



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:46 PM GMT

PDB ID : 4V5Q  
Title : The crystal structure of EF-Tu and G24A-tRNA-Trp bound to a near- cognate codon on the 70S ribosome  
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.  
Deposited on : 2010-12-07  
Resolution : 3.10 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

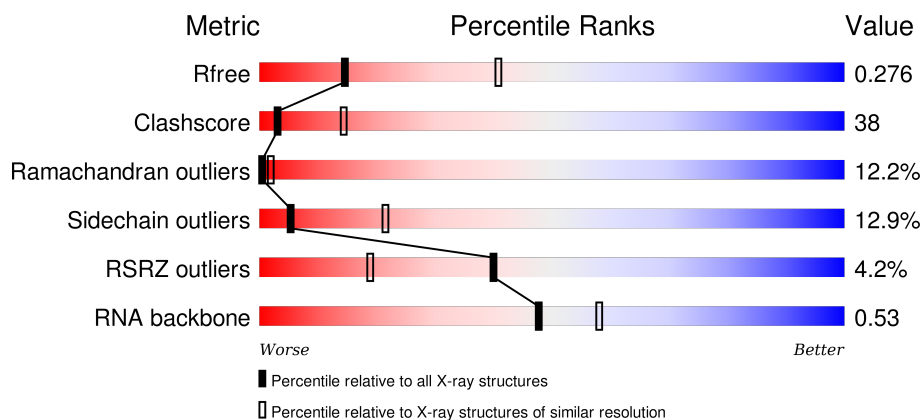
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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




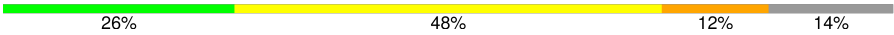
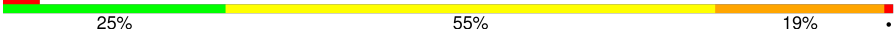
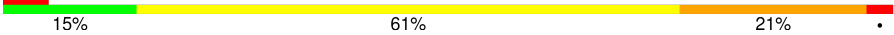

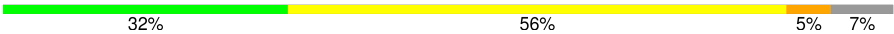
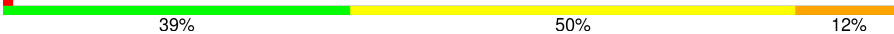
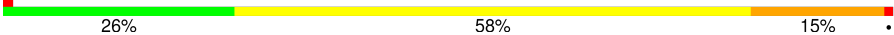
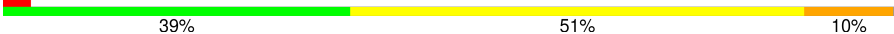
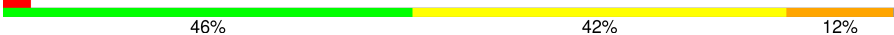

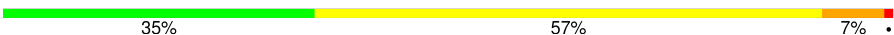
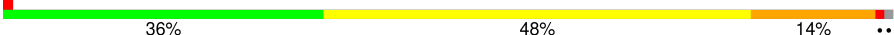
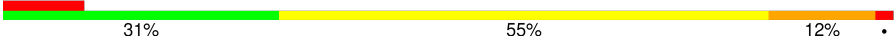
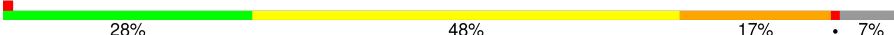
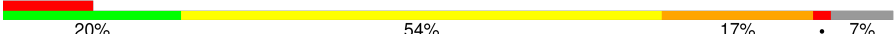





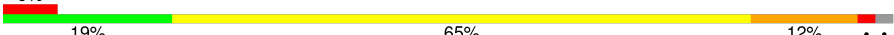

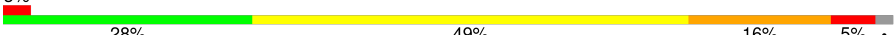

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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



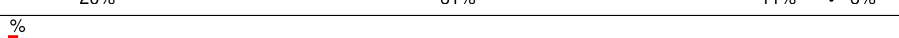
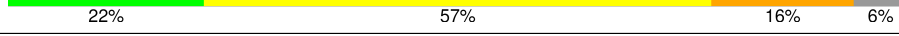
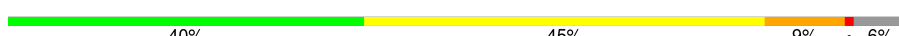
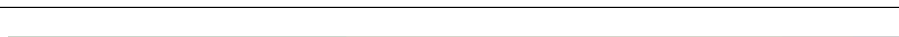
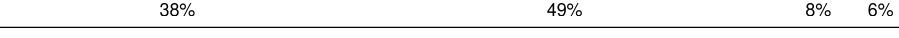
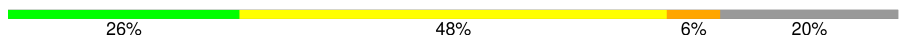

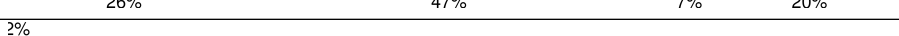
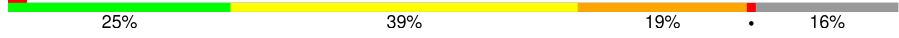
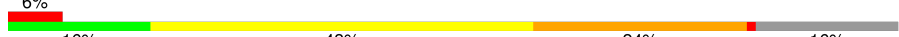
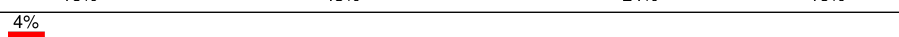
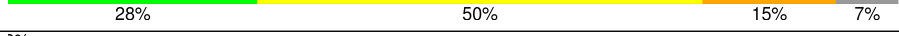

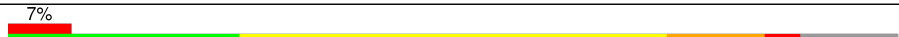
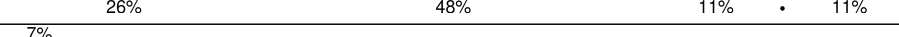
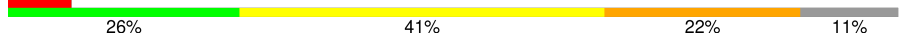

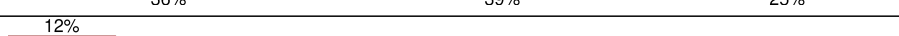
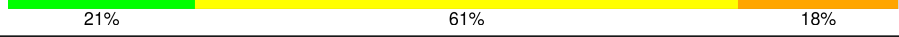
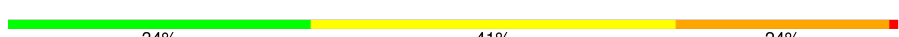
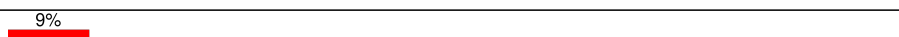
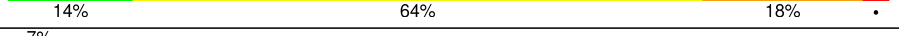

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
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	AW	76	
22	CV	76	
22	CW	76	
23	AX	27	
23	CX	27	
24	AY	77	
24	CY	77	
25	AZ	405	
25	CZ	405	
26	B0	85	
26	D0	85	

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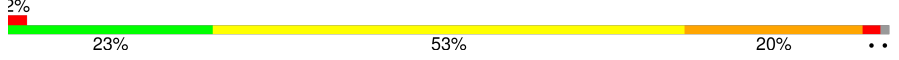
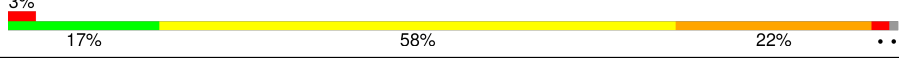
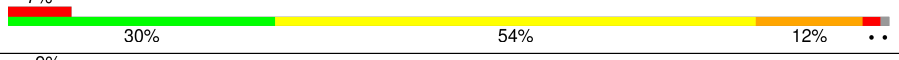
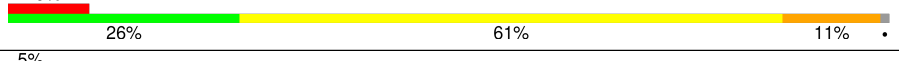
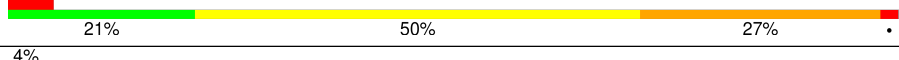
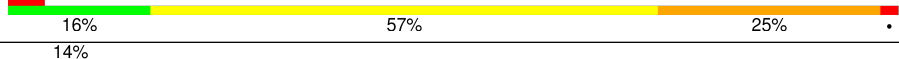
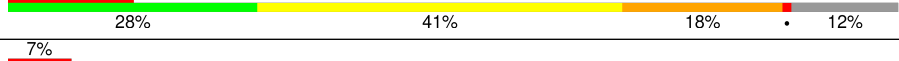
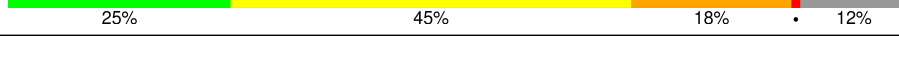
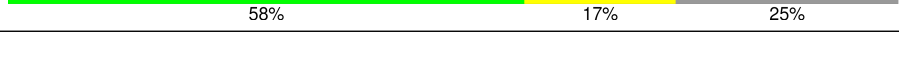
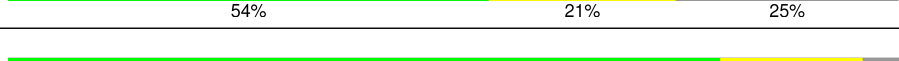
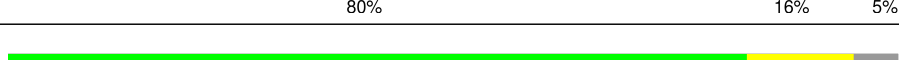
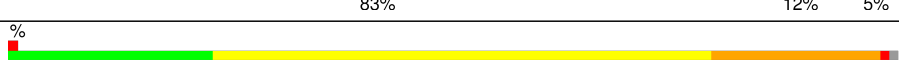
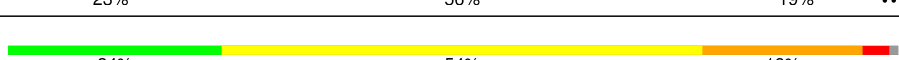
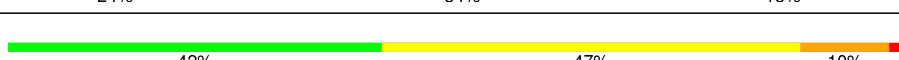
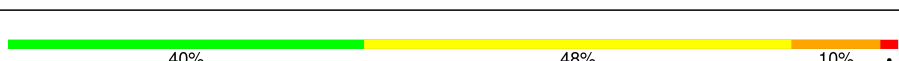
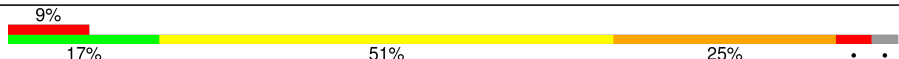
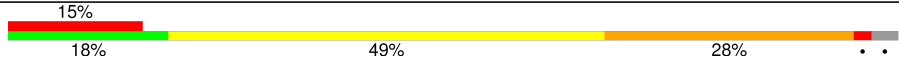


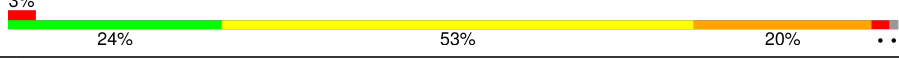
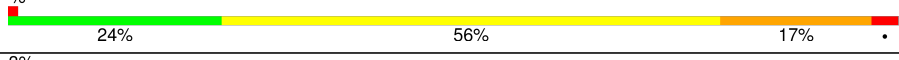

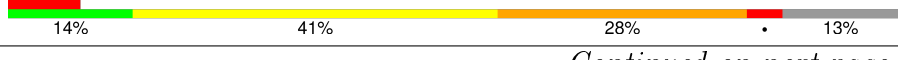



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Mol	Chain	Length	Quality of chain
27	B1	98	
27	D1	98	
28	B2	72	
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229	
39	BD	276	

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Mol	Chain	Length	Quality of chain
39	DD	276	
40	BE	206	
40	DE	206	
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	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	

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Mol	Chain	Length	Quality of chain
52	BT	146	
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	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	ZN	AN	101	-	-	X	-
60	GDP	AZ	501	-	-	X	-
60	GDP	CZ	501	-	-	X	-
61	KIR	CZ	502	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 307194 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 RRNA.

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	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
2	CB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	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	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			
5	CE	150	Total	C	N	O	S	0	0	0
			1146	724	217	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	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			794	499	156	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	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			
12	CL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	124	Total	C	N	O	S	0	0	0
			987	611	205	169	2			
13	CM	124	Total	C	N	O	S	0	0	0
			987	611	205	169	2			

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

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

- 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	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	CP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	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	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			
19	CS	78	Total	C	N	O	S	0	0	0
			629	403	114	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	24	Total	C	N	O	0	0	0
			208	128	50	30			
21	CU	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE.

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

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	17	Total	C	N	O	P	0	0	0
			361	164	68	113	16			
23	CX	17	Total	C	N	O	P	0	0	0
			361	164	68	113	16			

- Molecule 24 is a RNA chain called A-SITE TRNA G24A TRP-TRNA TRP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AY	77	Total	C	N	O	P	S	0	0	0
			1644	742	289	535	76	2			
24	CY	77	Total	C	N	O	P	S	0	0	0
			1644	742	289	535	76	2			

- Molecule 25 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AZ	385	Total	C	N	O	S	0	0	0
			2984	1885	524	563	12			
25	CZ	385	Total	C	N	O	S	0	0	0
			2984	1885	524	563	12			

- 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			
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	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			
27	D1	93	Total	C	N	O	S	0	0	0
			731	460	145	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	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			
29	D3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	44	Total	C	N	O	S	0	0	0
			340	218	57	61	4			
30	D4	44	Total	C	N	O	S	0	0	0
			340	218	57	61	4			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
33	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
34	D8	63	Total	C	N	O	S	0	0	0
			507	326	101	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
			62477	27807	11683	20087	2900			
36	DA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	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	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
40	DE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			
41	DF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	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			
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	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			
43	DH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O	0	0	0
			651	391	130	130			
44	DJ	130	Total	C	N	O	0	0	0
			651	391	130	130			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BK	140	Total	C	N	O	0	0	0
			700	420	140	140			
45	DK	140	Total	C	N	O	0	0	0
			700	420	140	140			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
46	DN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	98	Total	C	N	O		0	0	0
			770	486	154	130				
51	DS	98	Total	C	N	O		0	0	0
			770	486	154	130				

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
52	DT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BX	92	Total	C	N	O	0	0	0
			725	471	131	123			
56	DX	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			
57	DY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

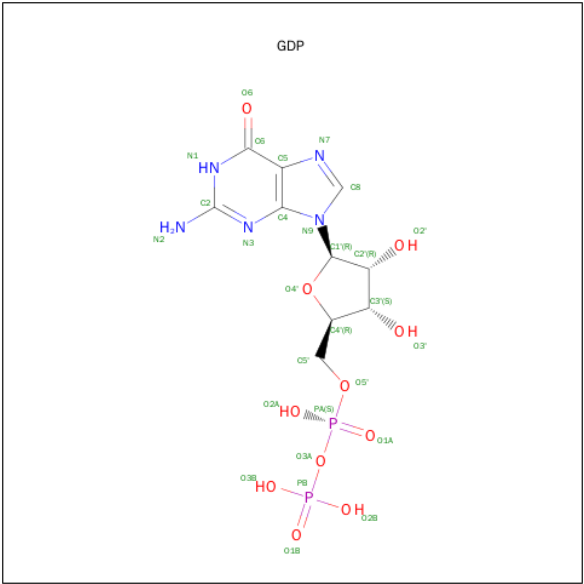
- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	183	Total	C	N	O	S	0	0	0
			1459	932	260	265	2			
58	DZ	183	Total	C	N	O	S	0	0	0
			1459	932	260	265	2			

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

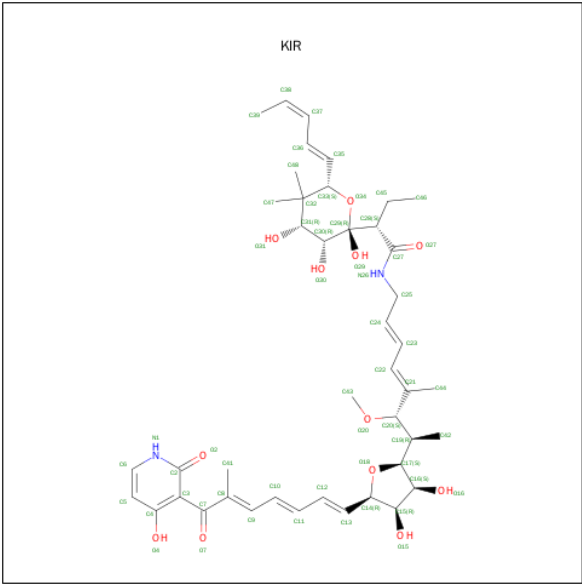
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

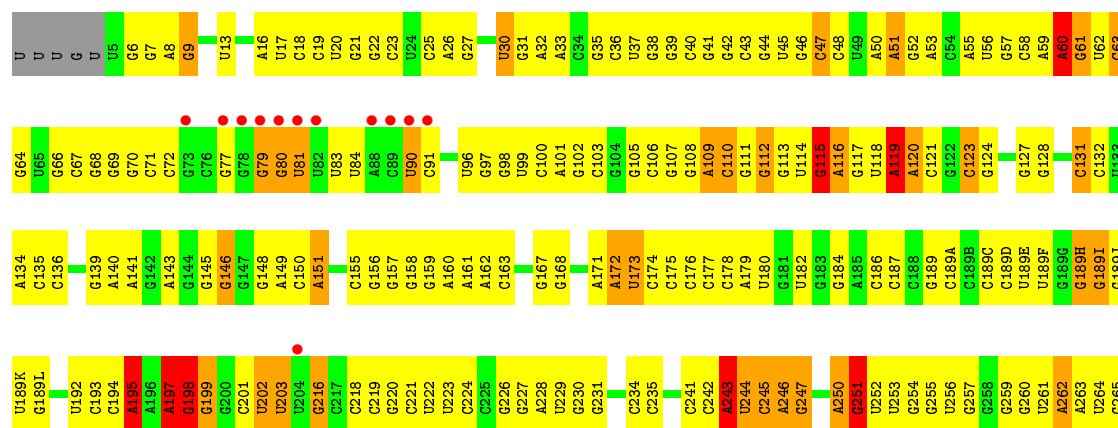
- Molecule 61 is KIRROMYCIN (three-letter code: KIR) (formula: C<sub>43</sub>H<sub>60</sub>N<sub>2</sub>O<sub>12</sub>).



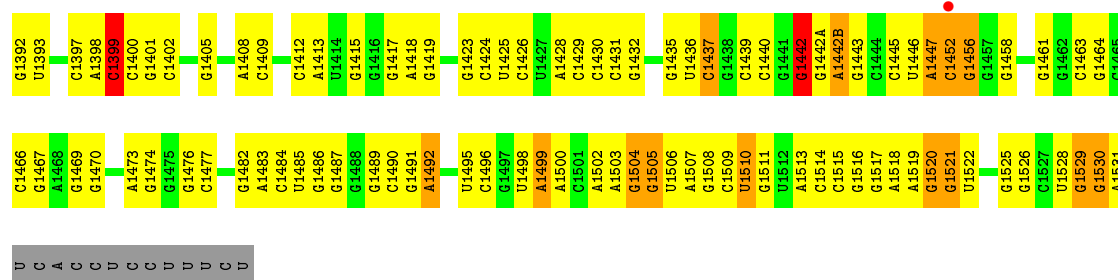
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AZ	1	Total	C	N	O		0	0
			57	43	2	12			
61	CZ	1	Total	C	N	O		0	0
			57	43	2	12			



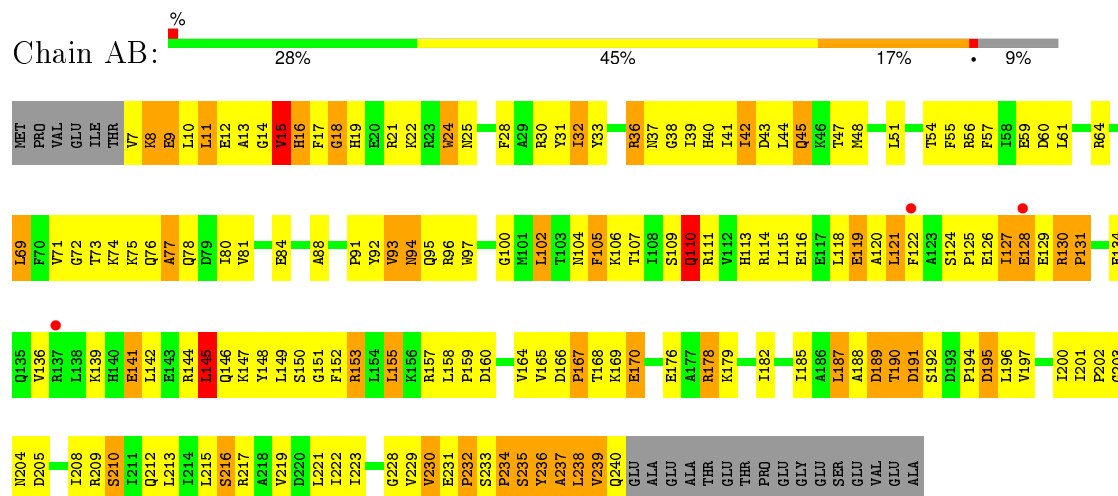




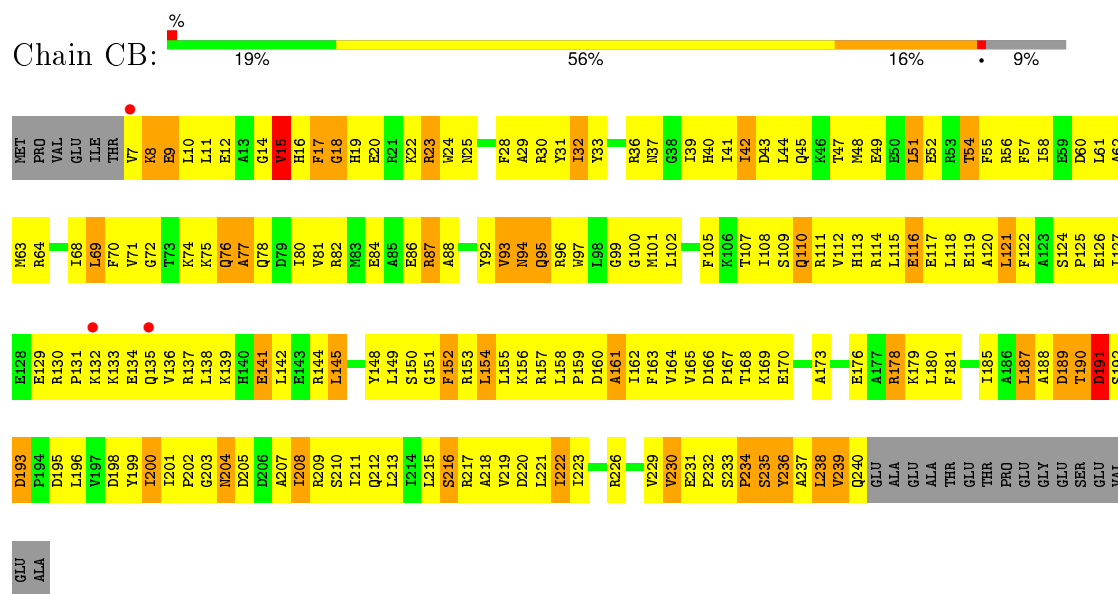




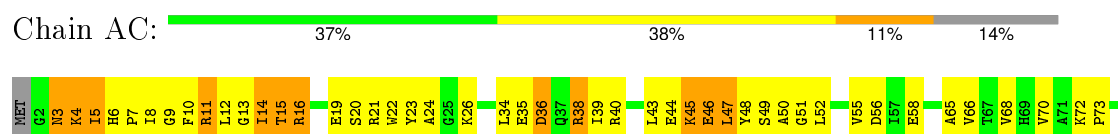
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

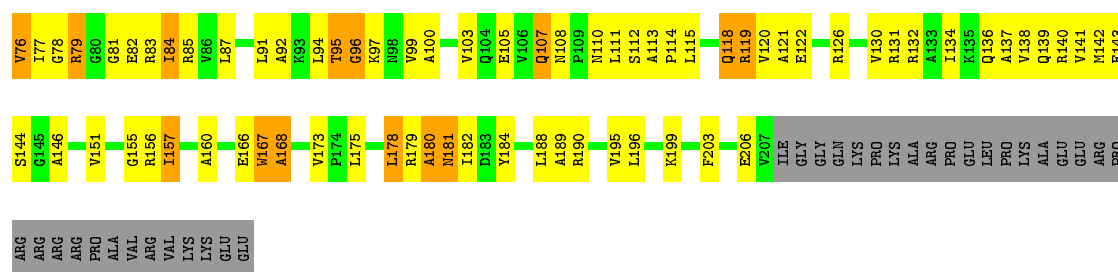


• Molecule 2: 30S RIBOSOMAL PROTEIN S2



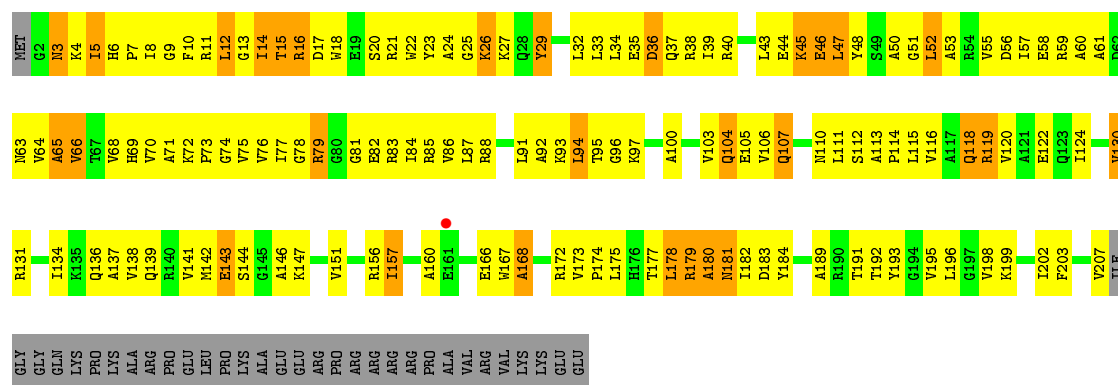
• Molecule 3: 30S RIBOSOMAL PROTEIN S3





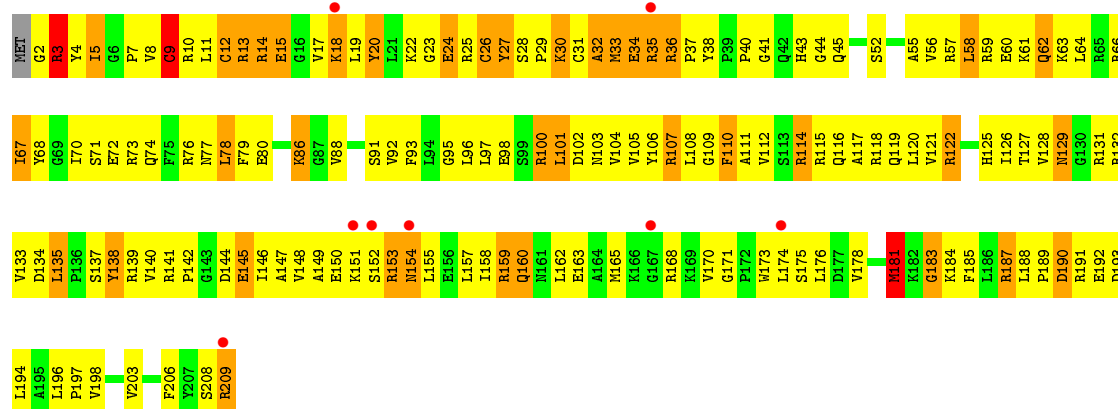
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC: 26% 48% 12% 14%



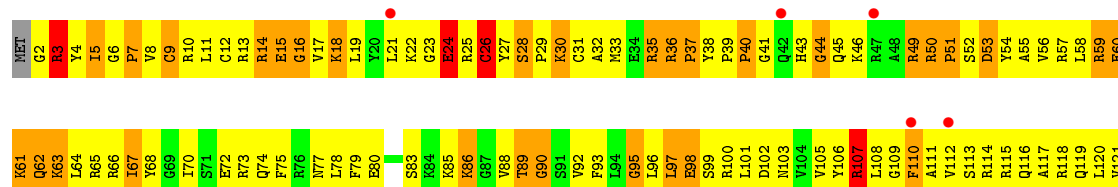
### • Molecule 4: 30S RIBOSOMAL PROTEIN S4

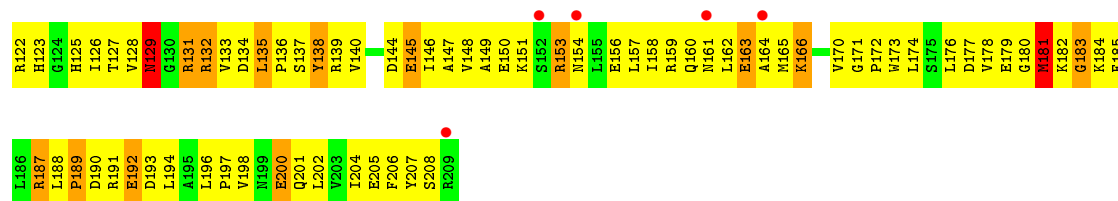
Chain AD: 4% 25% 55% 19%



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

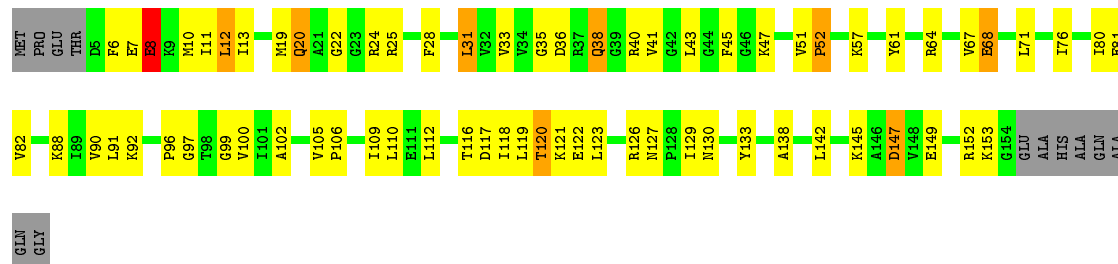
Chain CD: 5% 15% 61% 21%





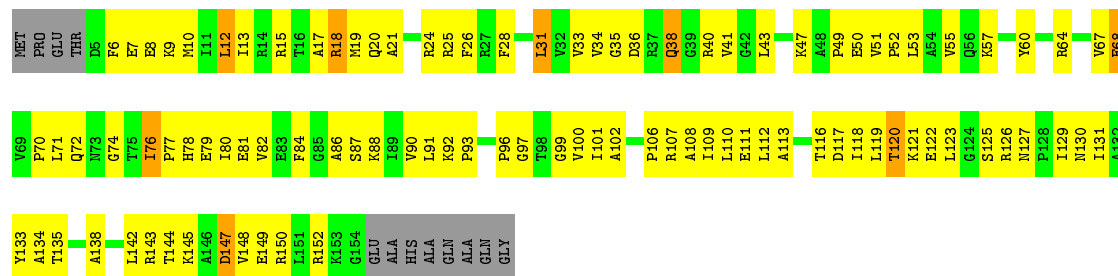
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE: 50% 37% 5% 7%



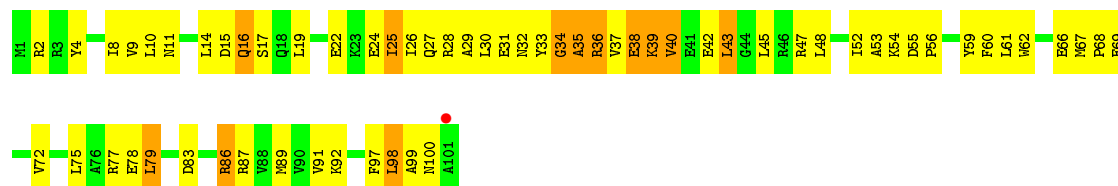
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE: 32% 56% 5% 7%



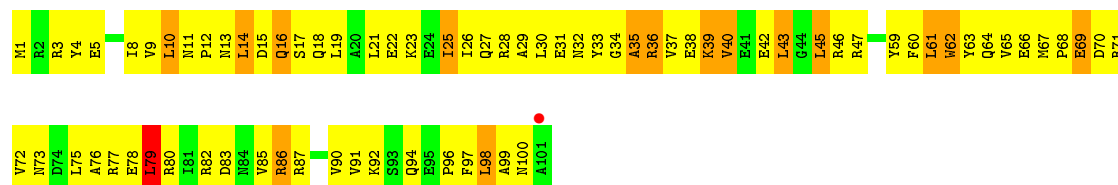
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF: 39% 50% 12%

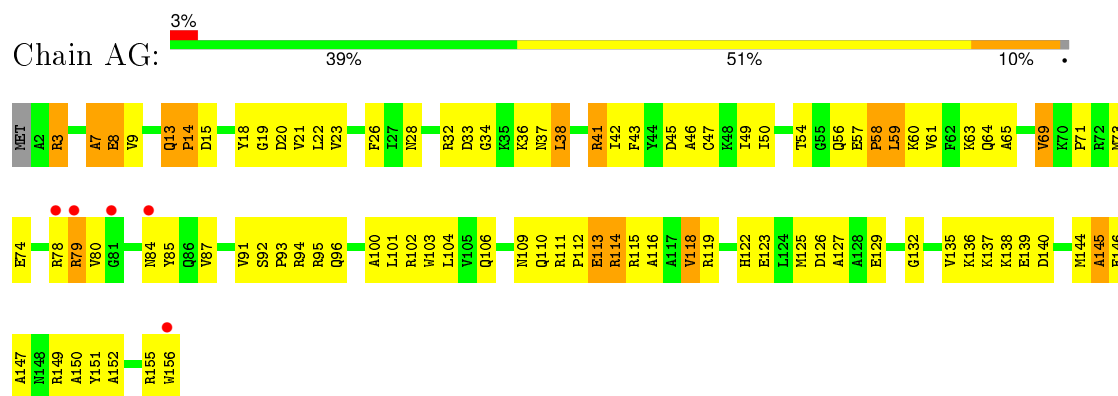


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

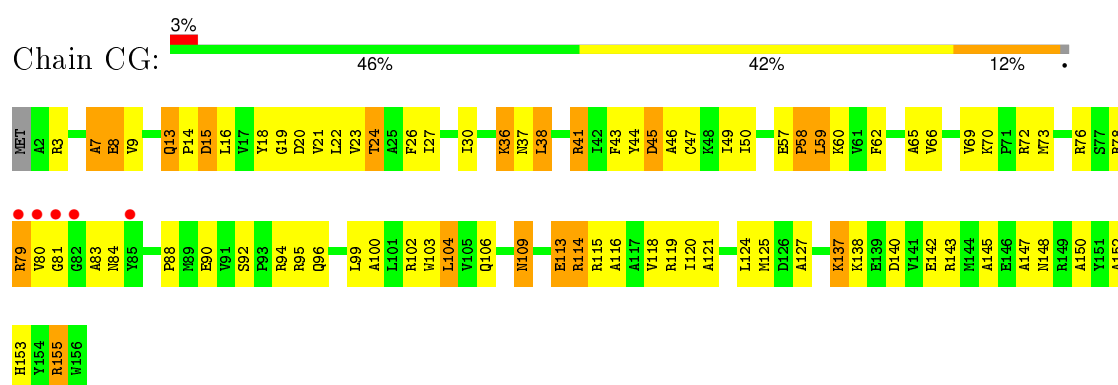
Chain CF: 26% 58% 15%



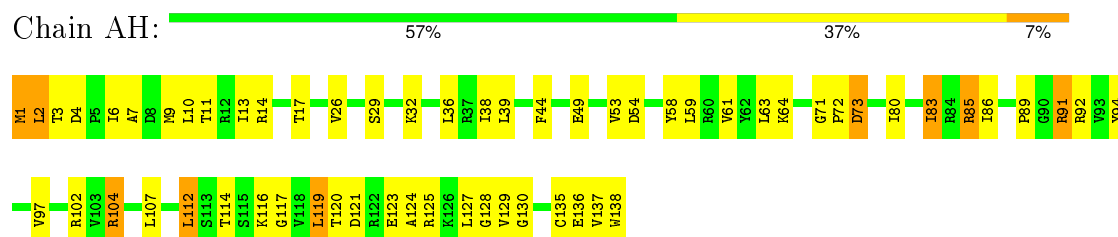
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



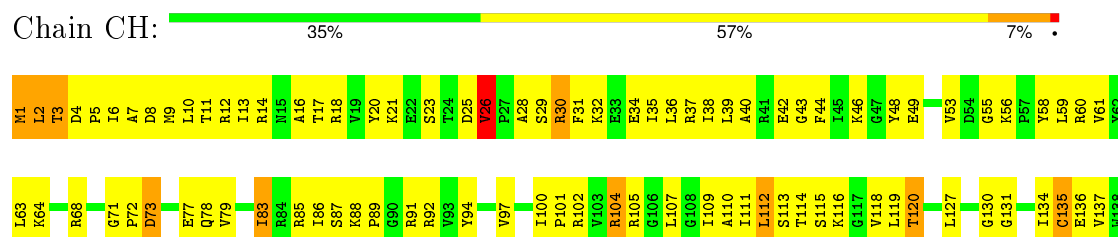
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



- Molecule 8: 30S RIBOSOMAL PROTEIN S8

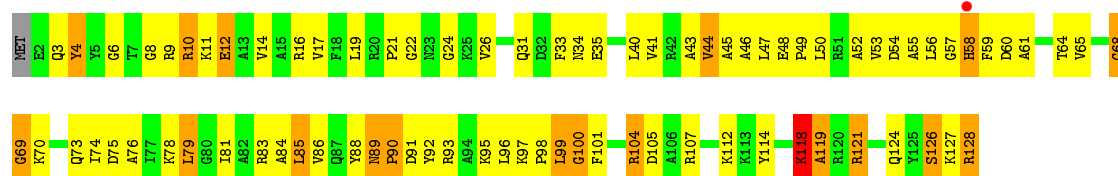


- Molecule 8: 30S RIBOSOMAL PROTEIN S8

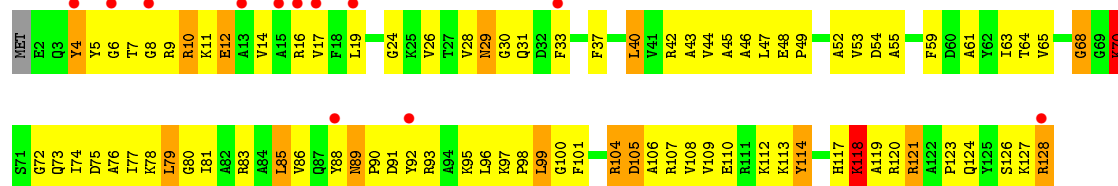


- Molecule 9: 30S RIBOSOMAL PROTEIN S9

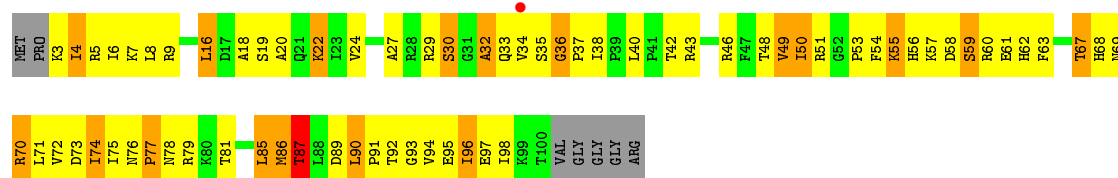




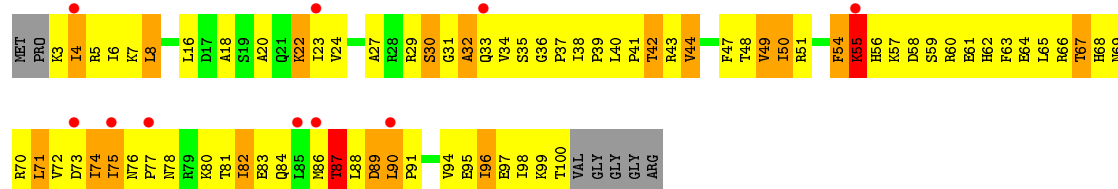
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



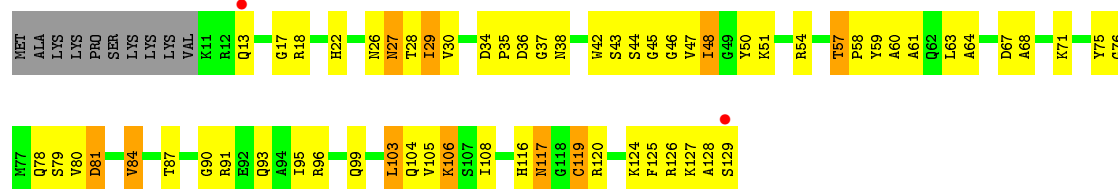
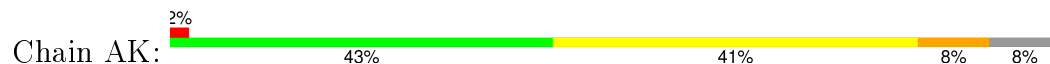
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S10



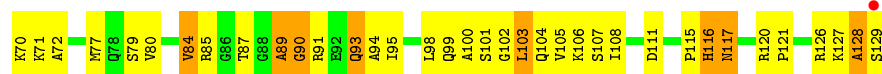
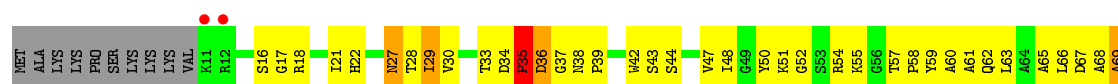
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



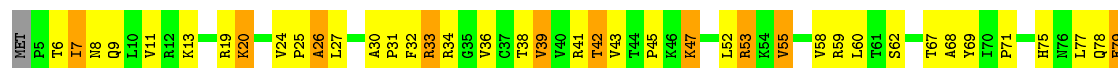
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



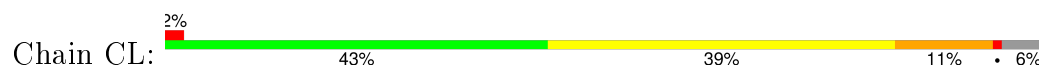




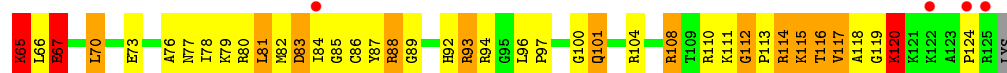
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



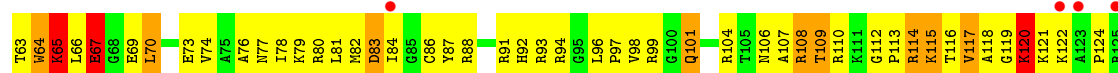
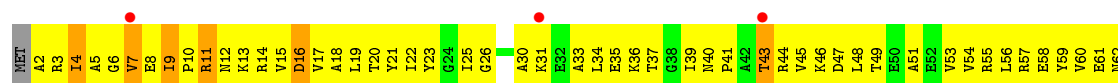
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

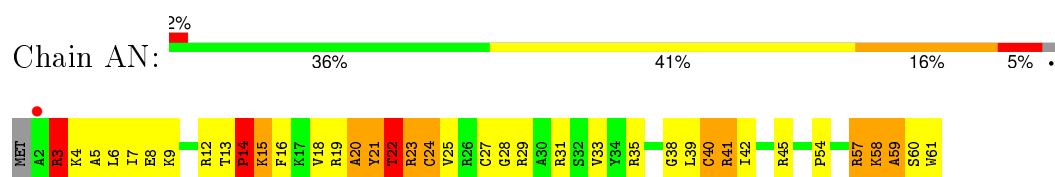


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

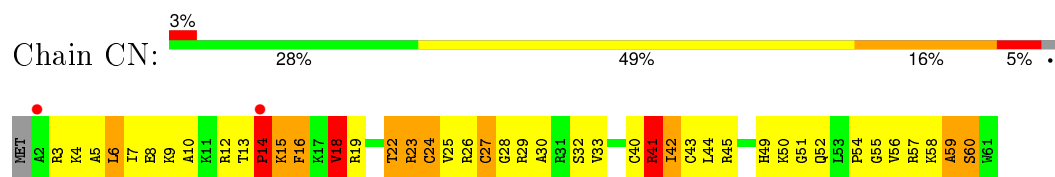


LYS

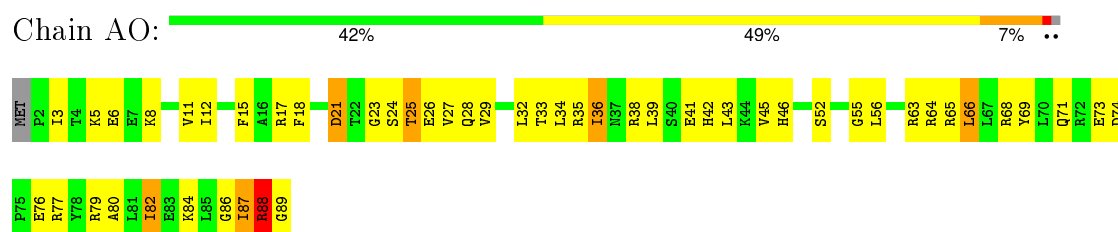
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



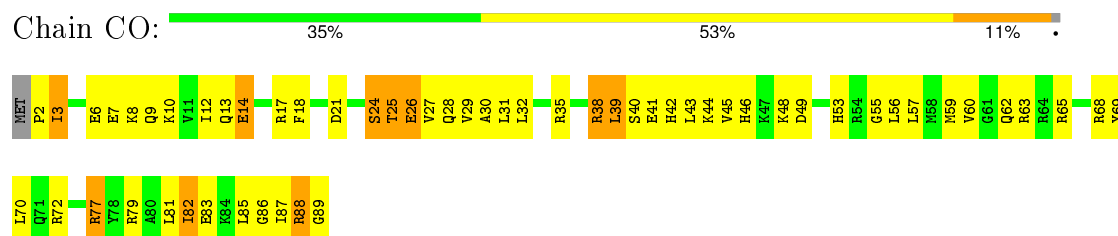
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



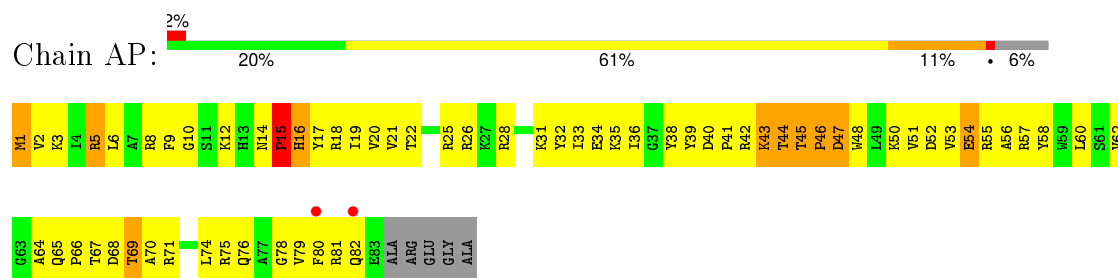
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



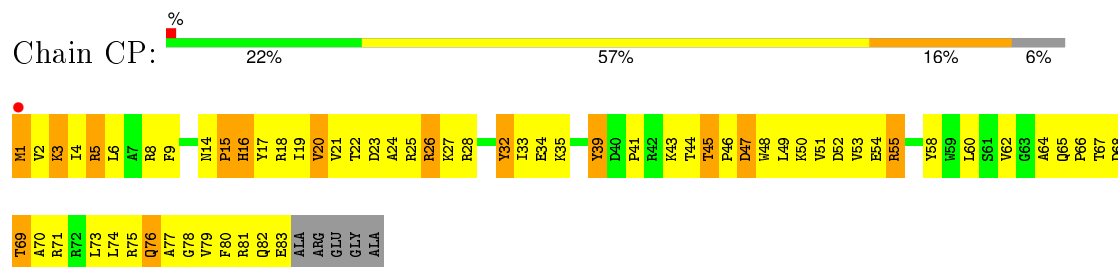
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



- Molecule 16: 30S RIBOSOMAL PROTEIN S16

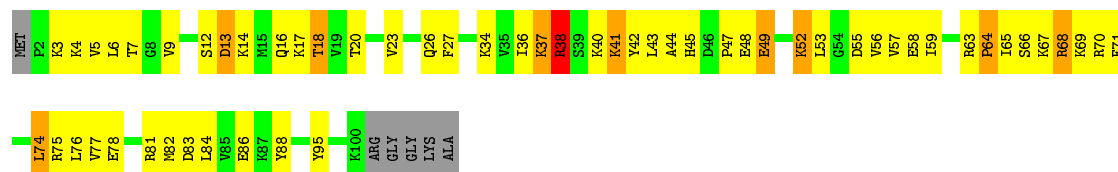


- Molecule 16: 30S RIBOSOMAL PROTEIN S16

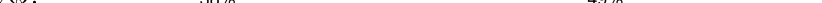


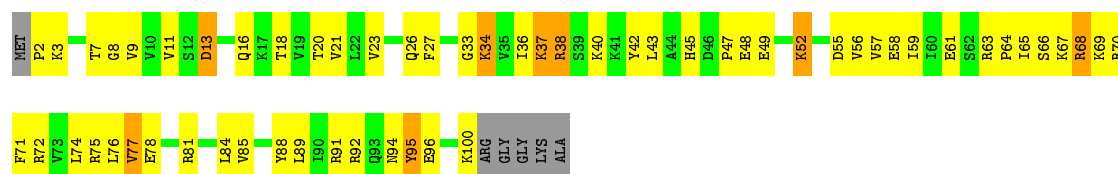
● Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:  40% 45% 9% • 6%

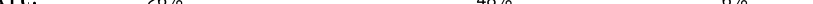


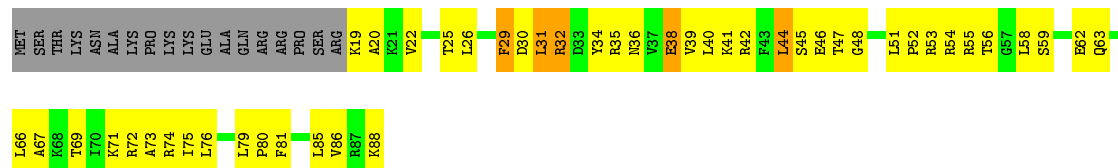
● Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ: 

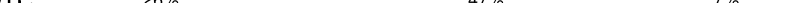


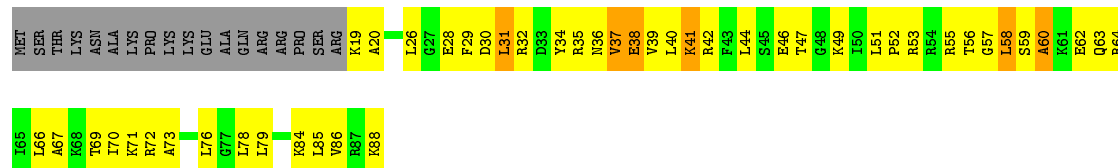
● Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR: 

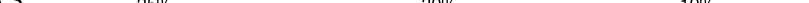


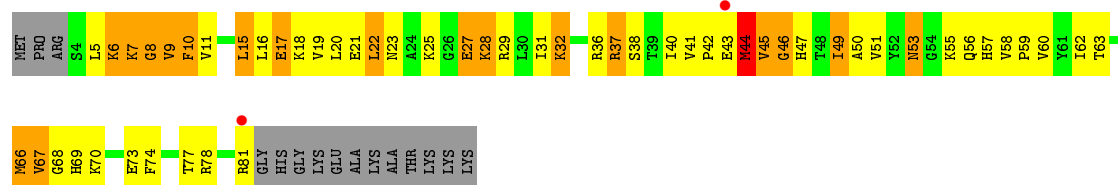
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR: 

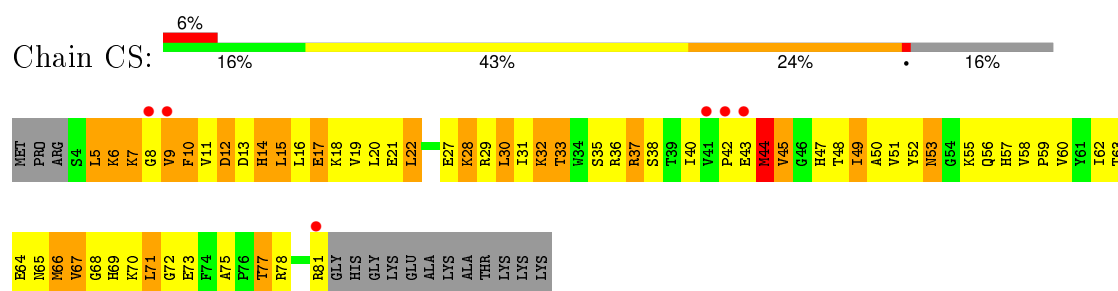


● Molecule 19: 30S RIBOSOMAL PROTEIN S19

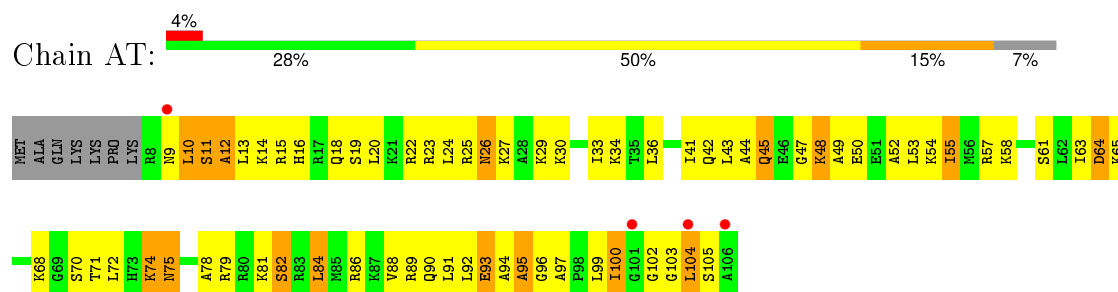
Chain AS: 



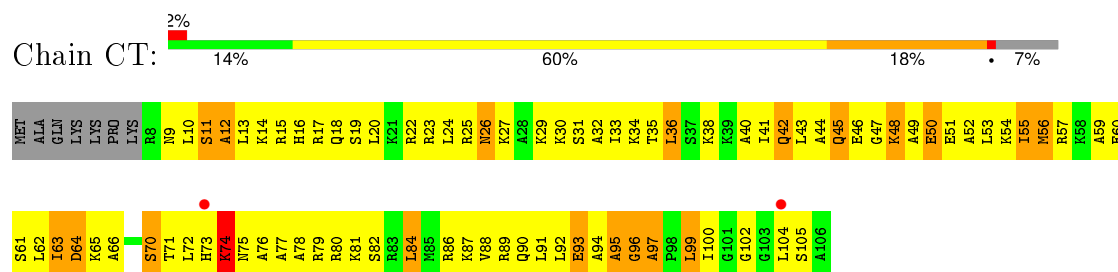
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



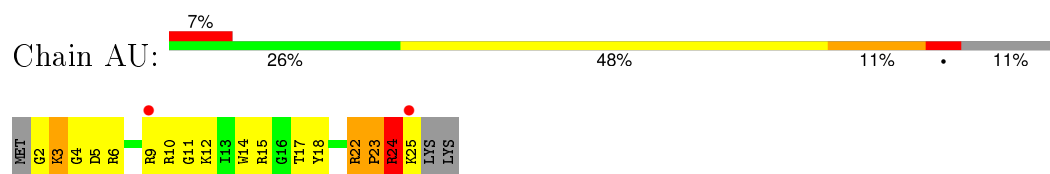
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



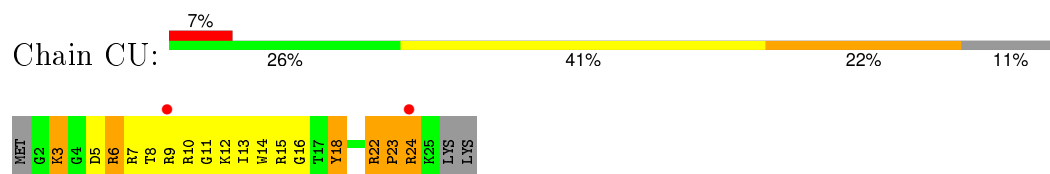
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



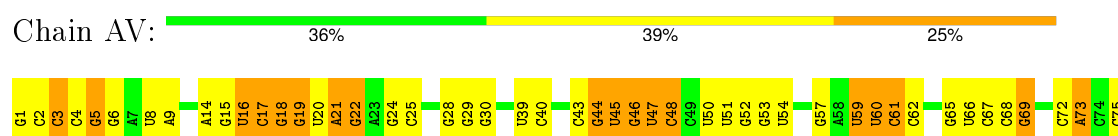
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

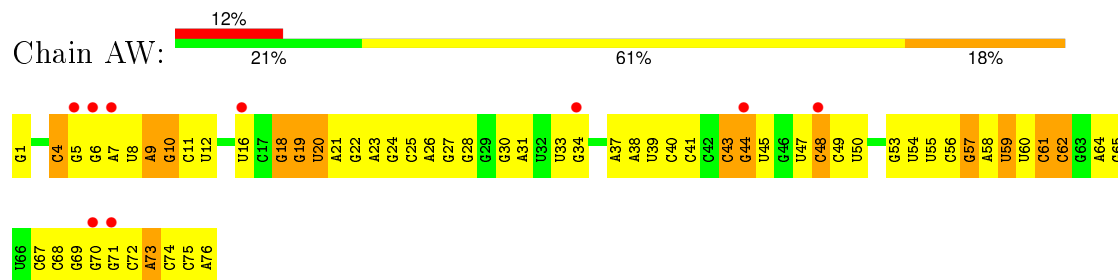


• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

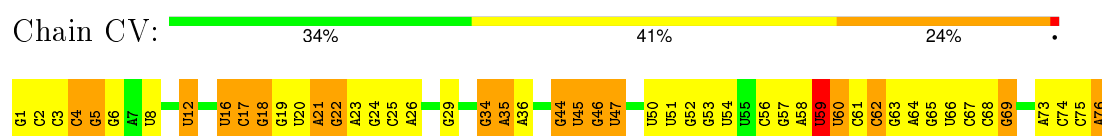


A76

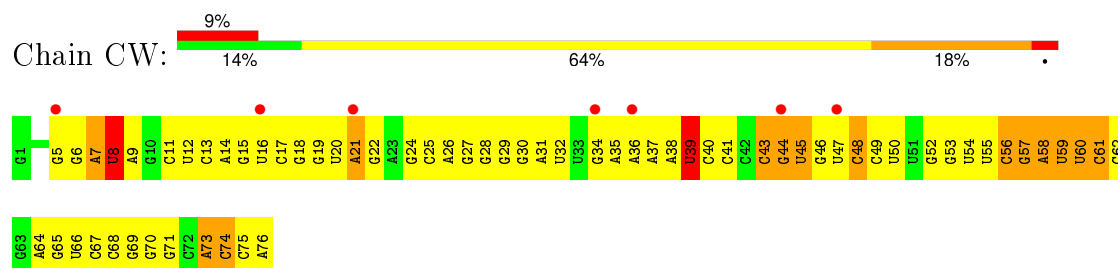
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



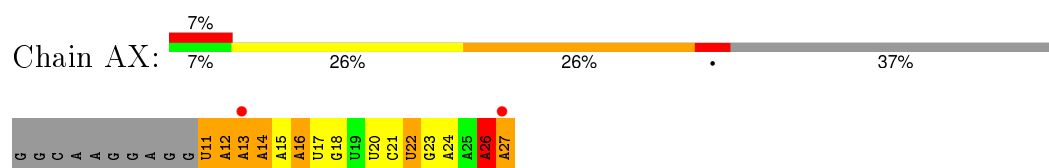
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



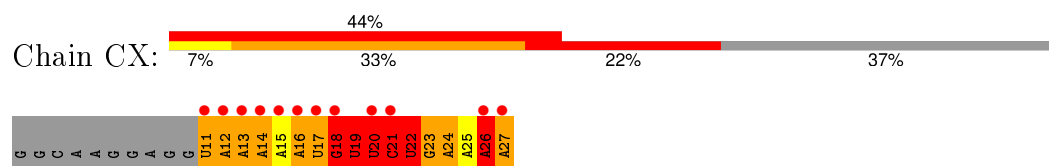
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



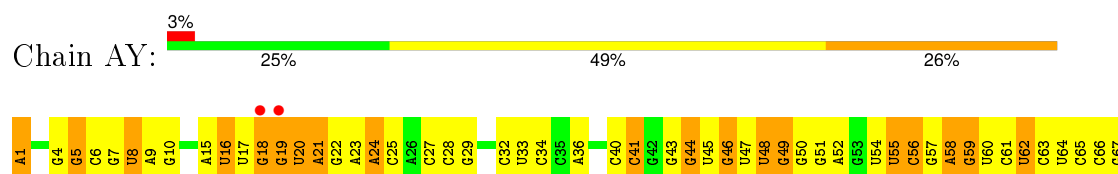
- Molecule 23: MRNA

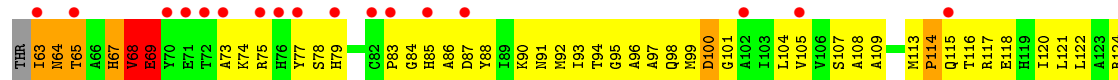


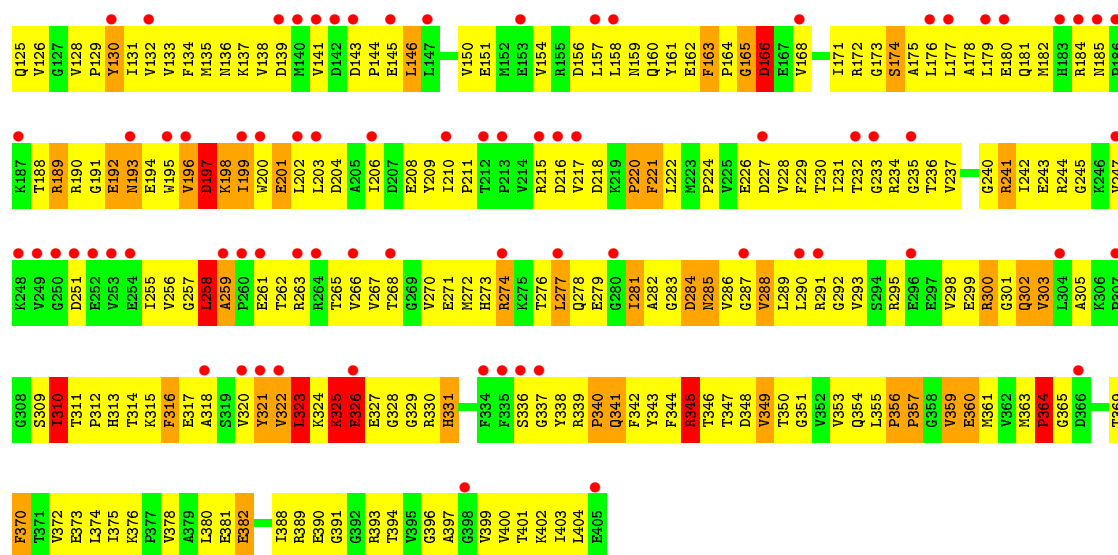
- Molecule 23: MRNA



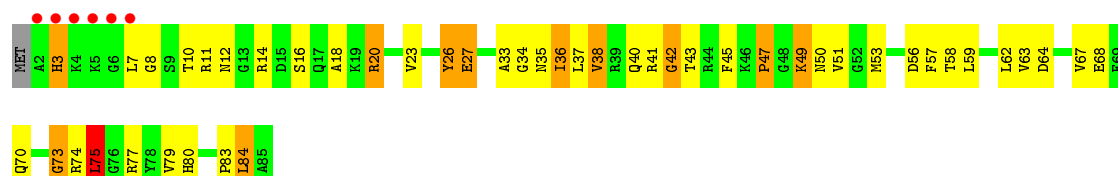
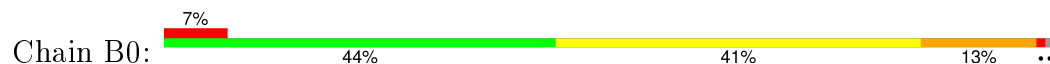
- Molecule 24: A-SITE TRNA G24A TRP-TRNA TRP



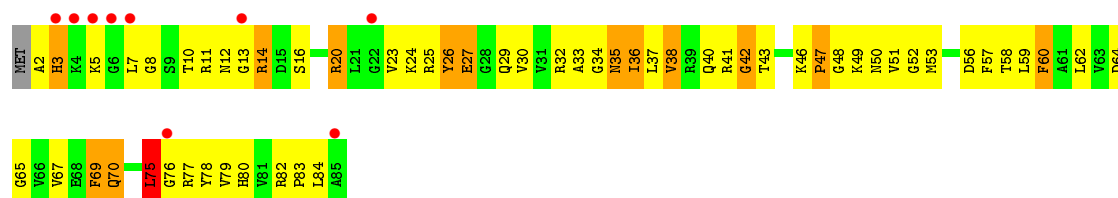




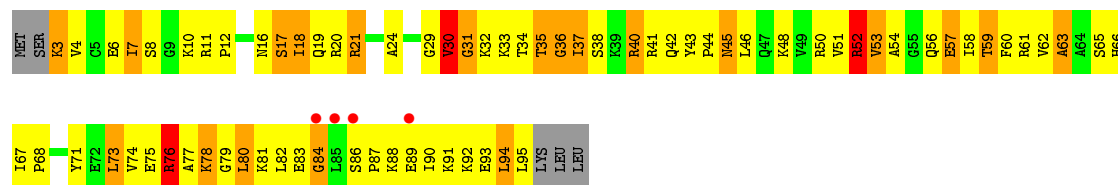
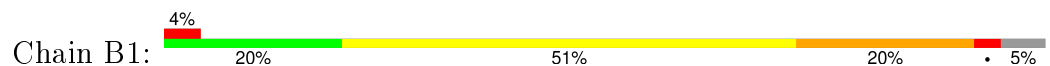
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



• Molecule 26: 50S RIBOSOMAL PROTEIN L27



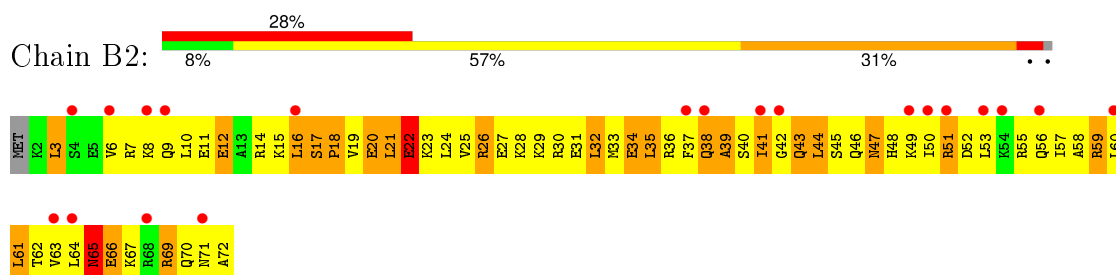
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



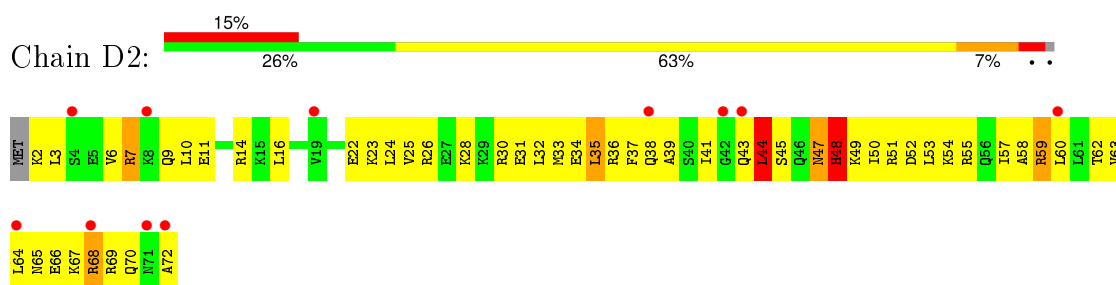
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



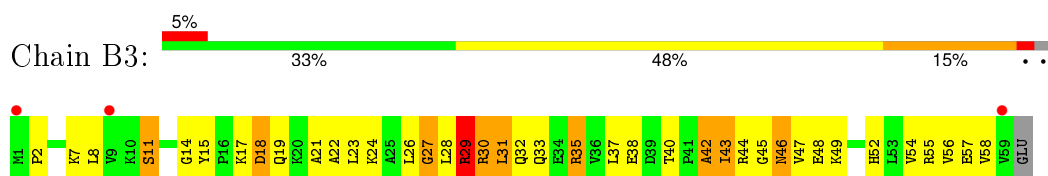
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



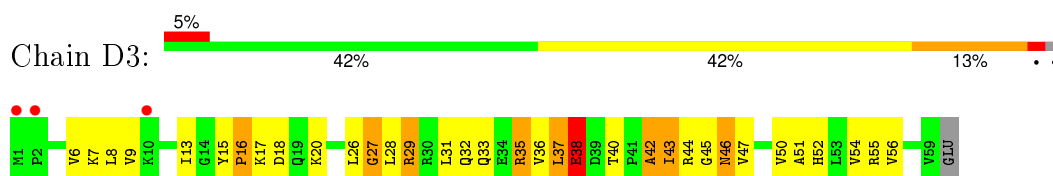
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



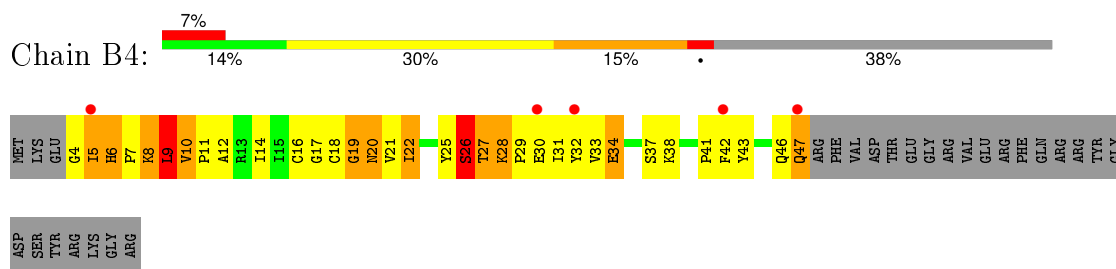
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



● Molecule 29: 50S RIBOSOMAL PROTEIN L30

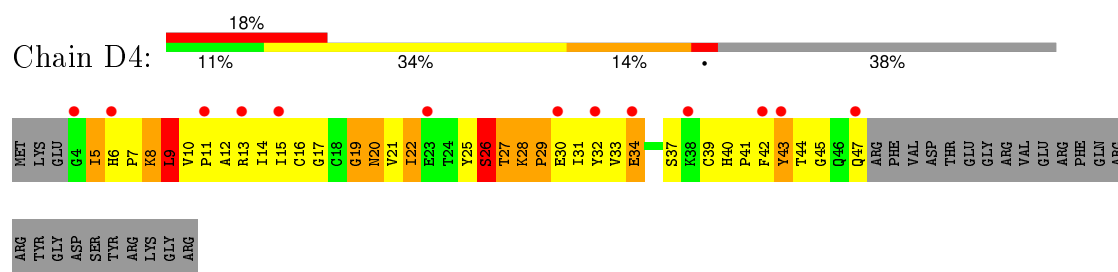


- Molecule 30: 50S RIBOSOMAL PROTEIN L31

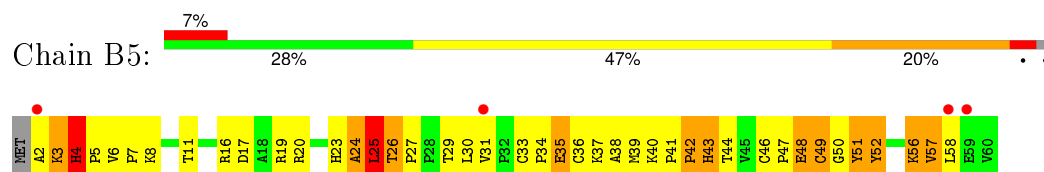


• Molecule 30: 50S RIBOSOMAL PROTEIN L31

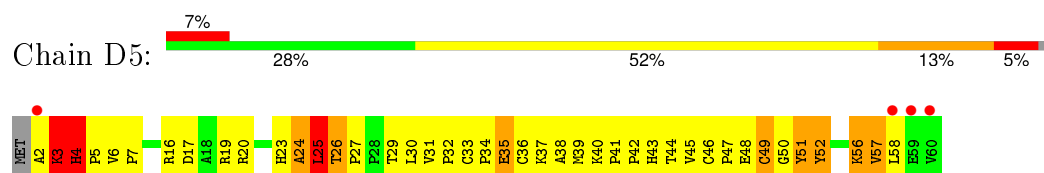




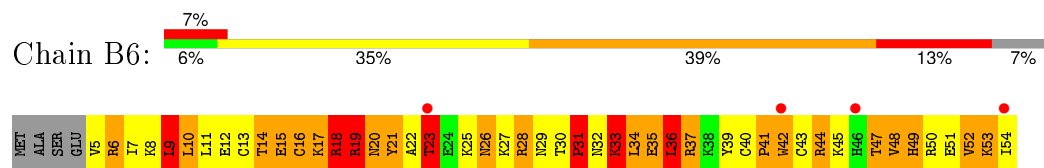
- Molecule 31: 50S RIBOSOMAL PROTEIN L32



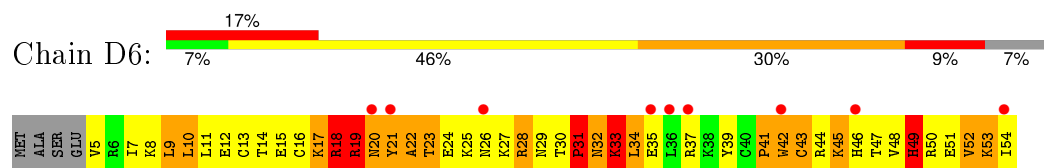
- Molecule 31: 50S RIBOSOMAL PROTEIN L32



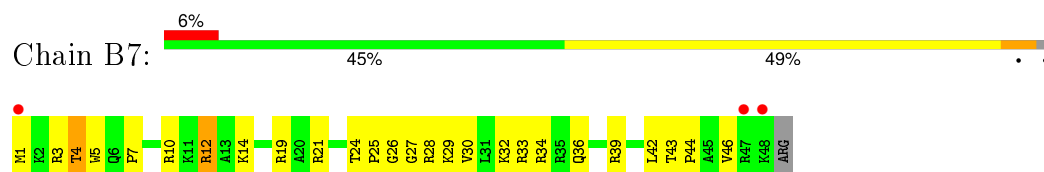
- Molecule 32: 50S RIBOSOMAL PROTEIN L33



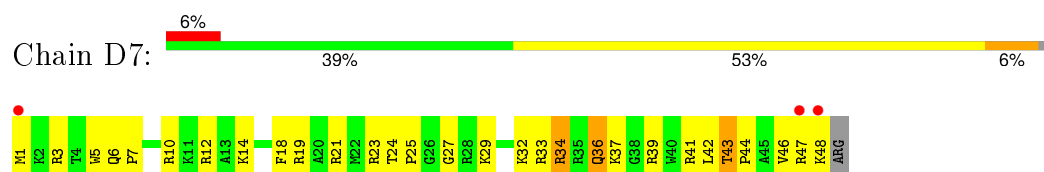
- Molecule 32: 50S RIBOSOMAL PROTEIN L33



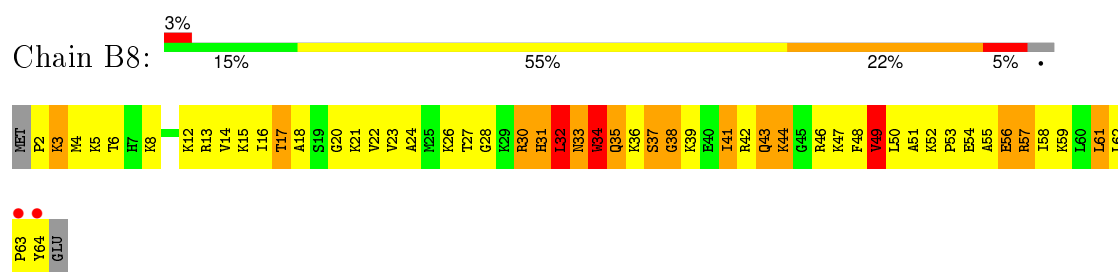
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



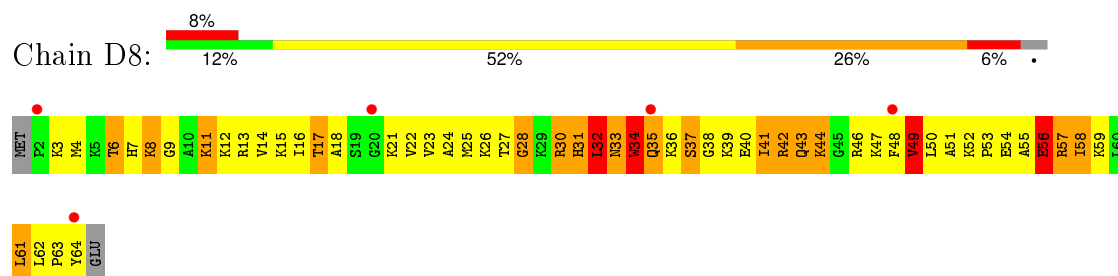
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



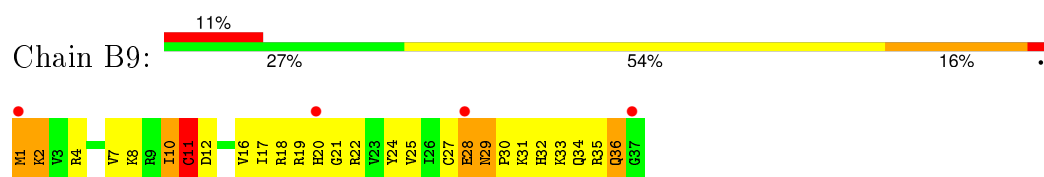
- Molecule 34: 50S RIBOSOMAL PROTEIN L35



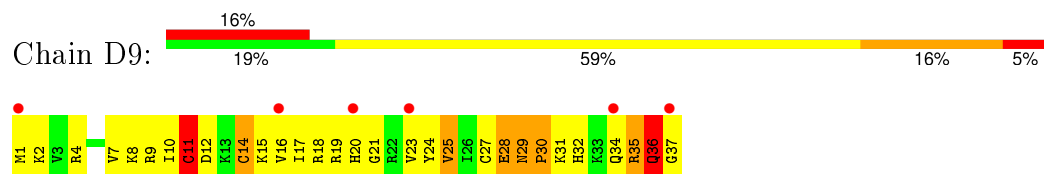
• Molecule 34: 50S RIBOSOMAL PROTEIN L35



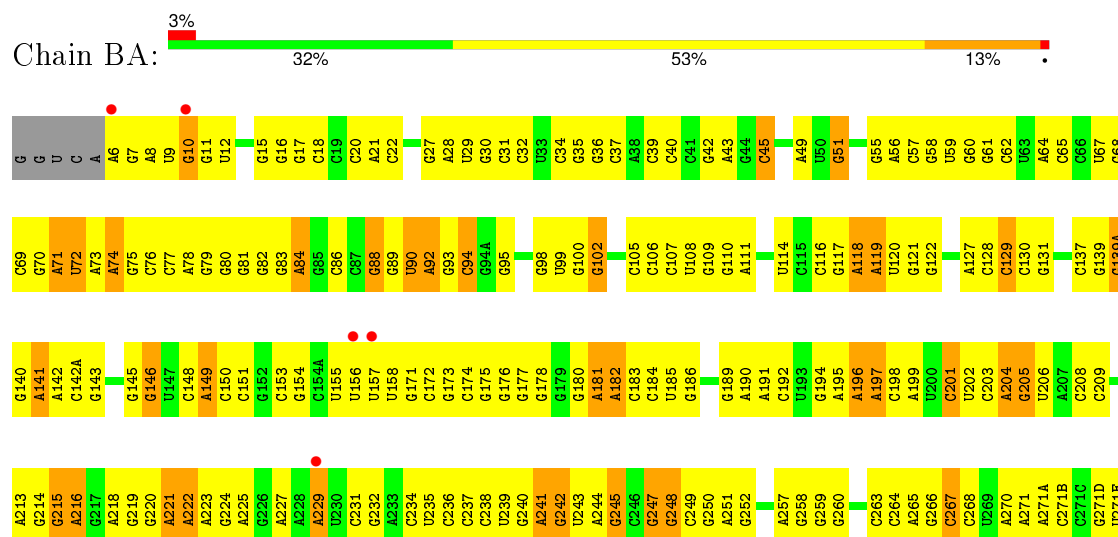
• Molecule 35: 50S RIBOSOMAL PROTEIN L36

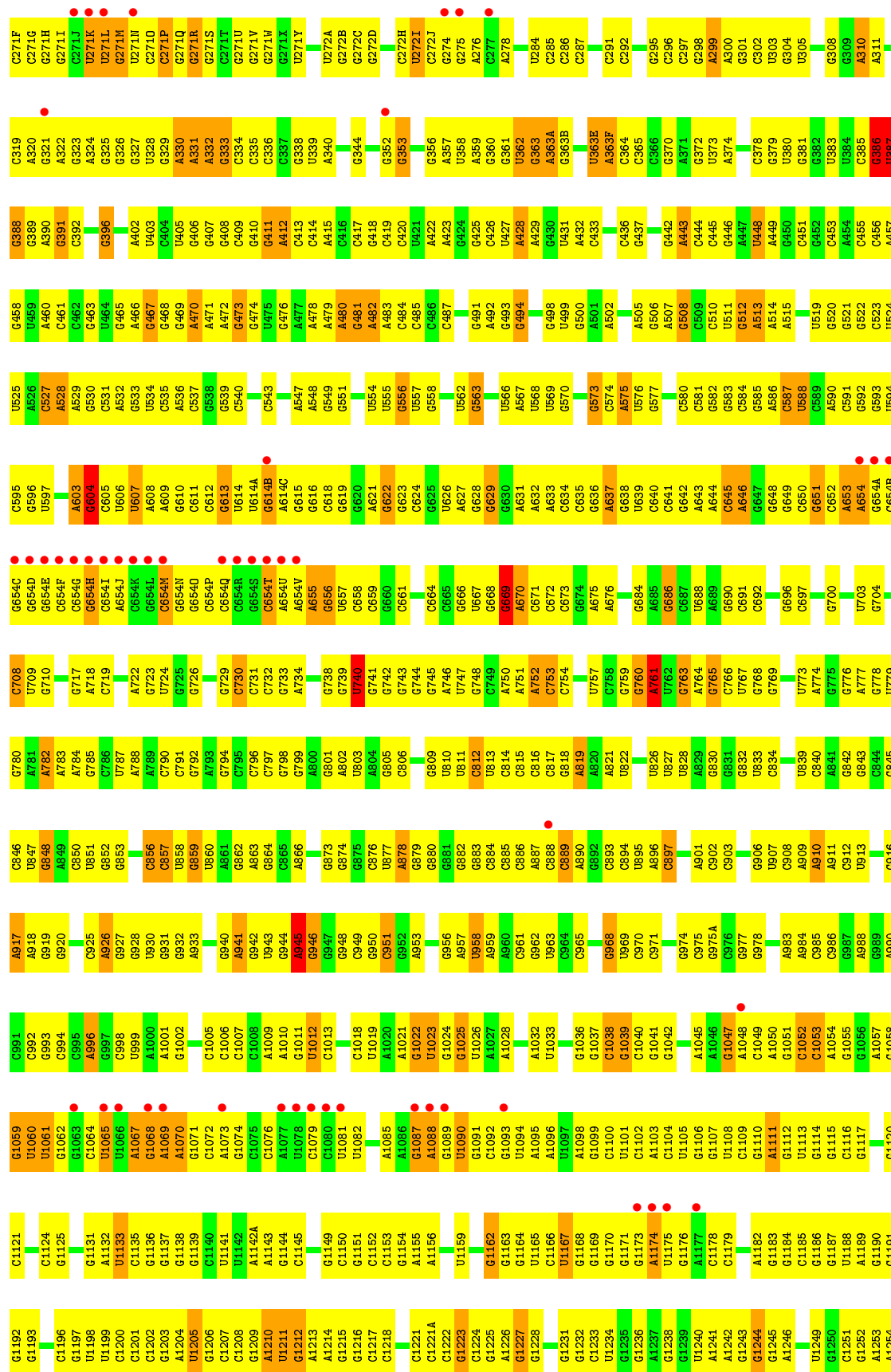


• Molecule 35: 50S RIBOSOMAL PROTEIN L36



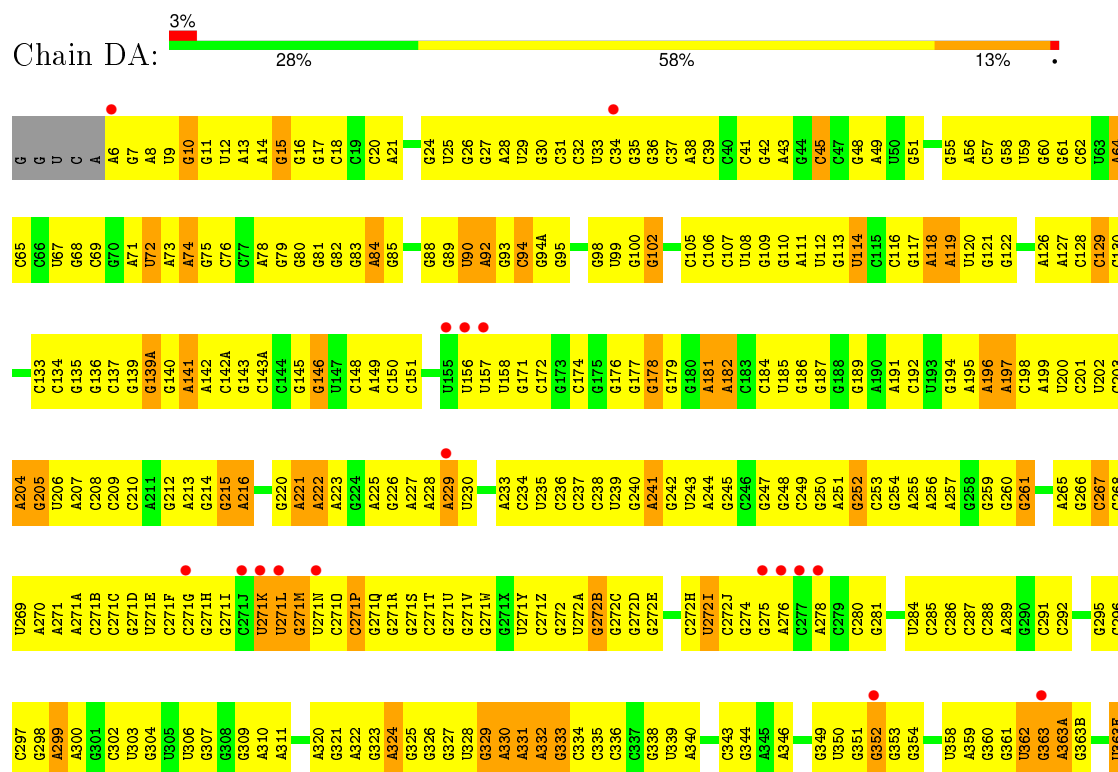
• Molecule 36: 23S RIBOSOMAL RNA





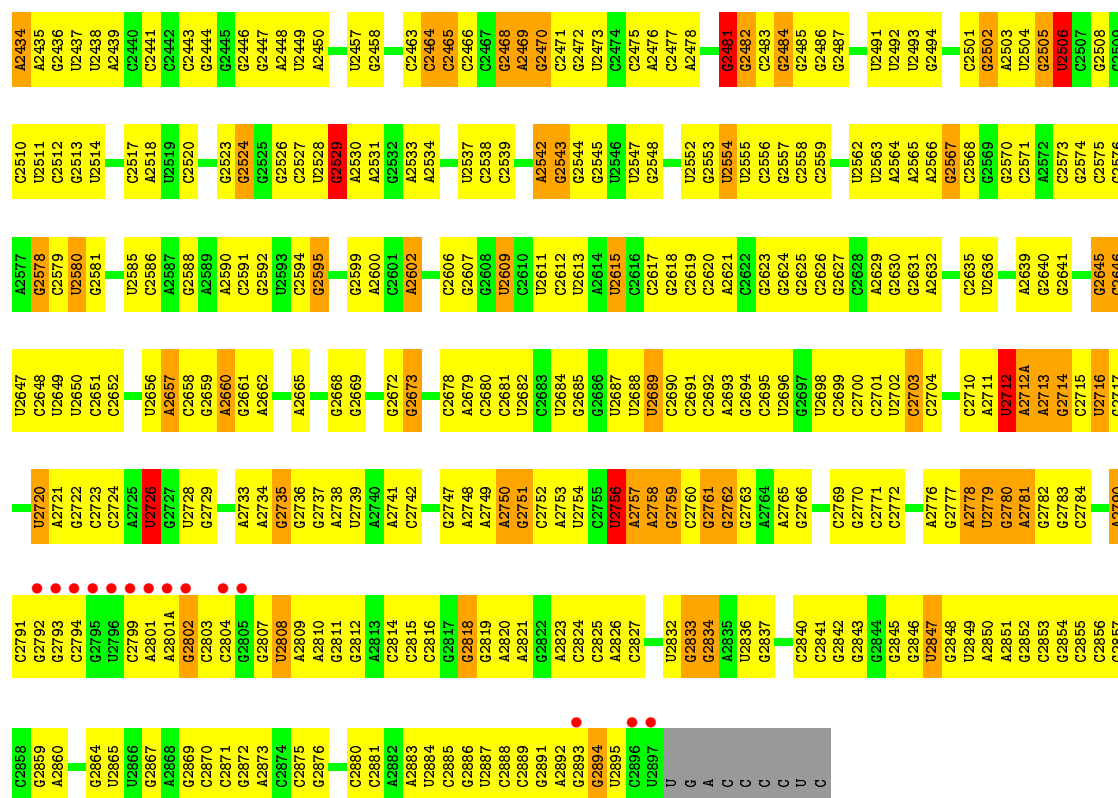


- Molecule 36: 23S RIBOSOMAL RNA



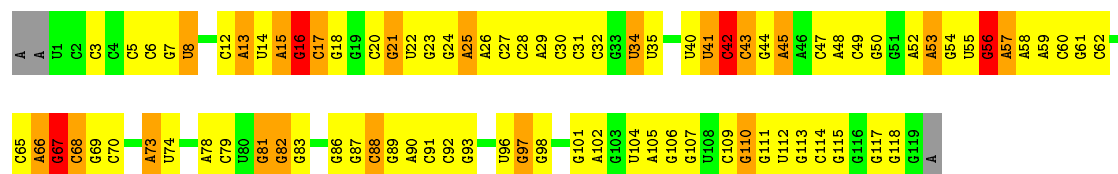
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G1314	G1245	A1177	G1107	G1047	A980	A900	U828	U757	A676	C634	C574	A506	C364
C1315	A1246	C1178	U1108	A1048	A981	A901	A829	C758	A677	C635	A575	G506	G365
U1316	A1247	C1179	C1109	A1049	A982	C902	G830	G759	C678	C636	U576	A507	C366
A1317	G1248	G1183	G1110	A1050	A983	C903	G831	G760	C679	A637	G577	G508	G370
C1318	U1248	G1184	A1111	G1051	A984	C904	G832	A761	A685	C638	A578	G442	A371
G1319	C1250	C1185	G1112	C1052	C985	U905	U833	U762	U686	U639	C579	A512	G372
C1320	G1186	G1187	U1113	C1053	C986	G906	C834	G763	G687	U639	C580	A513	U373
A1321	G1187	G1188	G1114	A1054	A987	U907	A835	A764	C688	C640	C581	A514	A374
C1322	A1188	G1189	G1115	G1055	A988	C908	G836	G765	A688	C645	C582	A515	C375
A1323	A1189	C1116	C1116	G1056	G989	A909	C837	G766	A689	C646	C583	C516	C376
G1324	U1255	G1190	G1120	A1057	A990	A910	C838	U767	G690	A646	C584	C517	C377
	G1256	G1191	G1121	G1058	C991	A911	U839	G768	C691	A647	C585	G518	C378
	C1257	G1192	C1121	G1059	C992	C912	C840	G769	C692	G648	A586	U519	G379
C1327	G1258	G1193	G1125	U1060	G993	U913		G770	C693	G649	C587	G520	U380
G1328	G1259		G1126	U1061	C994	C914	G845	G771	G694	C650	U588	G521	G381
U1329	C1260	G1196	A1126	G1062	C995	C915	C846	U772	U694	C651	C589	G522	G382
C1330	C1261	G1197	A1127	G1063	A996	G916	U847	G773	G695	C652	C590	C523	U383
A1331	A1262	U1198	G1131	C1064	G997	A917	G848	A774	C697	A653	C591	U524	U384
G1332	U1263	U1199	G1132	U1065	C998	A918	A849	G775	C698	G648	C592	G527	C385
	G1264	C1200	A1132	U1066	U999		C850	G776	U703	G654A	G593	C527	G386
A1336	A1265	C1201	U1133	A1067	A1000	C924	U851	A782	G704	C654B	U594	A528	U387
G1337	G1266	G1197	C1135	G1068	A1001	C925	G852	U783	A705	C654C	C595	A529	G388
A1338	A1267	U1197	G1136	A1069	A996	A926	U847	A784	G706	C654D	G596	G530	G389
	C1270	U1198	G1137	A1070	G997	G927	G848	G785	G707	C654E	U597	C531	A390
U1341	A1268	U1199	G1138	G1071	C1005	G928	C856		C708	C654F	G598	A532	G391
	G1271	C1202	A1139	C1072	C1006		C857		G709	C654G	G599	G533	C392
G1344	A1272	G1206	C1140	A1073	A1010	G932	U858	G786	U710	C654H	G600	U534	G396
C1345	U1273	C1207	U1141	G1074	A1011	A933	U859	U787	G711	C654I	C601	C535	G397
G1346	A1274	C1208	U1142	U1075	G1012	U940	U860	A789	G712	A654J	A596	A536	G398
A1347	G1275	A1210	A1142A	C1076	U1012	G941	A861	C790	G713	C654K	A603	C537	G399
C1348	A1276	U1211	A1143	U1077	C1013	A941	G862			C654L	G604	G540	G400
A1349	G1277	C1212	G1144	U1078	U1014	G942	A863	G792	C720	C654M	C605	A470	A401
C1350	A1278	A1213	C1145	C1079	U1014	U944	G864	A793	A722	C654N	U606	A471	A402
G1352	G1279	G1214		C1080	C1018	A945	A866	C796	G723	C654O	U607	C543	U403
A1353		G1215	G1149	U1081	U1019	G946		C797	U724	C654P	A608	A547	C404
A1354	A1286	G1216	C1150	U1082	A1020		G874			C654Q	A609	A548	U405
G1355	A1287	C1217	G1151	U1083	A1021	A953	G875	A802	G729	C654R	C610	G549	G406
C1356	U1288	C1218	C1152	A1084	G1022	G954	C876	U803	C730	C654S	C611	G551	G407
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A1308	A1308	A1241	A1173	U1103	G1042		C897						
G1309	G1309	G1242	U1174	C1104		G978	C898						
G1381	G1310	G1243	U1175	U1105	A1045								

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G2373	G2308	U2244	A2171	C2040	A1970	C1894	U1818	C1751	C1657	U1590	C1516	A1449	C1383
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A2376	A2311	A2247	C2174	C2043	G1973		A1821	C1754			G1519	U1485	C1386
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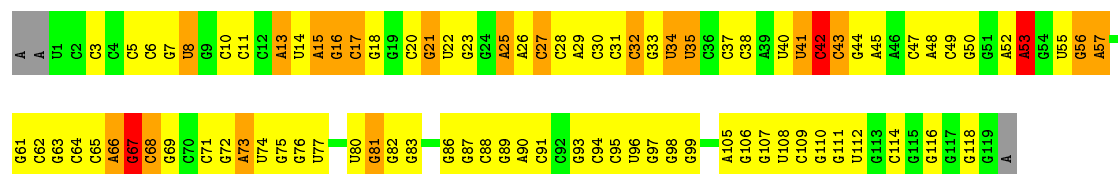
• Molecule 37: 5S RIBOSOMAL RNA

Chain BB: 26% 52% 16%



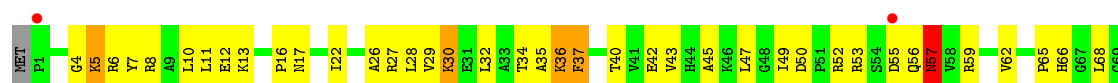
• Molecule 37: 5S RIBOSOMAL RNA

Chain DB: 25% 55% 16%

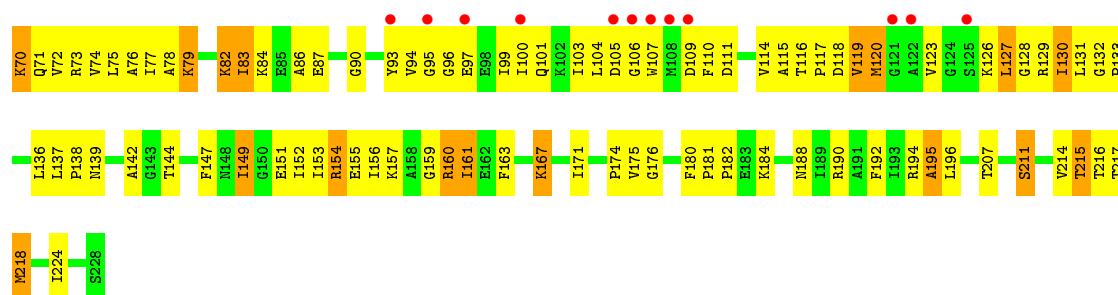


• Molecule 38: 50S RIBOSOMAL PROTEIN L1

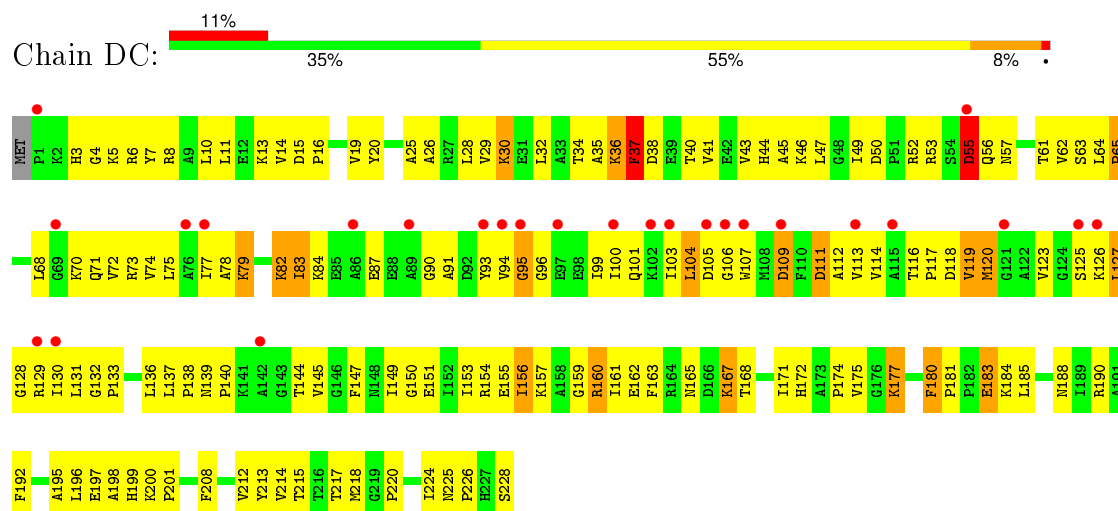
Chain BC: 6% 43% 47% 9%



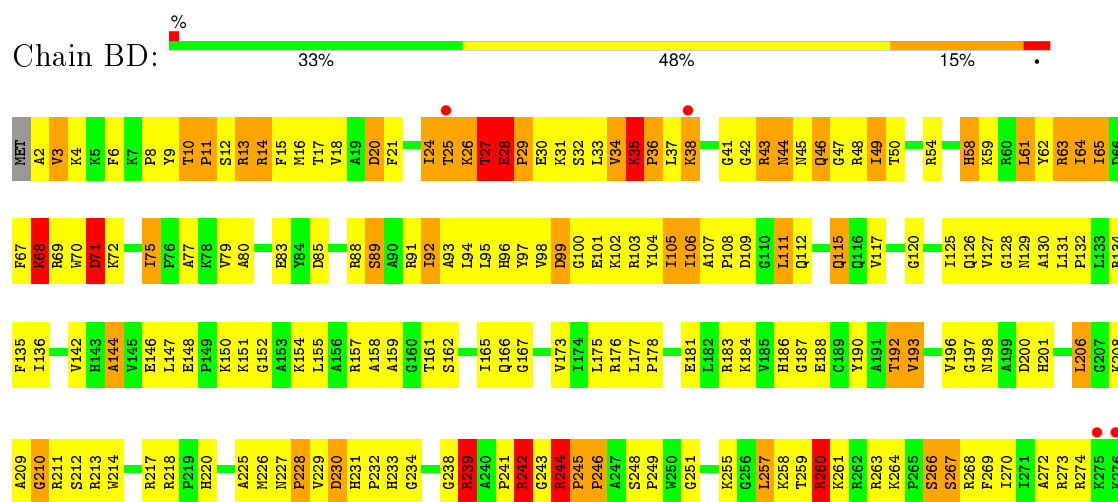




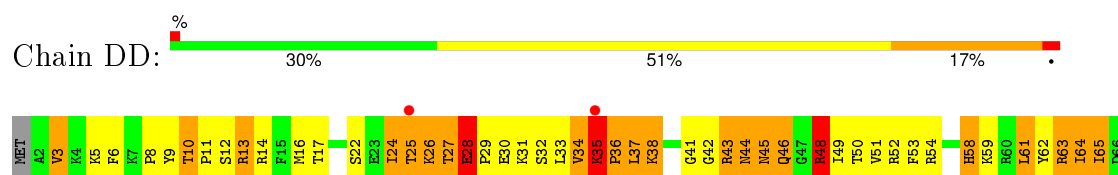
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

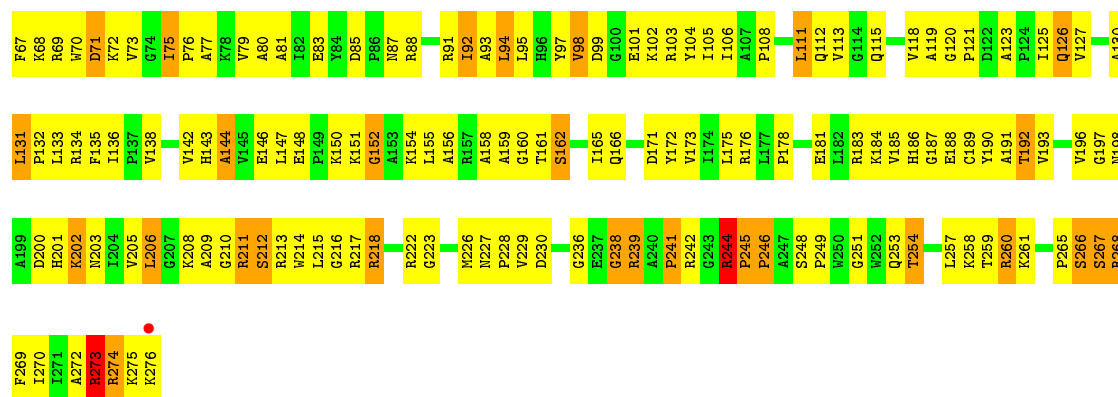


• Molecule 39: 50S RIBOSOMAL PROTEIN L2

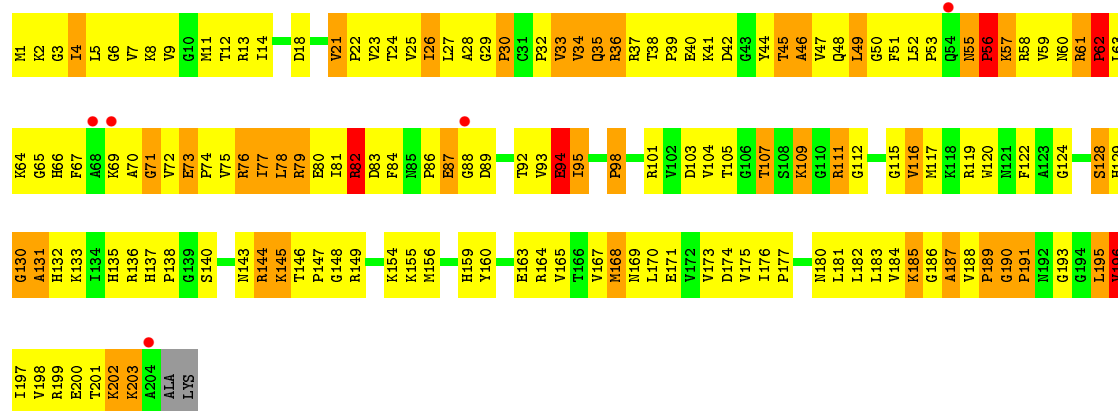


• Molecule 39: 50S RIBOSOMAL PROTEIN L2

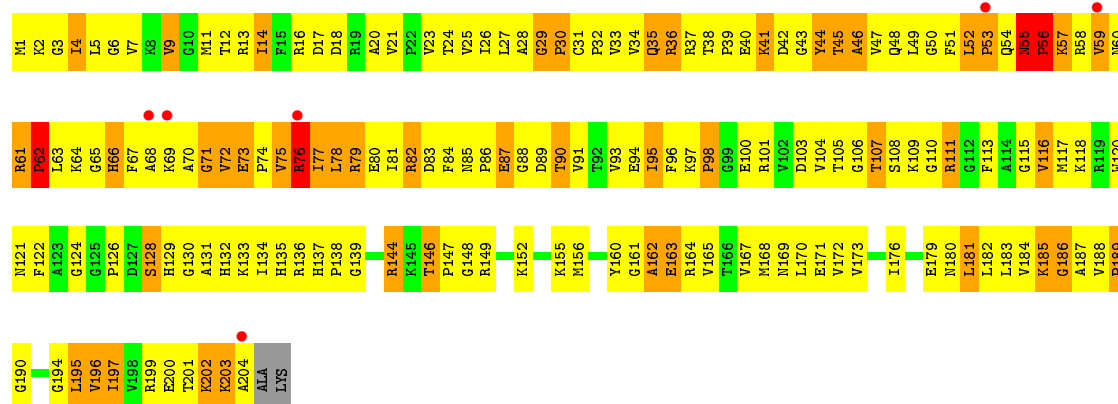




• Molecule 40: 50S RIBOSOMAL PROTEIN L3

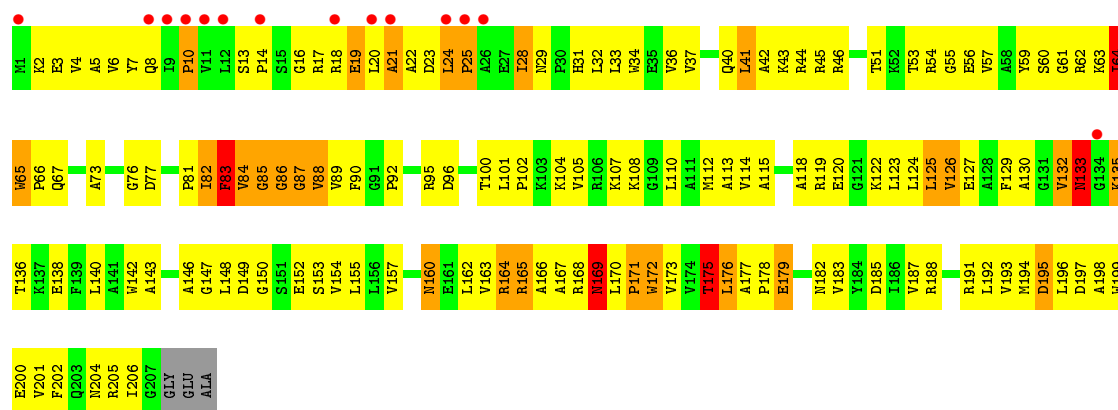


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

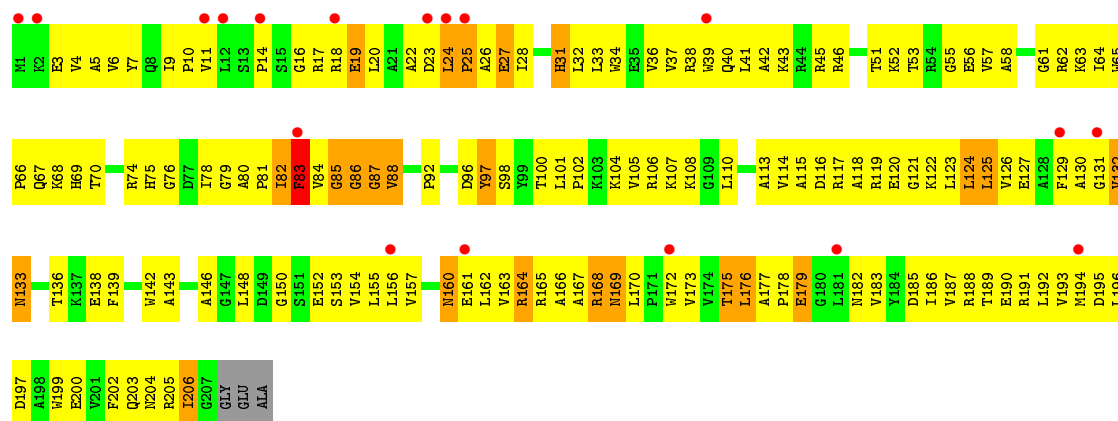


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

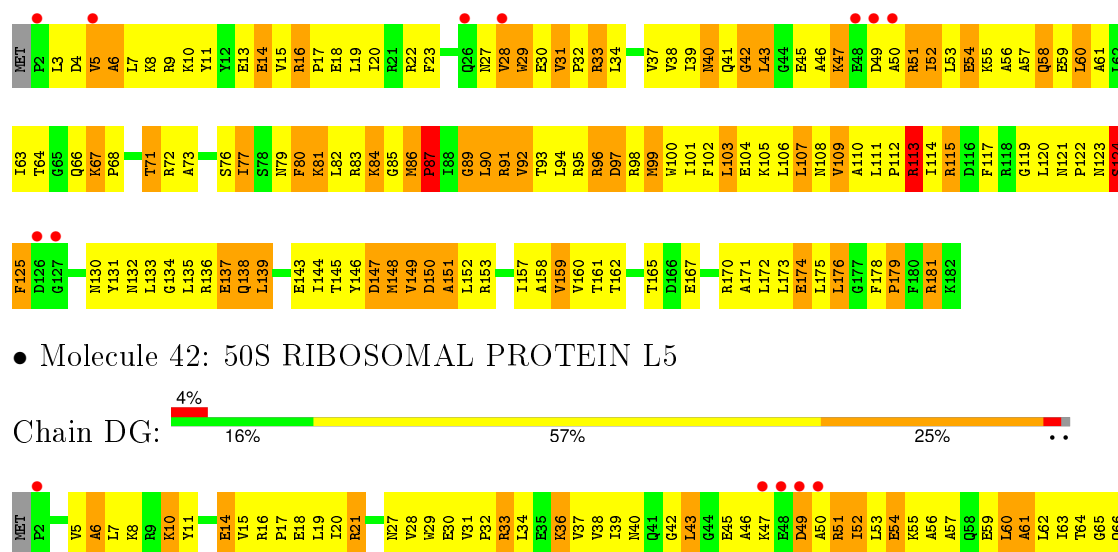




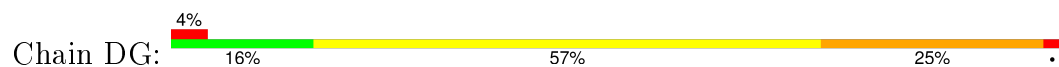
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

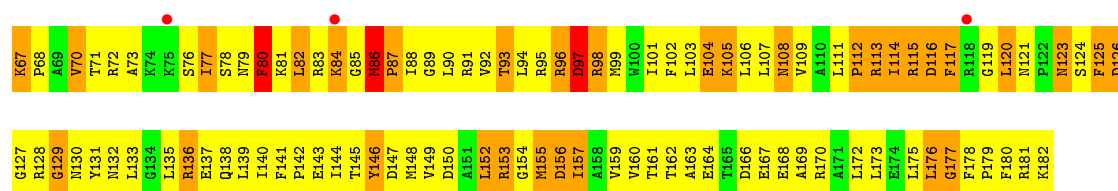


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

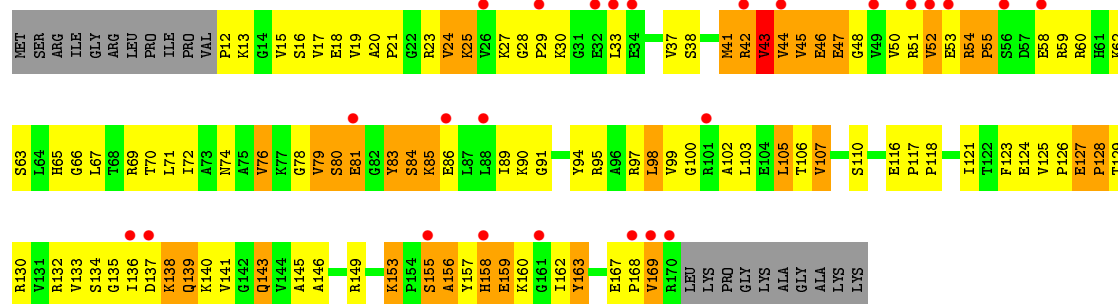


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

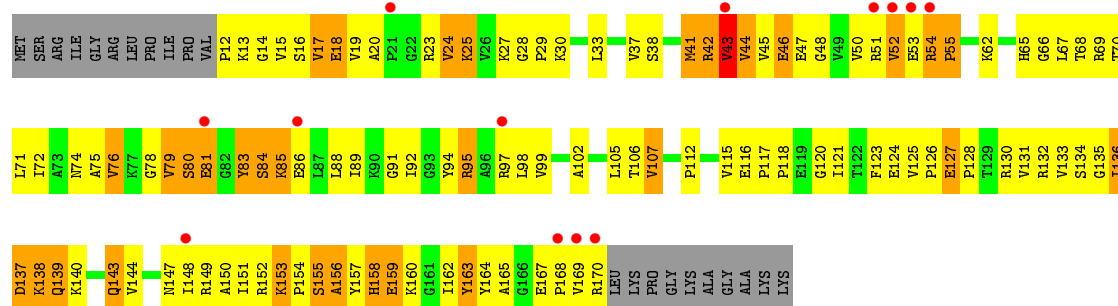




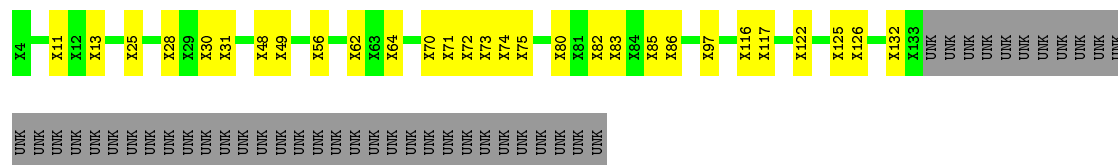
• Molecule 43: 50S RIBOSOMAL PROTEIN L6



• Molecule 43: 50S RIBOSOMAL PROTEIN L6



• Molecule 44: 50S RIBOSOMAL PROTEIN L10



• Molecule 44: 50S RIBOSOMAL PROTEIN L10





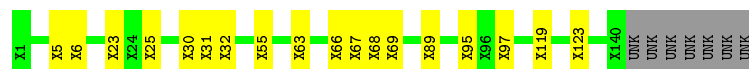
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK: 80% 16% 5%



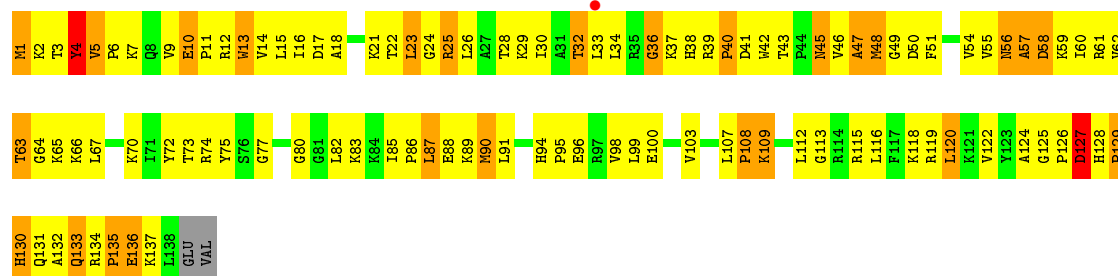
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain DK: 83% 12% 5%



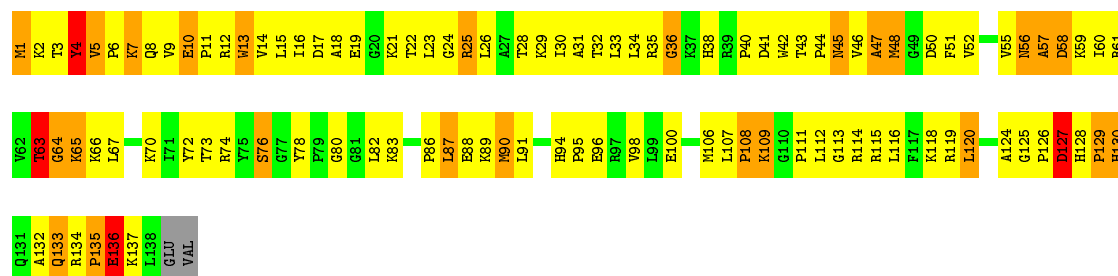
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN: 23% 56% 19% ..



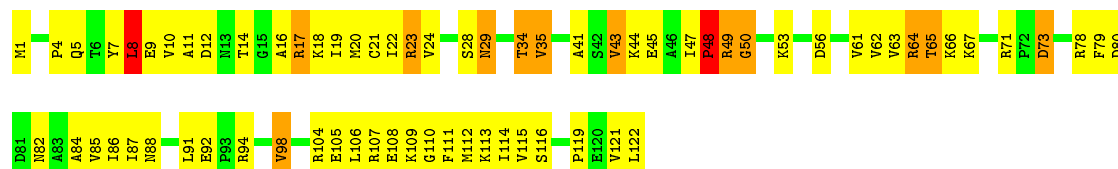
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN: 24% 54% 18% ..



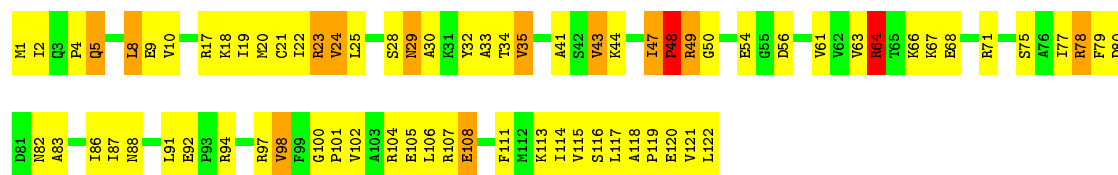
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO: 42% 47% 10% .




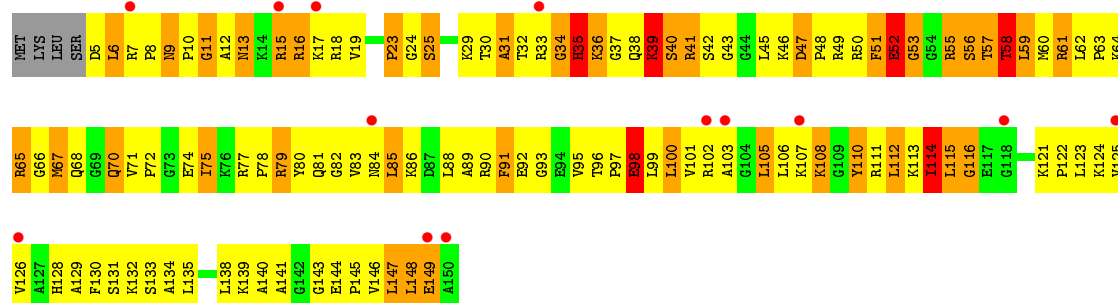
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO: 




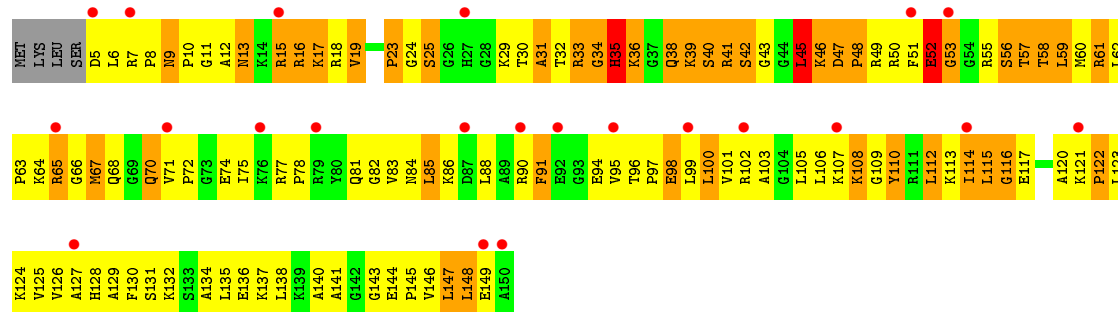
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP: 



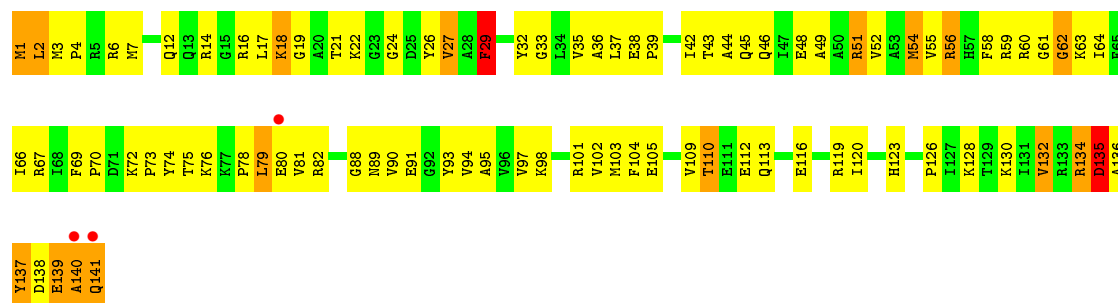
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP: 

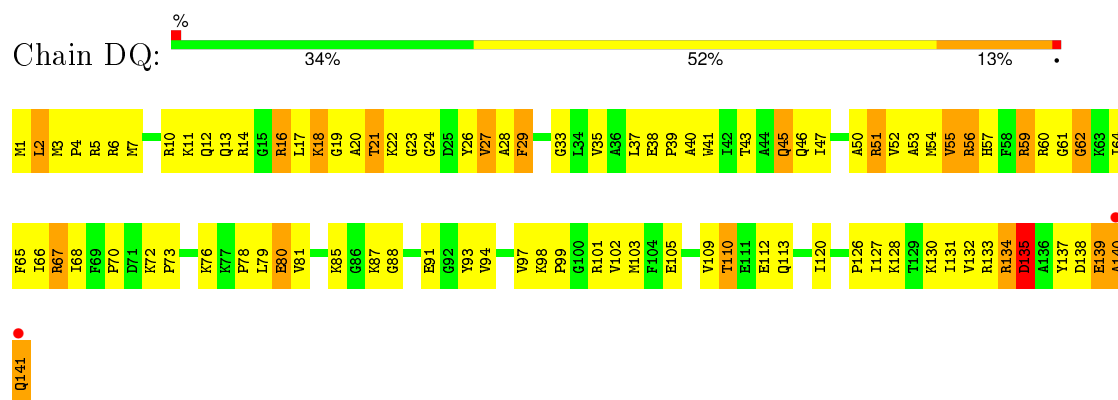


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

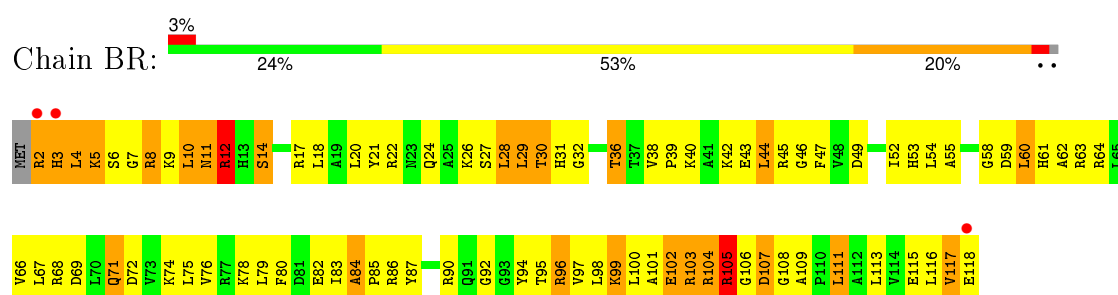
Chain BQ: 



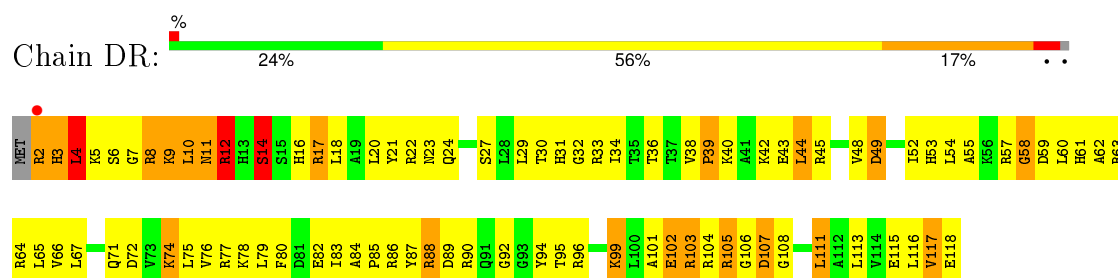
- Molecule 49: 50S RIBOSOMAL PROTEIN L16



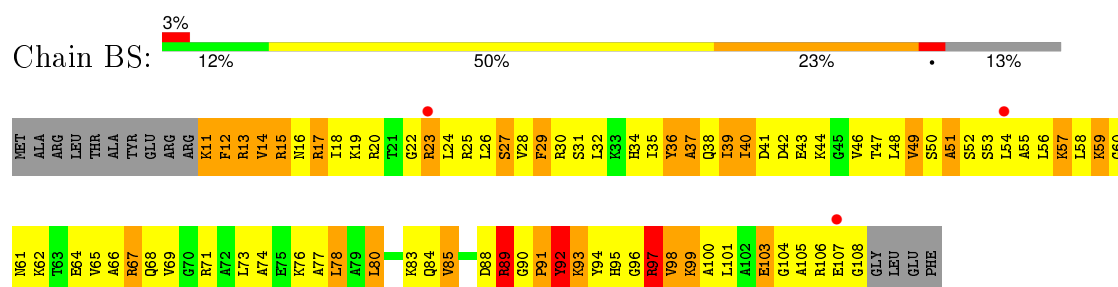
- Molecule 50: 50S RIBOSOMAL PROTEIN L17



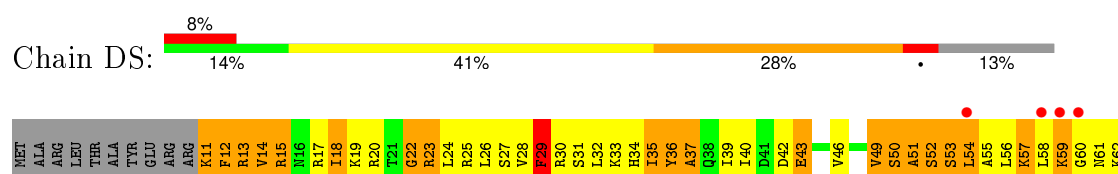
- Molecule 50: 50S RIBOSOMAL PROTEIN L17

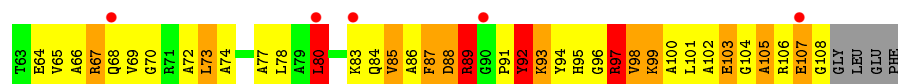


- Molecule 51: 50S RIBOSOMAL PROTEIN L18

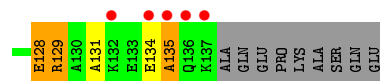
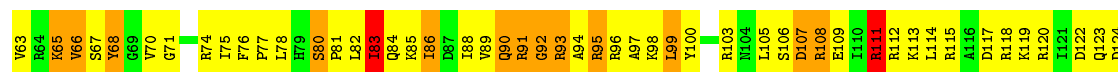
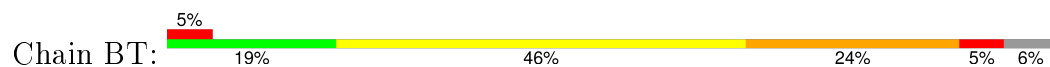


- Molecule 51: 50S RIBOSOMAL PROTEIN L18

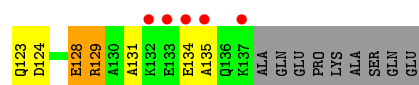
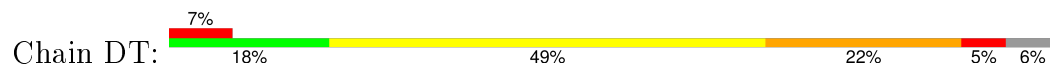




• Molecule 52: 50S RIBOSOMAL PROTEIN L19



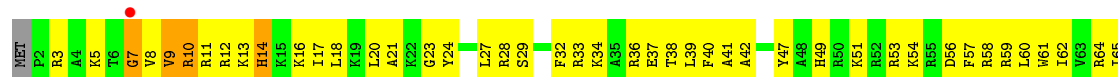
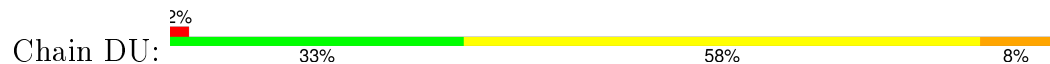
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



• Molecule 53: 50S RIBOSOMAL PROTEIN L20

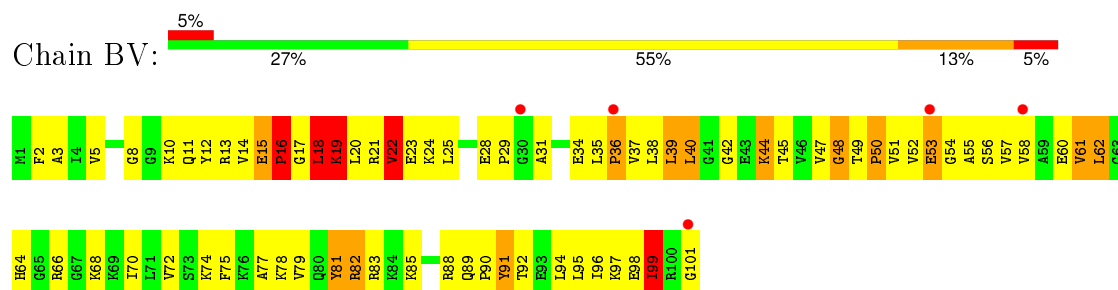


• Molecule 53: 50S RIBOSOMAL PROTEIN L20

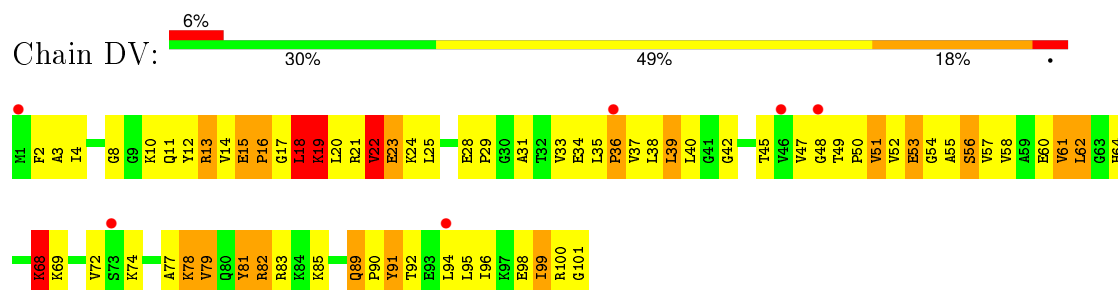




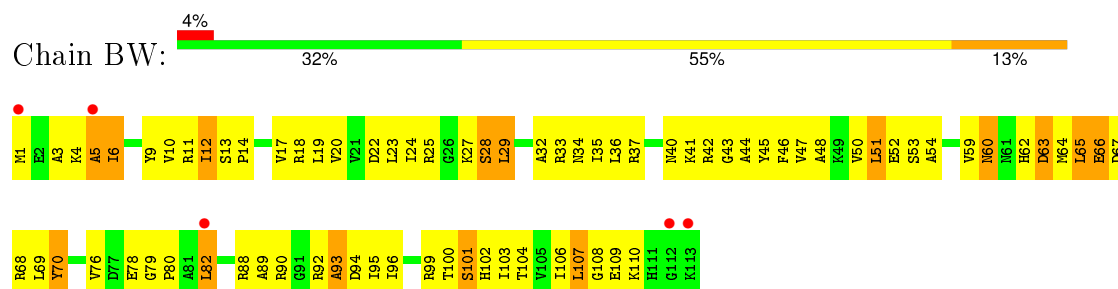
- Molecule 54: 50S RIBOSOMAL PROTEIN L21



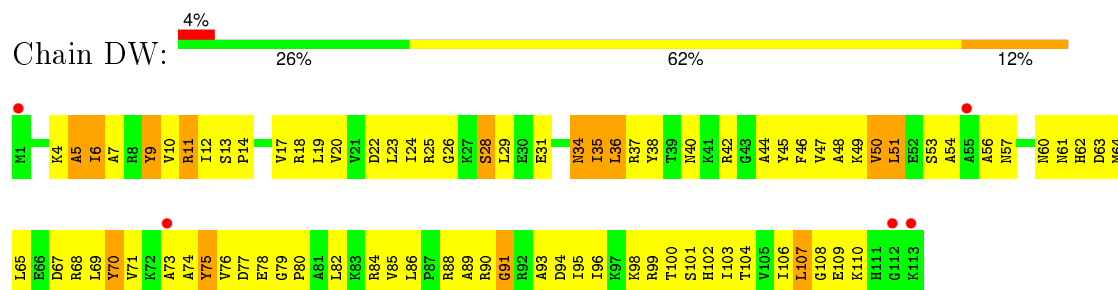
- Molecule 54: 50S RIBOSOMAL PROTEIN L21



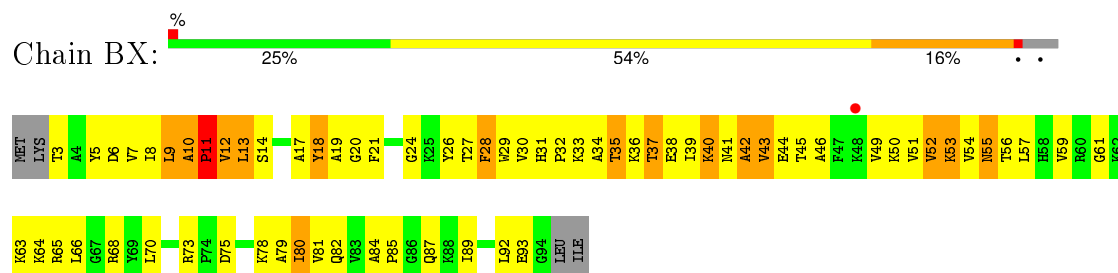
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



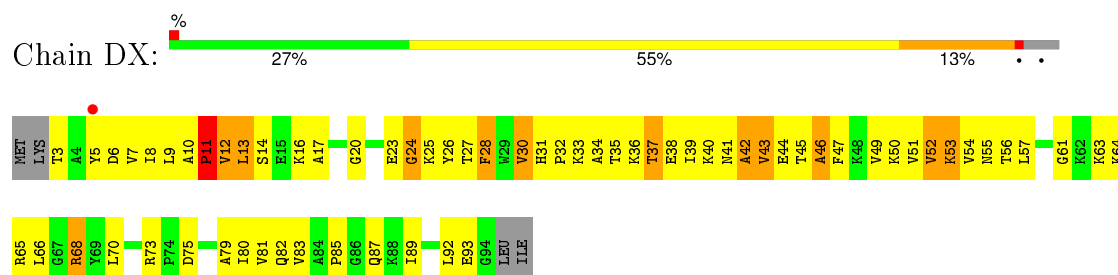
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



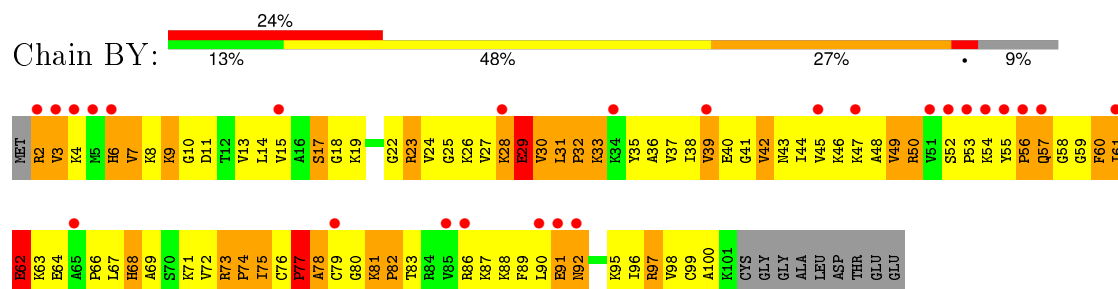
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



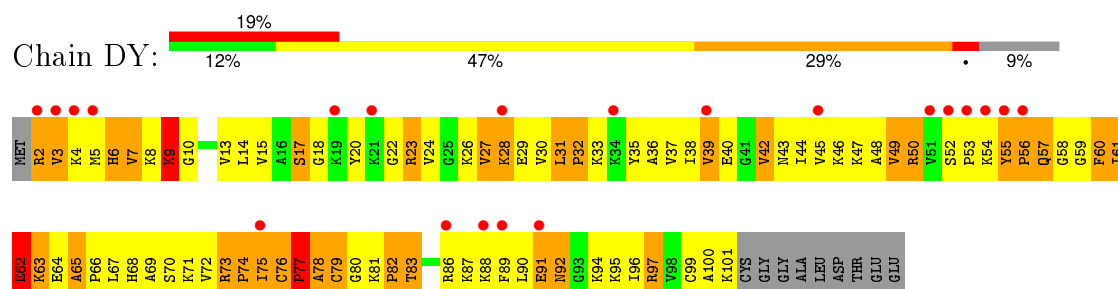
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



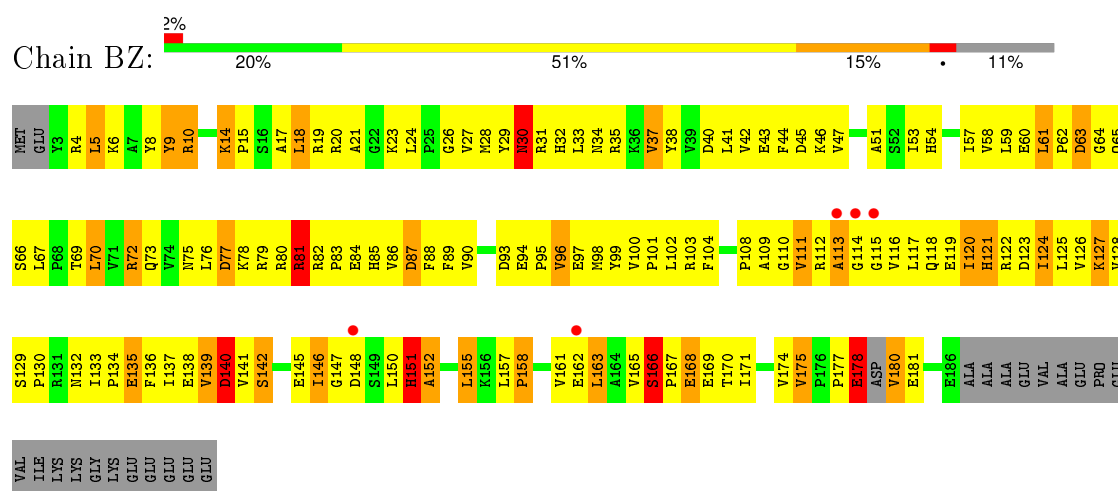
- Molecule 57: 50S RIBOSOMAL PROTEIN L24



- Molecule 57: 50S RIBOSOMAL PROTEIN L24



- Molecule 58: 50S RIBOSOMAL PROTEIN L25



- Molecule 58: 50S RIBOSOMAL PROTEIN L25



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	289.90Å 269.40Å 404.50Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-3.10) 91.8 (49.22-2.80)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.238 , 0.275 0.238 , 0.276	Depositor DCC
$R_{free}$ test set	55079 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 74.4	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	2 of 1394902 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	307194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: OMC, GDP, ZN, H2U, KIR, MIA, 4SU, 7MG, 5MU, PSU

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	0.67	10/36190 (0.0%)	0.79	44/56486 (0.1%)
1	CA	0.54	3/36190 (0.0%)	0.74	25/56486 (0.0%)
2	AB	0.55	0/1935	0.76	0/2609
2	CB	0.43	0/1935	0.70	0/2609
3	AC	0.65	1/1636 (0.1%)	0.83	0/2205
3	CC	0.43	0/1636	0.70	0/2205
4	AD	0.48	1/1733 (0.1%)	0.75	1/2318 (0.0%)
4	CD	0.44	1/1733 (0.1%)	0.71	0/2318
5	AE	0.65	1/1162 (0.1%)	0.81	0/1564
5	CE	0.52	0/1162	0.77	0/1564
6	AF	0.50	0/856	0.70	1/1154 (0.1%)
6	CF	0.38	0/856	0.67	0/1154
7	AG	0.52	0/1276	0.73	1/1709 (0.1%)
7	CG	0.39	0/1276	0.63	0/1709
8	AH	0.57	0/1136	0.80	0/1527
8	CH	0.49	0/1136	0.79	0/1527
9	AI	0.55	0/1029	0.82	0/1379
9	CI	0.41	0/1029	0.68	0/1379
10	AJ	0.55	0/807	0.85	0/1085
10	CJ	0.40	0/807	0.75	1/1085 (0.1%)
11	AK	0.60	1/900 (0.1%)	0.80	0/1213
11	CK	0.46	0/900	0.76	1/1213 (0.1%)
12	AL	0.52	0/986	0.82	1/1320 (0.1%)
12	CL	0.44	0/986	0.77	0/1320
13	AM	0.51	0/998	0.80	0/1336
13	CM	0.39	0/998	0.74	0/1336
14	AN	0.70	1/501 (0.2%)	0.98	1/664 (0.2%)
14	CN	0.53	1/501 (0.2%)	0.86	1/664 (0.2%)
15	AO	0.52	0/745	0.77	0/992
15	CO	0.44	0/745	0.66	0/992
16	AP	0.46	0/716	0.74	0/963
16	CP	0.40	0/716	0.70	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.54	0/836	0.76	0/1117
17	CQ	0.45	0/836	0.76	0/1117
18	AR	0.56	0/579	0.73	0/768
18	CR	0.46	0/579	0.72	0/768
19	AS	0.55	0/642	0.76	0/865
19	CS	0.40	0/642	0.76	0/865
20	AT	0.42	0/765	0.69	0/1007
20	CT	0.36	0/765	0.71	0/1007
21	AU	0.55	0/212	0.87	0/277
21	CU	0.48	0/212	0.80	0/277
22	AV	0.68	0/1809	0.79	0/2819
22	AW	0.47	0/1809	0.74	0/2819
22	CV	0.92	5/1809 (0.3%)	0.90	7/2819 (0.2%)
22	CW	0.41	0/1809	0.73	0/2819
23	AX	0.79	0/405	0.91	2/629 (0.3%)
23	CX	1.78	13/405 (3.2%)	1.64	16/629 (2.5%)
24	AY	0.49	1/1618 (0.1%)	0.71	0/2514
24	CY	0.64	2/1618 (0.1%)	0.76	0/2514
25	AZ	0.84	12/3042 (0.4%)	0.99	15/4129 (0.4%)
25	CZ	0.90	14/3042 (0.5%)	1.02	17/4129 (0.4%)
26	B0	0.47	0/671	0.78	0/892
26	D0	0.42	0/671	0.74	0/892
27	B1	0.51	0/738	0.81	1/981 (0.1%)
27	D1	0.42	0/738	0.76	0/981
28	B2	0.38	0/600	0.73	0/793
28	D2	0.35	0/600	0.60	0/793
29	B3	0.40	0/472	0.67	0/634
29	D3	0.38	0/472	0.68	0/634
30	B4	0.46	0/349	0.66	0/474
30	D4	0.51	0/349	0.62	0/474
31	B5	0.44	0/473	0.73	0/639
31	D5	0.43	0/473	0.74	0/639
32	B6	0.70	0/440	0.94	0/586
32	D6	0.58	0/440	0.85	0/586
33	B7	0.49	0/426	0.73	0/561
33	D7	0.44	0/426	0.74	1/561 (0.2%)
34	B8	0.58	0/515	0.89	1/679 (0.1%)
34	D8	0.52	0/515	0.87	1/679 (0.1%)
35	B9	0.56	0/310	0.73	0/407
35	D9	0.69	1/310 (0.3%)	0.81	0/407
36	BA	0.56	7/69976 (0.0%)	0.74	36/109244 (0.0%)
36	DA	0.51	3/69976 (0.0%)	0.73	25/109244 (0.0%)
37	BB	0.51	0/2853	0.77	3/4451 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DB	0.48	0/2853	0.76	0/4451
38	BC	0.46	2/1774 (0.1%)	0.65	0/2391
38	DC	0.41	2/1774 (0.1%)	0.61	0/2391
39	BD	0.62	0/2195	0.93	3/2955 (0.1%)
39	DD	0.51	0/2195	0.86	1/2955 (0.0%)
40	BE	0.46	0/1596	0.77	1/2153 (0.0%)
40	DE	0.45	0/1596	0.75	1/2153 (0.0%)
41	BF	0.40	0/1658	0.65	0/2244
41	DF	0.40	0/1658	0.64	0/2244
42	BG	0.48	0/1499	0.78	0/2016
42	DG	0.40	0/1499	0.70	0/2016
43	BH	0.37	0/1245	0.66	0/1682
43	DH	0.35	0/1245	0.66	0/1682
46	BN	0.39	0/1131	0.72	0/1525
46	DN	0.39	0/1131	0.70	0/1525
47	BO	0.53	0/943	0.74	1/1269 (0.1%)
47	DO	0.51	1/943 (0.1%)	0.74	0/1269
48	BP	0.46	0/1131	0.96	4/1504 (0.3%)
48	DP	0.42	0/1131	0.93	4/1504 (0.3%)
49	BQ	0.52	0/1143	0.73	0/1527
49	DQ	0.51	0/1143	0.69	0/1527
50	BR	0.41	0/974	0.81	2/1302 (0.2%)
50	DR	0.38	0/974	0.77	2/1302 (0.2%)
51	BS	0.45	0/778	0.79	0/1036
51	DS	0.41	0/778	0.76	1/1036 (0.1%)
52	BT	0.48	0/1155	0.78	1/1542 (0.1%)
52	DT	0.44	0/1155	0.77	1/1542 (0.1%)
53	BU	0.42	0/975	0.69	0/1297
53	DU	0.44	0/975	0.69	0/1297
54	BV	0.38	0/790	0.68	0/1057
54	DV	0.37	0/790	0.67	0/1057
55	BW	0.39	0/907	0.76	0/1216
55	DW	0.39	0/907	0.68	0/1216
56	BX	0.45	0/739	0.70	0/993
56	DX	0.41	0/739	0.67	0/993
57	BY	0.36	0/788	0.69	0/1051
57	DY	0.38	0/788	0.70	0/1051
58	BZ	0.50	0/1491	0.75	0/2024
58	DZ	0.46	0/1491	0.72	0/2024
All	All	0.55	83/330116 (0.0%)	0.75	224/493186 (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	90
1	CA	2	54
5	AE	0	1
22	AV	0	1
22	CV	0	2
22	CW	0	2
23	AX	0	2
23	CX	0	6
24	CY	0	1
25	AZ	0	2
25	CZ	0	2
36	BA	2	87
36	DA	0	79
37	BB	0	4
37	DB	0	3
39	BD	0	1
46	BN	0	1
All	All	5	338

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CV	34	G	C5-C6	-23.91	1.18	1.42
25	CZ	69	GLU	CB-CG	17.54	1.85	1.52
25	AZ	69	GLU	CB-CG	16.36	1.83	1.52
25	AZ	68	VAL	CA-C	12.52	1.85	1.52
25	CZ	68	VAL	CA-C	11.51	1.82	1.52

The worst 5 of 224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AZ	356	PRO	C-N-CD	-26.29	62.77	120.60
25	CZ	356	PRO	C-N-CD	-25.87	63.68	120.60
25	AZ	197	ASP	CB-CG-OD2	-14.50	105.25	118.30
25	AZ	69	GLU	N-CA-CB	-13.90	85.58	110.60
25	CZ	69	GLU	N-CA-CB	-13.63	86.07	110.60

All (5) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
1	AA	508	C	C3'
36	BA	1300	U	C3'
36	BA	1820	U	C3'
1	CA	508	C	C3'
1	CA	1399	C	C3'

5 of 338 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	108	G	Sidechain
1	AA	123	C	Sidechain
1	AA	13	U	Sidechain
1	AA	189(G)	G	Sidechain
1	AA	20	U	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	1034	0
1	CA	32329	0	16318	1281	0
2	AB	1900	0	1951	204	0
2	CB	1900	0	1951	237	0
3	AC	1612	0	1677	145	0
3	CC	1612	0	1677	183	0
4	AD	1703	0	1763	229	0
4	CD	1703	0	1763	265	0
5	AE	1146	0	1207	75	0
5	CE	1146	0	1207	108	0
6	AF	843	0	857	71	0
6	CF	843	0	857	94	0
7	AG	1257	0	1296	88	0
7	CG	1257	0	1296	87	0
8	AH	1116	0	1177	64	0
8	CH	1116	0	1177	92	0
9	AI	1010	0	1037	111	0
9	CI	1010	0	1037	117	0
10	AJ	794	0	840	126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	CJ	794	0	840	169	0
11	AK	885	0	904	67	0
11	CK	885	0	904	77	0
12	AL	970	0	1057	112	0
12	CL	970	0	1057	87	0
13	AM	987	0	1059	122	0
13	CM	987	0	1059	139	0
14	AN	492	0	531	62	0
14	CN	492	0	530	77	0
15	AO	734	0	771	47	0
15	CO	734	0	771	56	0
16	AP	700	0	720	92	0
16	CP	700	0	720	102	0
17	AQ	823	0	891	70	0
17	CQ	823	0	891	76	0
18	AR	574	0	644	51	0
18	CR	574	0	644	54	0
19	AS	629	0	652	81	0
19	CS	629	0	652	104	0
20	AT	763	0	861	105	0
20	CT	763	0	861	110	0
21	AU	208	0	221	32	0
21	CU	208	0	221	29	0
22	AV	1619	0	822	74	0
22	AW	1619	0	822	75	0
22	CV	1619	0	822	78	0
22	CW	1619	0	822	90	0
23	AX	361	0	184	27	0
23	CX	361	0	184	30	0
24	AY	1644	0	853	71	0
24	CY	1644	0	853	130	0
25	AZ	2984	0	2997	433	0
25	CZ	2984	0	2997	513	0
26	B0	662	0	688	75	0
26	D0	662	0	688	96	0
27	B1	731	0	808	88	0
27	D1	731	0	808	116	0
28	B2	598	0	653	179	0
28	D2	598	0	653	81	0
29	B3	467	0	523	57	0
29	D3	467	0	523	40	0
30	B4	340	0	336	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	D4	340	0	335	55	0
31	B5	459	0	480	82	0
31	D5	459	0	480	86	0
32	B6	433	0	461	143	0
32	D6	433	0	461	147	0
33	B7	418	0	467	35	0
33	D7	418	0	467	40	0
34	B8	507	0	576	118	0
34	D8	507	0	576	134	0
35	B9	307	0	335	35	0
35	D9	307	0	336	49	0
36	BA	62477	0	31497	2272	0
36	DA	62477	0	31497	2491	0
37	BB	2551	0	1295	108	0
37	DB	2551	0	1295	108	0
38	BC	1742	0	1800	152	0
38	DC	1742	0	1800	181	0
39	BD	2145	0	2234	297	0
39	DD	2145	0	2234	321	0
40	BE	1563	0	1629	227	0
40	DE	1563	0	1629	256	0
41	BF	1623	0	1677	197	0
41	DF	1623	0	1677	209	0
42	BG	1474	0	1535	241	0
42	DG	1474	0	1535	275	0
43	BH	1222	0	1282	171	0
43	DH	1222	0	1282	159	0
44	BJ	651	0	170	19	0
44	DJ	651	0	162	25	0
45	BK	700	0	175	15	0
45	DK	700	0	171	13	0
46	BN	1104	0	1180	160	0
46	DN	1104	0	1180	159	0
47	BO	933	0	996	92	0
47	DO	933	0	996	100	0
48	BP	1114	0	1187	291	0
48	DP	1114	0	1187	301	0
49	BQ	1122	0	1179	141	0
49	DQ	1122	0	1179	138	0
50	BR	960	0	1021	131	0
50	DR	960	0	1021	136	0
51	BS	770	0	832	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	DS	770	0	832	159	0
52	BT	1141	0	1202	234	0
52	DT	1141	0	1202	211	0
53	BU	958	0	1015	141	0
53	DU	958	0	1015	152	0
54	BV	779	0	852	135	0
54	DV	779	0	852	124	0
55	BW	896	0	953	100	0
55	DW	896	0	953	97	0
56	BX	725	0	778	98	0
56	DX	725	0	778	107	0
57	BY	775	0	870	176	0
57	DY	775	0	870	164	0
58	BZ	1459	0	1488	216	0
58	DZ	1459	0	1488	206	0
59	AD	1	0	0	0	0
59	AN	1	0	0	2	0
59	B4	1	0	0	0	0
59	B9	1	0	0	0	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D9	1	0	0	1	0
60	AZ	28	0	12	12	0
60	CZ	28	0	12	13	0
61	AZ	57	0	59	11	0
61	CZ	57	0	59	14	0
All	All	307194	0	208701	19683	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 38.

The worst 5 of 19683 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)
25:CZ:69:GLU:CG	25:CZ:69:GLU:CB	1.85	1.54
25:AZ:69:GLU:CB	25:AZ:69:GLU:CG	1.83	1.52
25:CZ:68:VAL:C	25:CZ:68:VAL:CA	1.82	1.46
25:AZ:68:VAL:C	25:AZ:68:VAL:CA	1.85	1.45
25:CZ:198:LYS:HE3	25:CZ:201:GLU:OE1	1.33	1.29

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	232/256 (91%)	168 (72%)	35 (15%)	29 (12%)	0	1
2	CB	232/256 (91%)	154 (66%)	50 (22%)	28 (12%)	0	2
3	AC	204/239 (85%)	161 (79%)	29 (14%)	14 (7%)	1	8
3	CC	204/239 (85%)	147 (72%)	40 (20%)	17 (8%)	1	6
4	AD	206/209 (99%)	139 (68%)	44 (21%)	23 (11%)	0	3
4	CD	206/209 (99%)	128 (62%)	44 (21%)	34 (16%)	0	0
5	AE	148/162 (91%)	138 (93%)	8 (5%)	2 (1%)	14	48
5	CE	148/162 (91%)	122 (82%)	25 (17%)	1 (1%)	26	65
6	AF	99/101 (98%)	78 (79%)	15 (15%)	6 (6%)	2	11
6	CF	99/101 (98%)	75 (76%)	13 (13%)	11 (11%)	0	3
7	AG	153/156 (98%)	121 (79%)	20 (13%)	12 (8%)	1	6
7	CG	153/156 (98%)	121 (79%)	24 (16%)	8 (5%)	2	15
8	AH	136/138 (99%)	124 (91%)	8 (6%)	4 (3%)	6	29
8	CH	136/138 (99%)	117 (86%)	12 (9%)	7 (5%)	2	15
9	AI	125/128 (98%)	85 (68%)	26 (21%)	14 (11%)	0	3
9	CI	125/128 (98%)	79 (63%)	31 (25%)	15 (12%)	0	2
10	AJ	96/105 (91%)	72 (75%)	15 (16%)	9 (9%)	1	4
10	CJ	96/105 (91%)	71 (74%)	16 (17%)	9 (9%)	1	4
11	AK	117/129 (91%)	103 (88%)	13 (11%)	1 (1%)	21	61
11	CK	117/129 (91%)	88 (75%)	23 (20%)	6 (5%)	2	15
12	AL	122/132 (92%)	97 (80%)	15 (12%)	10 (8%)	1	6
12	CL	122/132 (92%)	92 (75%)	22 (18%)	8 (7%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	AM	122/126 (97%)	75 (62%)	31 (25%)	16 (13%)	0	1
13	CM	122/126 (97%)	72 (59%)	35 (29%)	15 (12%)	0	2
14	AN	58/61 (95%)	40 (69%)	10 (17%)	8 (14%)	0	1
14	CN	58/61 (95%)	34 (59%)	15 (26%)	9 (16%)	0	0
15	AO	86/89 (97%)	68 (79%)	13 (15%)	5 (6%)	2	12
15	CO	86/89 (97%)	68 (79%)	15 (17%)	3 (4%)	4	24
16	AP	81/88 (92%)	50 (62%)	21 (26%)	10 (12%)	0	2
16	CP	81/88 (92%)	49 (60%)	22 (27%)	10 (12%)	0	2
17	AQ	97/105 (92%)	84 (87%)	9 (9%)	4 (4%)	3	20
17	CQ	97/105 (92%)	80 (82%)	11 (11%)	6 (6%)	2	10
18	AR	68/88 (77%)	52 (76%)	12 (18%)	4 (6%)	2	12
18	CR	68/88 (77%)	51 (75%)	12 (18%)	5 (7%)	1	7
19	AS	76/93 (82%)	50 (66%)	16 (21%)	10 (13%)	0	1
19	CS	76/93 (82%)	45 (59%)	20 (26%)	11 (14%)	0	1
20	AT	97/106 (92%)	62 (64%)	24 (25%)	11 (11%)	0	2
20	CT	97/106 (92%)	64 (66%)	19 (20%)	14 (14%)	0	1
21	AU	22/27 (82%)	16 (73%)	3 (14%)	3 (14%)	0	1
21	CU	22/27 (82%)	14 (64%)	5 (23%)	3 (14%)	0	1
25	AZ	381/405 (94%)	272 (71%)	66 (17%)	43 (11%)	0	2
25	CZ	381/405 (94%)	270 (71%)	68 (18%)	43 (11%)	0	2
26	B0	82/85 (96%)	65 (79%)	10 (12%)	7 (8%)	1	5
26	D0	82/85 (96%)	62 (76%)	12 (15%)	8 (10%)	1	4
27	B1	91/98 (93%)	58 (64%)	18 (20%)	15 (16%)	0	0
27	D1	91/98 (93%)	64 (70%)	12 (13%)	15 (16%)	0	0
28	B2	69/72 (96%)	34 (49%)	20 (29%)	15 (22%)	0	0
28	D2	69/72 (96%)	44 (64%)	19 (28%)	6 (9%)	1	5
29	B3	57/60 (95%)	42 (74%)	9 (16%)	6 (10%)	1	3
29	D3	57/60 (95%)	39 (68%)	10 (18%)	8 (14%)	0	1
30	B4	42/71 (59%)	25 (60%)	10 (24%)	7 (17%)	0	0
30	D4	42/71 (59%)	17 (40%)	17 (40%)	8 (19%)	0	0
31	B5	57/60 (95%)	40 (70%)	7 (12%)	10 (18%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	D5	57/60 (95%)	40 (70%)	8 (14%)	9 (16%)	0	0
32	B6	48/54 (89%)	20 (42%)	10 (21%)	18 (38%)	0	0
32	D6	48/54 (89%)	20 (42%)	14 (29%)	14 (29%)	0	0
33	B7	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
33	D7	46/49 (94%)	40 (87%)	6 (13%)	0	100	100
34	B8	61/65 (94%)	31 (51%)	18 (30%)	12 (20%)	0	0
34	D8	61/65 (94%)	27 (44%)	19 (31%)	15 (25%)	0	0
35	B9	35/37 (95%)	19 (54%)	11 (31%)	5 (14%)	0	1
35	D9	35/37 (95%)	17 (49%)	13 (37%)	5 (14%)	0	1
38	BC	226/229 (99%)	176 (78%)	33 (15%)	17 (8%)	1	7
38	DC	226/229 (99%)	170 (75%)	37 (16%)	19 (8%)	1	6
39	BD	273/276 (99%)	199 (73%)	46 (17%)	28 (10%)	1	4
39	DD	273/276 (99%)	197 (72%)	43 (16%)	33 (12%)	0	2
40	BE	202/206 (98%)	125 (62%)	45 (22%)	32 (16%)	0	0
40	DE	202/206 (98%)	129 (64%)	38 (19%)	35 (17%)	0	0
41	BF	205/210 (98%)	145 (71%)	34 (17%)	26 (13%)	0	1
41	DF	205/210 (98%)	129 (63%)	54 (26%)	22 (11%)	0	3
42	BG	179/182 (98%)	110 (62%)	33 (18%)	36 (20%)	0	0
42	DG	179/182 (98%)	99 (55%)	53 (30%)	27 (15%)	0	0
43	BH	157/180 (87%)	97 (62%)	31 (20%)	29 (18%)	0	0
43	DH	157/180 (87%)	99 (63%)	27 (17%)	31 (20%)	0	0
46	BN	136/140 (97%)	91 (67%)	27 (20%)	18 (13%)	0	1
46	DN	136/140 (97%)	89 (65%)	27 (20%)	20 (15%)	0	1
47	BO	120/122 (98%)	97 (81%)	15 (12%)	8 (7%)	1	9
47	DO	120/122 (98%)	97 (81%)	15 (12%)	8 (7%)	1	9
48	BP	144/150 (96%)	77 (54%)	36 (25%)	31 (22%)	0	0
48	DP	144/150 (96%)	78 (54%)	34 (24%)	32 (22%)	0	0
49	BQ	139/141 (99%)	112 (81%)	20 (14%)	7 (5%)	3	16
49	DQ	139/141 (99%)	112 (81%)	17 (12%)	10 (7%)	1	7
50	BR	115/118 (98%)	81 (70%)	15 (13%)	19 (16%)	0	0
50	DR	115/118 (98%)	73 (64%)	27 (24%)	15 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BS	96/112 (86%)	44 (46%)	29 (30%)	23 (24%)	0	0
51	DS	96/112 (86%)	44 (46%)	22 (23%)	30 (31%)	0	0
52	BT	135/146 (92%)	76 (56%)	28 (21%)	31 (23%)	0	0
52	DT	135/146 (92%)	71 (53%)	35 (26%)	29 (22%)	0	0
53	BU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	6
53	DU	115/118 (98%)	74 (64%)	34 (30%)	7 (6%)	2	11
54	BV	99/101 (98%)	65 (66%)	21 (21%)	13 (13%)	0	1
54	DV	99/101 (98%)	67 (68%)	19 (19%)	13 (13%)	0	1
55	BW	111/113 (98%)	78 (70%)	17 (15%)	16 (14%)	0	1
55	DW	111/113 (98%)	72 (65%)	23 (21%)	16 (14%)	0	1
56	BX	90/96 (94%)	63 (70%)	15 (17%)	12 (13%)	0	1
56	DX	90/96 (94%)	58 (64%)	22 (24%)	10 (11%)	0	3
57	BY	98/110 (89%)	43 (44%)	28 (29%)	27 (28%)	0	0
57	DY	98/110 (89%)	43 (44%)	26 (26%)	29 (30%)	0	0
58	BZ	181/206 (88%)	117 (65%)	38 (21%)	26 (14%)	0	1
58	DZ	181/206 (88%)	114 (63%)	42 (23%)	25 (14%)	0	1
All	All	12270/13100 (94%)	8441 (69%)	2326 (19%)	1503 (12%)	0	2

5 of 1503 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	8	LYS
2	AB	9	GLU
2	AB	15	VAL
2	AB	127	ILE
2	AB	131	PRO

### 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%)	178 (88%)	24 (12%)	6	25
2	CB	202/220 (92%)	177 (88%)	25 (12%)	6	23
3	AC	160/188 (85%)	142 (89%)	18 (11%)	7	28
3	CC	160/188 (85%)	144 (90%)	16 (10%)	9	34
4	AD	180/181 (99%)	151 (84%)	29 (16%)	3	13
4	CD	180/181 (99%)	153 (85%)	27 (15%)	3	15
5	AE	115/123 (94%)	106 (92%)	9 (8%)	16	49
5	CE	115/123 (94%)	105 (91%)	10 (9%)	13	44
6	AF	90/90 (100%)	79 (88%)	11 (12%)	6	24
6	CF	90/90 (100%)	77 (86%)	13 (14%)	4	17
7	AG	126/127 (99%)	113 (90%)	13 (10%)	9	32
7	CG	126/127 (99%)	116 (92%)	10 (8%)	15	49
8	AH	119/119 (100%)	108 (91%)	11 (9%)	11	40
8	CH	119/119 (100%)	112 (94%)	7 (6%)	24	60
9	AI	98/99 (99%)	89 (91%)	9 (9%)	11	40
9	CI	98/99 (99%)	88 (90%)	10 (10%)	9	33
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	6	22
10	CJ	88/92 (96%)	74 (84%)	14 (16%)	3	13
11	AK	90/99 (91%)	77 (86%)	13 (14%)	4	17
11	CK	90/99 (91%)	77 (86%)	13 (14%)	4	17
12	AL	104/109 (95%)	91 (88%)	13 (12%)	6	22
12	CL	104/109 (95%)	93 (89%)	11 (11%)	8	31
13	AM	99/101 (98%)	85 (86%)	14 (14%)	4	18
13	CM	99/101 (98%)	85 (86%)	14 (14%)	4	18
14	AN	49/50 (98%)	42 (86%)	7 (14%)	4	17
14	CN	49/50 (98%)	43 (88%)	6 (12%)	6	24
15	AO	79/80 (99%)	69 (87%)	10 (13%)	5	22
15	CO	79/80 (99%)	69 (87%)	10 (13%)	5	22
16	AP	72/74 (97%)	68 (94%)	4 (6%)	26	62
16	CP	72/74 (97%)	65 (90%)	7 (10%)	10	36
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	17	51
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	61	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	61/77 (79%)	54 (88%)	7 (12%)	7	27
18	CR	61/77 (79%)	54 (88%)	7 (12%)	7	27
19	AS	69/80 (86%)	58 (84%)	11 (16%)	3	13
19	CS	69/80 (86%)	54 (78%)	15 (22%)	1	5
20	AT	76/82 (93%)	66 (87%)	10 (13%)	5	20
20	CT	76/82 (93%)	67 (88%)	9 (12%)	6	25
21	AU	19/22 (86%)	17 (90%)	2 (10%)	8	31
21	CU	19/22 (86%)	16 (84%)	3 (16%)	3	13
25	AZ	322/338 (95%)	282 (88%)	40 (12%)	6	23
25	CZ	322/338 (95%)	281 (87%)	41 (13%)	5	22
26	B0	66/67 (98%)	53 (80%)	13 (20%)	1	7
26	D0	66/67 (98%)	55 (83%)	11 (17%)	3	11
27	B1	78/83 (94%)	68 (87%)	10 (13%)	5	21
27	D1	78/83 (94%)	70 (90%)	8 (10%)	9	32
28	B2	66/67 (98%)	55 (83%)	11 (17%)	3	11
28	D2	66/67 (98%)	60 (91%)	6 (9%)	12	40
29	B3	51/52 (98%)	44 (86%)	7 (14%)	4	19
29	D3	51/52 (98%)	45 (88%)	6 (12%)	6	25
30	B4	39/63 (62%)	28 (72%)	11 (28%)	0	1
30	D4	39/63 (62%)	29 (74%)	10 (26%)	0	2
31	B5	51/52 (98%)	44 (86%)	7 (14%)	4	19
31	D5	51/52 (98%)	45 (88%)	6 (12%)	6	25
32	B6	49/52 (94%)	32 (65%)	17 (35%)	0	0
32	D6	49/52 (94%)	36 (74%)	13 (26%)	0	2
33	B7	41/42 (98%)	37 (90%)	4 (10%)	10	36
33	D7	41/42 (98%)	35 (85%)	6 (15%)	4	16
34	B8	53/55 (96%)	43 (81%)	10 (19%)	2	8
34	D8	53/55 (96%)	43 (81%)	10 (19%)	2	8
35	B9	34/34 (100%)	28 (82%)	6 (18%)	2	10
35	D9	34/34 (100%)	29 (85%)	5 (15%)	4	16
38	BC	180/181 (99%)	168 (93%)	12 (7%)	20	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DC	180/181 (99%)	165 (92%)	15 (8%)	14	46
39	BD	217/218 (100%)	176 (81%)	41 (19%)	2	8
39	DD	217/218 (100%)	185 (85%)	32 (15%)	4	16
40	BE	165/166 (99%)	137 (83%)	28 (17%)	2	11
40	DE	165/166 (99%)	137 (83%)	28 (17%)	2	11
41	BF	165/166 (99%)	147 (89%)	18 (11%)	8	30
41	DF	165/166 (99%)	152 (92%)	13 (8%)	15	49
42	BG	155/156 (99%)	130 (84%)	25 (16%)	3	13
42	DG	155/156 (99%)	127 (82%)	28 (18%)	2	9
43	BH	132/148 (89%)	122 (92%)	10 (8%)	16	51
43	DH	132/148 (89%)	123 (93%)	9 (7%)	20	55
46	BN	117/119 (98%)	102 (87%)	15 (13%)	5	21
46	DN	117/119 (98%)	99 (85%)	18 (15%)	3	14
47	BO	100/100 (100%)	92 (92%)	8 (8%)	15	48
47	DO	100/100 (100%)	90 (90%)	10 (10%)	9	34
48	BP	112/116 (97%)	89 (80%)	23 (20%)	1	6
48	DP	112/116 (97%)	92 (82%)	20 (18%)	2	10
49	BQ	111/111 (100%)	94 (85%)	17 (15%)	3	14
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	5	22
50	BR	100/101 (99%)	88 (88%)	12 (12%)	6	24
50	DR	100/101 (99%)	89 (89%)	11 (11%)	8	30
51	BS	77/88 (88%)	65 (84%)	12 (16%)	3	14
51	DS	77/88 (88%)	61 (79%)	16 (21%)	1	6
52	BT	120/127 (94%)	101 (84%)	19 (16%)	3	13
52	DT	120/127 (94%)	102 (85%)	18 (15%)	3	15
53	BU	92/94 (98%)	84 (91%)	8 (9%)	13	44
53	DU	92/94 (98%)	85 (92%)	7 (8%)	16	51
54	BV	82/82 (100%)	69 (84%)	13 (16%)	3	13
54	DV	82/82 (100%)	66 (80%)	16 (20%)	2	7
55	BW	91/92 (99%)	85 (93%)	6 (7%)	21	56
55	DW	91/92 (99%)	85 (93%)	6 (7%)	21	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	BX	74/78 (95%)	65 (88%)	9 (12%)	6	24
56	DX	74/78 (95%)	68 (92%)	6 (8%)	15	47
57	BY	84/91 (92%)	72 (86%)	12 (14%)	4	17
57	DY	84/91 (92%)	73 (87%)	11 (13%)	5	21
58	BZ	161/179 (90%)	134 (83%)	27 (17%)	2	11
58	DZ	161/179 (90%)	138 (86%)	23 (14%)	4	17
All	All	10350/10856 (95%)	9014 (87%)	1336 (13%)	5	21

5 of 1336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	BT	99	LEU
4	CD	163	GLU
51	DS	12	PHE
54	BV	40	LEU
58	BZ	148	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 314 such sidechains are listed below:

Mol	Chain	Res	Type
55	BW	57	ASN
7	CG	84	ASN
49	DQ	45	GLN
56	BX	87	GLN
3	CC	3	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	227 (15%)	50 (3%)
1	CA	1503/1522 (98%)	229 (15%)	41 (2%)
22	AV	75/76 (98%)	20 (26%)	0
22	AW	75/76 (98%)	20 (26%)	0
22	CV	75/76 (98%)	19 (25%)	2 (2%)
22	CW	75/76 (98%)	22 (29%)	2 (2%)
23	AX	17/27 (62%)	8 (47%)	1 (5%)
23	CX	17/27 (62%)	9 (52%)	1 (5%)
24	AY	74/77 (96%)	24 (32%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	CY	74/77 (96%)	25 (33%)	1 (1%)
36	BA	2900/2915 (99%)	511 (17%)	48 (1%)
36	DA	2900/2915 (99%)	513 (17%)	43 (1%)
37	BB	118/122 (96%)	26 (22%)	4 (3%)
37	DB	118/122 (96%)	26 (22%)	4 (3%)
All	All	9524/9630 (98%)	1679 (17%)	198 (2%)

5 of 1679 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 198 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2145	C
1	CA	197	A
36	DA	1970	A
36	BA	2464	C
37	BB	16	G

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

18 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
24	H2U	AY	16	24	17,21,22	0.95	1 (5%)	23,30,33	1.83	4 (17%)
24	H2U	AY	17	24	17,21,22	0.91	0	23,30,33	1.85	5 (21%)
24	H2U	AY	20	24	17,21,22	0.95	1 (5%)	23,30,33	1.96	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	OMC	AY	32	24	13,22,23	0.88	0	20,31,34	1.05	2 (10%)
24	MIA	AY	37	24	21,31,32	1.38	1 (4%)	26,44,47	1.88	4 (15%)
24	7MG	AY	46	24	19,26,27	1.67	3 (15%)	24,39,42	2.27	3 (12%)
24	5MU	AY	54	24	12,22,23	1.33	3 (25%)	14,32,35	4.49	3 (21%)
24	PSU	AY	55	24	13,21,22	1.22	2 (15%)	18,30,33	3.65	6 (33%)
24	4SU	AY	8	24	11,21,22	1.74	2 (18%)	13,30,33	2.42	1 (7%)
24	H2U	CY	16	24	17,21,22	1.05	2 (11%)	23,30,33	1.85	4 (17%)
24	H2U	CY	17	24	17,21,22	0.98	0	23,30,33	1.91	5 (21%)
24	H2U	CY	20	24	17,21,22	0.96	0	23,30,33	1.99	6 (26%)
24	OMC	CY	32	24	13,22,23	0.89	0	20,31,34	1.05	2 (10%)
24	MIA	CY	37	24	21,31,32	1.55	3 (14%)	26,44,47	1.44	3 (11%)
24	7MG	CY	46	24	19,26,27	1.62	3 (15%)	24,39,42	2.26	3 (12%)
24	5MU	CY	54	24	12,22,23	1.34	3 (25%)	14,32,35	4.51	3 (21%)
24	PSU	CY	55	24	13,21,22	1.25	2 (15%)	18,30,33	3.80	6 (33%)
24	4SU	CY	8	24	11,21,22	1.81	2 (18%)	13,30,33	2.45	1 (7%)

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
24	H2U	AY	16	24	-	0/7/38/39	0/2/2/2
24	H2U	AY	17	24	-	0/7/38/39	0/2/2/2
24	H2U	AY	20	24	-	0/7/38/39	0/2/2/2
24	OMC	AY	32	24	-	0/5/27/28	0/2/2/2
24	MIA	AY	37	24	-	0/11/33/34	0/3/3/3
24	7MG	AY	46	24	-	0/7/37/38	0/3/3/3
24	5MU	AY	54	24	-	0/3/25/26	0/2/2/2
24	PSU	AY	55	24	-	0/7/25/26	0/2/2/2
24	4SU	AY	8	24	-	0/3/25/26	0/2/2/2
24	H2U	CY	16	24	-	0/7/38/39	0/2/2/2
24	H2U	CY	17	24	-	0/7/38/39	0/2/2/2
24	H2U	CY	20	24	-	0/7/38/39	0/2/2/2
24	OMC	CY	32	24	-	0/5/27/28	0/2/2/2
24	MIA	CY	37	24	-	0/11/33/34	0/3/3/3
24	7MG	CY	46	24	-	0/7/37/38	0/3/3/3
24	5MU	CY	54	24	-	0/3/25/26	0/2/2/2
24	PSU	CY	55	24	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	4SU	CY	8	24	-	0/3/25/26	0/2/2/2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	46	7MG	C8-N9	-4.92	1.38	1.45
24	CY	46	7MG	C8-N9	-4.80	1.38	1.45
24	CY	46	7MG	C8-N7	-2.74	1.31	1.43
24	AY	46	7MG	C8-N7	-2.73	1.31	1.43
24	CY	37	MIA	C12-N6	-2.27	1.40	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CY	55	PSU	N1-C2-N3	-12.97	120.06	128.33
24	AY	55	PSU	N1-C2-N3	-12.47	120.38	128.33
24	CY	54	5MU	C5-C4-N3	-8.95	115.17	125.14
24	AY	54	5MU	C5-C4-N3	-8.80	115.34	125.14
24	CY	8	4SU	C5-C4-N3	-8.56	115.24	123.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	16	H2U	1	0
24	AY	20	H2U	3	0
24	AY	32	OMC	1	0
24	AY	46	7MG	1	0
24	AY	54	5MU	3	0
24	AY	55	PSU	2	0
24	AY	8	4SU	3	0
24	CY	16	H2U	1	0
24	CY	20	H2U	3	0
24	CY	32	OMC	1	0
24	CY	46	7MG	1	0
24	CY	54	5MU	3	0
24	CY	55	PSU	2	0
24	CY	8	4SU	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 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	AZ	501	-	23,30,30	1.29	3 (13%)	30,47,47	1.87	7 (23%)
61	KIR	AZ	502	-	55,59,59	3.84	22 (40%)	53,84,84	1.75	12 (22%)
60	GDP	CZ	501	-	23,30,30	1.29	3 (13%)	30,47,47	1.83	8 (26%)
61	KIR	CZ	502	-	55,59,59	3.82	22 (40%)	53,84,84	1.73	11 (20%)

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	AZ	501	-	-	0/12/32/32	0/3/3/3
61	KIR	AZ	502	-	-	0/54/98/98	0/3/3/3
60	GDP	CZ	501	-	-	0/12/32/32	0/3/3/3
61	KIR	CZ	502	-	-	0/54/98/98	0/3/3/3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	502	KIR	O18-C17	-14.85	1.22	1.44
61	CZ	502	KIR	O18-C17	-14.14	1.23	1.44
61	CZ	502	KIR	O30-C30	-11.65	1.18	1.42
61	AZ	502	KIR	O30-C30	-11.46	1.18	1.42
61	AZ	502	KIR	O34-C33	-10.32	1.30	1.44

The worst 5 of 38 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AZ	501	GDP	PA-O3A-PB	-4.80	116.58	132.67
61	AZ	502	KIR	O29-C29-O34	-4.65	102.49	110.18
60	CZ	501	GDP	PA-O3A-PB	-4.63	117.13	132.67
60	CZ	501	GDP	N3-C2-N1	-4.60	120.44	127.44
60	AZ	501	GDP	N3-C2-N1	-4.45	120.67	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	AZ	501	GDP	12	0
61	AZ	502	KIR	11	0
60	CZ	501	GDP	13	0
61	CZ	502	KIR	14	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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%)	-0.26	30 (1%) 68 46	22, 58, 151, 200	0
1	CA	1504/1522 (98%)	-0.23	25 (1%) 73 52	39, 79, 157, 200	0
2	AB	234/256 (91%)	-0.30	3 (1%) 79 62	33, 66, 135, 154	0
2	CB	234/256 (91%)	-0.25	3 (1%) 79 62	50, 89, 142, 150	0
3	AC	206/239 (86%)	-0.58	0 100 100	25, 49, 78, 88	0
3	CC	206/239 (86%)	-0.42	1 (0%) 91 83	53, 80, 106, 113	0
4	AD	208/209 (99%)	0.10	8 (3%) 44 21	59, 88, 122, 126	0
4	CD	208/209 (99%)	0.18	10 (4%) 34 15	79, 105, 125, 135	0
5	AE	150/162 (92%)	-0.61	0 100 100	30, 45, 71, 97	0
5	CE	150/162 (92%)	-0.46	0 100 100	48, 63, 85, 102	0
6	AF	101/101 (100%)	-0.48	1 (0%) 84 69	48, 74, 94, 105	0
6	CF	101/101 (100%)	-0.12	1 (0%) 84 69	79, 98, 111, 119	0
7	AG	155/156 (99%)	-0.36	5 (3%) 51 27	39, 65, 96, 117	0
7	CG	155/156 (99%)	-0.06	5 (3%) 51 27	71, 95, 115, 127	0
8	AH	138/138 (100%)	-0.54	0 100 100	32, 49, 69, 74	0
8	CH	138/138 (100%)	-0.43	0 100 100	46, 64, 80, 87	0
9	AI	127/128 (99%)	-0.19	1 (0%) 87 75	32, 68, 111, 124	0
9	CI	127/128 (99%)	0.44	12 (9%) 11 4	66, 106, 132, 139	0
10	AJ	98/105 (93%)	-0.08	1 (1%) 84 69	33, 70, 112, 125	0
10	CJ	98/105 (93%)	0.46	10 (10%) 9 3	66, 109, 144, 148	0
11	AK	119/129 (92%)	-0.41	2 (1%) 73 52	32, 50, 92, 118	0
11	CK	119/129 (92%)	-0.21	3 (2%) 61 37	52, 76, 100, 120	0
12	AL	124/132 (93%)	-0.26	1 (0%) 87 75	33, 61, 85, 124	0
12	CL	124/132 (93%)	-0.15	2 (1%) 74 55	47, 72, 99, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	124/126 (98%)	-0.07	5 (4%) 42 20	43, 72, 103, 131	0
13	CM	124/126 (98%)	0.07	7 (5%) 28 11	76, 99, 122, 142	0
14	AN	60/61 (98%)	-0.27	1 (1%) 73 52	30, 53, 78, 84	0
14	CN	60/61 (98%)	0.07	2 (3%) 50 26	65, 83, 102, 105	0
15	AO	88/89 (98%)	-0.50	0 100 100	36, 54, 82, 88	0
15	CO	88/89 (98%)	-0.29	0 100 100	44, 68, 90, 98	0
16	AP	83/88 (94%)	0.01	2 (2%) 62 39	61, 74, 98, 133	0
16	CP	83/88 (94%)	0.19	1 (1%) 81 64	74, 90, 110, 132	0
17	AQ	99/105 (94%)	-0.36	0 100 100	40, 60, 79, 89	0
17	CQ	99/105 (94%)	-0.20	0 100 100	53, 71, 91, 102	0
18	AR	70/88 (79%)	-0.42	0 100 100	39, 60, 90, 99	0
18	CR	70/88 (79%)	-0.24	0 100 100	56, 81, 108, 118	0
19	AS	78/93 (83%)	-0.03	2 (2%) 59 35	52, 73, 117, 127	0
19	CS	78/93 (83%)	0.17	6 (7%) 16 5	81, 97, 126, 132	0
20	AT	99/106 (93%)	0.16	4 (4%) 42 20	55, 80, 126, 130	0
20	CT	99/106 (93%)	0.11	2 (2%) 68 46	74, 90, 120, 122	0
21	AU	24/27 (88%)	0.00	2 (8%) 14 5	41, 55, 79, 99	0
21	CU	24/27 (88%)	0.64	2 (8%) 14 5	74, 92, 105, 113	0
22	AV	76/76 (100%)	-0.45	0 100 100	35, 72, 107, 124	0
22	AW	76/76 (100%)	0.40	9 (11%) 6 2	64, 140, 185, 199	0
22	CV	76/76 (100%)	-0.28	0 100 100	51, 86, 120, 137	0
22	CW	76/76 (100%)	0.45	7 (9%) 11 4	94, 170, 191, 200	0
23	AX	17/27 (62%)	0.49	2 (11%) 6 2	31, 91, 142, 143	0
23	CX	17/27 (62%)	2.34	12 (70%) 0 0	69, 122, 155, 157	0
24	AY	68/77 (88%)	0.27	2 (2%) 55 31	57, 140, 177, 197	0
24	CY	68/77 (88%)	0.39	1 (1%) 76 58	73, 142, 175, 198	0
25	AZ	385/405 (95%)	0.67	33 (8%) 13 4	87, 124, 151, 169	0
25	CZ	385/405 (95%)	1.42	110 (28%) 1 0	111, 133, 156, 170	0
26	B0	84/85 (98%)	0.18	6 (7%) 19 7	58, 73, 107, 122	0
26	D0	84/85 (98%)	0.51	9 (10%) 8 3	69, 86, 113, 123	0
27	B1	93/98 (94%)	0.05	4 (4%) 39 18	45, 69, 129, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	D1	93/98 (94%)	0.18	1 (1%) 82 66	59, 86, 133, 139	0
28	B2	71/72 (98%)	1.43	20 (28%) 1 0	130, 143, 155, 158	0
28	D2	71/72 (98%)	0.53	11 (15%) 3 1	100, 122, 136, 143	0
29	B3	59/60 (98%)	0.23	3 (5%) 32 13	65, 81, 106, 122	0
29	D3	59/60 (98%)	0.33	3 (5%) 32 13	60, 93, 106, 126	0
30	B4	44/71 (61%)	0.70	5 (11%) 7 2	111, 140, 167, 173	0
30	D4	44/71 (61%)	1.21	13 (29%) 1 0	136, 163, 184, 186	0
31	B5	59/60 (98%)	0.18	4 (6%) 20 7	62, 87, 148, 163	0
31	D5	59/60 (98%)	0.27	4 (6%) 20 7	63, 92, 145, 154	0
32	B6	50/54 (92%)	0.54	4 (8%) 15 5	57, 84, 103, 110	0
32	D6	50/54 (92%)	0.98	9 (18%) 2 1	73, 97, 116, 122	0
33	B7	48/49 (97%)	0.16	3 (6%) 23 9	51, 64, 101, 121	0
33	D7	48/49 (97%)	0.12	3 (6%) 23 9	64, 73, 104, 125	0
34	B8	63/65 (96%)	0.26	2 (3%) 51 27	56, 73, 91, 115	0
34	D8	63/65 (96%)	0.42	5 (7%) 15 5	72, 85, 101, 120	0
35	B9	37/37 (100%)	0.61	4 (10%) 8 2	73, 85, 103, 104	0
35	D9	37/37 (100%)	1.18	6 (16%) 3 1	67, 96, 107, 120	0
36	BA	2901/2915 (99%)	-0.13	79 (2%) 58 34	26, 77, 181, 200	0
36	DA	2901/2915 (99%)	-0.08	80 (2%) 56 32	37, 87, 180, 200	0
37	BB	119/122 (97%)	-0.47	0 100 100	59, 85, 112, 132	0
37	DB	119/122 (97%)	-0.43	0 100 100	69, 101, 126, 132	0
38	BC	228/229 (99%)	0.04	14 (6%) 25 10	50, 79, 160, 173	0
38	DC	228/229 (99%)	0.51	26 (11%) 7 2	68, 103, 170, 180	0
39	BD	275/276 (99%)	-0.40	4 (1%) 76 58	30, 49, 83, 105	0
39	DD	275/276 (99%)	-0.30	3 (1%) 82 66	42, 61, 91, 111	0
40	BE	204/206 (99%)	0.01	5 (2%) 61 37	50, 79, 128, 140	0
40	DE	204/206 (99%)	0.03	6 (2%) 55 31	47, 84, 133, 138	0
41	BF	207/210 (98%)	0.35	14 (6%) 20 7	53, 112, 162, 170	0
41	DF	207/210 (98%)	0.46	18 (8%) 13 4	62, 118, 161, 170	0
42	BG	181/182 (99%)	-0.02	9 (4%) 32 13	63, 86, 117, 130	0
42	DG	181/182 (99%)	0.08	8 (4%) 38 17	89, 108, 136, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BH	159/180 (88%)	0.78	25 (15%) 3 1	93, 134, 152, 156	0
43	DH	159/180 (88%)	0.56	13 (8%) 14 5	87, 129, 146, 154	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	138/140 (98%)	-0.06	1 (0%) 89 78	63, 89, 125, 134	0
46	DN	138/140 (98%)	-0.16	0 100 100	69, 90, 125, 133	0
47	BO	122/122 (100%)	-0.43	0 100 100	46, 63, 77, 85	0
47	DO	122/122 (100%)	-0.37	0 100 100	47, 67, 83, 89	0
48	BP	146/150 (97%)	0.56	13 (8%) 12 4	55, 103, 133, 150	0
48	DP	146/150 (97%)	0.75	22 (15%) 3 1	64, 115, 137, 153	0
49	BQ	141/141 (100%)	-0.20	3 (2%) 67 44	46, 64, 86, 128	0
49	DQ	141/141 (100%)	-0.20	2 (1%) 78 60	51, 66, 90, 126	0
50	BR	117/118 (99%)	0.09	3 (2%) 59 35	60, 85, 107, 126	0
50	DR	117/118 (99%)	0.09	1 (0%) 85 72	57, 90, 105, 123	0
51	BS	98/112 (87%)	0.15	3 (3%) 52 28	63, 90, 116, 126	0
51	DS	98/112 (87%)	0.47	9 (9%) 11 4	77, 102, 126, 128	0
52	BT	137/146 (93%)	0.01	8 (5%) 26 11	58, 84, 142, 167	0
52	DT	137/146 (93%)	-0.00	10 (7%) 18 6	63, 90, 147, 169	0
53	BU	117/118 (99%)	-0.03	1 (0%) 85 72	64, 79, 111, 128	0
53	DU	117/118 (99%)	-0.01	2 (1%) 73 52	63, 86, 110, 124	0
54	BV	101/101 (100%)	0.31	5 (4%) 32 13	62, 116, 129, 136	0
54	DV	101/101 (100%)	0.41	6 (5%) 26 11	71, 115, 134, 136	0
55	BW	113/113 (100%)	0.13	5 (4%) 38 17	65, 90, 116, 141	0
55	DW	113/113 (100%)	0.34	5 (4%) 38 17	73, 93, 123, 145	0
56	BX	92/96 (95%)	0.24	1 (1%) 82 66	75, 95, 110, 118	0
56	DX	92/96 (95%)	0.23	1 (1%) 82 66	82, 100, 116, 120	0
57	BY	100/110 (90%)	1.30	26 (26%) 1 0	108, 134, 162, 168	0
57	DY	100/110 (90%)	1.19	21 (21%) 1 0	107, 136, 160, 169	0
58	BZ	183/206 (88%)	-0.11	5 (2%) 58 34	56, 83, 120, 132	0
58	DZ	183/206 (88%)	-0.03	5 (2%) 58 34	62, 88, 120, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	21996/23370 (94%)	-0.00	917 (4%) 40 19	22, 84, 151, 200	0

The worst 5 of 917 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	CZ	183	HIS	12.6
41	BF	24	LEU	11.7
25	AZ	85	HIS	11.1
49	BQ	141	GLN	10.7
36	BA	1077	A	9.7

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
24	MIA	AY	37	29/30	0.91	0.25	-	64,78,89,98	0
24	H2U	AY	16	20/21	0.61	0.47	-	196,198,199,200	0
24	OMC	AY	32	21/22	0.89	0.20	-	101,105,115,115	0
24	PSU	AY	55	20/21	0.77	0.25	-	156,161,162,162	0
24	H2U	AY	20	20/21	0.83	0.43	-	186,189,193,193	0
24	5MU	CY	54	21/22	0.84	0.26	-	139,149,151,155	0
24	MIA	CY	37	29/30	0.92	0.23	-	80,87,95,99	0
24	PSU	CY	55	20/21	0.69	0.29	-	158,161,162,162	0
24	H2U	CY	17	20/21	0.62	0.57	-	199,199,200,200	0
24	OMC	CY	32	21/22	0.87	0.29	-	108,114,121,121	0
24	7MG	AY	46	24/25	0.84	0.27	-	145,150,151,151	0
24	7MG	CY	46	24/25	0.85	0.30	-	148,153,154,154	0
24	5MU	AY	54	21/22	0.81	0.20	-	139,150,152,154	0
24	4SU	AY	8	20/21	0.77	0.21	-	142,144,146,146	0
24	H2U	CY	20	20/21	0.79	0.38	-	188,191,192,192	0
24	H2U	CY	16	20/21	0.60	0.44	-	194,198,199,199	0
24	H2U	AY	17	20/21	0.68	0.36	-	199,199,200,200	0
24	4SU	CY	8	20/21	0.81	0.27	-	143,145,147,148	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
61	KIR	CZ	502	57/57	0.67	0.61	3.17	122,131,140,141	0
61	KIR	AZ	502	57/57	0.81	0.36	0.83	115,122,129,130	0
59	ZN	AN	101	1/1	0.98	0.18	0.80	48,48,48,48	0
59	ZN	AD	301	1/1	0.99	0.27	0.47	74,74,74,74	0
60	GDP	AZ	501	28/28	0.69	0.31	0.29	129,133,138,138	0
59	ZN	CD	301	1/1	0.99	0.28	0.10	79,79,79,79	0
60	GDP	CZ	501	28/28	0.70	0.27	-0.30	137,140,141,141	0
59	ZN	CN	101	1/1	0.99	0.17	-0.58	77,77,77,77	0
59	ZN	D4	101	1/1	0.85	0.12	-0.89	196,196,196,196	0
59	ZN	B9	101	1/1	0.92	0.12	-0.95	113,113,113,113	0
59	ZN	B4	101	1/1	0.95	0.13	-0.97	112,112,112,112	0
59	ZN	D9	101	1/1	0.90	0.17	-1.19	141,141,141,141	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.