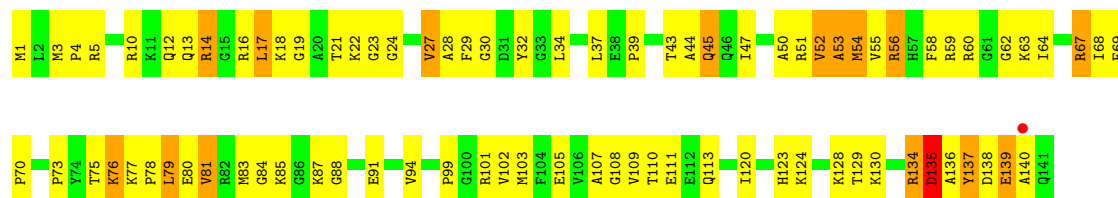
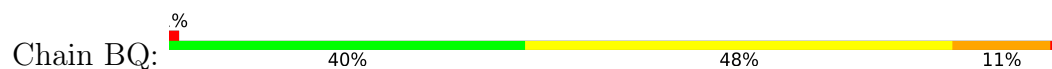
• Molecule 47: 50S RIBOSOMAL PROTEIN L15

Chain DP: 2% 15% 57% 23%

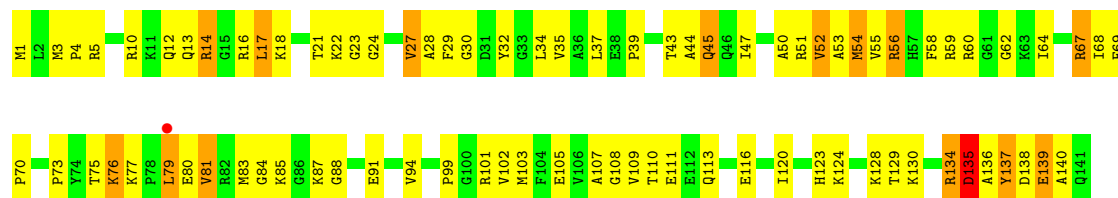
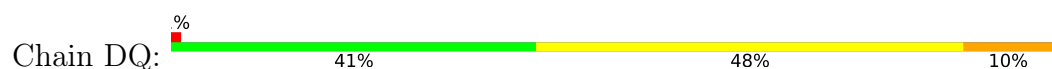




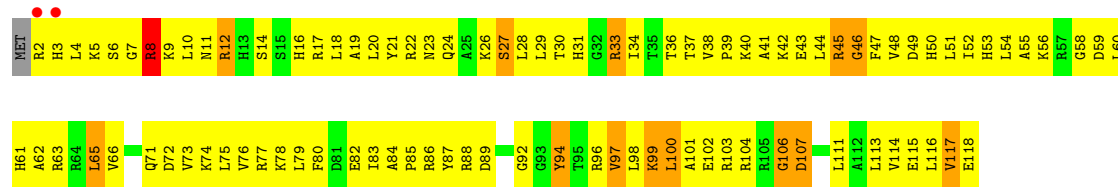
• Molecule 48: 50S RIBOSOMAL PROTEIN L16



• Molecule 48: 50S RIBOSOMAL PROTEIN L16



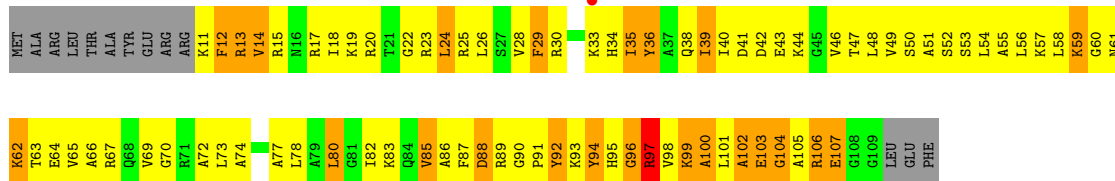
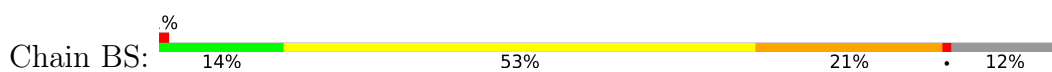
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



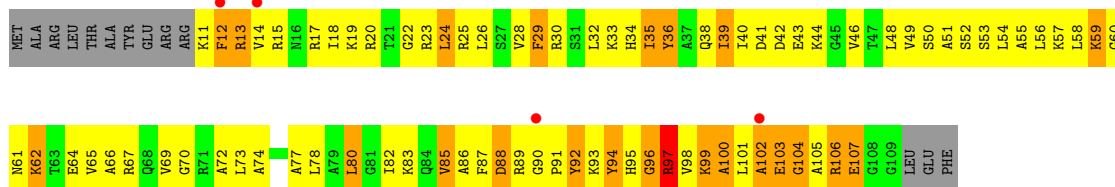
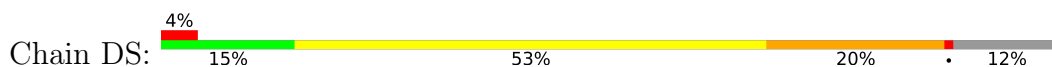
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



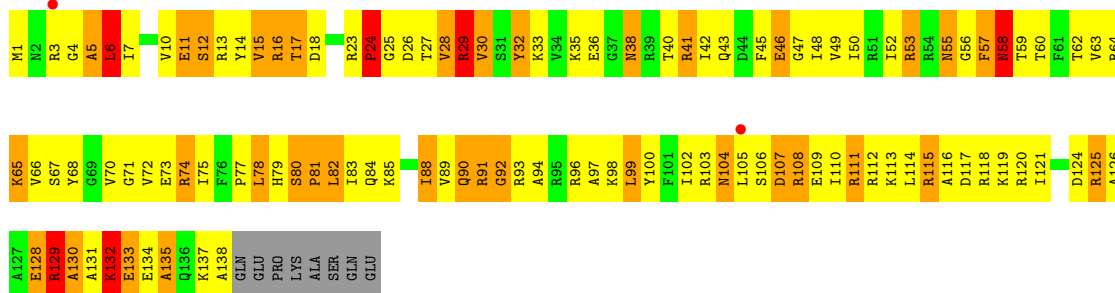
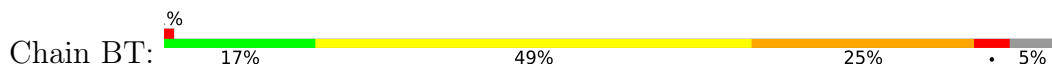
• Molecule 50: 50S RIBOSOMAL PROTEIN L18



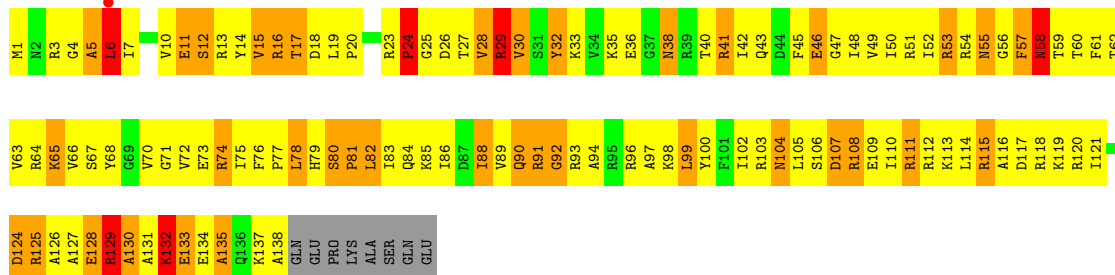
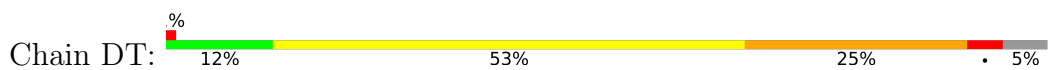
• Molecule 50: 50S RIBOSOMAL PROTEIN L18



• Molecule 51: 50S RIBOSOMAL PROTEIN L19

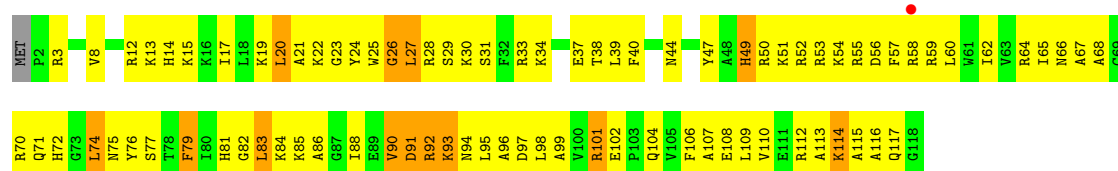


• Molecule 51: 50S RIBOSOMAL PROTEIN L19

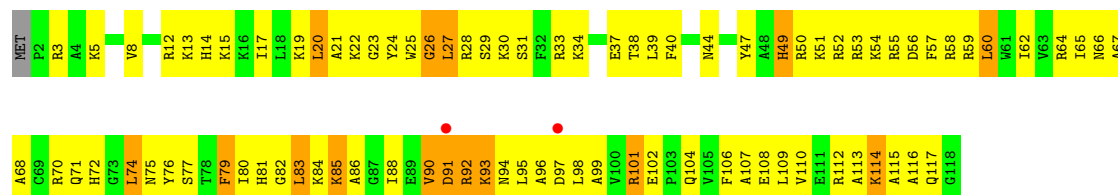


• Molecule 52: 50S RIBOSOMAL PROTEIN L20

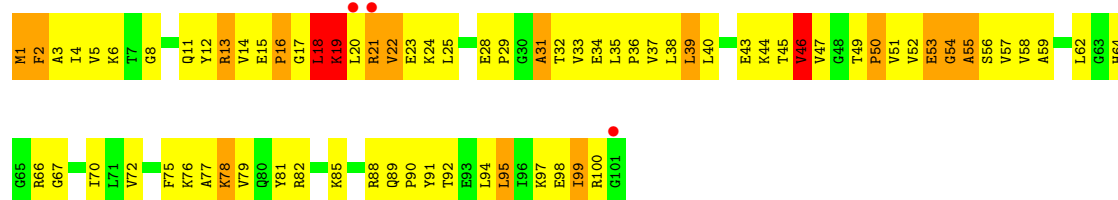




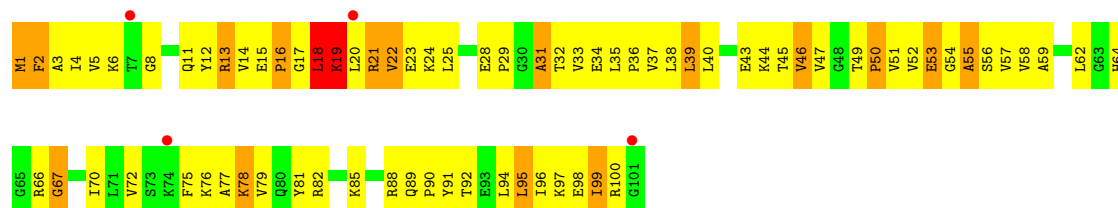
• Molecule 52: 50S RIBOSOMAL PROTEIN L20



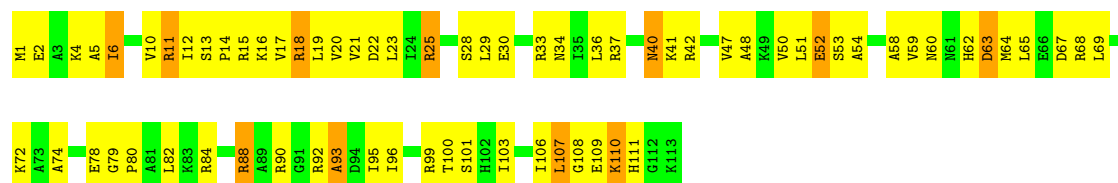
• Molecule 53: 50S RIBOSOMAL PROTEIN L21



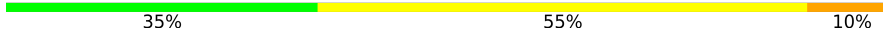
• Molecule 53: 50S RIBOSOMAL PROTEIN L21

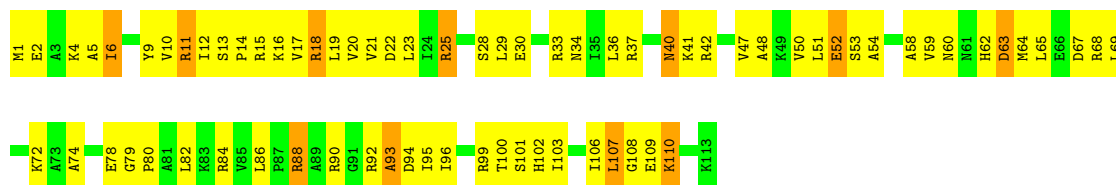


• Molecule 54: 50S RIBOSOMAL PROTEIN L22




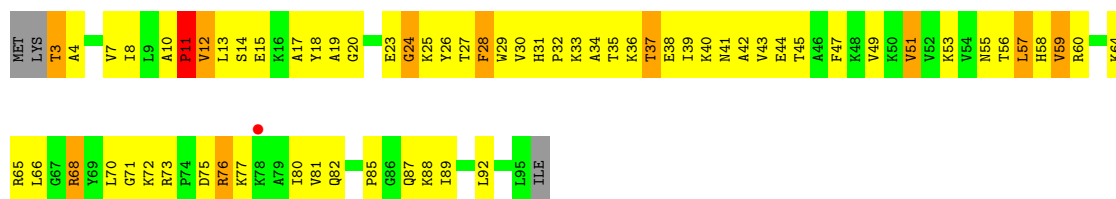
• Molecule 54: 50S RIBOSOMAL PROTEIN L22

Chain DW:  35% 55% 10%



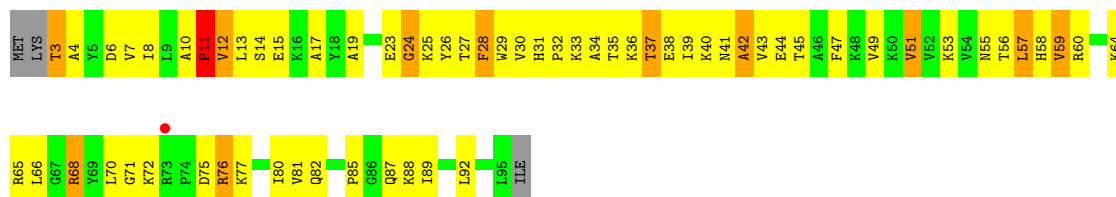
• Molecule 55: 50S RIBOSOMAL PROTEIN L23

Chain BX:  28% 57% 10%




• Molecule 55: 50S RIBOSOMAL PROTEIN L23

Chain DX:  30% 54% 11%




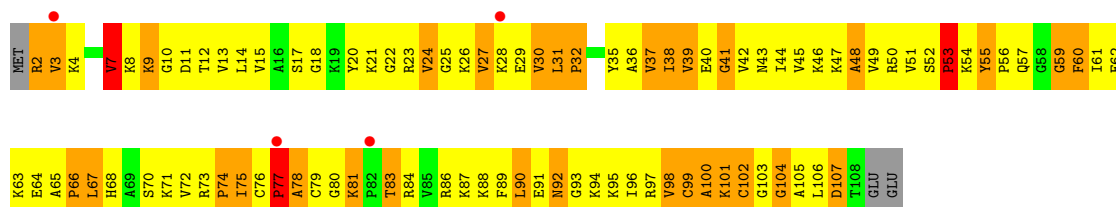
• Molecule 56: 50S RIBOSOMAL PROTEIN L24

Chain BY:  3% 11% 55% 29%

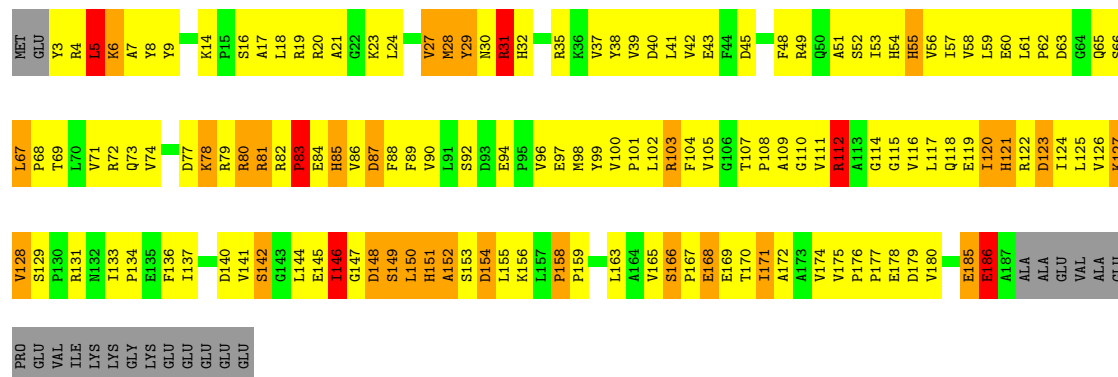


• Molecule 56: 50S RIBOSOMAL PROTEIN L24

Chain DY:  4% 10% 55% 29%



## ● Molecule 57: 50S RIBOSOMAL PROTEIN L25

Chain BZ:  20% 53% 14% 10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.214 , 0.249 0.215 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 98.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.54	0/36190	0.74	23/56486 (0.0%)
1	CA	0.51	0/36190	0.74	16/56486 (0.0%)
2	AB	0.44	0/1936	0.67	0/2611
2	CB	0.41	0/1936	0.68	0/2611
3	AC	0.48	0/1637	0.64	0/2207
3	CC	0.43	0/1637	0.64	0/2207
4	AD	0.39	0/1733	0.65	0/2318
4	CD	0.39	0/1733	0.65	0/2318
5	AE	0.49	0/1163	0.68	0/1566
5	CE	0.50	0/1163	0.68	0/1566
6	AF	0.40	0/856	0.63	0/1154
6	CF	0.38	0/856	0.64	0/1154
7	AG	0.40	0/1276	0.60	0/1709
7	CG	0.38	0/1276	0.61	0/1709
8	AH	0.45	0/1136	0.71	0/1527
8	CH	0.43	0/1136	0.70	0/1527
9	AI	0.42	0/1027	0.67	0/1373
9	CI	0.40	0/1027	0.66	0/1373
10	AJ	0.45	0/808	0.69	0/1087
10	CJ	0.42	0/808	0.69	0/1087
11	AK	0.45	0/900	0.70	0/1213
11	CK	0.41	0/900	0.69	0/1213
12	AL	0.47	0/987	0.71	0/1322
12	CL	0.45	0/987	0.70	0/1322
13	AM	0.39	0/999	0.67	0/1338
13	CM	0.38	0/999	0.67	0/1338
14	AN	0.47	0/501	0.67	0/664
14	CN	0.45	0/501	0.67	0/664
15	AO	0.40	0/745	0.62	0/992
15	CO	0.39	0/745	0.62	0/992
16	AP	0.39	0/717	0.63	0/965
16	CP	0.40	0/717	0.62	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.47	0/837	0.66	0/1119
17	CQ	0.44	0/837	0.66	0/1119
18	AR	0.45	0/579	0.67	0/768
18	CR	0.46	0/579	0.68	0/768
19	AS	0.43	0/643	0.68	1/867 (0.1%)
19	CS	0.41	0/643	0.68	1/867 (0.1%)
20	AT	0.38	0/765	0.64	0/1007
20	CT	0.36	0/765	0.65	0/1007
21	AU	0.47	0/213	0.61	0/279
21	CU	0.46	0/213	0.62	0/279
22	AV	0.52	0/1809	0.70	0/2819
22	CV	0.46	0/1809	0.69	0/2819
23	AW	0.36	0/1810	0.70	0/2821
23	CW	0.95	2/1810 (0.1%)	0.68	0/2821
24	AX	0.38	0/288	0.72	0/446
24	CX	0.69	1/288 (0.3%)	0.85	1/446 (0.2%)
25	AY	0.47	0/5313	0.69	0/7195
25	CY	0.45	0/5313	0.68	0/7195
26	B0	0.40	0/671	0.66	0/892
26	D0	0.40	0/671	0.66	0/892
27	B1	0.42	0/739	0.71	0/983
27	D1	0.41	0/739	0.67	0/983
28	B2	0.32	0/600	0.64	0/793
28	D2	0.33	0/600	0.61	0/793
29	B3	0.40	0/473	0.59	0/636
29	D3	0.40	0/473	0.60	0/636
30	B4	0.47	0/461	0.83	1/623 (0.2%)
30	D4	0.48	0/461	0.83	1/623 (0.2%)
31	B5	0.37	0/473	0.69	0/639
31	D5	0.39	0/473	0.69	0/639
32	B6	0.62	0/440	0.94	2/586 (0.3%)
32	D6	0.56	0/440	0.93	2/586 (0.3%)
33	B7	0.43	0/427	0.68	0/563
33	D7	0.44	0/427	0.67	0/563
34	B8	0.54	0/516	0.83	0/681
34	D8	0.51	0/516	0.82	0/681
35	B9	0.42	0/310	0.65	0/407
35	D9	0.43	0/310	0.66	0/407
36	BA	0.50	3/69972 (0.0%)	0.74	35/109237 (0.0%)
36	DA	0.49	3/69972 (0.0%)	0.73	36/109237 (0.0%)
37	BB	0.41	0/2853	0.72	1/4451 (0.0%)
37	DB	0.41	0/2853	0.72	1/4451 (0.0%)
38	BC	0.55	1/1774 (0.1%)	0.61	0/2391

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DC	0.41	0/1774	0.60	0/2391
39	BD	0.47	0/2195	0.77	1/2955 (0.0%)
39	DD	0.46	0/2195	0.76	1/2955 (0.0%)
40	BE	0.44	0/1597	0.70	0/2155
40	DE	0.44	0/1597	0.70	0/2155
41	BF	0.37	0/1659	0.62	0/2246
41	DF	0.36	0/1659	0.62	0/2246
42	BG	0.41	0/1498	0.74	1/2013 (0.0%)
42	DG	0.38	0/1498	0.69	0/2013
43	BH	0.36	0/1293	0.67	0/1746
43	DH	0.36	0/1293	0.67	0/1746
45	BN	0.35	0/1132	0.68	0/1527
45	DN	0.35	0/1132	0.68	0/1527
46	BO	0.44	0/943	0.66	0/1269
46	DO	0.44	0/943	0.66	0/1269
47	BP	0.41	0/1131	0.87	3/1504 (0.2%)
47	DP	0.40	0/1131	0.87	3/1504 (0.2%)
48	BQ	0.43	0/1143	0.63	0/1527
48	DQ	0.43	0/1143	0.63	0/1527
49	BR	0.37	0/974	0.66	0/1302
49	DR	0.36	0/974	0.66	0/1302
50	BS	0.39	0/779	0.68	0/1038
50	DS	0.37	0/779	0.67	0/1038
51	BT	0.45	0/1156	0.77	1/1544 (0.1%)
51	DT	0.45	0/1156	0.77	1/1544 (0.1%)
52	BU	0.39	0/975	0.64	0/1297
52	DU	0.40	0/975	0.64	0/1297
53	BV	0.36	0/790	0.67	0/1057
53	DV	0.35	0/790	0.68	0/1057
54	BW	0.36	0/907	0.62	0/1216
54	DW	0.35	0/907	0.62	0/1216
55	BX	0.40	0/740	0.65	0/995
55	DX	0.41	0/740	0.64	0/995
56	BY	0.39	0/824	0.62	0/1100
56	DY	0.39	0/824	0.62	0/1100
57	BZ	0.44	0/1500	0.67	0/2037
57	DZ	0.41	0/1500	0.70	0/2037
All	All	0.48	10/331626 (0.0%)	0.72	132/494526 (0.0%)

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 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CW	38	A	O3'-P	37.35	2.06	1.61
38	BC	54	ARG	C-N	-15.66	0.98	1.34
24	CX	19	A	O3'-P	-9.03	1.50	1.61
36	BA	272(I)	U	N1-C2	7.87	1.45	1.38
36	DA	272(I)	U	N1-C2	7.37	1.45	1.38

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BA	1992	G	C2'-C3'-O3'	10.46	132.51	109.50
36	DA	1992	G	C2'-C3'-O3'	10.39	132.37	109.50
1	AA	1498	U	C2'-C3'-O3'	9.73	130.91	109.50
1	CA	1498	U	C2'-C3'-O3'	9.60	130.62	109.50
36	BA	1799	G	C2'-C3'-O3'	9.35	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	1169	0
1	CA	32329	0	16318	1210	0
2	AB	1901	0	1951	223	0
2	CB	1901	0	1951	225	0
3	AC	1613	0	1677	185	0
3	CC	1613	0	1677	191	0
4	AD	1703	0	1763	171	0
4	CD	1703	0	1763	178	0
5	AE	1147	0	1207	115	0
5	CE	1147	0	1207	112	0
6	AF	843	0	857	76	0
6	CF	843	0	857	79	0
7	AG	1257	0	1296	89	0
7	CG	1257	0	1296	93	0
8	AH	1116	0	1177	89	0
8	CH	1116	0	1177	88	0
9	AI	1010	0	1035	139	0
9	CI	1010	0	1035	137	0
10	AJ	795	0	840	154	0
10	CJ	795	0	840	159	0
11	AK	885	0	904	56	0
11	CK	885	0	904	63	0
12	AL	971	0	1057	142	0
12	CL	971	0	1057	145	0
13	AM	988	0	1059	156	0
13	CM	988	0	1059	154	0
14	AN	492	0	529	64	0
14	CN	492	0	529	63	0
15	AO	734	0	771	69	0
15	CO	734	0	771	73	0
16	AP	701	0	720	66	0
16	CP	701	0	720	67	0
17	AQ	824	0	891	57	0
17	CQ	824	0	891	65	0
18	AR	574	0	644	79	0
18	CR	574	0	644	79	0
19	AS	630	0	652	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	630	0	652	108	0
20	AT	763	0	861	97	0
20	CT	763	0	861	94	0
21	AU	209	0	221	18	0
21	CU	209	0	221	17	0
22	AV	1619	0	822	60	0
22	CV	1619	0	822	58	0
23	AW	1641	0	839	126	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	857	0
25	CY	5215	0	5287	809	0
26	B0	662	0	688	98	0
26	D0	662	0	688	99	0
27	B1	732	0	808	126	0
27	D1	732	0	808	112	0
28	B2	598	0	653	84	0
28	D2	598	0	653	113	0
29	B3	468	0	523	59	0
29	D3	468	0	523	64	0
30	B4	451	0	449	93	0
30	D4	451	0	449	88	0
31	B5	459	0	480	101	0
31	D5	459	0	480	99	0
32	B6	433	0	461	150	0
32	D6	433	0	461	149	0
33	B7	419	0	467	38	0
33	D7	419	0	467	36	0
34	B8	508	0	576	96	0
34	D8	508	0	576	101	0
35	B9	307	0	335	30	0
35	D9	307	0	335	27	0
36	BA	62474	0	31497	2601	0
36	DA	62474	0	31497	2636	0
37	BB	2551	0	1295	132	0
37	DB	2551	0	1295	139	0
38	BC	1742	0	1797	158	0
38	DC	1742	0	1798	160	0
39	BD	2145	0	2234	304	0
39	DD	2145	0	2234	315	0
40	BE	1564	0	1629	249	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DE	1564	0	1629	244	0
41	BF	1624	0	1677	237	0
41	DF	1624	0	1677	232	0
42	BG	1474	0	1534	241	0
42	DG	1474	0	1534	261	0
43	BH	1269	0	1337	178	0
43	DH	1269	0	1337	176	0
44	BJ	851	0	194	31	0
44	DJ	851	0	195	32	0
45	BN	1105	0	1180	183	0
45	DN	1105	0	1180	184	0
46	BO	933	0	996	109	0
46	DO	933	0	996	102	0
47	BP	1114	0	1187	296	0
47	DP	1114	0	1187	297	0
48	BQ	1122	0	1179	134	0
48	DQ	1122	0	1179	123	0
49	BR	960	0	1021	150	0
49	DR	960	0	1021	152	0
50	BS	771	0	832	153	0
50	DS	771	0	832	146	0
51	BT	1142	0	1202	242	0
51	DT	1142	0	1202	241	0
52	BU	958	0	1015	133	0
52	DU	958	0	1015	139	0
53	BV	779	0	852	140	0
53	DV	779	0	852	140	0
54	BW	896	0	953	100	0
54	DW	896	0	953	99	0
55	BX	726	0	778	79	0
55	DX	726	0	778	83	0
56	BY	811	0	901	175	0
56	DY	811	0	901	179	0
57	BZ	1468	0	1492	200	0
57	DZ	1468	0	1492	219	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

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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	13	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	21259	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 41.

The worst 5 of 21259 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

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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

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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

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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

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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%)	184 (91%)	18 (9%)	8	31
2	CB	202/220 (92%)	183 (91%)	19 (9%)	7	29
3	AC	160/188 (85%)	139 (87%)	21 (13%)	3	18
3	CC	160/188 (85%)	139 (87%)	21 (13%)	3	18
4	AD	180/181 (99%)	160 (89%)	20 (11%)	5	24
4	CD	180/181 (99%)	160 (89%)	20 (11%)	5	24
5	AE	115/123 (94%)	104 (90%)	11 (10%)	7	28
5	CE	115/123 (94%)	104 (90%)	11 (10%)	7	28
6	AF	90/90 (100%)	83 (92%)	7 (8%)	10	36
6	CF	90/90 (100%)	83 (92%)	7 (8%)	10	36
7	AG	126/127 (99%)	117 (93%)	9 (7%)	12	39
7	CG	126/127 (99%)	118 (94%)	8 (6%)	15	42
8	AH	119/119 (100%)	110 (92%)	9 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	119/119 (100%)	110 (92%)	9 (8%)	11	37
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%)	77 (88%)	11 (12%)	3	19
10	CJ	88/92 (96%)	76 (86%)	12 (14%)	3	18
11	AK	90/99 (91%)	87 (97%)	3 (3%)	33	57
11	CK	90/99 (91%)	87 (97%)	3 (3%)	33	57
12	AL	104/109 (95%)	93 (89%)	11 (11%)	5	25
12	CL	104/109 (95%)	93 (89%)	11 (11%)	5	25
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%)	44 (90%)	5 (10%)	6	26
14	CN	49/50 (98%)	44 (90%)	5 (10%)	6	26
15	AO	79/80 (99%)	73 (92%)	6 (8%)	11	37
15	CO	79/80 (99%)	73 (92%)	6 (8%)	11	37
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%)	89 (95%)	5 (5%)	19	46
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	14	42
18	AR	61/77 (79%)	58 (95%)	3 (5%)	21	47
18	CR	61/77 (79%)	58 (95%)	3 (5%)	21	47
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%)	66 (87%)	10 (13%)	3	18
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%)	495 (88%)	68 (12%)	4	20
25	CY	563/582 (97%)	498 (88%)	65 (12%)	4	22
26	B0	66/67 (98%)	59 (89%)	7 (11%)	5	25
26	D0	66/67 (98%)	59 (89%)	7 (11%)	5	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	B1	78/83 (94%)	68 (87%)	10 (13%)	3	19
27	D1	78/83 (94%)	72 (92%)	6 (8%)	10	37
28	B2	66/67 (98%)	60 (91%)	6 (9%)	7	30
28	D2	66/67 (98%)	61 (92%)	5 (8%)	11	37
29	B3	51/52 (98%)	48 (94%)	3 (6%)	16	44
29	D3	51/52 (98%)	48 (94%)	3 (6%)	16	44
30	B4	51/63 (81%)	39 (76%)	12 (24%)	0	4
30	D4	51/63 (81%)	39 (76%)	12 (24%)	0	4
31	B5	51/52 (98%)	47 (92%)	4 (8%)	10	36
31	D5	51/52 (98%)	47 (92%)	4 (8%)	10	36
32	B6	49/52 (94%)	39 (80%)	10 (20%)	1	7
32	D6	49/52 (94%)	39 (80%)	10 (20%)	1	7
33	B7	41/42 (98%)	36 (88%)	5 (12%)	4	20
33	D7	41/42 (98%)	36 (88%)	5 (12%)	4	20
34	B8	53/55 (96%)	45 (85%)	8 (15%)	2	15
34	D8	53/55 (96%)	44 (83%)	9 (17%)	1	11
35	B9	34/34 (100%)	32 (94%)	2 (6%)	16	44
35	D9	34/34 (100%)	32 (94%)	2 (6%)	16	44
38	BC	180/181 (99%)	169 (94%)	11 (6%)	15	43
38	DC	180/181 (99%)	168 (93%)	12 (7%)	13	40
39	BD	217/218 (100%)	182 (84%)	35 (16%)	2	13
39	DD	217/218 (100%)	182 (84%)	35 (16%)	2	13
40	BE	165/166 (99%)	140 (85%)	25 (15%)	2	14
40	DE	165/166 (99%)	140 (85%)	25 (15%)	2	14
41	BF	165/166 (99%)	154 (93%)	11 (7%)	13	40
41	DF	165/166 (99%)	154 (93%)	11 (7%)	13	40
42	BG	155/156 (99%)	127 (82%)	28 (18%)	1	9
42	DG	155/156 (99%)	126 (81%)	29 (19%)	1	8
43	BH	136/148 (92%)	125 (92%)	11 (8%)	9	34
43	DH	136/148 (92%)	125 (92%)	11 (8%)	9	34
45	BN	117/119 (98%)	103 (88%)	14 (12%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DN	117/119 (98%)	103 (88%)	14 (12%)	4	20
46	BO	100/100 (100%)	94 (94%)	6 (6%)	16	43
46	DO	100/100 (100%)	94 (94%)	6 (6%)	16	43
47	BP	112/116 (97%)	93 (83%)	19 (17%)	1	11
47	DP	112/116 (97%)	92 (82%)	20 (18%)	1	9
48	BQ	111/111 (100%)	101 (91%)	10 (9%)	8	31
48	DQ	111/111 (100%)	101 (91%)	10 (9%)	8	31
49	BR	100/101 (99%)	89 (89%)	11 (11%)	5	24
49	DR	100/101 (99%)	87 (87%)	13 (13%)	3	19
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%)	96 (80%)	24 (20%)	1	7
51	DT	120/127 (94%)	96 (80%)	24 (20%)	1	7
52	BU	92/94 (98%)	82 (89%)	10 (11%)	5	24
52	DU	92/94 (98%)	81 (88%)	11 (12%)	4	20
53	BV	82/82 (100%)	72 (88%)	10 (12%)	4	20
53	DV	82/82 (100%)	73 (89%)	9 (11%)	5	24
54	BW	91/92 (99%)	86 (94%)	5 (6%)	18	45
54	DW	91/92 (99%)	86 (94%)	5 (6%)	18	45
55	BX	74/78 (95%)	65 (88%)	9 (12%)	4	20
55	DX	74/78 (95%)	65 (88%)	9 (12%)	4	20
56	BY	87/91 (96%)	76 (87%)	11 (13%)	3	19
56	DY	87/91 (96%)	76 (87%)	11 (13%)	3	19
57	BZ	162/179 (90%)	137 (85%)	25 (15%)	2	14
57	DZ	162/179 (90%)	145 (90%)	17 (10%)	5	25
All	All	10872/11344 (96%)	9687 (89%)	1185 (11%)	5	24

5 of 1185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	DD	67	PHE
54	DW	88	ARG
40	DE	26	ILE

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Mol	Chain	Res	Type
39	DD	65	ILE
45	DN	109	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 349 such sidechains are listed below:

Mol	Chain	Res	Type
20	CT	42	GLN
40	DE	48	GLN
25	CY	137	ASN
30	D4	6	HIS
42	DG	27	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	254 (16%)	36 (2%)
1	CA	1503/1522 (98%)	252 (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%)	588 (20%)	61 (2%)
36	DA	2900/2915 (99%)	585 (20%)	63 (2%)
37	BB	118/122 (96%)	25 (21%)	0
37	DB	118/122 (96%)	25 (21%)	0
All	All	9368/9474 (98%)	1826 (19%)	202 (2%)

5 of 1826 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	28,32,35	0.37	0
23	5MU	AW	54	23	19,22,23	0.27	0	28,32,35	0.29	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

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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	CY	702	61	24,30,30	1.35	3 (12%)	30,47,47	1.55	7 (23%)
59	FUA	CY	701	-	39,40,40	1.67	7 (17%)	49,64,64	1.44	9 (18%)
59	FUA	AY	701	-	39,40,40	1.68	7 (17%)	49,64,64	1.51	5 (10%)
60	GDP	AY	702	61	24,30,30	1.19	2 (8%)	30,47,47	1.44	4 (13%)

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	CY	702	61	-	0/12/32/32	0/3/3/3
59	FUA	CY	701	-	-	9/15/92/92	0/4/4/4
59	FUA	AY	701	-	-	6/15/92/92	0/4/4/4
60	GDP	AY	702	61	-	2/12/32/32	0/3/3/3

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	-4.50	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AY	701	FUA	C23-C22	-4.38	1.39	1.51
59	AY	701	FUA	C23-C24	-4.27	1.39	1.53
59	CY	701	FUA	C23-C24	-4.26	1.39	1.53
59	AY	701	FUA	C29-C22	4.19	1.53	1.47

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AY	701	FUA	C13-C12-C11	-4.33	105.84	111.90
59	CY	701	FUA	C16-O2-C31	-4.20	110.67	117.06
60	CY	702	GDP	PA-O3A-PB	-4.03	119.01	132.83
59	AY	701	FUA	C16-O2-C31	-3.91	111.12	117.06
60	AY	702	GDP	PA-O3A-PB	-3.57	120.58	132.83

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-C29
59	AY	701	FUA	C17-C22-C23-C24
59	AY	701	FUA	C29-C22-C23-C24
59	CY	701	FUA	C13-C17-C22-C29
59	CY	701	FUA	C17-C22-C23-C24

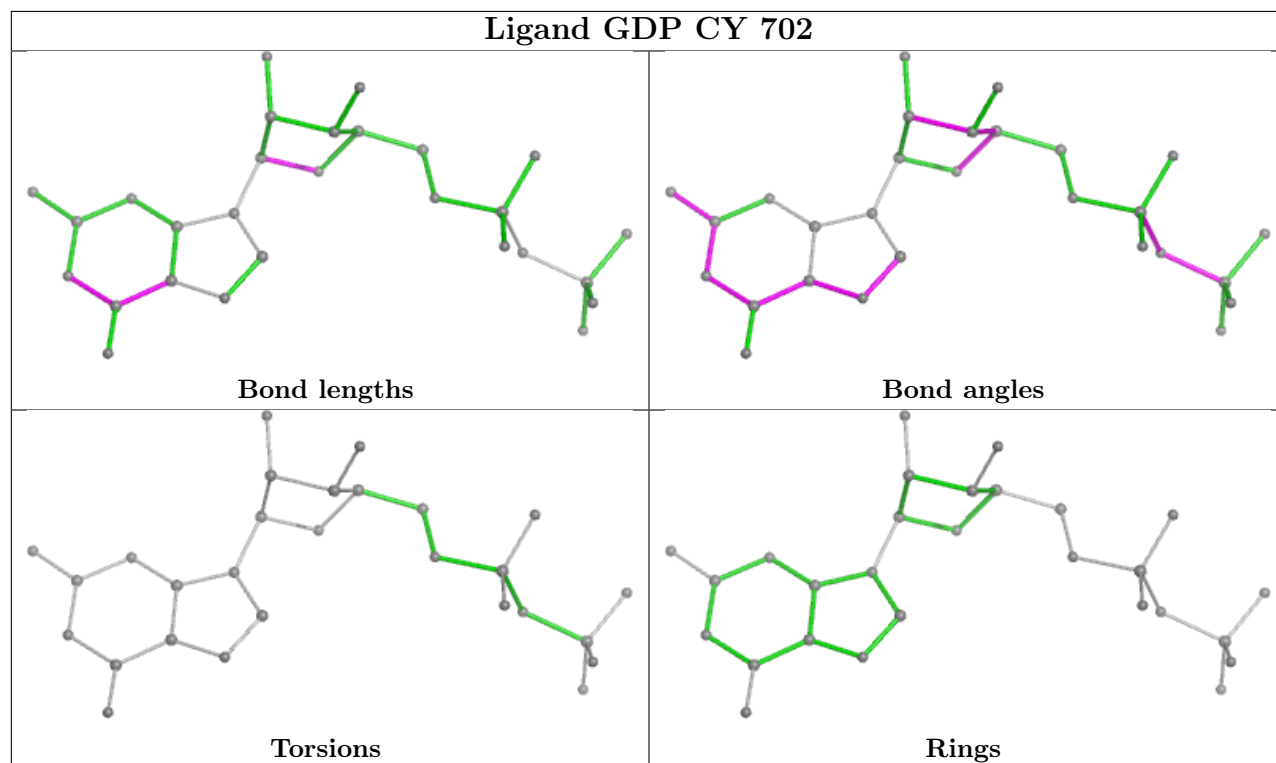
There are no ring outliers.

4 monomers are involved in 64 short contacts:

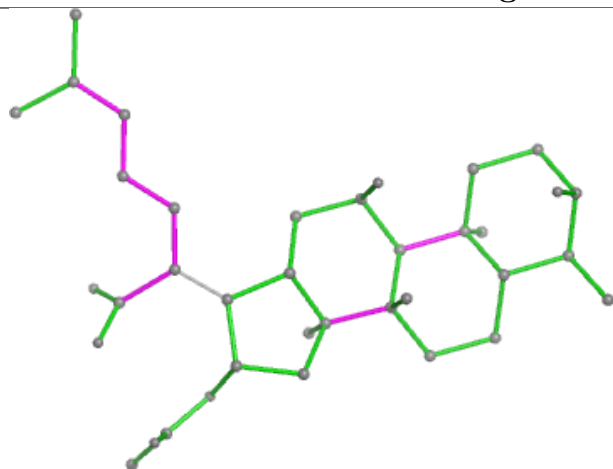
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	CY	702	GDP	10	0
59	CY	701	FUA	26	0
59	AY	701	FUA	15	0
60	AY	702	GDP	13	0

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

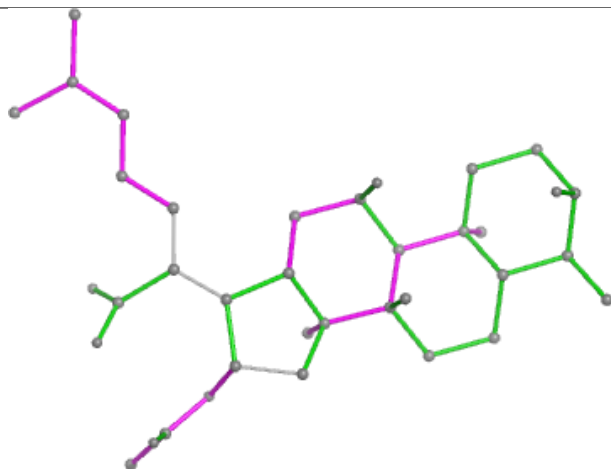
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



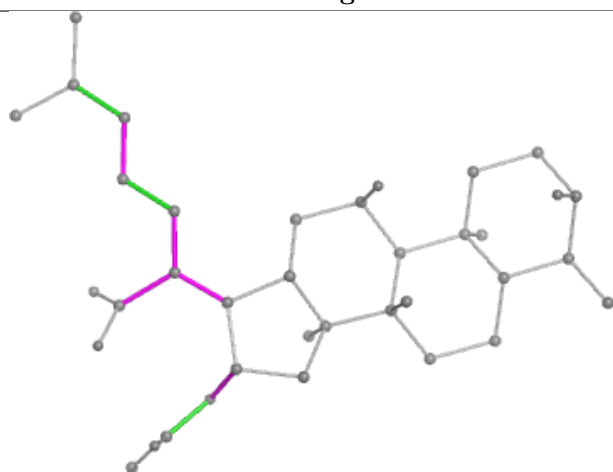
## Ligand FUA CY 701



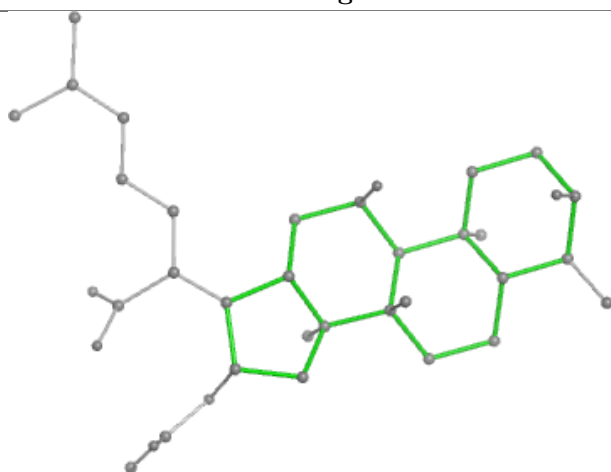
Bond lengths



Bond angles

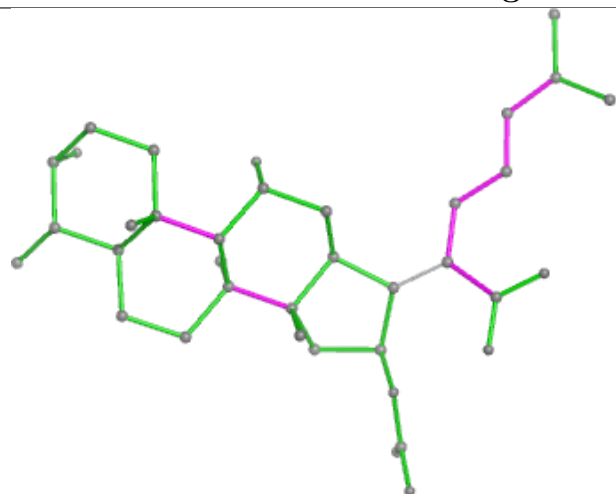


Torsions

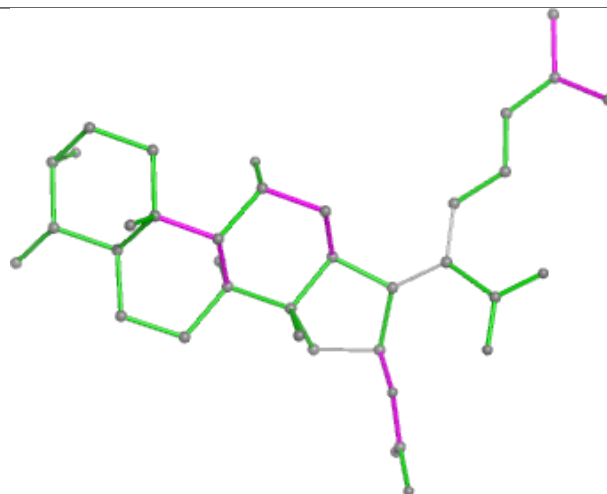


Rings

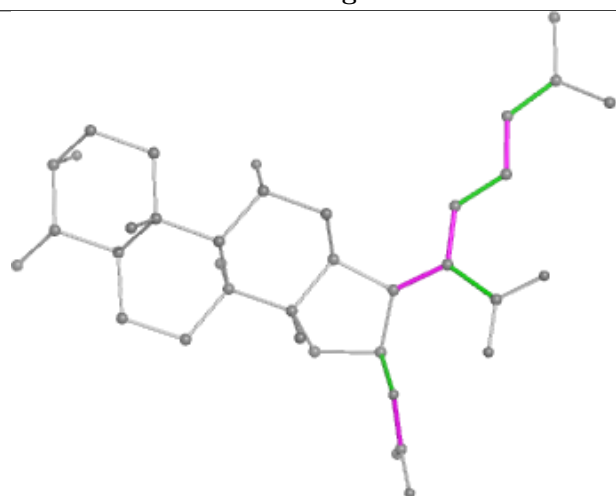
## Ligand FUA AY 701



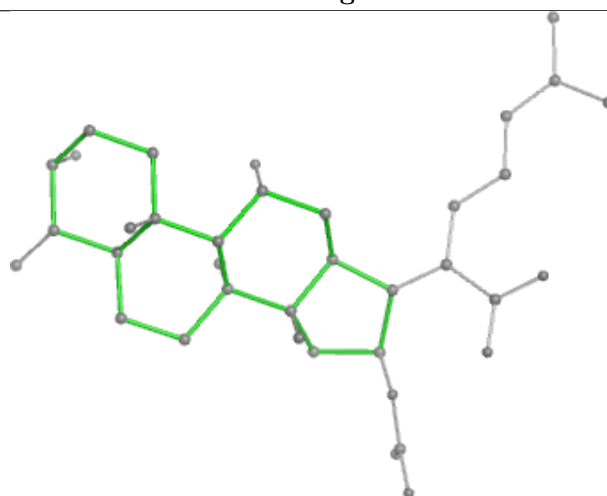
Bond lengths



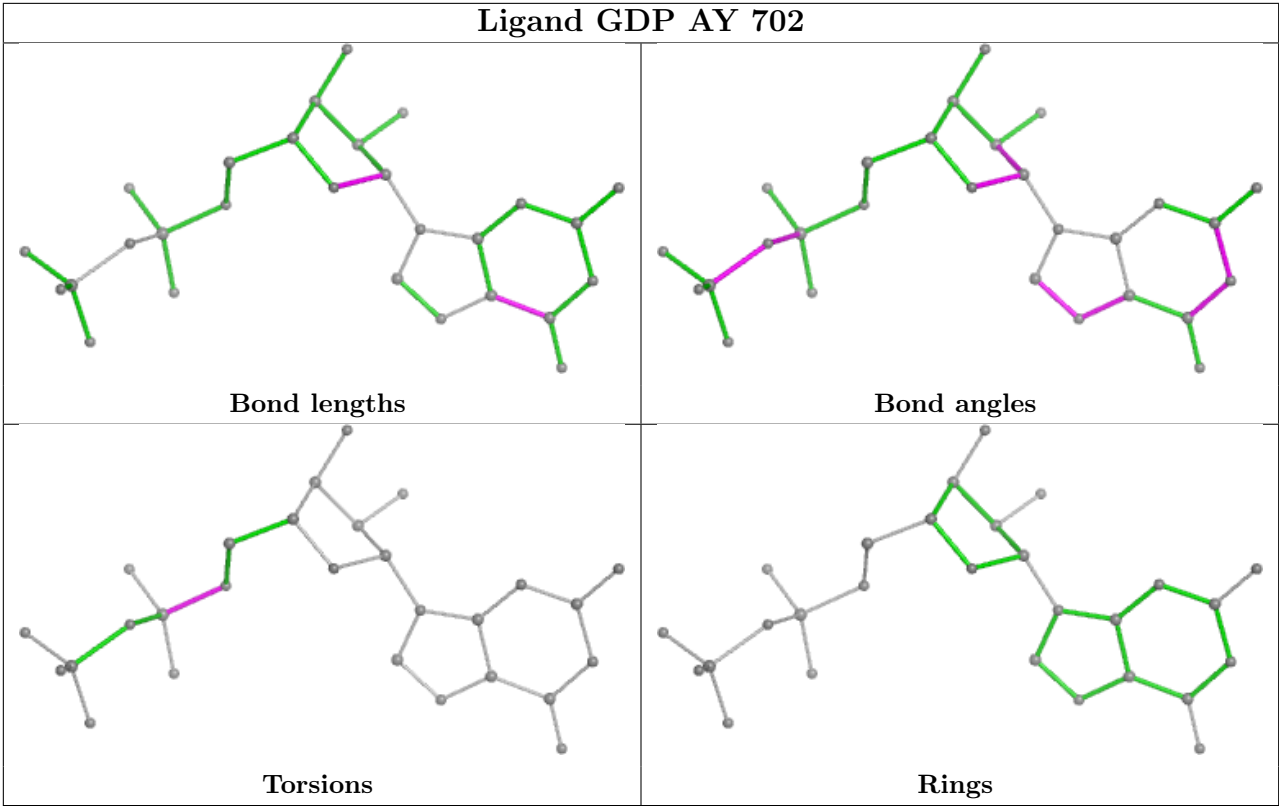
Bond angles



Torsions



Rings



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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	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

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	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%)	0.37	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

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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, 95<sup>th</sup> 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 <sup>2</sup> )	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
59	FUA	CY	701	37/37	0.18	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	0.81	0.14	55,55,55,55	0
58	ZN	D4	1000	1/1	0.83	0.10	200,200,200,200	0
58	ZN	B4	101	1/1	0.89	0.08	172,172,172,172	0
60	GDP	AY	702	28/28	0.90	0.10	93,97,99,99	0
61	MG	CY	703	1/1	0.93	0.11	46,46,46,46	0
60	GDP	CY	702	28/28	0.94	0.07	96,102,109,110	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

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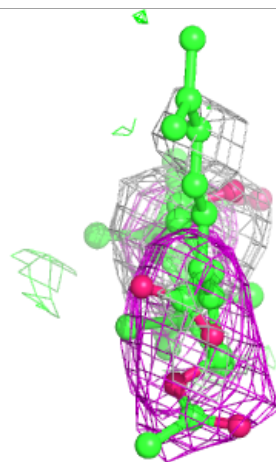
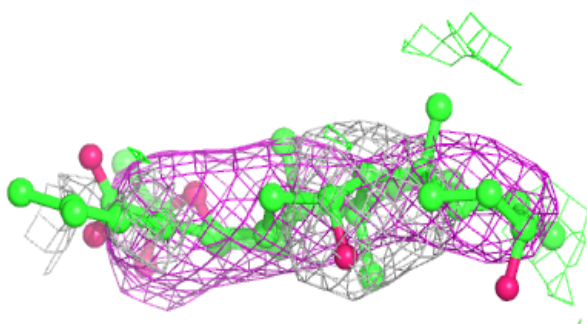
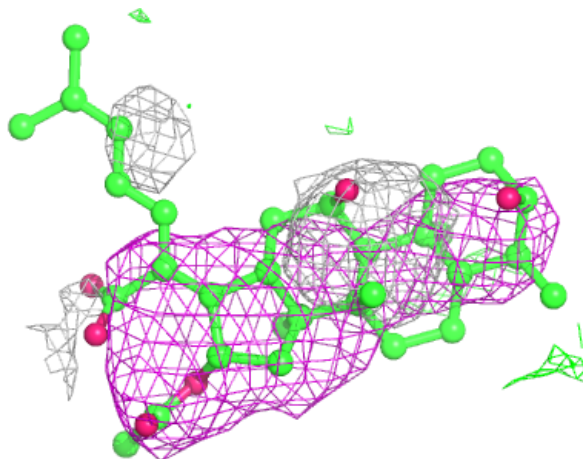
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
58	ZN	B9	101	1/1	0.99	0.02	93,93,93,93	0
58	ZN	D9	1000	1/1	1.00	0.03	123,123,123,123	0

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.

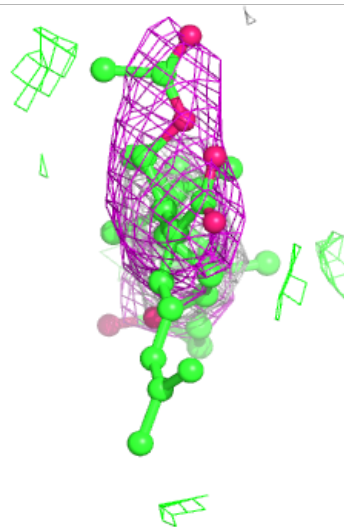
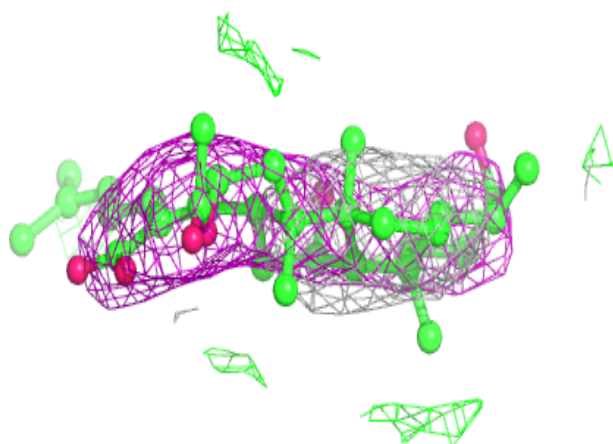
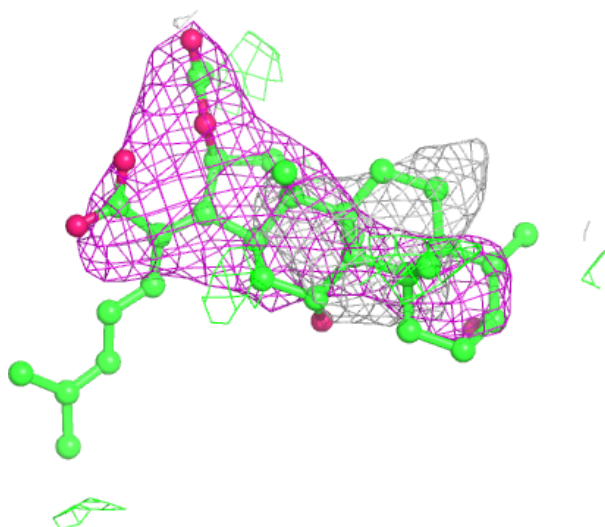
**Electron density around FUA CY 701:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FUA AY 701:**

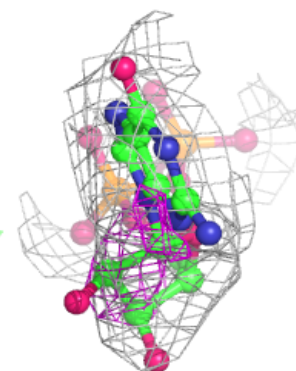
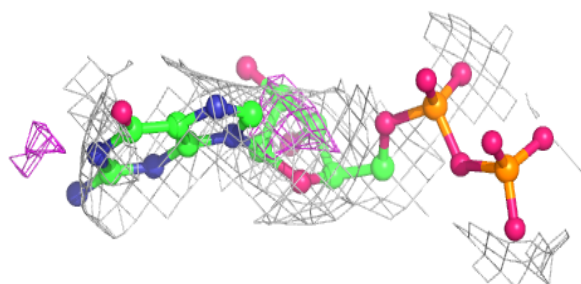
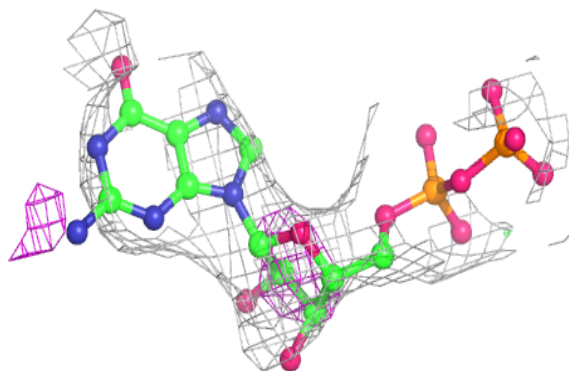
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



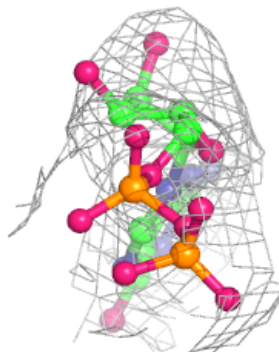
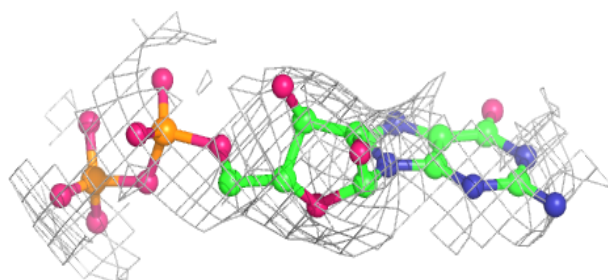
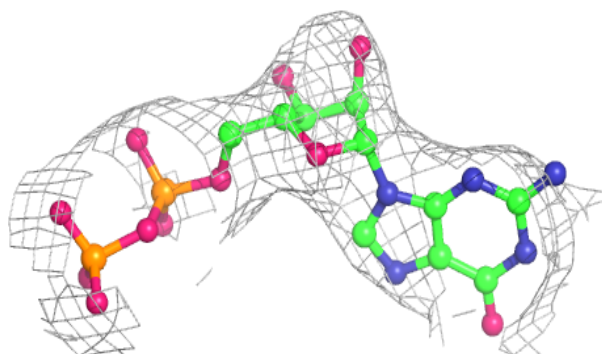


**Electron density around GDP AY 702:**

$2mF_o - DF_c$  (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.