



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:03 PM GMT

PDB ID : 4V5S
Title : The crystal structure of EF-Tu and G24A-tRNA-Trp bound to a 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

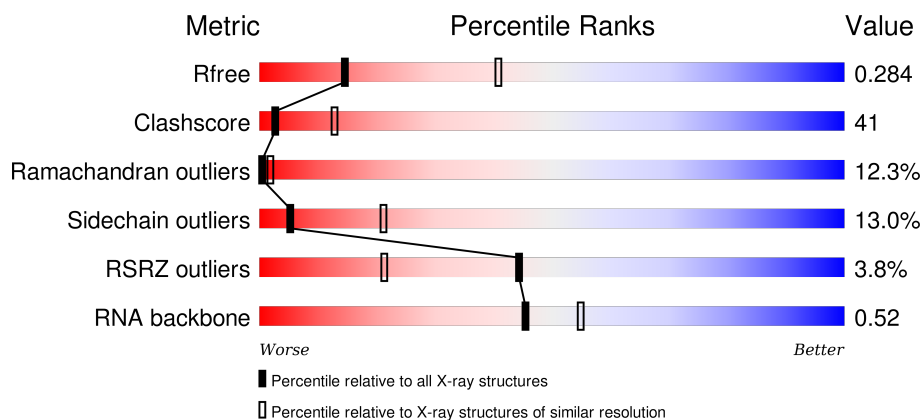
1 Overall quality at a glance

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 ≥ 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	




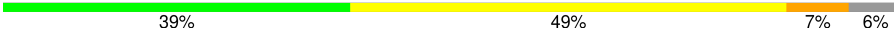
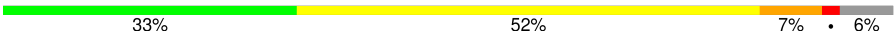
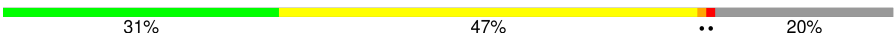
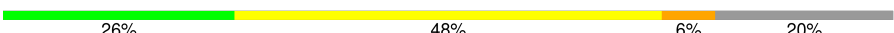
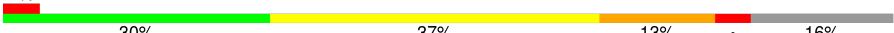
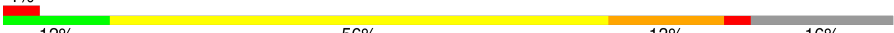





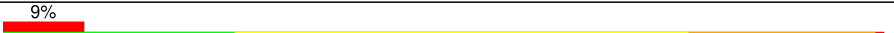



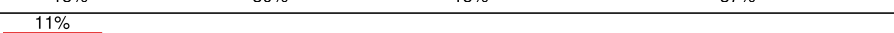
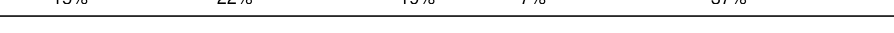


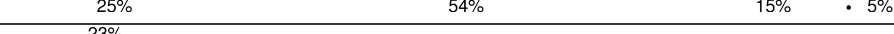
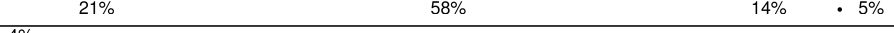

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	131	
12	CL	131	
13	AM	126	
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	


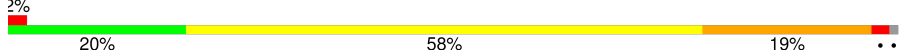
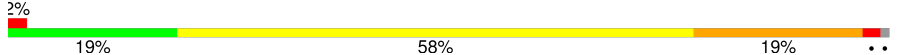
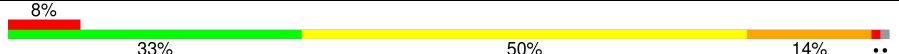
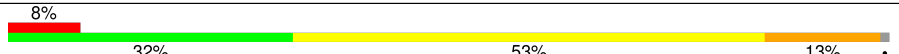
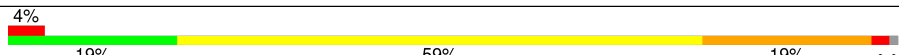
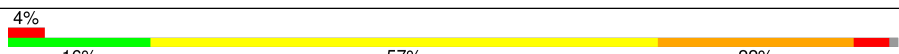
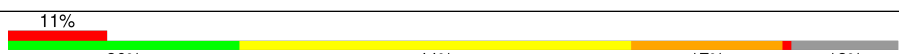
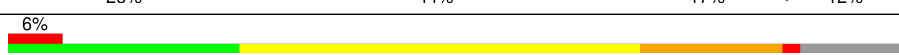
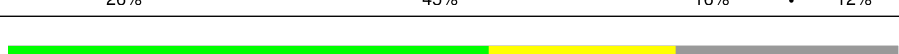

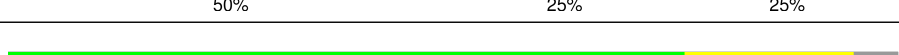

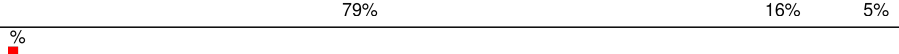
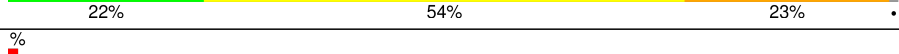
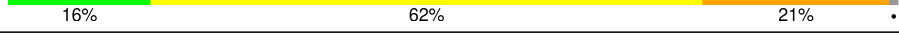
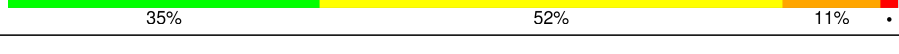
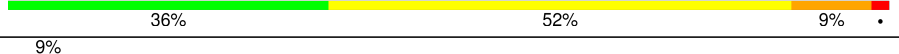
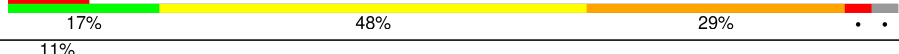
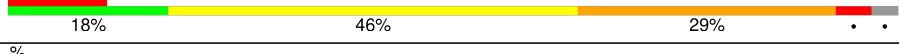

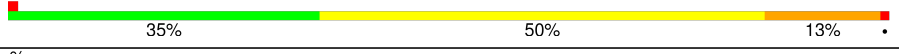
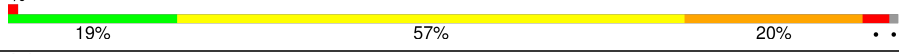
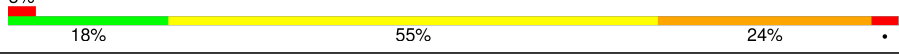

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Mol	Chain	Length	Quality of chain
27	B1	98	
27	D1	98	
28	B2	72	
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
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
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 307196 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
			362	164	68	114	16			
23	CX	17	Total	C	N	O	P	0	0	0
			362	164	68	114	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			

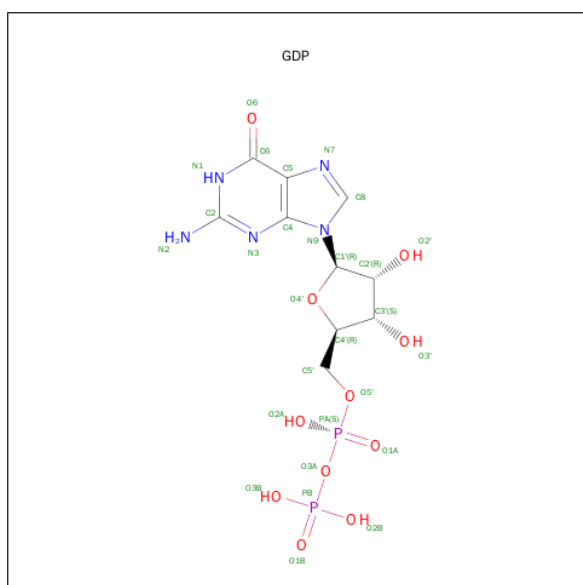
- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

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).

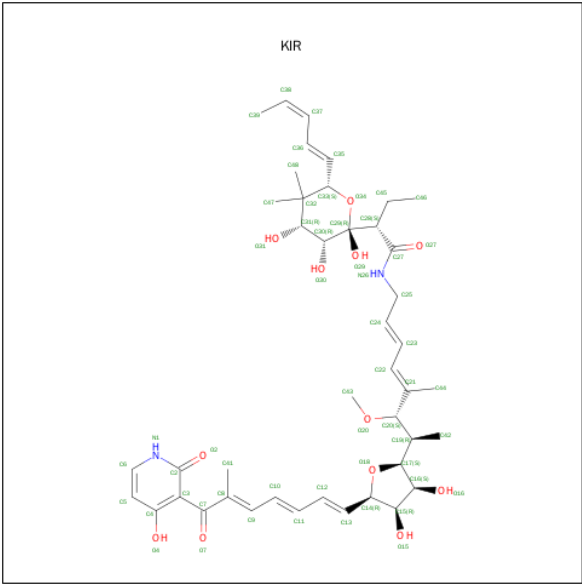
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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		

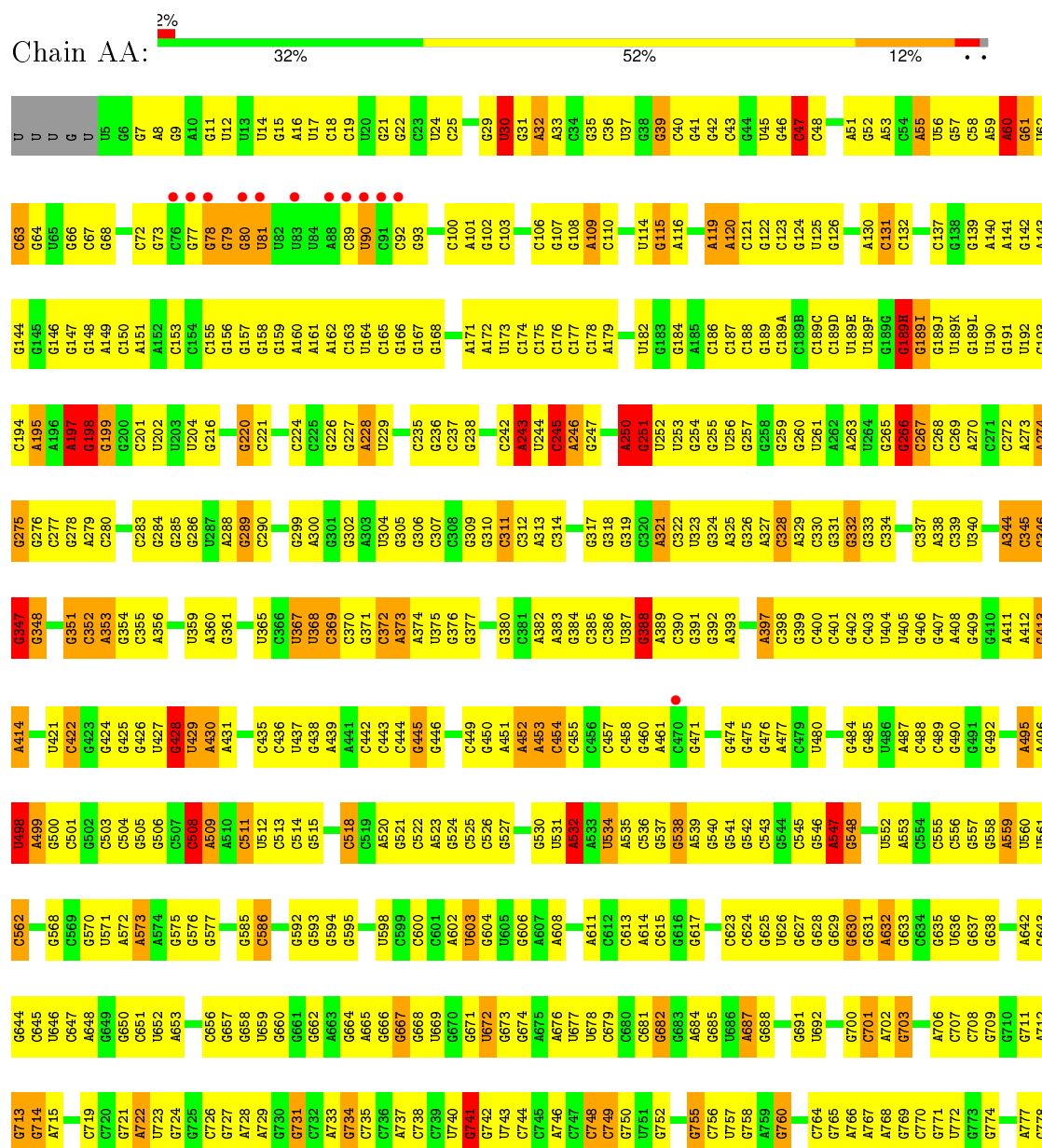
- Molecule 61 is KIRROMYCIN (three-letter code: KIR) (formula: C₄₃H₆₀N₂O₁₂).

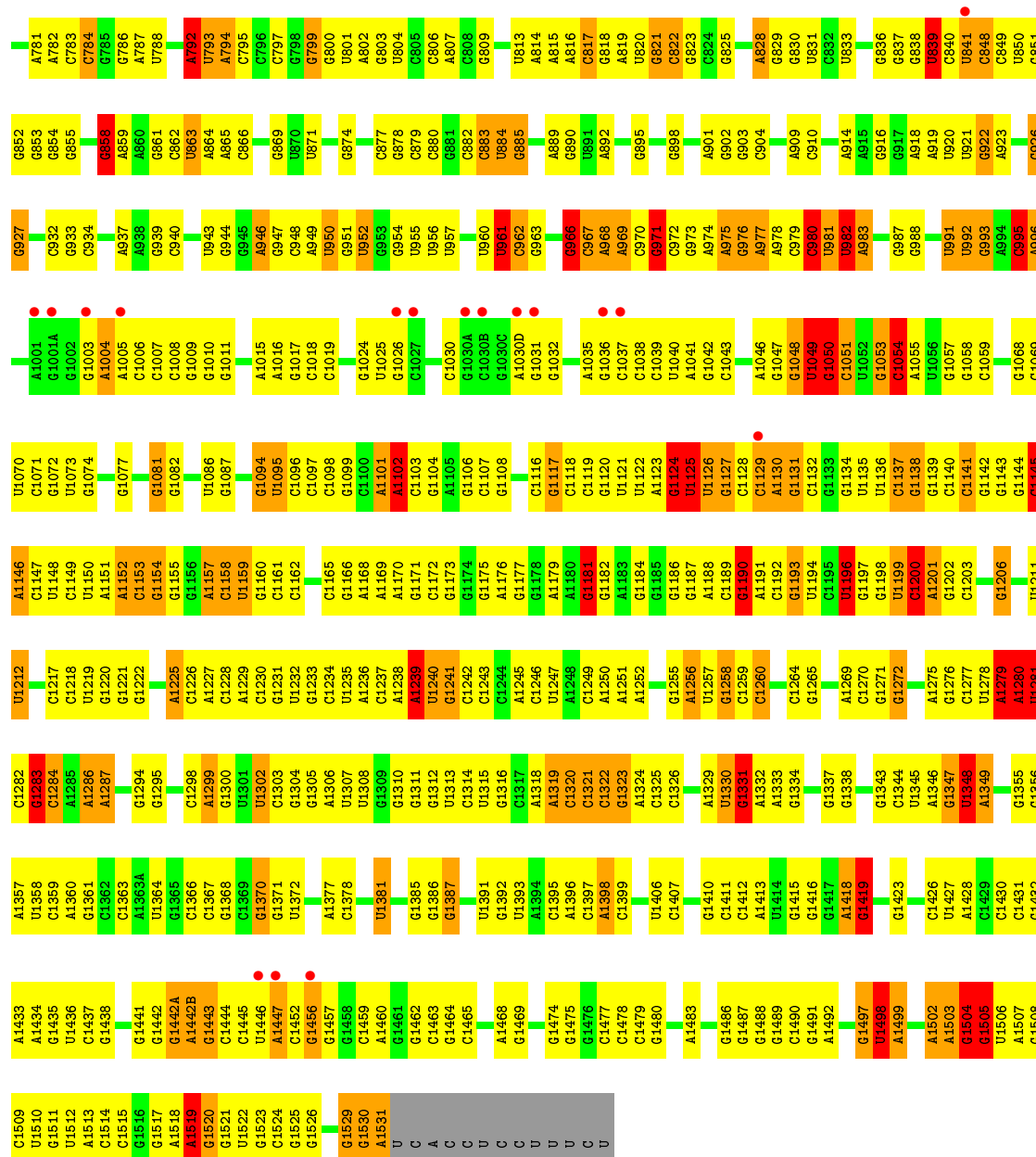


3 Residue-property plots

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

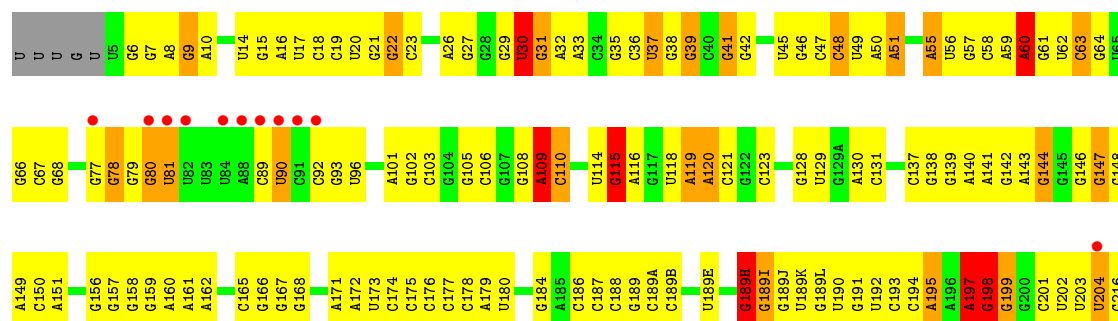
• Molecule 1: 16S RRNA



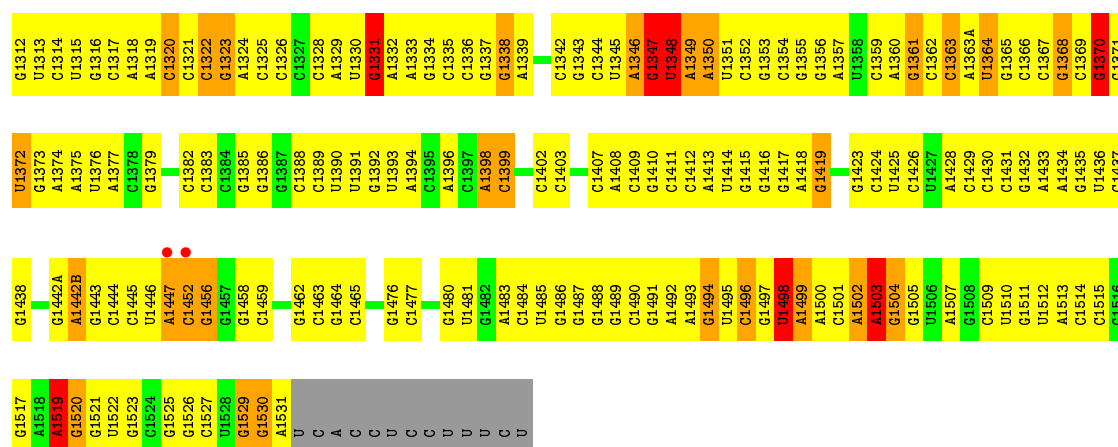


Molecule 1: 16S rRNA

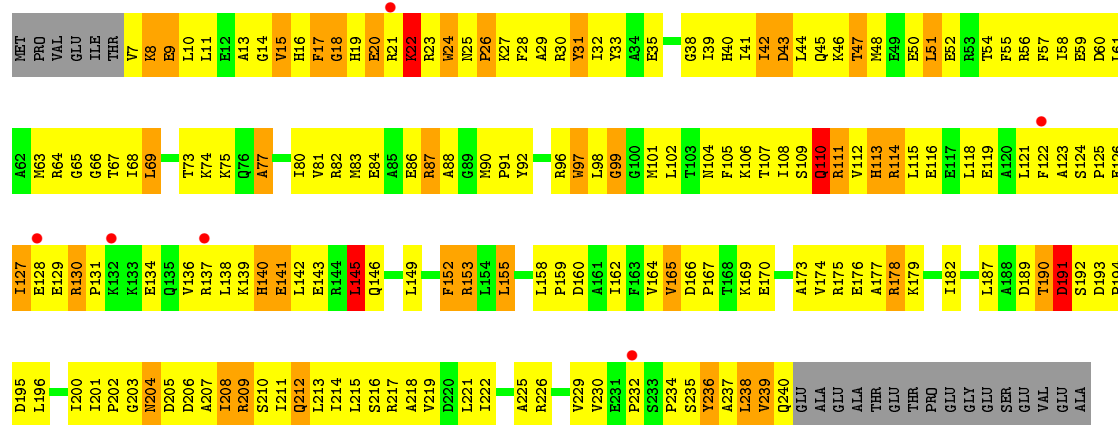
Chain CA: 26% 57% 13%



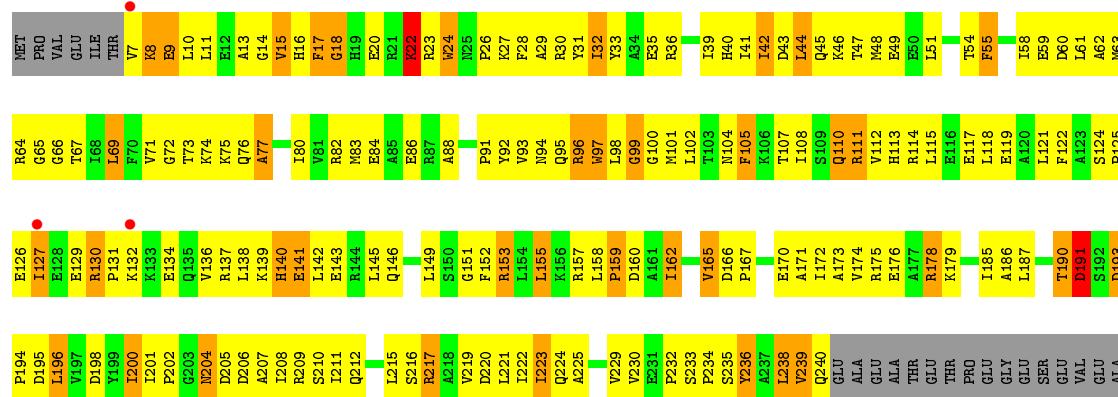
G1249	G1184	G1120	G1054	A923	U841	A777	C708	G638	G566	G492	C418	G351	G285	G220
A1260	G1185	G1123	A1055	C924	C848	G778	G711	G643	G567	G493	C419	C352	A288	C221
A1261	G1186	G1124	U1056	G925	C849	G779	G712	G644	G568	U494	U420	A353	G289	U222
	G1187	G1125	G1057	G926		A780	G713	G645		A495	G422	G355	C290	U223
	A1188	U1126	G1058	G927	G853	A781	G714	G646	A572	U496	G423	A356	C291	C224
A1265	G1189	G1127	G1059	G928	G854	A782	G715	G647	A573	A499	G424	G357	C292	C225
A1266	G1190	C1128	C1060	G929	G858	C783	G716		A574	G500	G425	U358	C293	G226
A1267		C1129	U1061	C930	A859	C784	G717		G575	C501	G426	U359	U294	G227
C1268	G1193	G1130	U1062		A860	G785	G718	G650	G576	G502	U427	A360	C295	A228
	U1196	A1131	G1065	C933	A861	G786	G719	G651	G577	G503	G428	G361	U296	U229
	G1197	G1132	U1066	A935	C862	U788	G720	U652	G585	C504	U429	G297	C297	G230
C1263	G1198	G1133	A1067	C936	U863	U789	G721	G653	G586	G505	U430	U365	A298	
C1264	U1199	G1134	G1068	A937	A864	A790	A722	A555		G506	A431	C366	G299	C234
G1265	C1200	U1135	C1069	A938	A865	G791	U723	G656	G592	C507		U367	A300	C235
G1266	A1201	U1136	U1070	G939	C866	A792	G724	G657	G593	C508	U434	U368	G301	G236
G1267	G1202	G1137	C1071	C940	G867	U793	G725	G658	G594	A509	C435	C369	G302	C237
A1268	C1203	U1138	G1072	G941	G869	A794	G726	U659	G595	A510	C436	C370	A303	
A1269	A1204	G1139	U1073	G942	U870	C795	G727	G660	G596	C511	U437	G371	U304	C242
C1270	U1205	C1140	C1007	U943	U871	C796		G661	C597		G438	G372	G305	
G1271	G1206	C1141	C1008	G944	G874	C797	G731	G662	U603		A439	A373		
G1272	G1207	G1142	G1009	G945	C877	U801	C732	A663	G604	C518	A441	A374	G309	U244
G1273	C1208	G1143	G1010	A946	G878		A733	G664	C599	C519	A442	U375	G310	C245
		G1144	G1011	G947	C879	U804	G735	A665	C600	A520	C443	G376	C311	A246
U1211	U1212	C1145	C948	G948			C736	G667	U603	A521	C444	G377	C312	G247
G1274		A1146	A949	A949	C882		C737		G604	A522	C445	G378	A313	U248
G1275		C1147	U1015	U950	C883	A807	A737	G673	G605	A523	G446	G379	C314	U249
C1276		U1148	G1016	G951	C884	C908	C738	G674	U605	C524	G447	C380	A315	G251
A1277	G1215	U1149	G1017	U952	U884	G809	G739		G606	C525	A448	C381		
A1280	C1217	U1150	G1018	G953	G885	G810	U740		A611	C526	C449	A382	G319	G254
U1281	C1218	A1151	U1090	G954	G886	C811	G741	G677	A608	G527	G450	A383	C320	G255
C1282	U1219	A1152	U1091	U955	G887	C812		U678	A609	G530	A451	G384	A321	U256
G1283	G1220	C1153	A1092	U956	G888	U813	C744	G679	G610	U531	A452	C385	C322	G257
A1284	G1221	G1154	U1025	U957	A889	A814	C745	C680	A611	A532	A453	C386	U323	G258
C1285	G1222		G1094	A958	G890	A815	A746	C681	C612	A533	G454	U387	G324	G259
A1286		A1157	U1095	A959	G891	A816	C747	G682	C613	U534	C455	A388	A325	G260
A1287	A1225	G1158	C1096	U960	U892	C817	C748	G683	A614	A535	C456	A389	G326	U261
A1288	C1226	U1159	C1097	U961	C893	G818	C749	A684	C615	G536	C457	C390	A327	A262
A1289	A1227	G1160	C1098	G962	A900	A819	G750	G685	G616	G537	C458	G391	C328	A263
	C1228	C1161	G1099	G963	A901	U820	U751	U686	G617	G538	G460	A393	C330	U264
		C1162	C1100	A964	G902	C821		A687	C618	A539		G394	G331	G265
U1292	G1230	G1165	A1101	A965		C822	C754	G688	U619	G540	G471		G332	C267
G1294	G1231	A1166	C1102	G966	G906	G823	G755	C689	C620	G541	A472		G333	C268
G1295	U1232	G1168	G1103	C967	A907	C824	C756	G690	A621	G542	G473		C334	C269
C1296	G1233	A1169	G1104	A968	A908	G825	U757	G691	A622	C543	G474			
C1298	U1234	G1170	G1105	A969	A909	C826	G758	U692	C623	G544	G475		C337	A270
A1299	A1235	G1171	C1106	C970	C910	U827	A759	G693	C624	G545	G476		C338	C271
G1300	C1237	C1172	C1107	G971	U911	A828	G760	A694	G625	G546	U460		A339	C272
U1301	A1238	G1173	C1108	G972	C912	G829		A695	U626	G547	U461		U340	A273
		G1174	C1109	G973	A913	G830	G763	A696	G627	G548	G481		C341	G275
U1302	A1239	G1175	A1110	A974	A914	U831	G764	U697	G628	G549		C403	C342	G276
C1303	U1240	G1176	C1111	A975	A915	C832	G765	G698	G629	C555	G483		C343	G277
G1304	G1177	A1178	C1112	G976	A916	U833	A766	C699	G630	C556	G484		U343	C278
G1305	C1242	G1179	C1113	A977	G916	C834	A767	G700	G631	C557	G485		A344	G279
A1306	G1178	G1178	C1114	G978	G917	U835		G701	A632	G558	U486		G345	A279
C1244	C1244	U1179	G1115	C979	A918	G836	C770	A702	G633	G559	A487		G346	C280
A1245	A1245	A1180	C1116	C980	A919	G837	G771	G703	C634	A560	C488		G347	G281
C1246	U1247	G1181	G1117	U981	A920	G838	G774	A706	G635	U561	C489		G348	A282
G1310		C1182	C1118	U982	U921	U839			U666		G490		A349	C283
G1311	A1248	A1183	C1119	A983	G922	C840		C707	G637	C562	G491		G350	G284



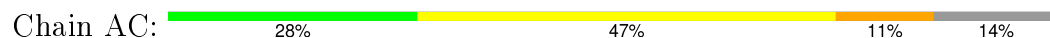
• Molecule 2: 30S RIBOSOMAL PROBLEM S2

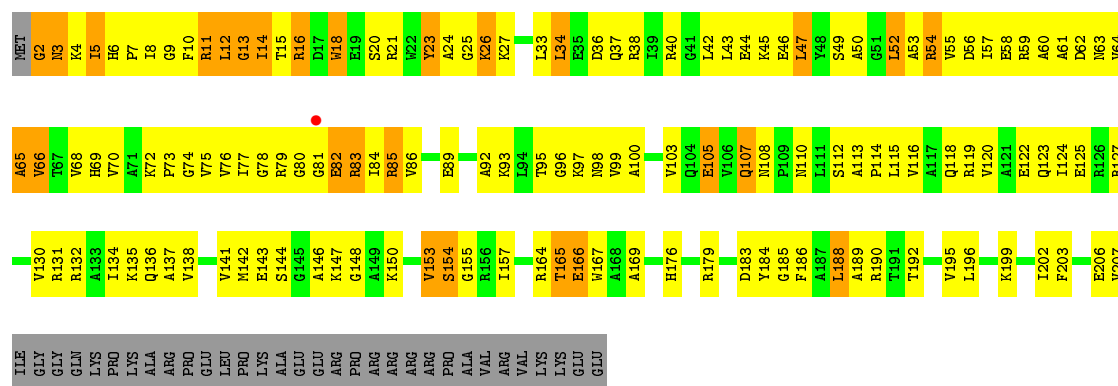


• Molecule 2: 30S RIBOSOMAL PROBLEM S2



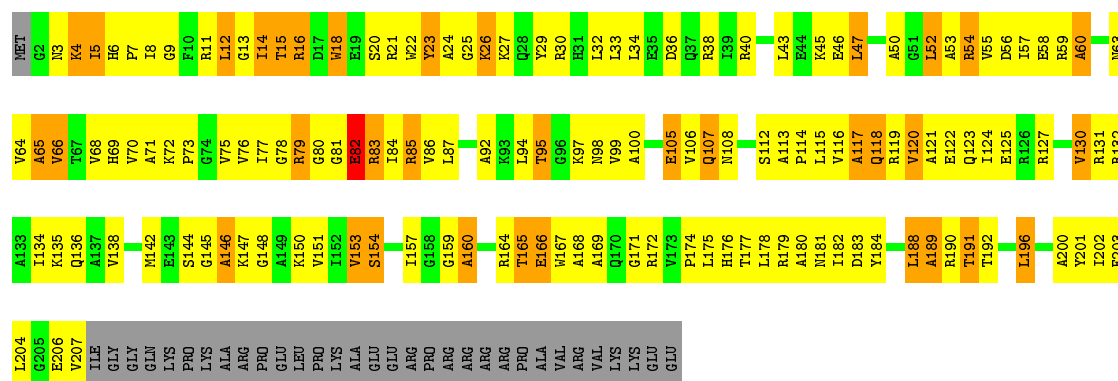
• Molecule 3: 30S RIBOSOMAL PROBLEM S3





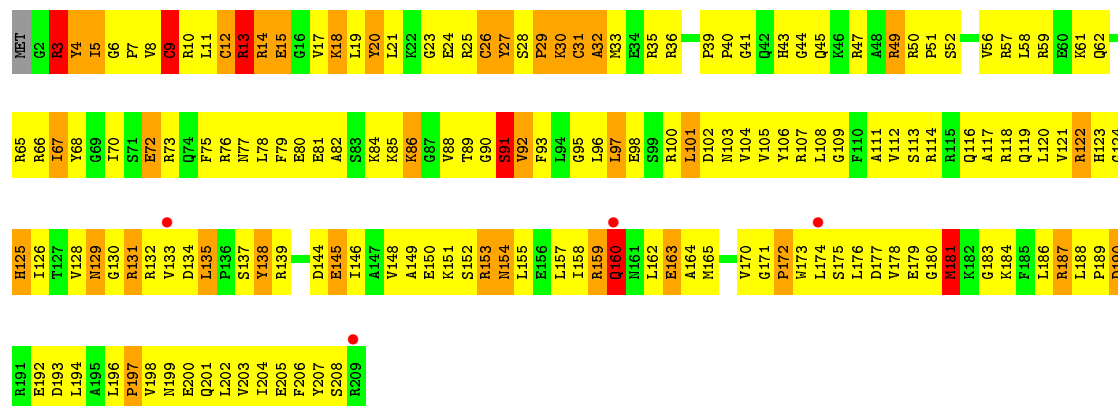
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC: 26% 46% 15% 14%



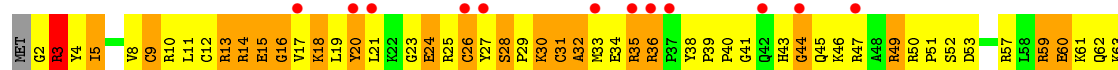
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

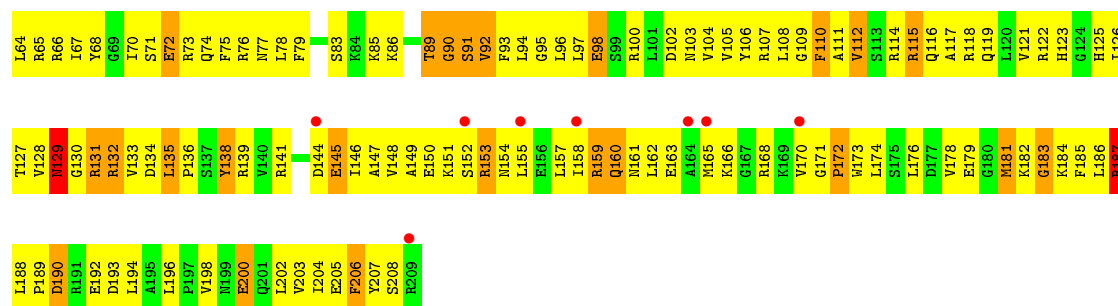
Chain AD: 2% 20% 60% 17%



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

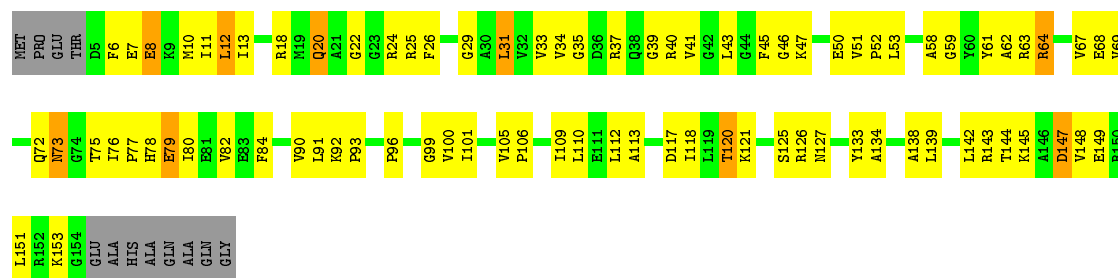
Chain CD: 10% 19% 59% 21%





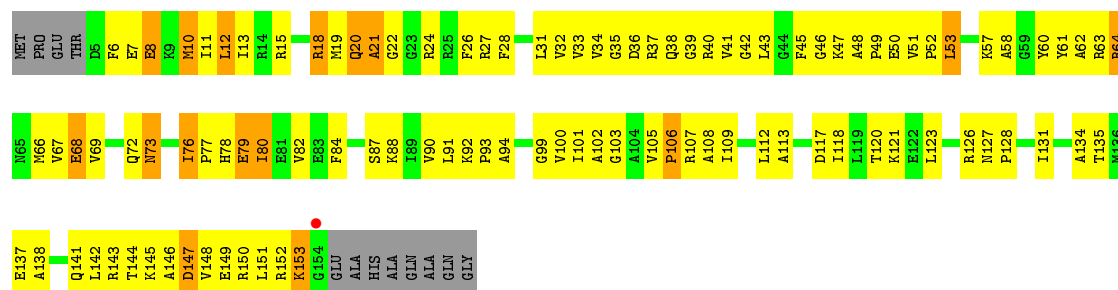
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE: 41% 46% 6% 7%



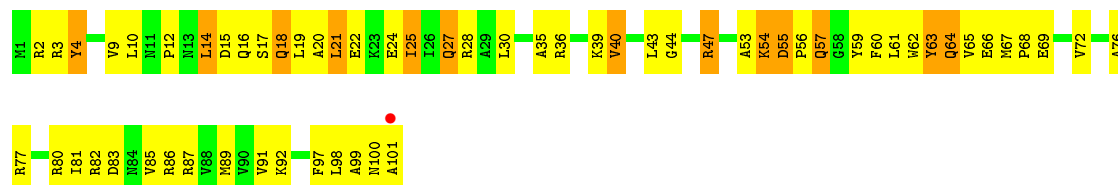
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE: 28% 54% 10% 7%



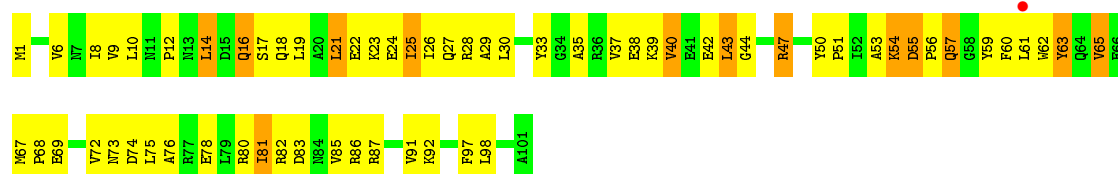
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF: 40% 48% 13%

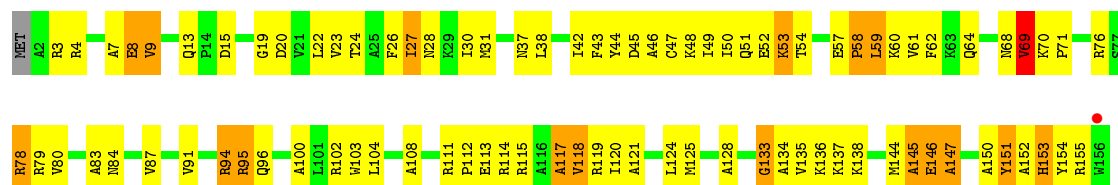
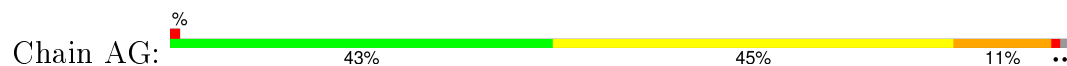


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF: 37% 50% 13%



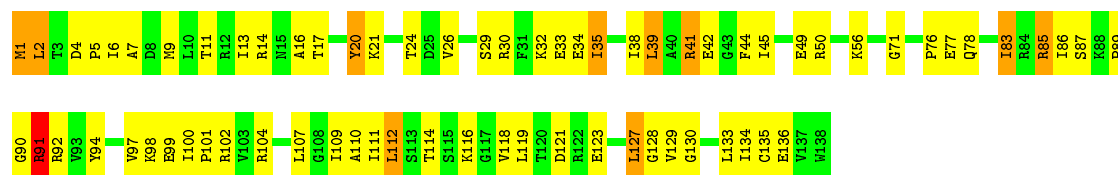
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



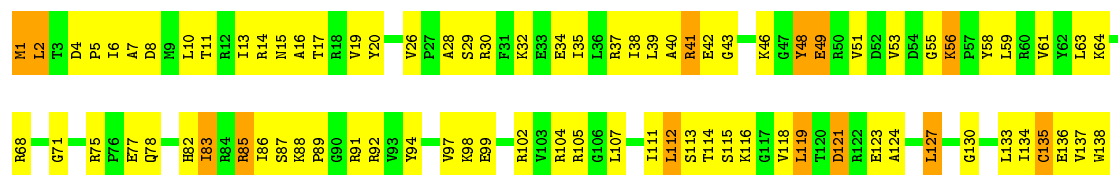
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



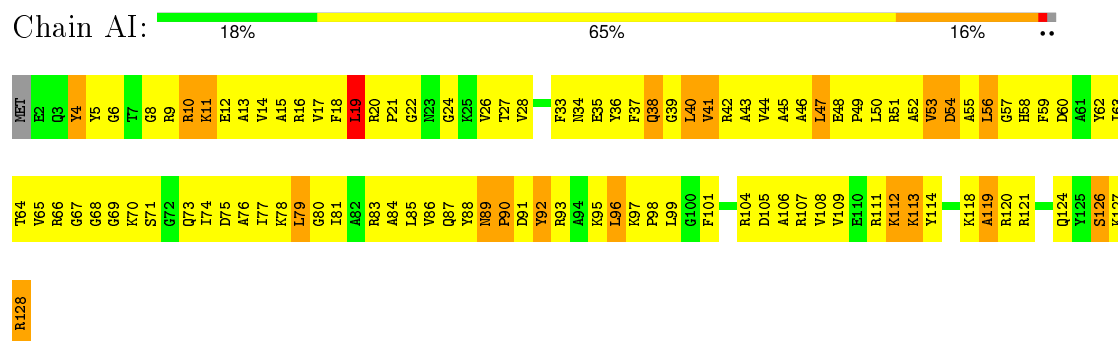
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



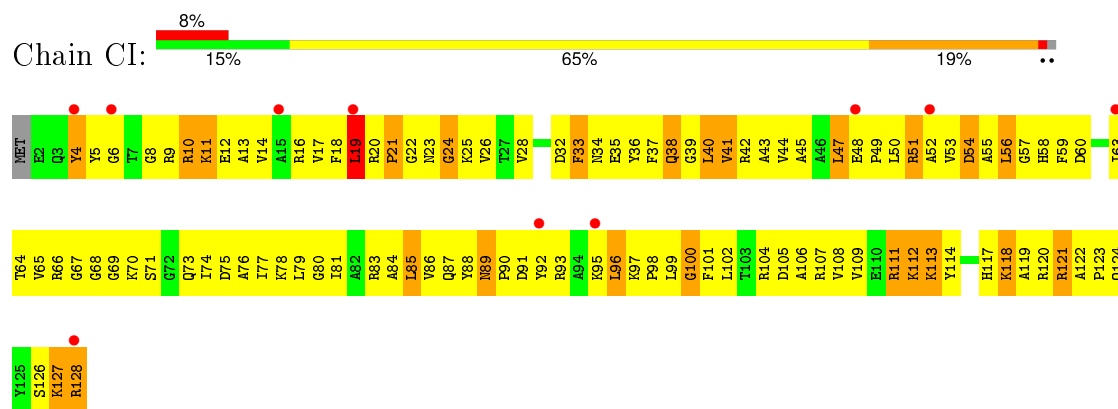
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



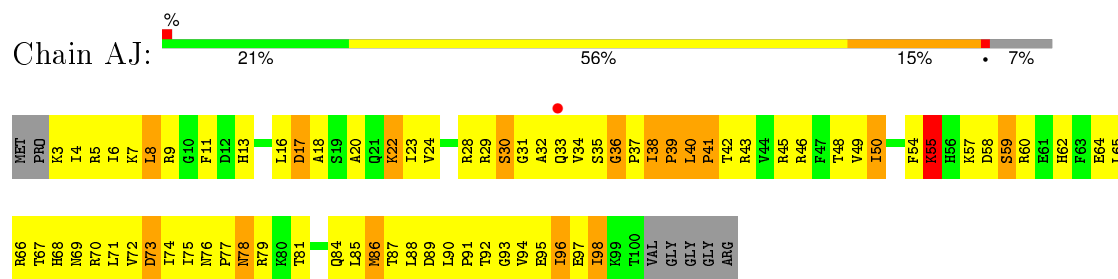
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



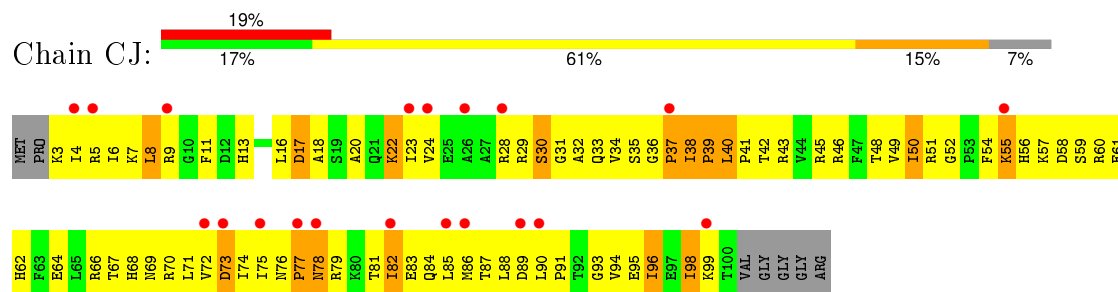
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

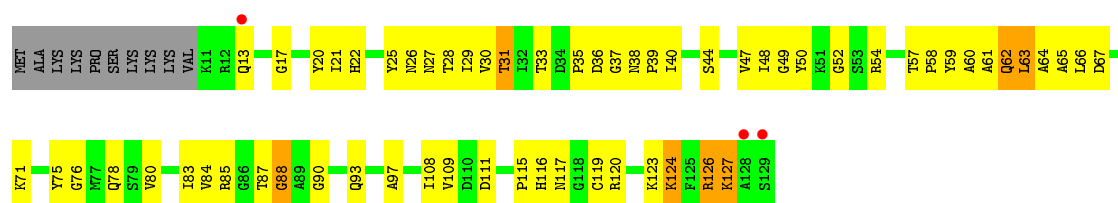


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

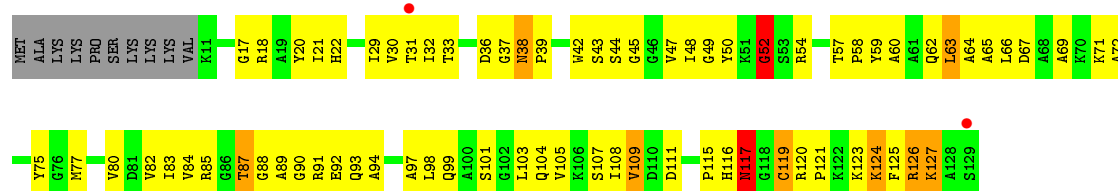


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

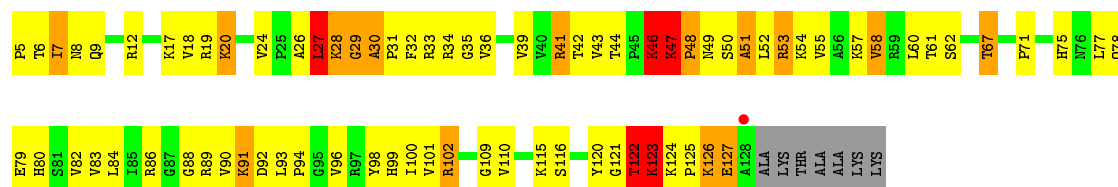




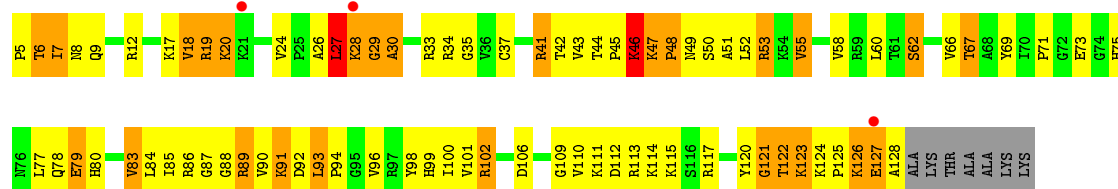
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



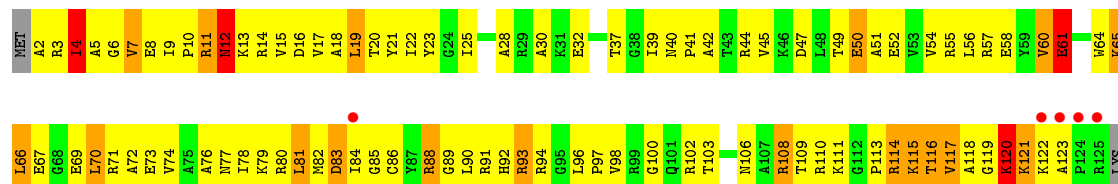
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



- Molecule 12: 30S RIBOSOMAL PROTEIN S12

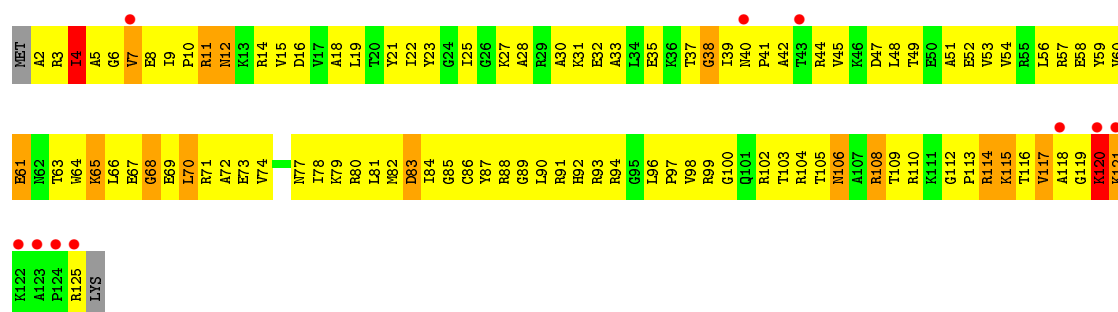


- Molecule 13: 30S RIBOSOMAL PROTEIN S13

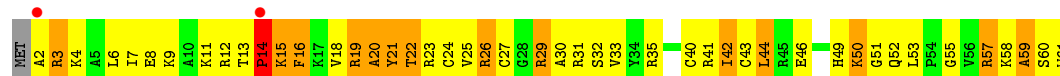


- Molecule 13: 30S RIBOSOMAL PROTEIN S13

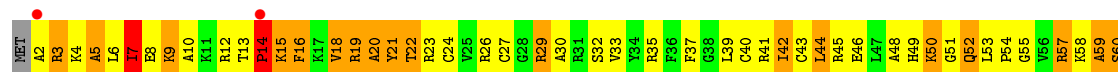
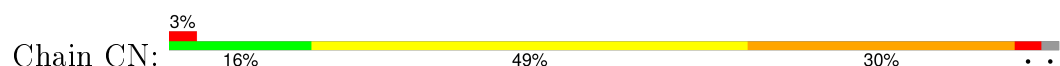




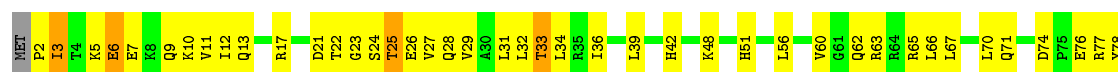
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



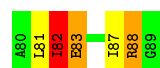
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

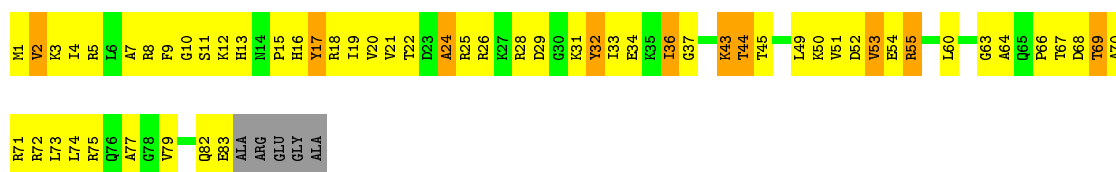


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

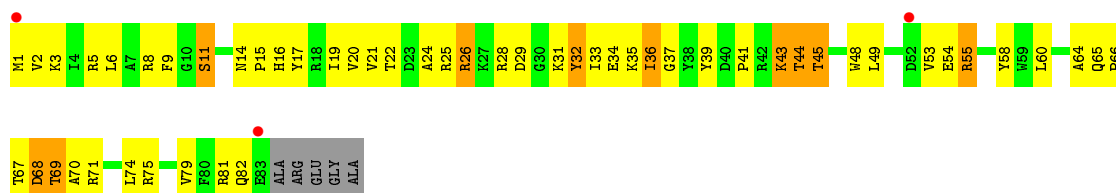


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

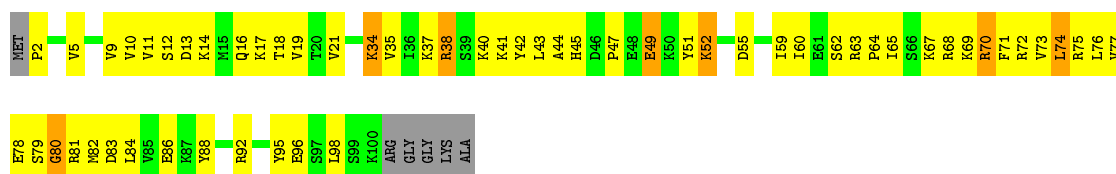




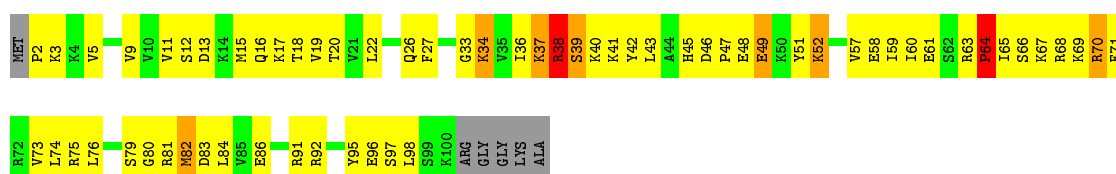
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



• Molecule 17: 30S RIBOSOMAL PROTEIN S17



• Molecule 17: 30S RIBOSOMAL PROTEIN S17



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

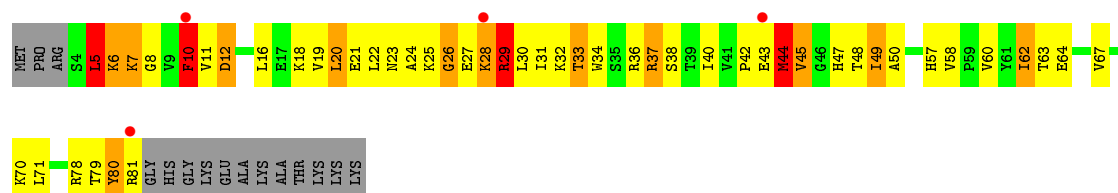


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

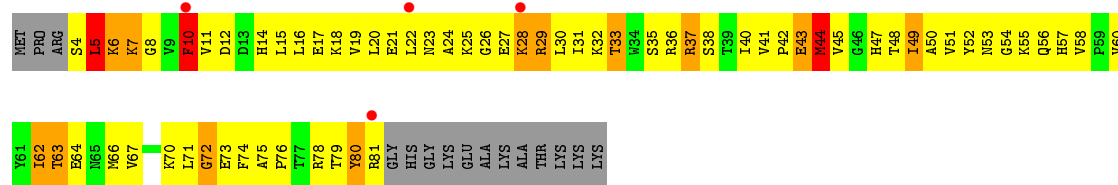
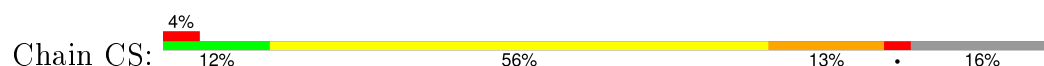




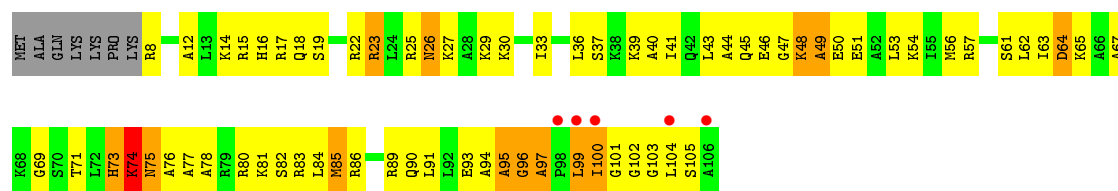
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



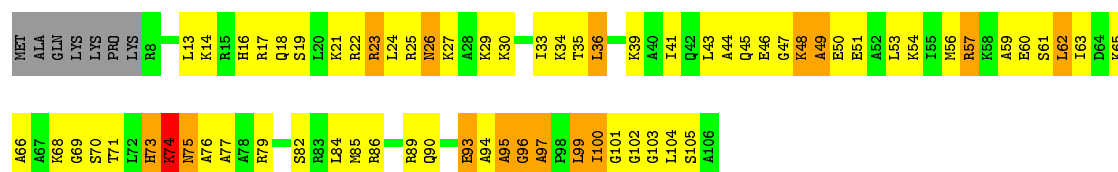
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

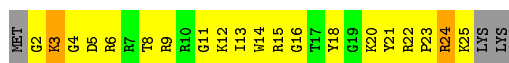


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

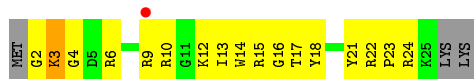
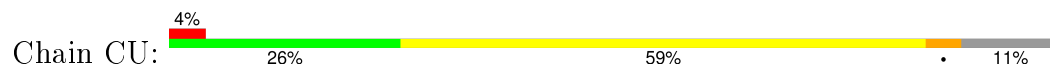


• Molecule 21: 30S RIBOSOMAL PROTEIN THX

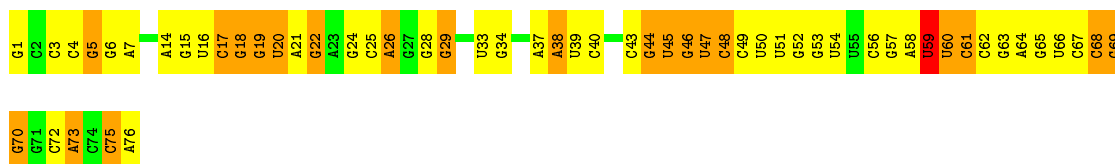




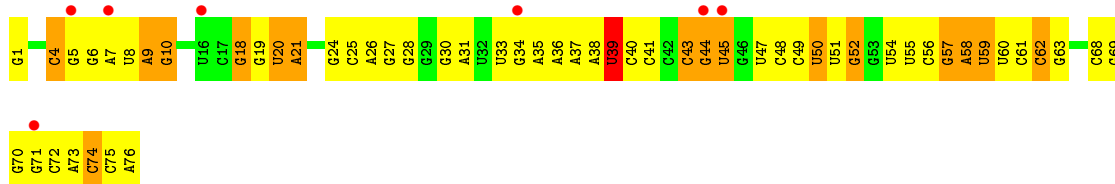
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



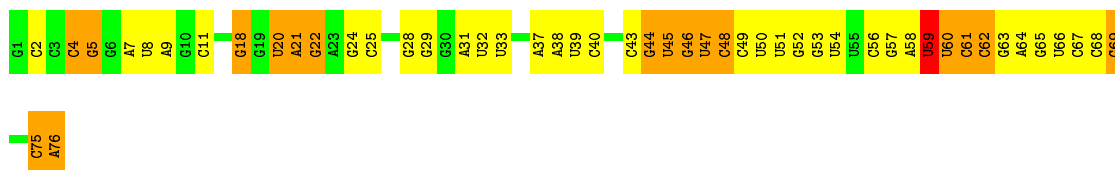
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



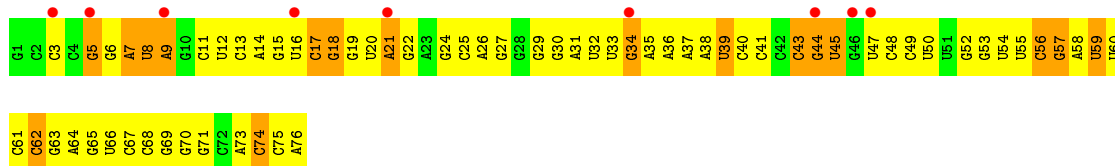
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



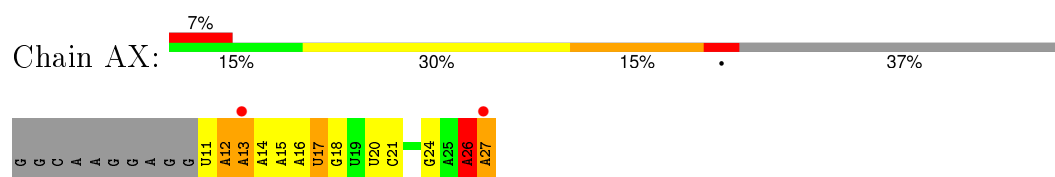
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



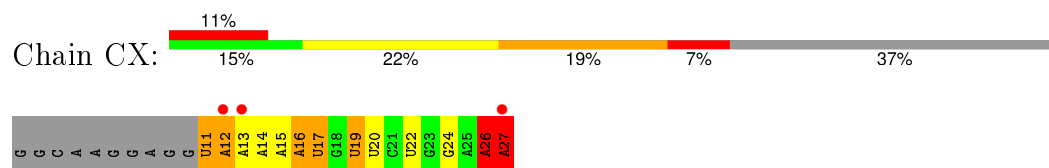
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



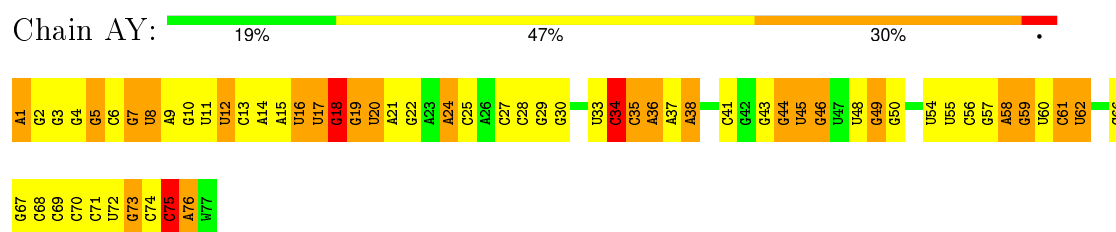
- Molecule 23: MRNA



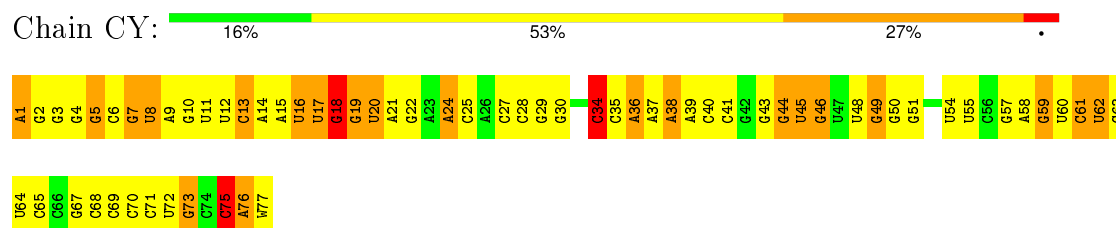
- Molecule 23: MRNA



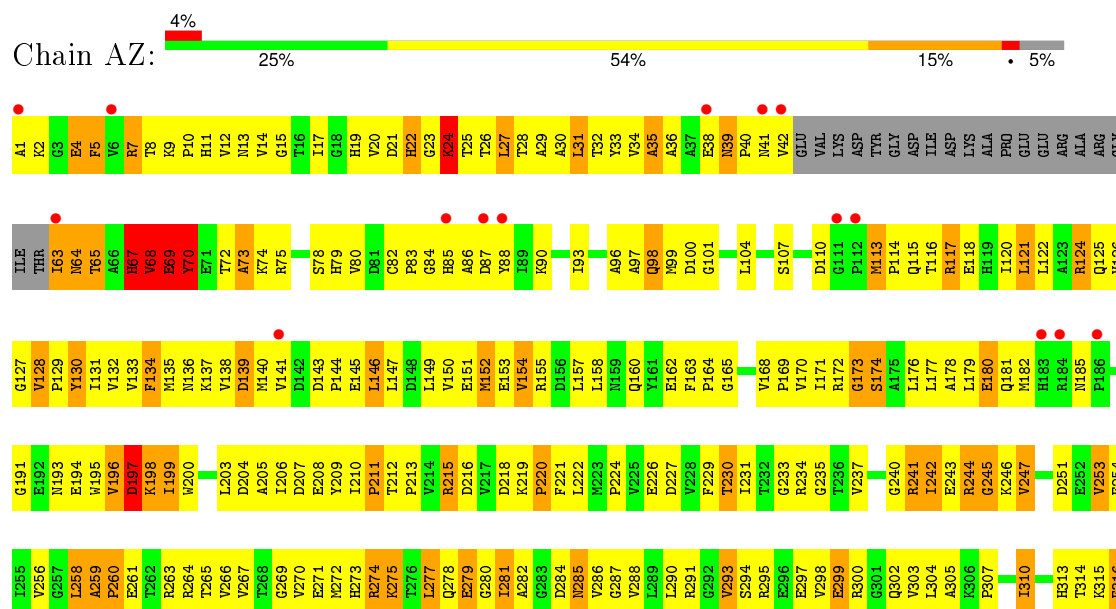
- Molecule 24: A-SITE TRNA G24A TRP-TRNA TRP

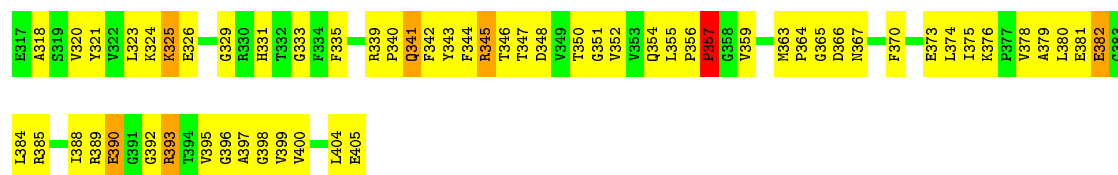


- Molecule 24: A-SITE TRNA G24A TRP-TRNA TRP

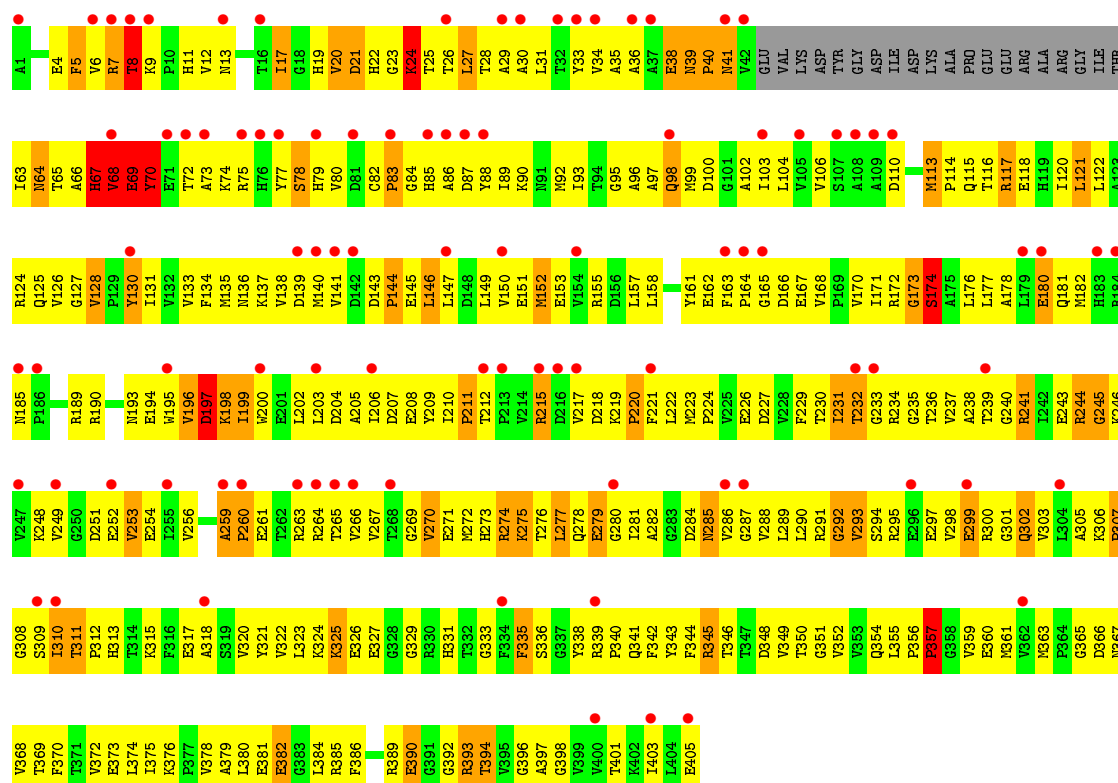


- Molecule 25: ELONGATION FACTOR TU

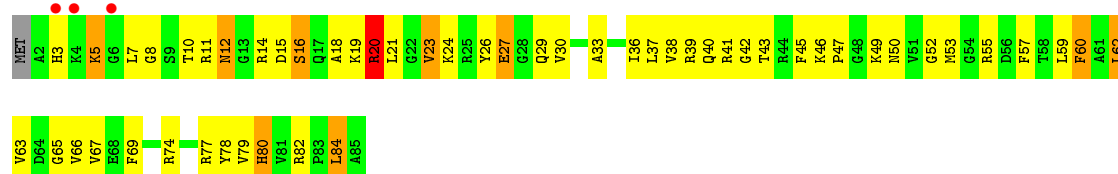




• Molecule 25: ELONGATION FACTOR TU



• Molecule 26: 50S RIBOSOMAL PROTEIN L27



• Molecule 26: 50S RIBOSOMAL PROTEIN L27





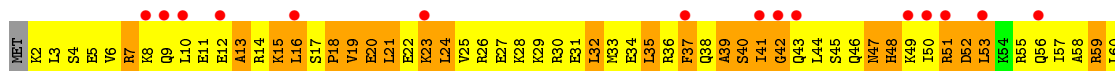
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



• Molecule 27: 50S RIBOSOMAL PROTEIN L28



• Molecule 28: 50S RIBOSOMAL PROTEIN L29



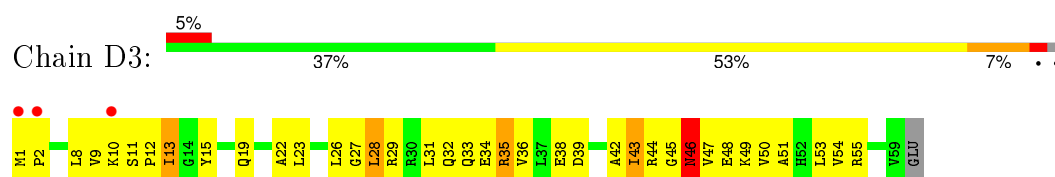
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



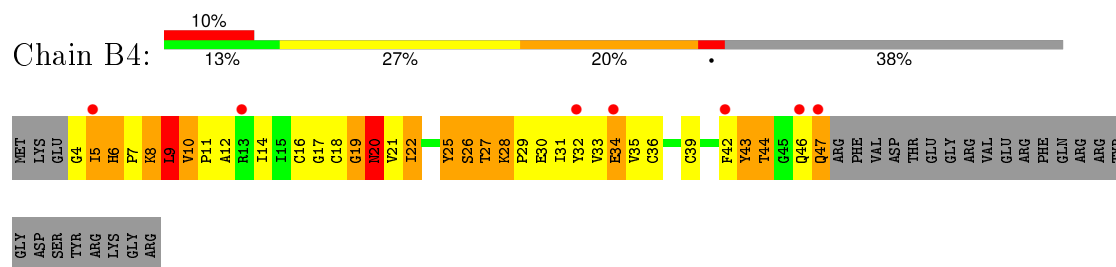
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



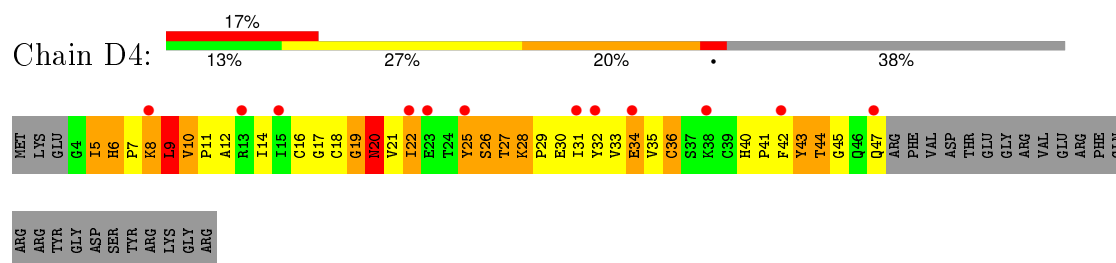
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



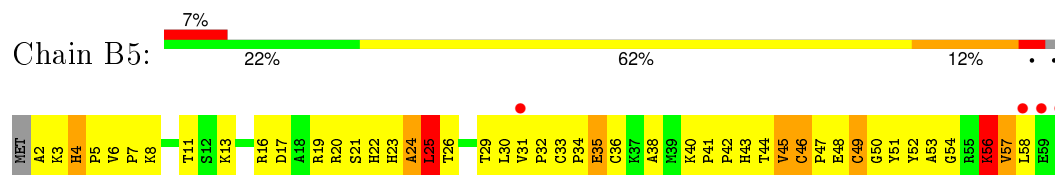
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



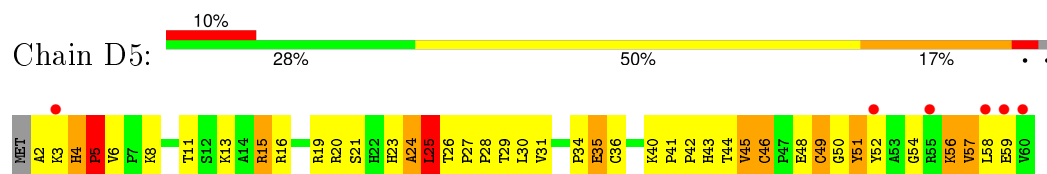
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



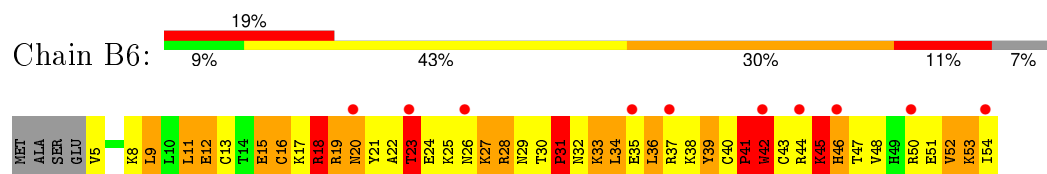
• Molecule 31: 50S RIBOSOMAL PROTEIN L32



• Molecule 31: 50S RIBOSOMAL PROTEIN L32

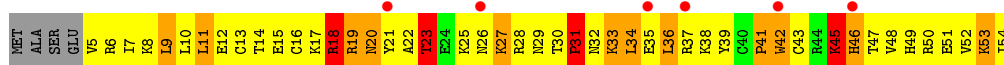


• Molecule 32: 50S RIBOSOMAL PROTEIN L33



• Molecule 32: 50S RIBOSOMAL PROTEIN L33





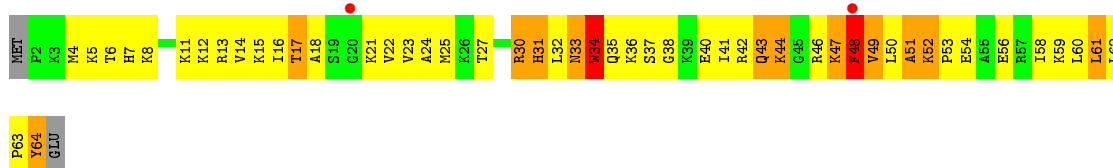
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



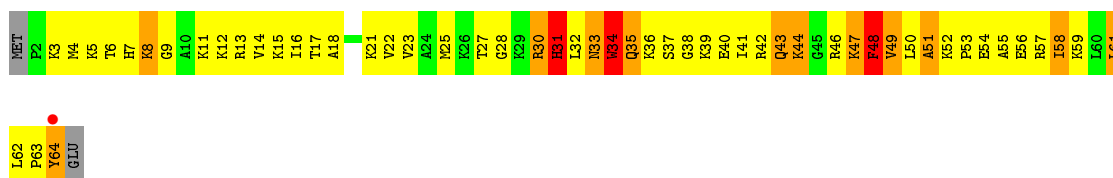
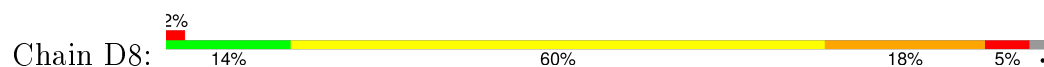
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



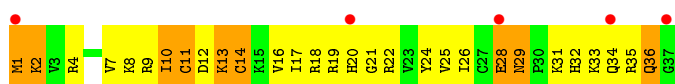
- Molecule 34: 50S RIBOSOMAL PROTEIN L35



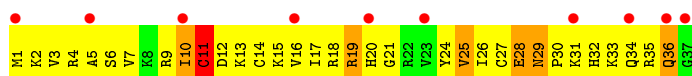
- Molecule 34: 50S RIBOSOMAL PROTEIN L35



- Molecule 35: 50S RIBOSOMAL PROTEIN L36

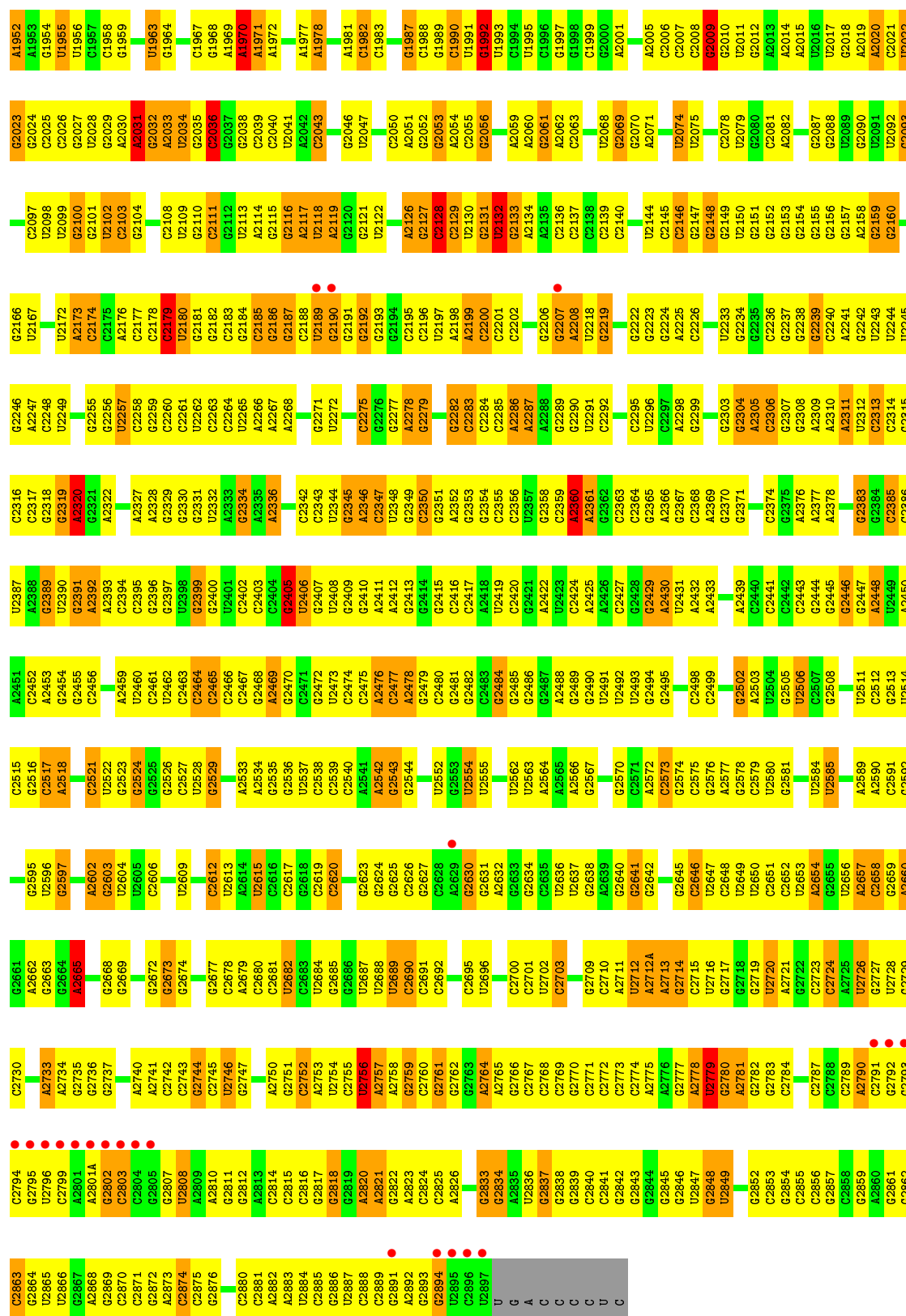


- Molecule 35: 50S RIBOSOMAL PROTEIN L36



Chain BA: 3% 28% 56% 15%

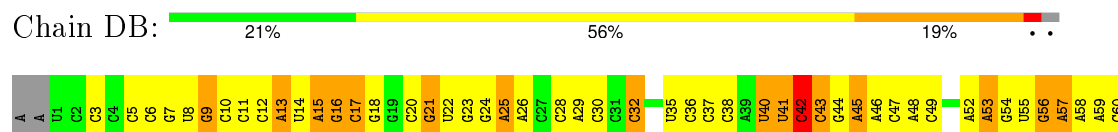
G1865	U1796	G1711	U1639	A1569	A1494	G1424	G1358	C1289	C1234	C1161	A1095	A1028	A960	C893
C1866	C1797	C1712	C1640	A1570	A1495	G1425	G1359	U1292	G1225	C1162	A1096	A1029	C961	C894
A1877	G1799	U1713	A1641	A1571	A1496	G1426	A1360	U1293	A1226	A1162	U1097	A1030	G962	C895
G1878	C1800	G1572	G1642	A1572	A1497	A1427	A1361	C1293	G1227	G1163	G1098	G1031	U963	U895
G1879	G1801	G1573	G1643	G1573	C1498	C1428	G1361	U1294	G1228	U1164	G1099	U1032	C964	A896
C1880	A1802	U1576	G1647	U1576	G1500	U1431	C1362	C1295	G1229	U1165	C1100	U1033	C965	C897
A1803	A1803	C1577	C1648	C1577	G1501	U1432	C1363	G1296	C1230	C1166	U1101	G1034	C965	C898
C1804	C1804	U1578	A1502	U1578	A1502	U1433	C1364	C1297	G1232	U1167	C1102	G1037	G968	C899
U1805	U1805	A1579	G1651	A1579	U1503	U1434	A1365	U1300	G1233	G1168	A1103	U1038	U969	C903
A1809	A1809	A1580	A1652	A1580	C1504	A1434	G1368	A1301	C1234	G1169	C1104	C1038	C970	C904
A1810	A1810	G1582	G1653	G1582	G1505	G1440	G1369	A1302	G1235	U1171	G1106	C1040	G974	U905
C1811	C1811	A1583	A1654	A1583	C1506	G1441	U1372	G1303	G1236	G1173	G1107	G1041	C975	G906
U1812	U1812	C1584	A1655	C1584	A1507	G1442	U1373	C1304	U1240	A1174	U1108	G1042	C975	G907
G1813	G1813	C1585	C1656	C1585	U1508	G1443	A1374	C1305	U1241	U1175	C1109	G1043	G977	A909
A1814	A1814	C1586	C1657	C1586	C1509	A1445	G1375	C1306	A1242	U1176	G1110	G1044	G978	A910
G1816	G1816	G1748	U1659	A1587	A1509A	C1445A	C1376	A1307	A1243	A1177	G1111	A1045	G979	A911
U1817	U1817	A1749	C1660	C1588	A1509B	C1446	C1377	A1308	G1243	C1178	G1112	A1046	C980	C912
A1818	A1818	G1750	G1661	C1589	G1511	G1447	G1377	G1309	G1244	C1179	U1113	G1047	U980	U913
C1819	C1819	C1751	C1662	U1590	C1511	G1448	A1378	G1310	G1245	C1180	G1114	A1048	C914	C914
U1820	U1820	G1752	U1512	C1591	U1512	A1449	A1379	G1311	A1246	C1181	G1115	C1049	C983	C915
A1821	A1821	C1753	C1663	C1592	C1516	A1452	G1380	U1312	A1247	A1182	C1116	A1050	A984	G916
G1822	G1822	G1754	A1664	G1593	G1517	U1453	G1381	U1313	G1248	G1183	G1117	G1051	C985	A917
C1823	C1823	A1755	A1665	G1594	U1518	U1454	G1382	C1314	U1249	C1184	G1120	C1052	C986	A918
U1824	U1824	G1756	G1666	G1595	G1517	U1455	C1383	G1315	G1250	C1185	G1121	C1053	C987	C919
G1825	G1825	U1757	G1667	A1596	U1518	G1456	A1384	C1318	C1251	G1186	G1122	A1054	A988	G920
A1826	A1826	C1758	A1668	A1597	U1523	A1457	G1385	G1319	G1252	U1187	G1122	A1057	G989	G921
C1827	C1827	U1759	U1669	C1598	G1524	C1458	C1386	C1320	A1253	U1188	A990	G1058	A990	U922
G1828	G1828	A1760	C1670	C1599	G1525	A1459	G1387	A1321	U1254	A1189	G1124	G1059	C991	C923
A1829	A1829	C1761	U1671	C1600	G1526	A1460	G1389	A1322	U1255	G1190	G1125	G1060	C992	C928
C1830	C1830	A1762	U1601	G1601	G1527	G1461	U1390	U1323	G1256	G1191	U1130	U1060	G993	U930
U1831	U1831	G1763	A1602	U1602	A1528	C1462	U1394	G1324	C1257	G1192	U1131	U1061	A996	G931
G1832	G1832	C1764	A1603	A1603	A1528A	G1463	A1395	C1327	C1258	G1193	G1132	G1062	A997	G932
U1833	U1833	U1765	C1678	A1608	G1529	G1466	U1396	G1328	G1260	C1196	U1133	C1064	C998	A933
A1834	A1834	C1766	U1679	A1609	C1530	C1467	U1397	U1329	U1263	G1197	G1136	U1065	U999	G934
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U1837	U1837	C1771	G1682	C1612	U1534	G1470	G1400	G1332	G1266	C1203	G1139	A1069	G1002	G939
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A1858	A1858	U1786	C1699	G1628	G1485	G1485	G1413	G1346	A1278	G1216	C1150	A1082	U1020	G952
G1859	G1859	A1787	G1699	A1554	A1486	G1487	G1416	U1347	G1279	C1217	G1151	G1087	A1021	A953
U1944	U1944	C1788	A1701	A1632	G1488	C1417	C1418	A1349	G1283	C1218	C1152	A1088	G1022	G954
G1945	G1945	A1789	U1702	A1633	U1489	U1489	G1413	C1350	A1284	G1219	C1153	G1089	U1023	C955
U1946	U1946	C1790	G1703	A1634	A1490	A1490	A1419	C1351	G1285	A1220	G1154	U1090	U1024	C956
C1947	C1947	A1791	G1635	G1635	G1491	G1491	U1420	U1352	A1286	C1221	A1155	G1091	G1025	A957
G1948	G1948	U1794	U1709	C1638	G1492	G1492	U1421	A1353	A1287	C1222	A1156	C1092	U1026	U958
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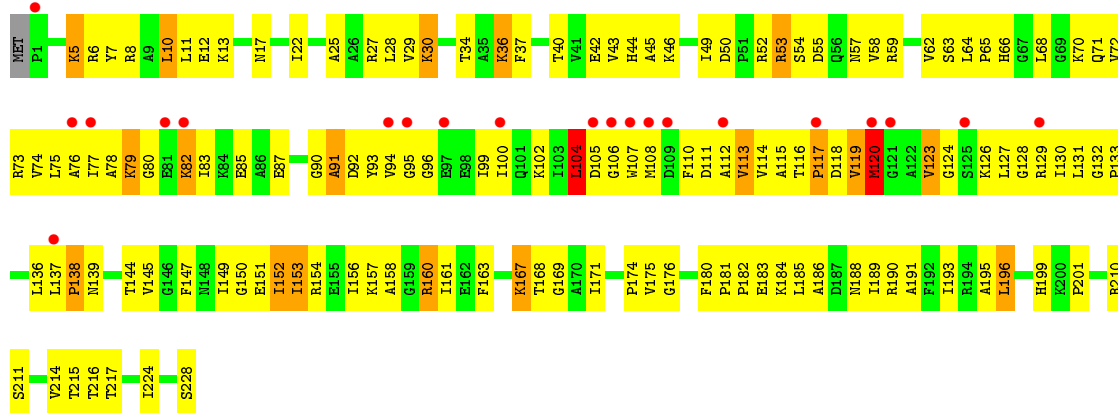


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A2018	U1033	A1096	U1226	A1365	U1433	C1509	A1571	A1641	U1710	C1794	G1865	C1947	C2018
A2019	U1034	A1097	G1227	A1366	A1434	C1509B	A1572	G1642	C1710	C1795	C1866	C1948	A2019
A2020	U1035	A1098	G1227	A1367	G1441	A1509A	G1573	G1643	C1711	U1796	A1876	G1949	A2020
C2021	G1036	G1099	G1231	G1368	G1442	G1510	C1574	C1644	C1712	U1797	A1877	U1951	C2021
U2022	C1037	C1100	G1232	G1369	G1443	C1511	U1578	G1647	U1713	U1798	G1878	U1952	U2022
G2023	U1038	U1101	C1233	G1374	G1444	U1515	A1579	C1648	G1714	G1799	C1879	A1953	G2023
G2024	G1039	U1101	G1233	C1375	A1445	C1516	A1580	G1649	G1718	C1800	C1880	A1954	G2024
C2025	U1040	C1102	G1233	C1376	A1456A	G1517	G1581	G1650	U1719	G1801	C1881	C1954	C2025
G2026	G1041	C1104	G1237	C1377	G1446	U1518	A1582	G1651	U1720	A1802	C1882	U1955	C2026
G2027		U1105	G1238	A1378	G1447	U1518	A1583	G1652	G1721	C1803	G1883	U1956	G2027
U2028		G1106	A1242	A1379	G1448	U1523	C1584	G1653	A1722	U1804	A1884	C1957	U2028
G2029	A1045	G1107	A1243	A1380	A1449	U1524	A1586	A1654	U1729	U1805	A1885	C1958	G2029
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G2031	G1047	G1107	A1244	G1382	U1454	C1525	A1587	G1656	G1740	A1810	C1887	U1963	G2031
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C2039	G1057	G1117	G1253	U1390	G1466	C1532	A1596	A1665	C1751	U1820	A1900	A1972	C2039
C2040	G1058		G1254	G1467	C1467	G1534	A1597	G1666	C1752	A1821	A1901	G1973	C2040
C2043	G1059	G1120	U1255	A1395	G1468	U1534	C1598	G1667	A1755	G1822	G1902	C1974	C2043
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	G1063	G1125	G1259	C1399	A1471	G1538	U1602	U1672		C1830	C1908		
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A1085	A1085	C1146	G1285	A1214	G1418	G1556	G1627	C1691	U1779	G1850	U1928	G2003	C2073
G1087	G1087	A1148	A1286	G1215	G1419	C1557	G1628	U1692	A1780	U1851	G1930	G2004	U2074
A1088	A1088	C1149	U1288	G1216	U1420	A1558	G1629	U1693	C1781	C1852	U1931	C2006	U2075
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G1093	G1093		C1297	C1430	C1428	C1565	C1637	A1700		G1860	A1936	G2011	U2086
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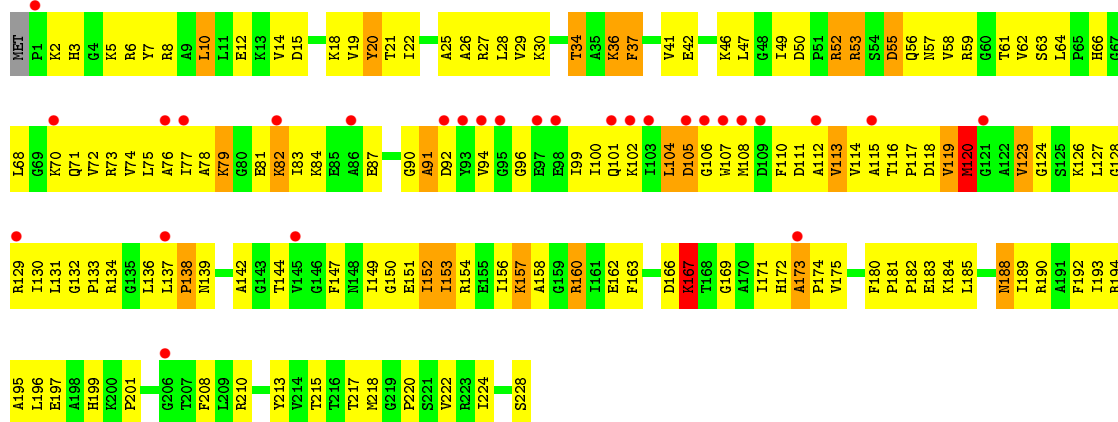




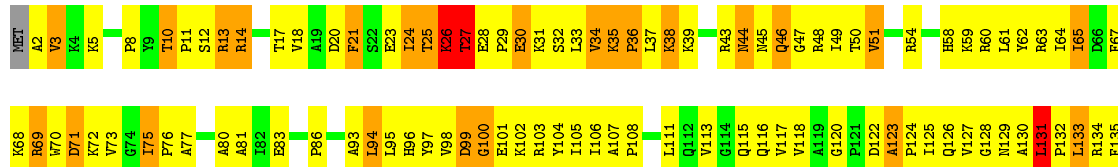
● Molecule 38: 50S RIBOSOMAL PROTEIN L1

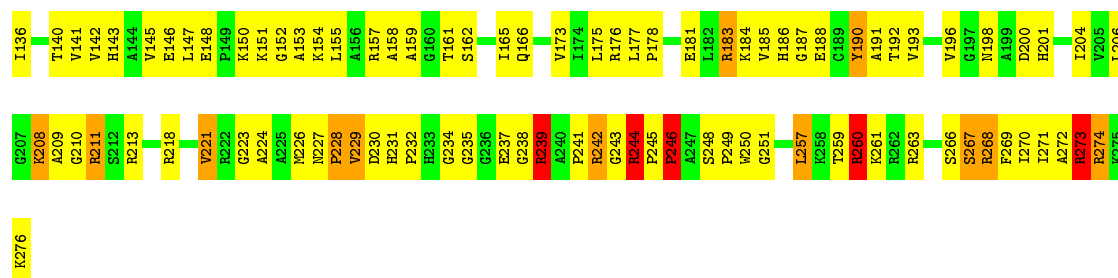


● Molecule 38: 50S RIBOSOMAL PROTEIN L1



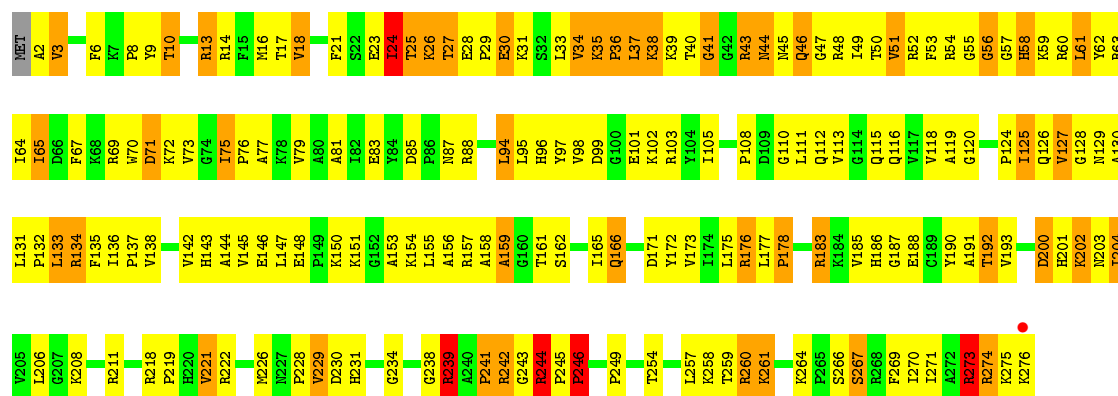
● Molecule 39: 50S RIBOSOMAL PROTEIN L2





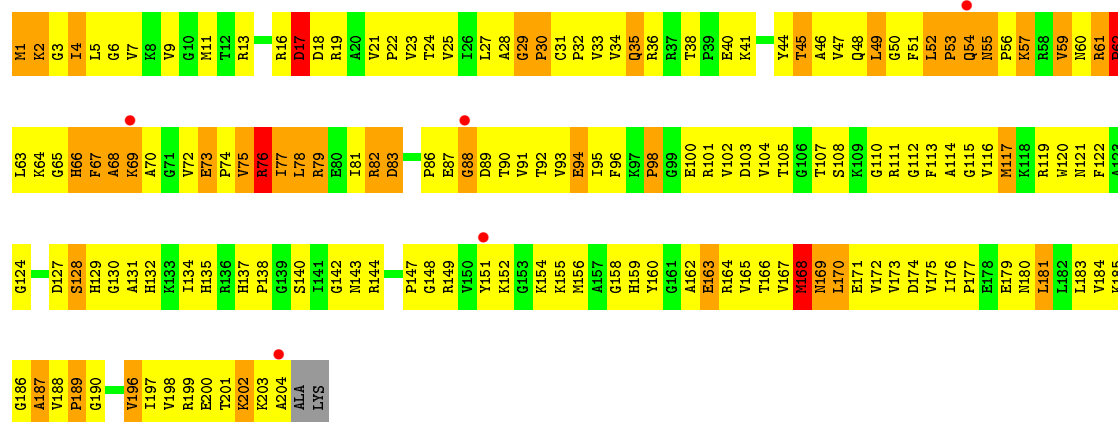
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

Chain DD: 34% 47% 17%



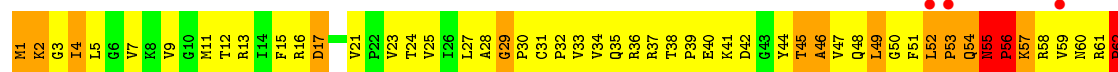
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

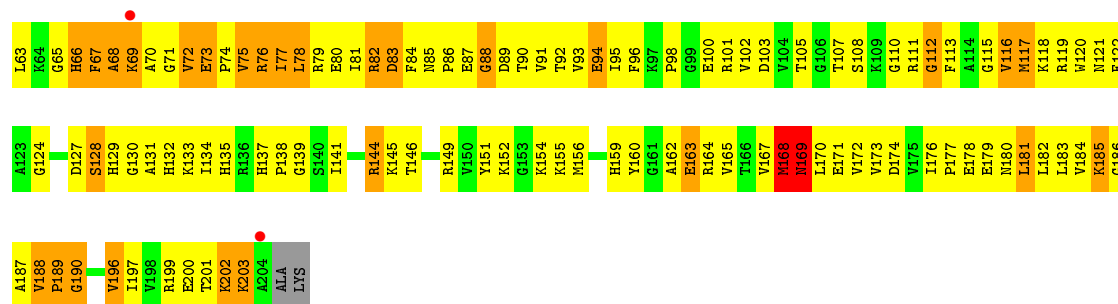
Chain BE: 2% 20% 58% 19%



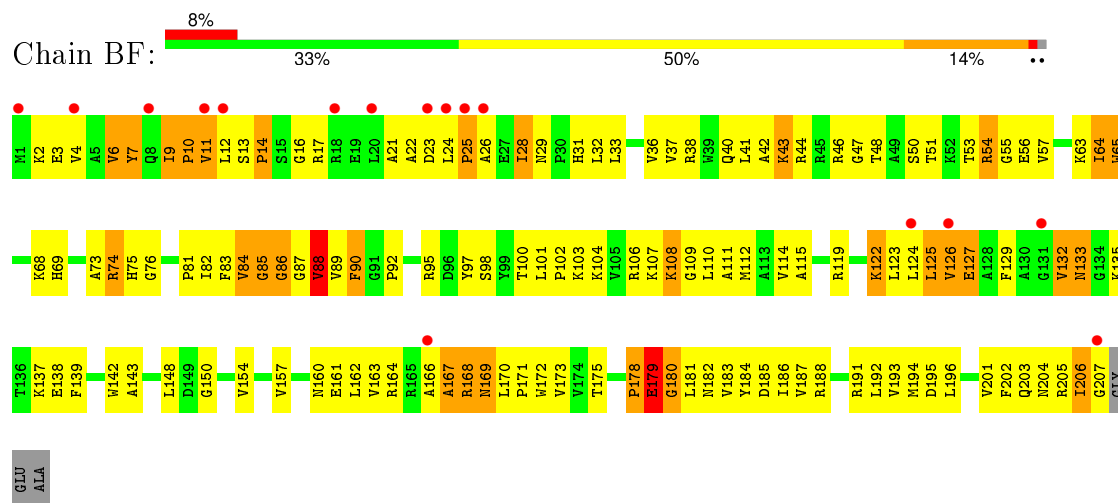
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain DE: 2% 19% 58% 19%

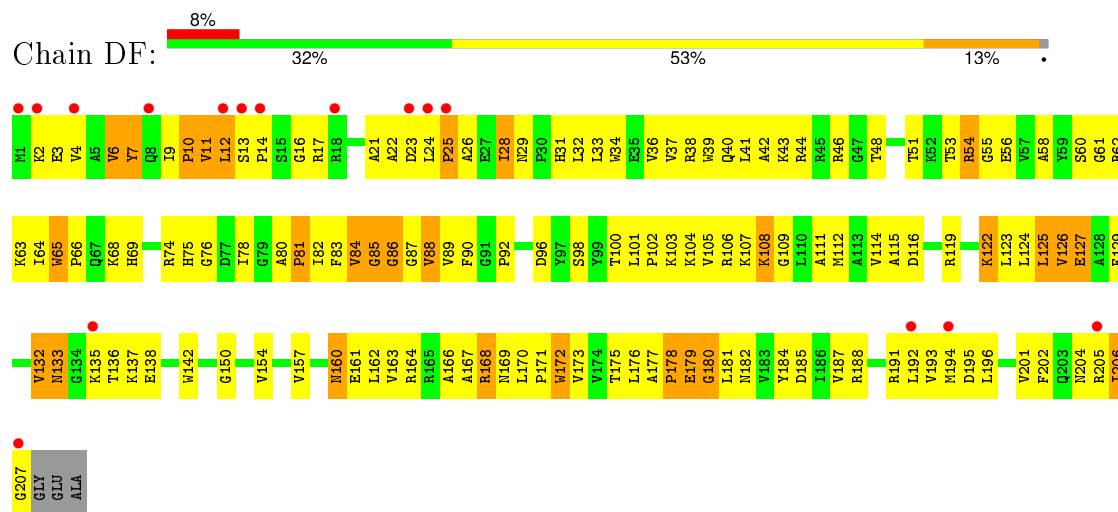




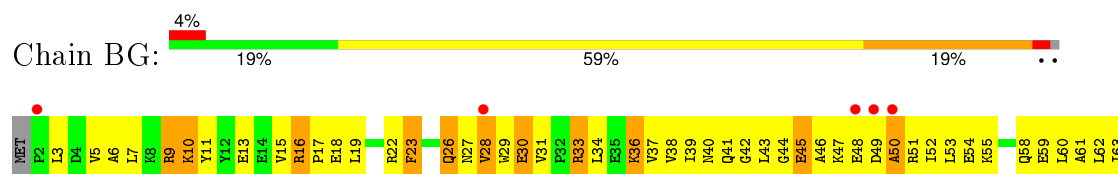
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

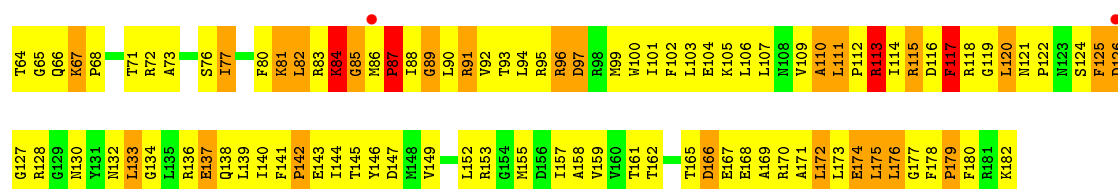


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

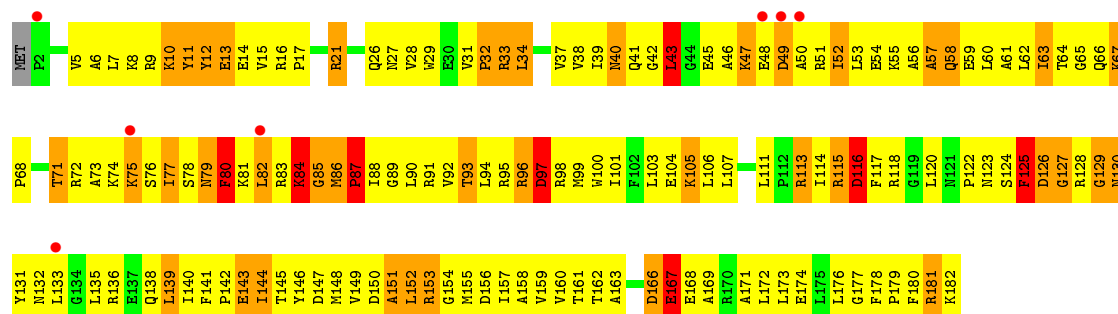
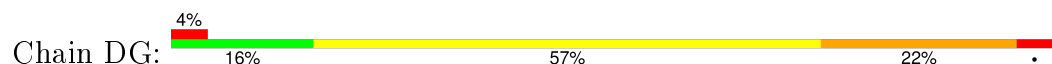


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

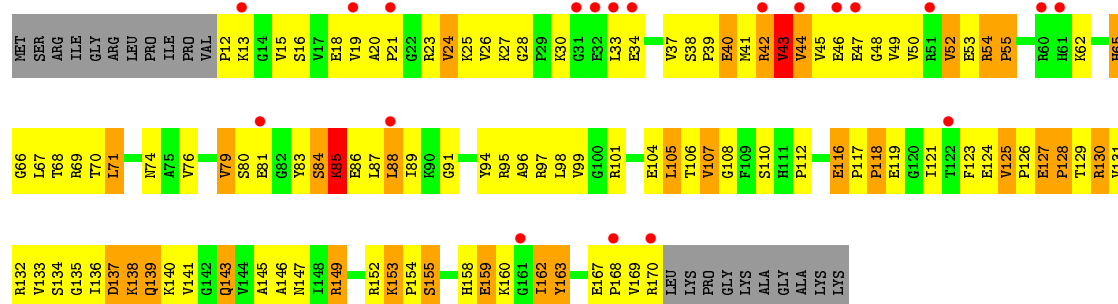




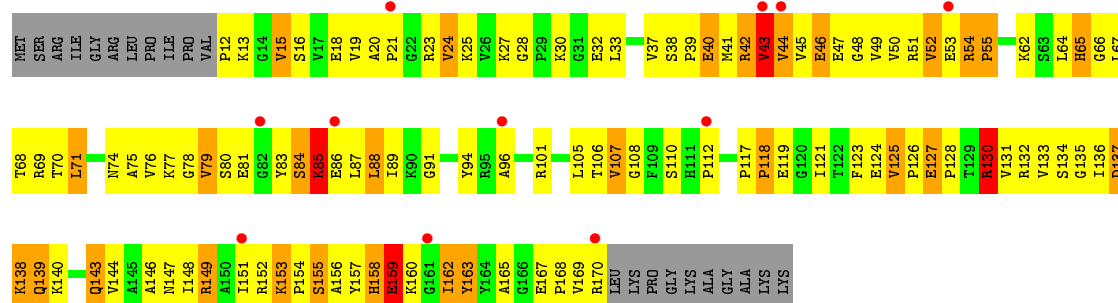
• Molecule 42: 50S RIBOSOMAL PROTEIN L5



• Molecule 43: 50S RIBOSOMAL PROTEIN L6

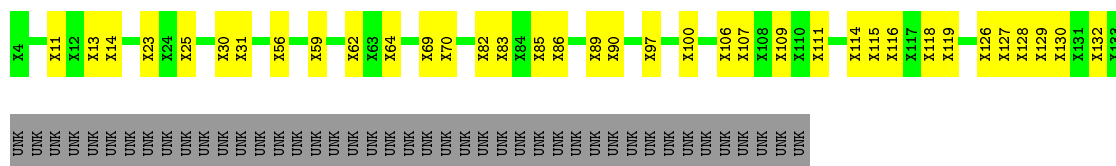


• Molecule 43: 50S RIBOSOMAL PROTEIN L6



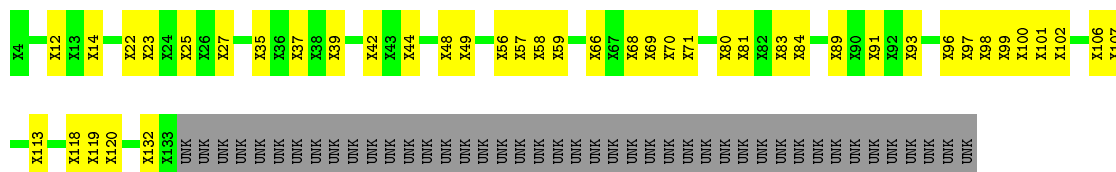
• Molecule 44: 50S RIBOSOMAL PROTEIN L10





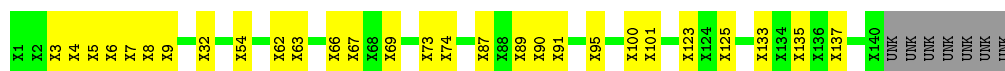
• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain DJ: 50% 25% 25%



• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK: 76% 19% 5%



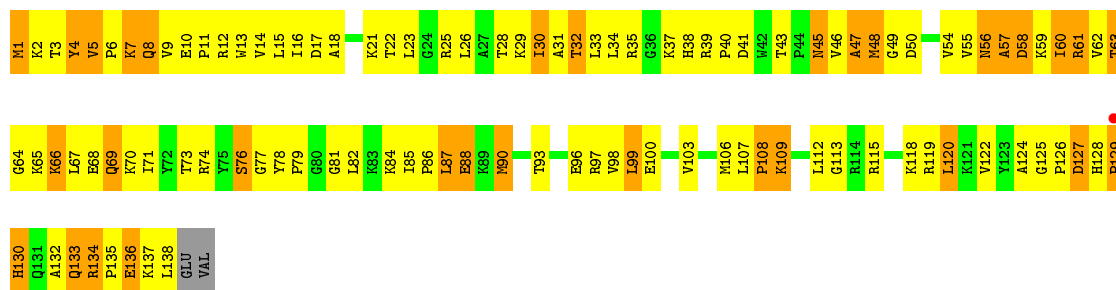
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain DK: 79% 16% 5%



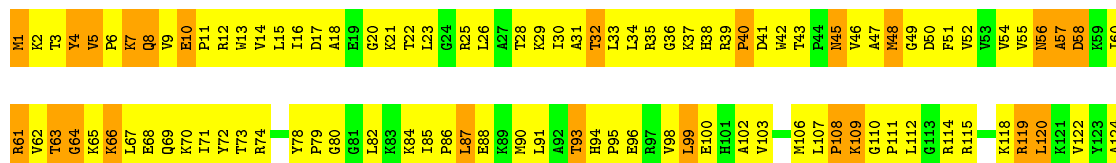
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

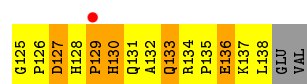
Chain BN: 22% 54% 23%



• Molecule 46: 50S RIBOSOMAL PROTEIN L13

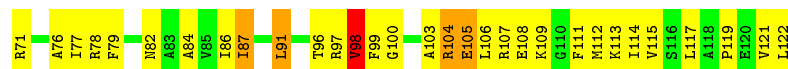
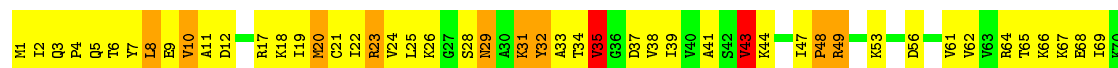
Chain DN: 16% 62% 21%





• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO: 35% 52% 11%



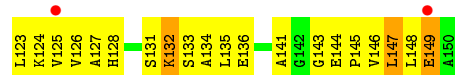
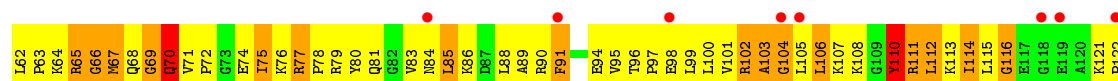
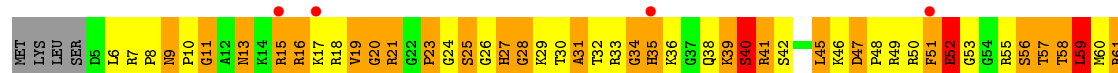
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO: 36% 52% 9%



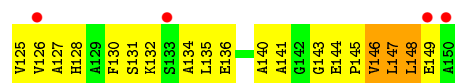
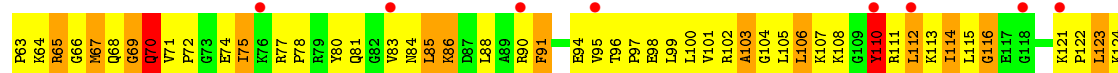
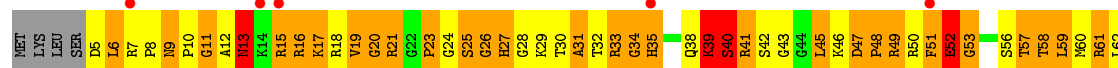
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP: 9% 17% 48% 29%

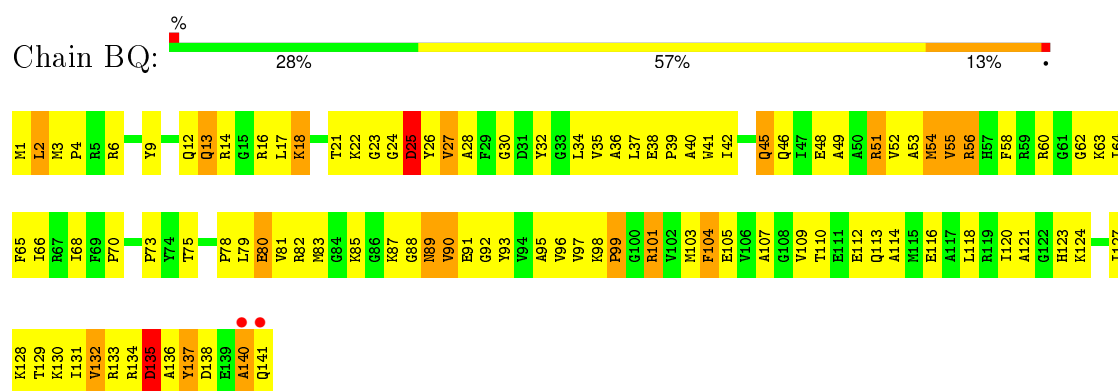


• Molecule 48: 50S RIBOSOMAL PROTEIN L15

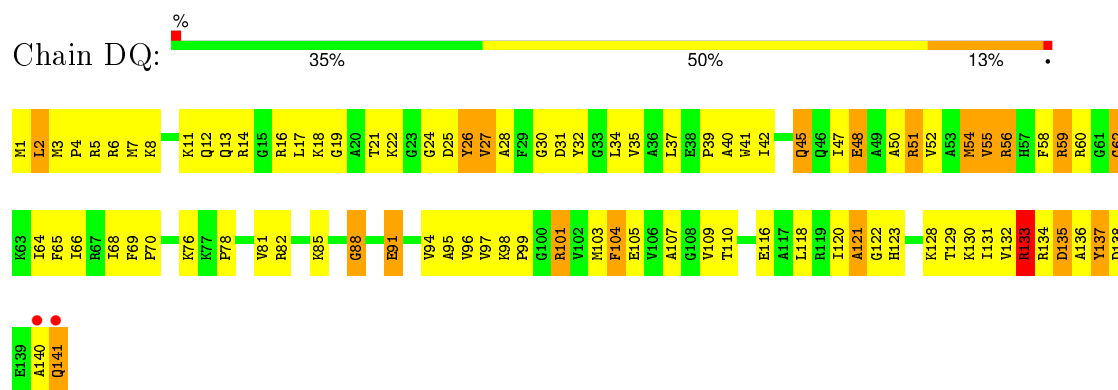
Chain DP: 11% 18% 46% 29%



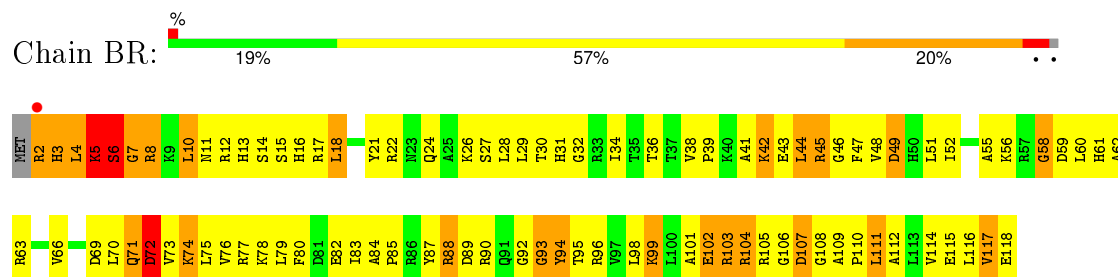
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



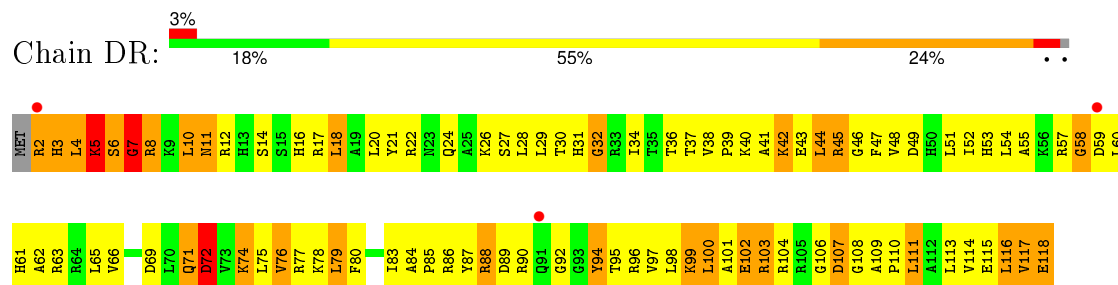
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



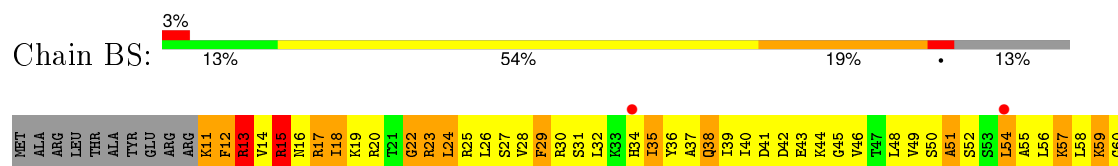
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

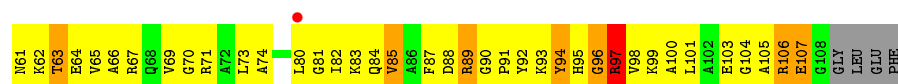


• Molecule 50: 50S RIBOSOMAL PROTEIN L17

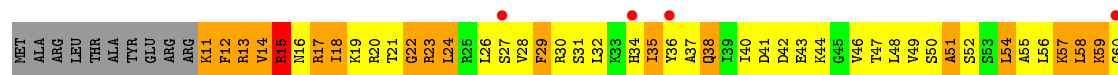


• Molecule 51: 50S RIBOSOMAL PROTEIN L18

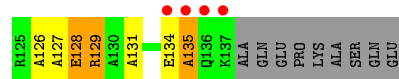
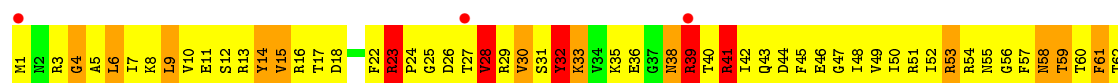
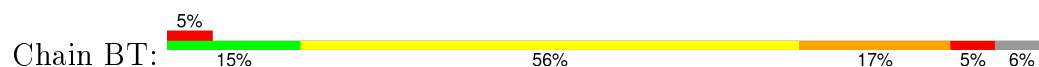




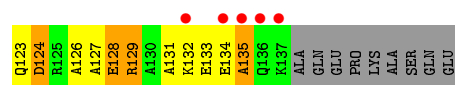
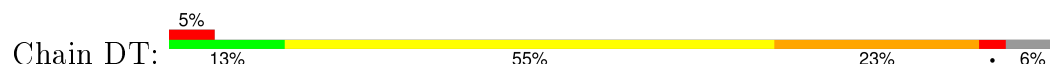
• Molecule 51: 50S RIBOSOMAL PROTEIN L18



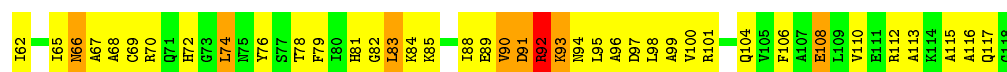
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



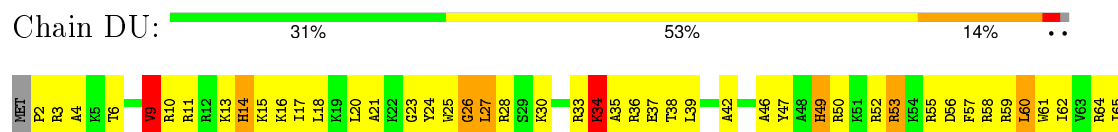
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



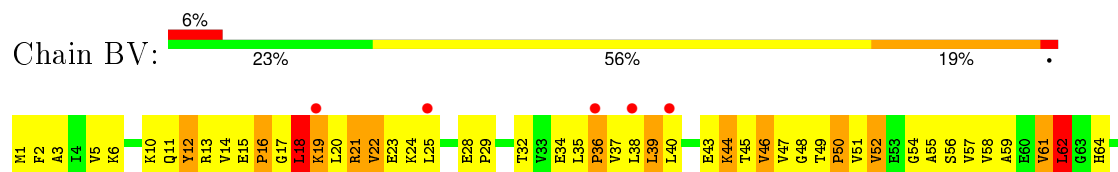
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



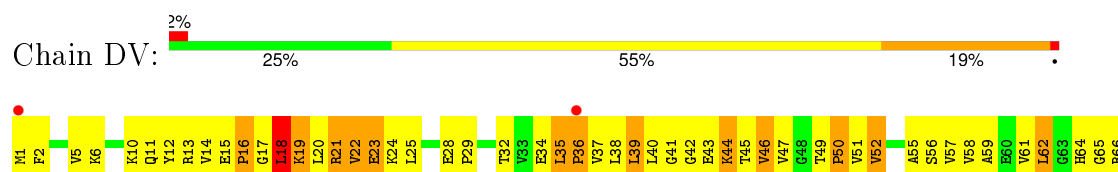
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



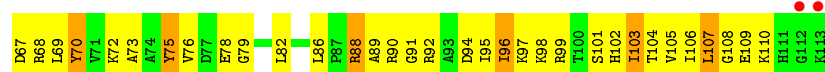
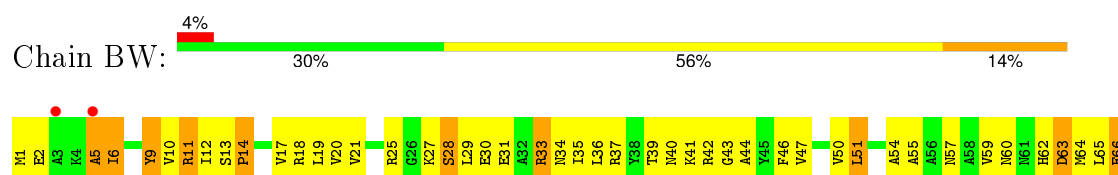
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



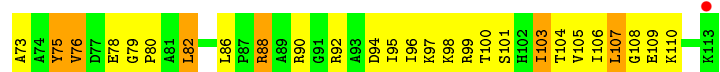
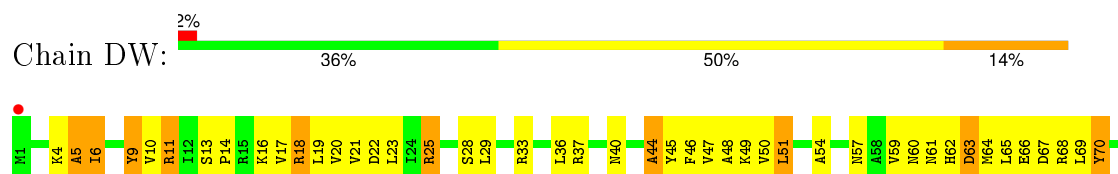
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



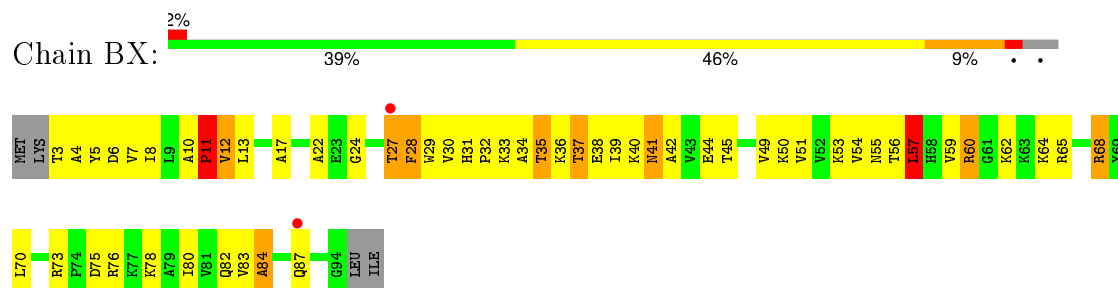
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



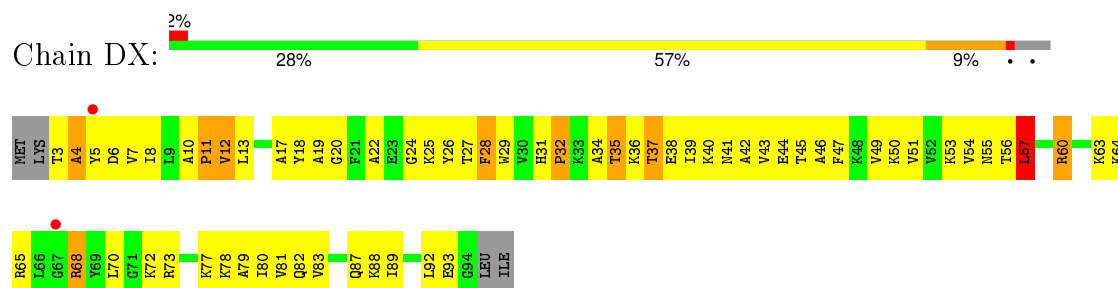
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



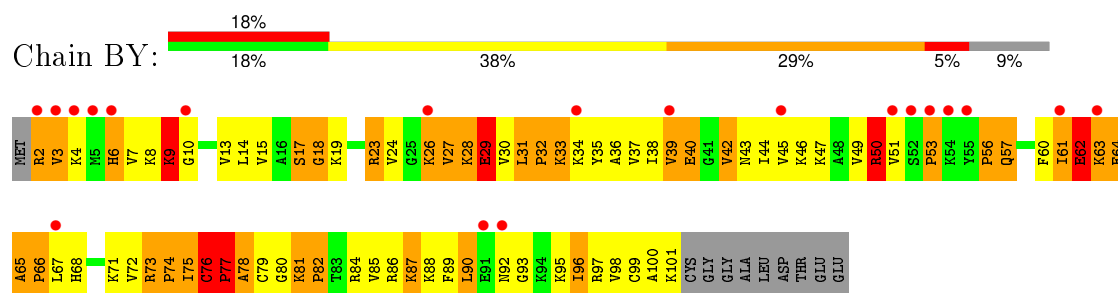
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



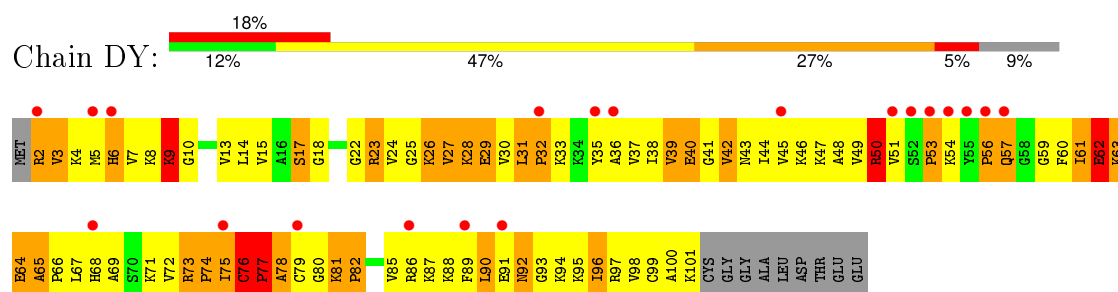
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



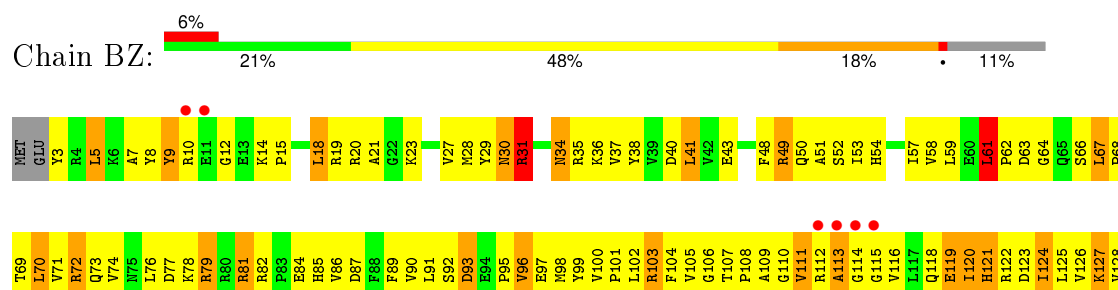
• Molecule 57: 50S RIBOSOMAL PROTEIN L24



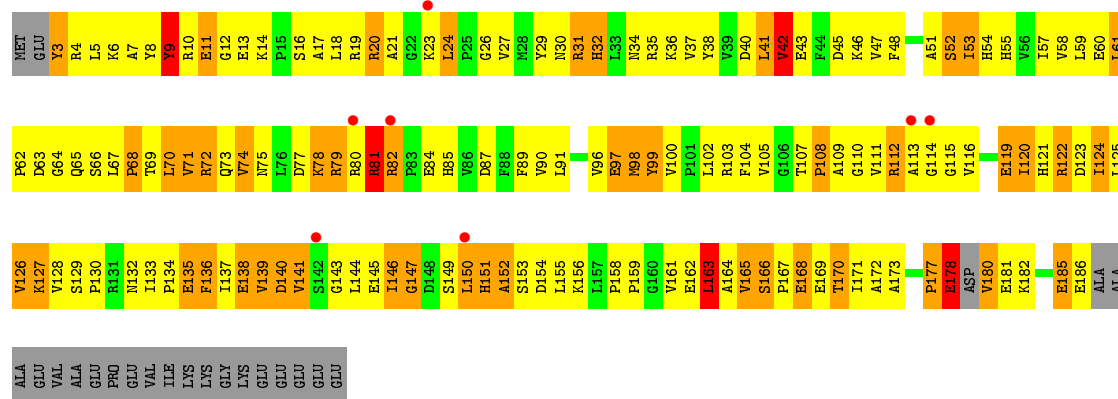
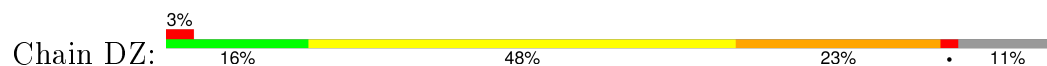
• Molecule 57: 50S RIBOSOMAL PROTEIN L24



• Molecule 58: 50S RIBOSOMAL PROTEIN L25



• Molecule 58: 50S RIBOSOMAL PROTEIN L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	289.80Å 269.10Å 403.90Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.83 – 2.93	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-3.10) 89.6 (49.83-2.93)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.96Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.247 , 0.285 0.246 , 0.284	Depositor DCC
R_{free} test set	54184 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 70.6	EDS
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	2 of 1182846 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	307196	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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	0.63	5/36190 (0.0%)	0.80	59/56486 (0.1%)
1	CA	0.60	4/36190 (0.0%)	0.78	33/56486 (0.1%)
2	AB	0.51	0/1935	0.76	2/2609 (0.1%)
2	CB	0.49	0/1935	0.76	0/2609
3	AC	0.57	1/1636 (0.1%)	0.81	0/2205
3	CC	0.54	0/1636	0.76	0/2205
4	AD	0.51	0/1733	0.81	2/2318 (0.1%)
4	CD	0.56	0/1733	0.84	1/2318 (0.0%)
5	AE	0.58	0/1162	0.85	0/1564
5	CE	0.56	0/1162	0.84	0/1564
6	AF	0.45	0/856	0.70	0/1154
6	CF	0.45	0/856	0.74	0/1154
7	AG	0.46	0/1276	0.68	2/1709 (0.1%)
7	CG	0.50	0/1276	0.63	0/1709
8	AH	0.51	0/1136	0.80	0/1527
8	CH	0.51	0/1136	0.80	0/1527
9	AI	0.50	0/1029	0.77	0/1379
9	CI	0.49	0/1029	0.74	0/1379
10	AJ	0.51	0/807	0.80	0/1085
10	CJ	0.48	0/807	0.74	0/1085
11	AK	0.56	0/900	0.84	1/1213 (0.1%)
11	CK	0.51	0/900	0.77	1/1213 (0.1%)
12	AL	0.53	0/986	0.90	2/1320 (0.2%)
12	CL	0.54	0/986	0.87	1/1320 (0.1%)
13	AM	0.43	0/998	0.75	0/1336
13	CM	0.42	0/998	0.75	0/1336
14	AN	0.56	0/501	0.87	1/664 (0.2%)
14	CN	0.70	0/501	0.92	0/664
15	AO	0.49	0/745	0.71	0/992
15	CO	0.50	0/745	0.71	0/992
16	AP	0.44	0/716	0.73	0/963
16	CP	0.40	0/716	0.71	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.47	0/836	0.73	0/1117
17	CQ	0.48	0/836	0.76	0/1117
18	AR	0.54	0/579	0.76	0/768
18	CR	0.52	0/579	0.76	0/768
19	AS	0.49	0/642	0.74	1/865 (0.1%)
19	CS	0.45	0/642	0.71	0/865
20	AT	0.40	0/765	0.72	0/1007
20	CT	0.37	0/765	0.70	0/1007
21	AU	0.43	0/212	0.75	0/277
21	CU	0.60	0/212	0.81	0/277
22	AV	0.64	0/1809	0.80	1/2819 (0.0%)
22	AW	0.47	1/1809 (0.1%)	0.74	0/2819
22	CV	0.58	0/1809	0.79	1/2819 (0.0%)
22	CW	0.40	0/1809	0.73	0/2819
23	AX	0.80	0/406	0.89	2/631 (0.3%)
23	CX	0.78	0/406	0.94	2/631 (0.3%)
24	AY	0.80	7/1618 (0.4%)	0.91	7/2514 (0.3%)
24	CY	0.76	4/1618 (0.2%)	0.91	7/2514 (0.3%)
25	AZ	0.72	7/3042 (0.2%)	0.84	8/4129 (0.2%)
25	CZ	0.79	6/3042 (0.2%)	0.88	7/4129 (0.2%)
26	B0	0.44	0/671	0.68	0/892
26	D0	0.45	0/671	0.72	0/892
27	B1	0.47	0/738	0.77	0/981
27	D1	0.42	0/738	0.70	0/981
28	B2	0.39	0/600	0.77	0/793
28	D2	0.34	0/600	0.66	0/793
29	B3	0.43	0/472	0.69	0/634
29	D3	0.39	0/472	0.71	0/634
30	B4	0.53	0/349	0.67	0/474
30	D4	0.52	0/349	0.65	0/474
31	B5	0.44	0/473	0.76	0/639
31	D5	0.43	0/473	0.77	0/639
32	B6	0.62	0/440	0.93	0/586
32	D6	0.60	0/440	0.91	0/586
33	B7	0.51	0/426	0.74	0/561
33	D7	0.47	0/426	0.71	0/561
34	B8	0.59	0/515	0.87	0/679
34	D8	0.56	0/515	0.87	0/679
35	B9	0.53	0/310	0.74	0/407
35	D9	0.61	0/310	0.92	0/407
36	BA	0.55	2/69976 (0.0%)	0.75	50/109244 (0.0%)
36	DA	0.54	3/69976 (0.0%)	0.75	43/109244 (0.0%)
37	BB	0.47	0/2853	0.75	0/4451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DB	0.49	0/2853	0.75	0/4451
38	BC	0.42	1/1774 (0.1%)	0.68	0/2391
38	DC	0.46	2/1774 (0.1%)	0.65	0/2391
39	BD	0.55	0/2195	0.89	4/2955 (0.1%)
39	DD	0.55	0/2195	0.90	5/2955 (0.2%)
40	BE	0.47	0/1596	0.76	0/2153
40	DE	0.49	0/1596	0.78	1/2153 (0.0%)
41	BF	0.41	0/1658	0.69	0/2244
41	DF	0.39	0/1658	0.67	0/2244
42	BG	0.43	0/1499	0.72	0/2016
42	DG	0.39	0/1499	0.71	0/2016
43	BH	0.40	0/1245	0.68	0/1682
43	DH	0.38	0/1245	0.71	0/1682
46	BN	0.44	0/1131	0.74	0/1525
46	DN	0.41	0/1131	0.72	0/1525
47	BO	0.52	0/943	0.76	1/1269 (0.1%)
47	DO	0.51	0/943	0.77	0/1269
48	BP	0.48	0/1131	1.00	6/1504 (0.4%)
48	DP	0.46	0/1131	1.00	6/1504 (0.4%)
49	BQ	0.51	0/1143	0.77	0/1527
49	DQ	0.50	0/1143	0.79	0/1527
50	BR	0.40	0/974	0.77	0/1302
50	DR	0.39	0/974	0.74	2/1302 (0.2%)
51	BS	0.41	0/778	0.74	0/1036
51	DS	0.41	0/778	0.70	0/1036
52	BT	0.44	0/1155	0.78	2/1542 (0.1%)
52	DT	0.43	0/1155	0.76	1/1542 (0.1%)
53	BU	0.46	0/975	0.75	0/1297
53	DU	0.49	0/975	0.74	0/1297
54	BV	0.40	0/790	0.75	0/1057
54	DV	0.41	0/790	0.73	0/1057
55	BW	0.39	0/907	0.70	0/1216
55	DW	0.40	0/907	0.67	0/1216
56	BX	0.45	0/739	0.70	1/993 (0.1%)
56	DX	0.45	0/739	0.72	1/993 (0.1%)
57	BY	0.38	0/788	0.70	0/1051
57	DY	0.38	0/788	0.73	1/1051 (0.1%)
58	BZ	0.46	0/1491	0.80	1/2024 (0.0%)
58	DZ	0.46	0/1491	0.74	1/2024 (0.0%)
All	All	0.55	43/330118 (0.0%)	0.77	267/493190 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	6	89
1	CA	4	91
8	AH	0	1
8	CH	0	1
19	AS	0	1
22	AV	0	7
22	CV	0	1
22	CW	0	1
23	AX	0	1
23	CX	0	4
24	AY	2	1
24	CY	2	2
25	AZ	0	2
25	CZ	0	2
36	BA	0	123
36	DA	1	104
37	BB	0	3
37	DB	0	3
39	BD	0	1
49	BQ	0	1
49	DQ	0	1
All	All	15	440

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	DA	761	A	C5-C6	-10.85	1.31	1.41
24	AY	34	C	C5-C6	10.54	1.42	1.34
25	AZ	69	GLU	N-CA	9.82	1.66	1.46
25	CZ	67	HIS	C-O	9.21	1.40	1.23
25	CZ	69	GLU	N-CA	8.60	1.63	1.46

The worst 5 of 267 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1054	C	N1-C1'-C2'	12.37	130.09	114.00
1	AA	1054	C	N3-C2-O2	12.20	130.44	121.90
1	AA	1498	U	C2'-C3'-O3'	11.43	134.65	109.50
1	CA	1054	C	N1-C1'-C2'	11.34	128.74	114.00
1	CA	1503	A	N9-C1'-C2'	-11.14	99.52	114.00

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	243	A	C3'
1	AA	508	C	C3'
1	AA	687	A	C3'
1	AA	968	A	C3'
1	AA	1498	U	C3'

5 of 440 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	114	U	Sidechain
1	AA	122	G	Sidechain
1	AA	14	U	Sidechain
1	AA	189(H)	G	Sidechain
1	AA	47	C	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1145	0
1	CA	32329	0	16317	1397	0
2	AB	1900	0	1951	238	3
2	CB	1900	0	1951	239	3
3	AC	1612	0	1677	194	0
3	CC	1612	0	1677	201	0
4	AD	1703	0	1765	249	0
4	CD	1703	0	1763	265	0
5	AE	1146	0	1207	111	0
5	CE	1146	0	1207	159	0
6	AF	843	0	857	75	0
6	CF	843	0	857	82	0
7	AG	1257	0	1296	81	0
7	CG	1257	0	1296	109	0
8	AH	1116	0	1177	72	0
8	CH	1116	0	1177	99	0
9	AI	1010	0	1037	145	0
9	CI	1010	0	1037	159	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	794	0	840	146	0
10	CJ	794	0	840	155	0
11	AK	885	0	904	58	0
11	CK	885	0	904	86	0
12	AL	970	0	1057	118	0
12	CL	970	0	1057	124	0
13	AM	987	0	1059	158	0
13	CM	987	0	1059	179	0
14	AN	492	0	529	70	0
14	CN	492	0	530	115	0
15	AO	734	0	771	64	0
15	CO	734	0	771	61	0
16	AP	700	0	720	71	0
16	CP	700	0	720	77	0
17	AQ	823	0	891	63	0
17	CQ	823	0	891	73	0
18	AR	574	0	644	51	0
18	CR	574	0	644	77	0
19	AS	629	0	652	73	0
19	CS	629	0	652	98	0
20	AT	763	0	861	84	0
20	CT	763	0	861	88	0
21	AU	208	0	221	28	0
21	CU	208	0	221	23	0
22	AV	1619	0	822	88	0
22	AW	1619	0	822	89	0
22	CV	1619	0	822	64	0
22	CW	1619	0	822	97	0
23	AX	362	0	184	13	0
23	CX	362	0	184	11	0
24	AY	1644	0	853	74	0
24	CY	1644	0	853	92	0
25	AZ	2984	0	2997	411	0
25	CZ	2984	0	2997	510	0
26	B0	662	0	688	90	0
26	D0	662	0	688	104	0
27	B1	731	0	808	104	0
27	D1	731	0	808	101	0
28	B2	598	0	653	192	0
28	D2	598	0	653	98	0
29	B3	467	0	523	58	0
29	D3	467	0	523	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B4	340	0	336	62	0
30	D4	340	0	337	55	0
31	B5	459	0	480	90	0
31	D5	459	0	480	73	0
32	B6	433	0	461	134	0
32	D6	433	0	461	134	0
33	B7	418	0	467	37	0
33	D7	418	0	467	31	0
34	B8	507	0	576	115	0
34	D8	507	0	576	130	0
35	B9	307	0	336	53	0
35	D9	307	0	338	83	0
36	BA	62477	0	31497	2437	0
36	DA	62477	0	31497	2528	0
37	BB	2551	0	1295	127	0
37	DB	2551	0	1295	122	0
38	BC	1742	0	1800	167	3
38	DC	1742	0	1800	184	3
39	BD	2145	0	2234	266	0
39	DD	2145	0	2234	290	0
40	BE	1563	0	1629	263	0
40	DE	1563	0	1629	276	0
41	BF	1623	0	1677	212	0
41	DF	1623	0	1677	226	0
42	BG	1474	0	1535	247	0
42	DG	1474	0	1535	278	0
43	BH	1222	0	1282	178	0
43	DH	1222	0	1282	193	0
44	BJ	651	0	170	25	0
44	DJ	651	0	157	32	0
45	BK	700	0	180	17	0
45	DK	700	0	176	16	0
46	BN	1104	0	1180	178	0
46	DN	1104	0	1180	205	0
47	BO	933	0	996	116	0
47	DO	933	0	996	108	0
48	BP	1114	0	1187	292	0
48	DP	1114	0	1187	290	0
49	BQ	1122	0	1179	166	0
49	DQ	1122	0	1179	165	0
50	BR	960	0	1021	150	0
50	DR	960	0	1021	154	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	BS	770	0	832	148	0
51	DS	770	0	832	140	0
52	BT	1141	0	1202	257	0
52	DT	1141	0	1202	227	0
53	BU	958	0	1015	165	0
53	DU	958	0	1015	154	0
54	BV	779	0	852	122	0
54	DV	779	0	852	122	0
55	BW	896	0	953	98	0
55	DW	896	0	953	93	0
56	BX	725	0	778	91	0
56	DX	725	0	778	108	0
57	BY	775	0	870	165	0
57	DY	775	0	870	168	0
58	BZ	1459	0	1488	216	0
58	DZ	1459	0	1488	254	0
59	AD	1	0	0	0	0
59	AN	1	0	0	0	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	7	0
60	CZ	28	0	12	17	0
61	AZ	57	0	58	5	0
61	CZ	57	0	58	7	0
All	All	307196	0	208708	20881	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

The worst 5 of 20881 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:AZ:357:PRO:CB	25:AZ:357:PRO:CG	1.77	1.43
38:DC:100:ILE:HG23	38:DC:127:LEU:CD1	1.68	1.23
4:CD:187:ARG:NH1	4:CD:187:ARG:HB3	1.52	1.22
15:AO:87:ILE:HG22	15:AO:88:ARG:H	1.08	1.18
24:CY:76:A:H1'	25:CZ:287:GLY:HA3	1.26	1.18

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:65:GLY:O	38:DC:27:ARG:NH2[2_646]	1.45	0.75
2:AB:65:GLY:O	38:BC:27:ARG:NH2[2_445]	1.59	0.61
2:CB:66:GLY:CA	38:DC:27:ARG:NH2[2_646]	1.87	0.33
2:AB:66:GLY:CA	38:BC:27:ARG:NH2[2_445]	1.94	0.26
2:CB:65:GLY:C	38:DC:27:ARG:NH2[2_646]	2.04	0.16

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%)	163 (70%)	43 (18%)	26 (11%)	0	3
2	CB	232/256 (91%)	157 (68%)	52 (22%)	23 (10%)	1	4
3	AC	204/239 (85%)	148 (72%)	37 (18%)	19 (9%)	1	4
3	CC	204/239 (85%)	136 (67%)	43 (21%)	25 (12%)	0	2
4	AD	206/209 (99%)	130 (63%)	48 (23%)	28 (14%)	0	1
4	CD	206/209 (99%)	124 (60%)	53 (26%)	29 (14%)	0	1
5	AE	148/162 (91%)	131 (88%)	13 (9%)	4 (3%)	6	31
5	CE	148/162 (91%)	125 (84%)	18 (12%)	5 (3%)	5	25
6	AF	99/101 (98%)	79 (80%)	14 (14%)	6 (6%)	2	11
6	CF	99/101 (98%)	76 (77%)	16 (16%)	7 (7%)	1	8
7	AG	153/156 (98%)	113 (74%)	27 (18%)	13 (8%)	1	5
7	CG	153/156 (98%)	113 (74%)	23 (15%)	17 (11%)	0	3
8	AH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	6	29
8	CH	136/138 (99%)	118 (87%)	13 (10%)	5 (4%)	4	23
9	AI	125/128 (98%)	79 (63%)	29 (23%)	17 (14%)	0	1
9	CI	125/128 (98%)	81 (65%)	25 (20%)	19 (15%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	96/105 (91%)	69 (72%)	19 (20%)	8 (8%)	1	6
10	CJ	96/105 (91%)	71 (74%)	17 (18%)	8 (8%)	1	6
11	AK	117/129 (91%)	98 (84%)	13 (11%)	6 (5%)	2	15
11	CK	117/129 (91%)	88 (75%)	22 (19%)	7 (6%)	2	11
12	AL	122/131 (93%)	93 (76%)	17 (14%)	12 (10%)	1	4
12	CL	122/131 (93%)	86 (70%)	19 (16%)	17 (14%)	0	1
13	AM	122/126 (97%)	70 (57%)	34 (28%)	18 (15%)	0	1
13	CM	122/126 (97%)	72 (59%)	36 (30%)	14 (12%)	0	2
14	AN	58/61 (95%)	39 (67%)	8 (14%)	11 (19%)	0	0
14	CN	58/61 (95%)	29 (50%)	14 (24%)	15 (26%)	0	0
15	AO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	4	24
15	CO	86/89 (97%)	64 (74%)	18 (21%)	4 (5%)	3	17
16	AP	81/88 (92%)	63 (78%)	14 (17%)	4 (5%)	3	16
16	CP	81/88 (92%)	60 (74%)	15 (18%)	6 (7%)	1	7
17	AQ	97/105 (92%)	82 (84%)	11 (11%)	4 (4%)	3	20
17	CQ	97/105 (92%)	77 (79%)	13 (13%)	7 (7%)	1	7
18	AR	68/88 (77%)	45 (66%)	19 (28%)	4 (6%)	2	12
18	CR	68/88 (77%)	49 (72%)	15 (22%)	4 (6%)	2	12
19	AS	76/93 (82%)	47 (62%)	20 (26%)	9 (12%)	0	2
19	CS	76/93 (82%)	41 (54%)	25 (33%)	10 (13%)	0	1
20	AT	97/106 (92%)	65 (67%)	20 (21%)	12 (12%)	0	1
20	CT	97/106 (92%)	67 (69%)	19 (20%)	11 (11%)	0	2
21	AU	22/27 (82%)	19 (86%)	2 (9%)	1 (4%)	3	17
21	CU	22/27 (82%)	15 (68%)	6 (27%)	1 (4%)	3	17
25	AZ	381/405 (94%)	268 (70%)	74 (19%)	39 (10%)	1	4
25	CZ	381/405 (94%)	275 (72%)	61 (16%)	45 (12%)	0	2
26	B0	82/85 (96%)	61 (74%)	16 (20%)	5 (6%)	2	11
26	D0	82/85 (96%)	63 (77%)	16 (20%)	3 (4%)	4	23
27	B1	91/98 (93%)	60 (66%)	19 (21%)	12 (13%)	0	1
27	D1	91/98 (93%)	62 (68%)	15 (16%)	14 (15%)	0	0
28	B2	69/72 (96%)	36 (52%)	14 (20%)	19 (28%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	D2	69/72 (96%)	43 (62%)	19 (28%)	7 (10%)	1	4
29	B3	57/60 (95%)	39 (68%)	10 (18%)	8 (14%)	0	1
29	D3	57/60 (95%)	43 (75%)	7 (12%)	7 (12%)	0	2
30	B4	42/71 (59%)	24 (57%)	10 (24%)	8 (19%)	0	0
30	D4	42/71 (59%)	19 (45%)	13 (31%)	10 (24%)	0	0
31	B5	57/60 (95%)	33 (58%)	14 (25%)	10 (18%)	0	0
31	D5	57/60 (95%)	35 (61%)	13 (23%)	9 (16%)	0	0
32	B6	48/54 (89%)	20 (42%)	11 (23%)	17 (35%)	0	0
32	D6	48/54 (89%)	23 (48%)	13 (27%)	12 (25%)	0	0
33	B7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	8	36
33	D7	46/49 (94%)	31 (67%)	14 (30%)	1 (2%)	8	36
34	B8	61/65 (94%)	39 (64%)	15 (25%)	7 (12%)	0	2
34	D8	61/65 (94%)	40 (66%)	12 (20%)	9 (15%)	0	1
35	B9	35/37 (95%)	18 (51%)	12 (34%)	5 (14%)	0	1
35	D9	35/37 (95%)	18 (51%)	10 (29%)	7 (20%)	0	0
38	BC	226/229 (99%)	159 (70%)	52 (23%)	15 (7%)	1	9
38	DC	226/229 (99%)	153 (68%)	54 (24%)	19 (8%)	1	6
39	BD	273/276 (99%)	194 (71%)	51 (19%)	28 (10%)	1	4
39	DD	273/276 (99%)	200 (73%)	47 (17%)	26 (10%)	1	4
40	BE	202/206 (98%)	133 (66%)	41 (20%)	28 (14%)	0	1
40	DE	202/206 (98%)	134 (66%)	37 (18%)	31 (15%)	0	0
41	BF	205/210 (98%)	137 (67%)	40 (20%)	28 (14%)	0	1
41	DF	205/210 (98%)	140 (68%)	37 (18%)	28 (14%)	0	1
42	BG	179/182 (98%)	109 (61%)	44 (25%)	26 (14%)	0	1
42	DG	179/182 (98%)	103 (58%)	40 (22%)	36 (20%)	0	0
43	BH	157/180 (87%)	94 (60%)	40 (26%)	23 (15%)	0	1
43	DH	157/180 (87%)	94 (60%)	39 (25%)	24 (15%)	0	0
46	BN	136/140 (97%)	85 (62%)	29 (21%)	22 (16%)	0	0
46	DN	136/140 (97%)	89 (65%)	27 (20%)	20 (15%)	0	1
47	BO	120/122 (98%)	102 (85%)	10 (8%)	8 (7%)	1	9
47	DO	120/122 (98%)	99 (82%)	14 (12%)	7 (6%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	BP	144/150 (96%)	66 (46%)	39 (27%)	39 (27%)	0	0
48	DP	144/150 (96%)	68 (47%)	39 (27%)	37 (26%)	0	0
49	BQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	4
49	DQ	139/141 (99%)	102 (73%)	29 (21%)	8 (6%)	2	12
50	BR	115/118 (98%)	79 (69%)	17 (15%)	19 (16%)	0	0
50	DR	115/118 (98%)	69 (60%)	24 (21%)	22 (19%)	0	0
51	BS	96/112 (86%)	53 (55%)	24 (25%)	19 (20%)	0	0
51	DS	96/112 (86%)	52 (54%)	23 (24%)	21 (22%)	0	0
52	BT	135/146 (92%)	79 (58%)	32 (24%)	24 (18%)	0	0
52	DT	135/146 (92%)	77 (57%)	34 (25%)	24 (18%)	0	0
53	BU	115/118 (98%)	75 (65%)	27 (24%)	13 (11%)	0	2
53	DU	115/118 (98%)	76 (66%)	25 (22%)	14 (12%)	0	2
54	BV	99/101 (98%)	63 (64%)	23 (23%)	13 (13%)	0	1
54	DV	99/101 (98%)	61 (62%)	26 (26%)	12 (12%)	0	2
55	BW	111/113 (98%)	79 (71%)	21 (19%)	11 (10%)	1	4
55	DW	111/113 (98%)	81 (73%)	20 (18%)	10 (9%)	1	5
56	BX	90/96 (94%)	64 (71%)	21 (23%)	5 (6%)	2	13
56	DX	90/96 (94%)	64 (71%)	19 (21%)	7 (8%)	1	6
57	BY	98/110 (89%)	39 (40%)	27 (28%)	32 (33%)	0	0
57	DY	98/110 (89%)	43 (44%)	26 (26%)	29 (30%)	0	0
58	BZ	181/206 (88%)	114 (63%)	39 (22%)	28 (16%)	0	0
58	DZ	181/206 (88%)	106 (59%)	34 (19%)	41 (23%)	0	0
All	All	12270/13098 (94%)	8296 (68%)	2465 (20%)	1509 (12%)	0	2

5 of 1509 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	8	LYS
2	AB	9	GLU
2	AB	15	VAL
2	AB	18	GLY
2	AB	77	ALA

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%)	174 (86%)	28 (14%)	4	19
2	CB	202/220 (92%)	173 (86%)	29 (14%)	4	17
3	AC	160/188 (85%)	139 (87%)	21 (13%)	5	21
3	CC	160/188 (85%)	141 (88%)	19 (12%)	6	25
4	AD	180/181 (99%)	150 (83%)	30 (17%)	3	11
4	CD	180/181 (99%)	151 (84%)	29 (16%)	3	13
5	AE	115/123 (94%)	104 (90%)	11 (10%)	10	37
5	CE	115/123 (94%)	103 (90%)	12 (10%)	9	32
6	AF	90/90 (100%)	76 (84%)	14 (16%)	3	14
6	CF	90/90 (100%)	77 (86%)	13 (14%)	4	17
7	AG	126/127 (99%)	116 (92%)	10 (8%)	15	49
7	CG	126/127 (99%)	118 (94%)	8 (6%)	22	58
8	AH	119/119 (100%)	105 (88%)	14 (12%)	6	25
8	CH	119/119 (100%)	106 (89%)	13 (11%)	8	30
9	AI	98/99 (99%)	84 (86%)	14 (14%)	4	17
9	CI	98/99 (99%)	86 (88%)	12 (12%)	6	24
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	7	28
10	CJ	88/92 (96%)	79 (90%)	9 (10%)	9	33
11	AK	90/99 (91%)	84 (93%)	6 (7%)	20	56
11	CK	90/99 (91%)	81 (90%)	9 (10%)	9	34
12	AL	104/108 (96%)	84 (81%)	20 (19%)	2	8
12	CL	104/108 (96%)	84 (81%)	20 (19%)	2	8
13	AM	99/101 (98%)	85 (86%)	14 (14%)	4	18
13	CM	99/101 (98%)	90 (91%)	9 (9%)	12	40
14	AN	49/50 (98%)	41 (84%)	8 (16%)	3	12
14	CN	49/50 (98%)	40 (82%)	9 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	79/80 (99%)	73 (92%)	6 (8%)	16	51
15	CO	79/80 (99%)	69 (87%)	10 (13%)	5	22
16	AP	72/74 (97%)	64 (89%)	8 (11%)	8	29
16	CP	72/74 (97%)	66 (92%)	6 (8%)	14	46
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	13	45
17	CQ	94/97 (97%)	85 (90%)	9 (10%)	10	37
18	AR	61/77 (79%)	55 (90%)	6 (10%)	10	36
18	CR	61/77 (79%)	54 (88%)	7 (12%)	7	27
19	AS	69/80 (86%)	56 (81%)	13 (19%)	2	8
19	CS	69/80 (86%)	57 (83%)	12 (17%)	2	11
20	AT	76/82 (93%)	70 (92%)	6 (8%)	15	49
20	CT	76/82 (93%)	69 (91%)	7 (9%)	11	40
21	AU	19/22 (86%)	18 (95%)	1 (5%)	28	64
21	CU	19/22 (86%)	17 (90%)	2 (10%)	8	31
25	AZ	322/338 (95%)	281 (87%)	41 (13%)	5	22
25	CZ	322/338 (95%)	284 (88%)	38 (12%)	6	25
26	B0	66/67 (98%)	57 (86%)	9 (14%)	5	19
26	D0	66/67 (98%)	56 (85%)	10 (15%)	3	14
27	B1	78/83 (94%)	67 (86%)	11 (14%)	4	18
27	D1	78/83 (94%)	64 (82%)	14 (18%)	2	10
28	B2	66/67 (98%)	54 (82%)	12 (18%)	2	9
28	D2	66/67 (98%)	60 (91%)	6 (9%)	12	40
29	B3	51/52 (98%)	46 (90%)	5 (10%)	10	36
29	D3	51/52 (98%)	47 (92%)	4 (8%)	16	49
30	B4	39/63 (62%)	28 (72%)	11 (28%)	0	1
30	D4	39/63 (62%)	28 (72%)	11 (28%)	0	1
31	B5	51/52 (98%)	48 (94%)	3 (6%)	24	60
31	D5	51/52 (98%)	45 (88%)	6 (12%)	6	25
32	B6	49/52 (94%)	38 (78%)	11 (22%)	1	4
32	D6	49/52 (94%)	40 (82%)	9 (18%)	2	9
33	B7	41/42 (98%)	34 (83%)	7 (17%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	D7	41/42 (98%)	34 (83%)	7 (17%)	2	11
34	B8	53/55 (96%)	43 (81%)	10 (19%)	2	8
34	D8	53/55 (96%)	44 (83%)	9 (17%)	2	11
35	B9	34/34 (100%)	28 (82%)	6 (18%)	2	10
35	D9	34/34 (100%)	31 (91%)	3 (9%)	12	43
38	BC	180/181 (99%)	164 (91%)	16 (9%)	12	42
38	DC	180/181 (99%)	167 (93%)	13 (7%)	18	53
39	BD	217/218 (100%)	185 (85%)	32 (15%)	4	16
39	DD	217/218 (100%)	185 (85%)	32 (15%)	4	16
40	BE	165/166 (99%)	142 (86%)	23 (14%)	4	19
40	DE	165/166 (99%)	139 (84%)	26 (16%)	3	13
41	BF	165/166 (99%)	156 (94%)	9 (6%)	27	63
41	DF	165/166 (99%)	158 (96%)	7 (4%)	36	73
42	BG	155/156 (99%)	133 (86%)	22 (14%)	4	18
42	DG	155/156 (99%)	131 (84%)	24 (16%)	3	14
43	BH	132/148 (89%)	117 (89%)	15 (11%)	7	28
43	DH	132/148 (89%)	115 (87%)	17 (13%)	5	21
46	BN	117/119 (98%)	102 (87%)	15 (13%)	5	21
46	DN	117/119 (98%)	104 (89%)	13 (11%)	8	29
47	BO	100/100 (100%)	88 (88%)	12 (12%)	6	24
47	DO	100/100 (100%)	90 (90%)	10 (10%)	9	34
48	BP	112/116 (97%)	95 (85%)	17 (15%)	3	14
48	DP	112/116 (97%)	90 (80%)	22 (20%)	1	7
49	BQ	111/111 (100%)	97 (87%)	14 (13%)	5	22
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	5	22
50	BR	100/101 (99%)	86 (86%)	14 (14%)	4	18
50	DR	100/101 (99%)	86 (86%)	14 (14%)	4	18
51	BS	77/88 (88%)	66 (86%)	11 (14%)	4	17
51	DS	77/88 (88%)	66 (86%)	11 (14%)	4	17
52	BT	120/127 (94%)	98 (82%)	22 (18%)	2	9
52	DT	120/127 (94%)	99 (82%)	21 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	BU	92/94 (98%)	82 (89%)	10 (11%)	8	30
53	DU	92/94 (98%)	83 (90%)	9 (10%)	10	36
54	BV	82/82 (100%)	66 (80%)	16 (20%)	2	7
54	DV	82/82 (100%)	69 (84%)	13 (16%)	3	13
55	BW	91/92 (99%)	80 (88%)	11 (12%)	6	24
55	DW	91/92 (99%)	81 (89%)	10 (11%)	8	30
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%)	71 (84%)	13 (16%)	3	14
57	DY	84/91 (92%)	71 (84%)	13 (16%)	3	14
58	BZ	161/179 (90%)	137 (85%)	24 (15%)	4	15
58	DZ	161/179 (90%)	133 (83%)	28 (17%)	2	11
All	All	10350/10854 (95%)	9007 (87%)	1343 (13%)	5	21

5 of 1343 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	BV	13	ARG
4	CD	179	GLU
51	DS	99	LYS
55	BW	39	THR
2	CB	32	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 317 such sidechains are listed below:

Mol	Chain	Res	Type
53	BU	66	ASN
5	CE	78	HIS
48	DP	38	GLN
54	BV	64	HIS
2	CB	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	236 (15%)	51 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	CA	1503/1522 (98%)	237 (15%)	46 (3%)
22	AV	75/76 (98%)	17 (22%)	1 (1%)
22	AW	75/76 (98%)	21 (28%)	0
22	CV	75/76 (98%)	21 (28%)	0
22	CW	75/76 (98%)	21 (28%)	2 (2%)
23	AX	16/27 (59%)	5 (31%)	0
23	CX	17/27 (62%)	6 (35%)	1 (5%)
24	AY	74/77 (96%)	29 (39%)	4 (5%)
24	CY	74/77 (96%)	27 (36%)	3 (4%)
36	BA	2900/2915 (99%)	525 (18%)	49 (1%)
36	DA	2900/2915 (99%)	520 (17%)	46 (1%)
37	BB	118/122 (96%)	26 (22%)	2 (1%)
37	DB	118/122 (96%)	24 (20%)	3 (2%)
All	All	9523/9630 (98%)	1715 (18%)	208 (2%)

5 of 1715 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 208 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2036	C
1	CA	266	G
36	DA	2033	A
36	BA	2131	G
37	BB	56	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	0.97	0	23,30,33	1.88	4 (17%)
24	H2U	AY	17	24	17,21,22	0.89	0	23,30,33	1.92	5 (21%)
24	H2U	AY	20	24	17,21,22	1.05	1 (5%)	23,30,33	1.87	6 (26%)
24	OMC	AY	32	24	13,22,23	0.77	0	20,31,34	1.02	2 (10%)
24	MIA	AY	37	24	21,31,32	1.45	4 (19%)	26,44,47	2.41	4 (15%)
24	7MG	AY	46	24	19,26,27	1.61	3 (15%)	24,39,42	2.30	3 (12%)
24	5MU	AY	54	24	12,22,23	1.38	3 (25%)	14,32,35	4.48	3 (21%)
24	PSU	AY	55	24	13,21,22	1.24	3 (23%)	18,30,33	3.69	8 (44%)
24	4SU	AY	8	24	11,21,22	1.62	4 (36%)	13,30,33	2.36	1 (7%)
24	H2U	CY	16	24	17,21,22	1.00	0	23,30,33	1.84	4 (17%)
24	H2U	CY	17	24	17,21,22	0.96	1 (5%)	23,30,33	1.89	4 (17%)
24	H2U	CY	20	24	17,21,22	1.09	2 (11%)	23,30,33	1.92	6 (26%)
24	OMC	CY	32	24	13,22,23	0.76	0	20,31,34	0.99	2 (10%)
24	MIA	CY	37	24	21,31,32	2.13	4 (19%)	26,44,47	2.28	5 (19%)
24	7MG	CY	46	24	19,26,27	1.62	3 (15%)	24,39,42	2.31	3 (12%)
24	5MU	CY	54	24	12,22,23	1.33	3 (25%)	14,32,35	4.49	3 (21%)
24	PSU	CY	55	24	13,21,22	1.06	2 (15%)	18,30,33	3.80	8 (44%)
24	4SU	CY	8	24	11,21,22	1.67	3 (27%)	13,30,33	2.33	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

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

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	46	7MG	C8-N9	-5.00	1.38	1.45
24	AY	46	7MG	C8-N9	-4.58	1.38	1.45
24	CY	37	MIA	C12-N6	-2.88	1.39	1.46
24	AY	37	MIA	C12-N6	-2.87	1.39	1.46
24	CY	46	7MG	C8-N7	-2.76	1.30	1.43

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CY	55	PSU	N1-C2-N3	-12.65	120.26	128.33
24	AY	55	PSU	N1-C2-N3	-12.20	120.55	128.33
24	CY	54	5MU	C5-C4-N3	-8.96	115.16	125.14
24	AY	54	5MU	C5-C4-N3	-8.92	115.21	125.14
24	AY	8	4SU	C5-C4-N3	-8.26	115.54	123.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	16	H2U	1	0
24	AY	17	H2U	1	0
24	AY	20	H2U	3	0
24	AY	37	MIA	1	0
24	AY	46	7MG	3	0
24	AY	54	5MU	3	0
24	AY	55	PSU	1	0
24	AY	8	4SU	5	0
24	CY	16	H2U	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CY	17	H2U	1	0
24	CY	20	H2U	3	0
24	CY	37	MIA	1	0
24	CY	46	7MG	4	0
24	CY	54	5MU	2	0
24	CY	55	PSU	1	0
24	CY	8	4SU	4	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	2.13	4 (17%)	30,47,47	2.51	10 (33%)
61	KIR	AZ	502	-	55,59,59	3.81	22 (40%)	53,84,84	1.73	11 (20%)
60	GDP	CZ	501	-	23,30,30	1.82	5 (21%)	30,47,47	2.19	8 (26%)
61	KIR	CZ	502	-	55,59,59	3.90	23 (41%)	53,84,84	1.66	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 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CZ	502	KIR	O18-C17	-14.37	1.22	1.44
61	AZ	502	KIR	O18-C17	-14.20	1.23	1.44
61	CZ	502	KIR	O30-C30	-12.09	1.17	1.42
61	AZ	502	KIR	O30-C30	-12.05	1.17	1.42
61	AZ	502	KIR	O34-C33	-11.26	1.29	1.44

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AZ	501	GDP	C4-C5-N7	-7.26	102.80	109.48
60	CZ	501	GDP	C5-C6-N1	-6.33	114.93	123.59
60	AZ	501	GDP	N3-C2-N1	-5.31	119.35	127.44
61	CZ	502	KIR	O29-C29-O34	-5.30	101.42	110.18
61	AZ	502	KIR	O29-C29-O34	-5.12	101.72	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	AZ	501	GDP	7	0
61	AZ	502	KIR	5	0
60	CZ	501	GDP	17	0
61	CZ	502	KIR	7	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	-0.22	29 (1%) 70 48	21, 54, 143, 200	0
1	CA	1504/1522 (98%)	-0.16	16 (1%) 82 66	31, 70, 146, 200	0
2	AB	234/256 (91%)	-0.28	6 (2%) 59 35	31, 60, 136, 149	0
2	CB	234/256 (91%)	-0.18	3 (1%) 79 62	46, 81, 139, 148	0
3	AC	206/239 (86%)	-0.51	1 (0%) 91 83	20, 46, 78, 89	0
3	CC	206/239 (86%)	-0.26	0 100 100	49, 74, 96, 100	0
4	AD	208/209 (99%)	0.19	4 (1%) 70 48	45, 83, 112, 119	0
4	CD	208/209 (99%)	0.38	20 (9%) 10 3	64, 95, 118, 126	0
5	AE	150/162 (92%)	-0.55	0 100 100	25, 42, 69, 86	0
5	CE	150/162 (92%)	-0.37	1 (0%) 89 78	43, 58, 82, 100	0
6	AF	101/101 (100%)	-0.40	1 (0%) 84 69	44, 70, 86, 94	0
6	CF	101/101 (100%)	-0.17	1 (0%) 84 69	64, 86, 97, 101	0
7	AG	155/156 (99%)	-0.31	1 (0%) 90 80	37, 66, 97, 113	0
7	CG	155/156 (99%)	0.07	8 (5%) 31 13	67, 87, 107, 122	0
8	AH	138/138 (100%)	-0.54	0 100 100	31, 47, 68, 75	0
8	CH	138/138 (100%)	-0.40	0 100 100	41, 61, 75, 84	0
9	AI	127/128 (99%)	-0.08	0 100 100	32, 72, 111, 123	0
9	CI	127/128 (99%)	0.42	10 (7%) 15 5	59, 97, 119, 124	0
10	AJ	98/105 (93%)	0.14	1 (1%) 84 69	30, 73, 126, 129	0
10	CJ	98/105 (93%)	0.77	20 (20%) 1 0	57, 102, 133, 137	0
11	AK	119/129 (92%)	-0.34	3 (2%) 61 37	29, 45, 78, 105	0
11	CK	119/129 (92%)	-0.23	2 (1%) 73 52	43, 66, 91, 106	0
12	AL	124/131 (94%)	-0.35	1 (0%) 87 75	24, 49, 70, 103	0
12	CL	124/131 (94%)	-0.26	3 (2%) 62 39	38, 54, 78, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	124/126 (98%)	0.04	5 (4%) 42 20	46, 82, 106, 147	0
13	CM	124/126 (98%)	0.29	10 (8%) 15 5	67, 92, 114, 148	0
14	AN	60/61 (98%)	-0.14	2 (3%) 50 26	28, 51, 84, 90	0
14	CN	60/61 (98%)	0.44	2 (3%) 50 26	65, 78, 98, 105	0
15	AO	88/89 (98%)	-0.35	0 100 100	31, 51, 79, 85	0
15	CO	88/89 (98%)	-0.20	0 100 100	41, 63, 85, 92	0
16	AP	83/88 (94%)	-0.04	0 100 100	48, 67, 85, 123	0
16	CP	83/88 (94%)	0.01	3 (3%) 46 23	62, 77, 92, 122	0
17	AQ	99/105 (94%)	-0.33	0 100 100	40, 58, 77, 85	0
17	CQ	99/105 (94%)	-0.25	0 100 100	44, 65, 85, 93	0
18	AR	70/88 (79%)	-0.47	0 100 100	35, 55, 88, 104	0
18	CR	70/88 (79%)	-0.27	0 100 100	47, 73, 100, 113	0
19	AS	78/93 (83%)	0.16	4 (5%) 32 13	48, 75, 119, 122	0
19	CS	78/93 (83%)	0.26	4 (5%) 32 13	71, 91, 120, 124	0
20	AT	99/106 (93%)	0.14	5 (5%) 32 13	65, 83, 117, 119	0
20	CT	99/106 (93%)	0.11	0 100 100	64, 84, 117, 118	0
21	AU	24/27 (88%)	-0.10	0 100 100	45, 61, 75, 90	0
21	CU	24/27 (88%)	0.48	1 (4%) 40 19	67, 79, 92, 94	0
22	AV	76/76 (100%)	-0.36	0 100 100	35, 70, 102, 112	0
22	AW	76/76 (100%)	0.37	7 (9%) 11 4	63, 136, 178, 190	0
22	CV	76/76 (100%)	-0.34	0 100 100	48, 76, 115, 128	0
22	CW	76/76 (100%)	0.52	9 (11%) 6 2	71, 165, 186, 196	0
23	AX	17/27 (62%)	0.50	2 (11%) 6 2	30, 82, 132, 133	0
23	CX	17/27 (62%)	0.93	3 (17%) 2 1	36, 99, 145, 145	0
24	AY	68/77 (88%)	-0.03	0 100 100	37, 108, 152, 185	0
24	CY	68/77 (88%)	0.03	0 100 100	45, 111, 145, 185	0
25	AZ	385/405 (95%)	0.18	15 (3%) 43 21	63, 105, 134, 163	0
25	CZ	385/405 (95%)	1.24	94 (24%) 1 0	93, 117, 143, 169	0
26	B0	84/85 (98%)	0.21	3 (3%) 46 23	62, 73, 100, 114	0
26	D0	84/85 (98%)	0.38	3 (3%) 46 23	66, 79, 101, 111	0
27	B1	93/98 (94%)	0.08	2 (2%) 65 42	47, 63, 120, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D1	93/98 (94%)	0.13	1 (1%) 82 66	51, 74, 115, 120	0
28	B2	71/72 (98%)	1.38	19 (26%) 1 0	122, 140, 151, 153	0
28	D2	71/72 (98%)	0.23	4 (5%) 28 11	90, 106, 126, 139	0
29	B3	59/60 (98%)	0.40	1 (1%) 73 52	59, 79, 101, 116	0
29	D3	59/60 (98%)	0.30	3 (5%) 32 13	58, 80, 97, 114	0
30	B4	44/71 (61%)	1.10	7 (15%) 3 1	102, 156, 180, 186	0
30	D4	44/71 (61%)	1.25	12 (27%) 1 0	113, 165, 186, 187	0
31	B5	59/60 (98%)	0.31	4 (6%) 20 7	52, 86, 150, 164	0
31	D5	59/60 (98%)	0.15	6 (10%) 9 3	55, 80, 148, 161	0
32	B6	50/54 (92%)	0.77	10 (20%) 1 0	55, 88, 106, 112	0
32	D6	50/54 (92%)	0.68	6 (12%) 6 2	57, 95, 107, 113	0
33	B7	48/49 (97%)	0.20	2 (4%) 40 19	47, 61, 95, 116	0
33	D7	48/49 (97%)	-0.10	0 100 100	47, 61, 91, 109	0
34	B8	63/65 (96%)	0.18	2 (3%) 51 27	55, 72, 84, 112	0
34	D8	63/65 (96%)	0.09	1 (1%) 74 55	56, 73, 85, 109	0
35	B9	37/37 (100%)	1.03	5 (13%) 4 2	79, 98, 112, 116	0
35	D9	37/37 (100%)	1.72	10 (27%) 1 0	84, 104, 115, 119	0
36	BA	2901/2915 (99%)	-0.05	85 (2%) 55 31	25, 74, 176, 200	0
36	DA	2901/2915 (99%)	-0.06	76 (2%) 59 35	32, 76, 175, 200	0
37	BB	119/122 (97%)	-0.25	0 100 100	54, 97, 123, 144	0
37	DB	119/122 (97%)	-0.25	0 100 100	61, 104, 128, 140	0
38	BC	228/229 (99%)	0.29	21 (9%) 11 4	40, 73, 163, 176	0
38	DC	228/229 (99%)	0.51	28 (12%) 5 2	64, 87, 166, 174	0
39	BD	275/276 (99%)	-0.38	0 100 100	28, 48, 78, 93	0
39	DD	275/276 (99%)	-0.32	1 (0%) 93 85	28, 53, 80, 94	0
40	BE	204/206 (99%)	0.08	5 (2%) 61 37	46, 73, 120, 129	0
40	DE	204/206 (99%)	-0.01	5 (2%) 61 37	39, 72, 122, 132	0
41	BF	207/210 (98%)	0.38	16 (7%) 16 5	42, 102, 155, 162	0
41	DF	207/210 (98%)	0.32	16 (7%) 16 5	47, 105, 155, 161	0
42	BG	181/182 (99%)	-0.00	7 (3%) 43 21	66, 85, 120, 134	0
42	DG	181/182 (99%)	0.20	7 (3%) 43 21	89, 108, 130, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BH	159/180 (88%)	0.78	20 (12%) 5 2	85, 123, 148, 152	0
43	DH	159/180 (88%)	0.60	11 (6%) 20 7	85, 123, 145, 150	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	138/140 (98%)	0.00	1 (0%) 89 78	56, 86, 130, 138	0
46	DN	138/140 (98%)	0.03	1 (0%) 89 78	61, 83, 132, 136	0
47	BO	122/122 (100%)	-0.36	0 100 100	43, 60, 73, 82	0
47	DO	122/122 (100%)	-0.39	0 100 100	40, 60, 73, 77	0
48	BP	146/150 (97%)	0.62	14 (9%) 10 3	49, 98, 124, 145	0
48	DP	146/150 (97%)	0.64	17 (11%) 6 2	47, 102, 126, 141	0
49	BQ	141/141 (100%)	-0.21	2 (1%) 78 60	47, 61, 84, 125	0
49	DQ	141/141 (100%)	-0.19	2 (1%) 78 60	43, 60, 87, 122	0
50	BR	117/118 (99%)	0.17	1 (0%) 85 72	55, 84, 101, 108	0
50	DR	117/118 (99%)	0.06	3 (2%) 59 35	52, 79, 97, 106	0
51	BS	98/112 (87%)	0.32	3 (3%) 52 28	69, 101, 122, 126	0
51	DS	98/112 (87%)	0.70	8 (8%) 14 5	86, 106, 124, 126	0
52	BT	137/146 (93%)	0.11	7 (5%) 32 13	54, 84, 135, 163	0
52	DT	137/146 (93%)	-0.04	7 (5%) 32 13	56, 81, 137, 160	0
53	BU	117/118 (99%)	-0.11	0 100 100	60, 74, 102, 111	0
53	DU	117/118 (99%)	-0.17	0 100 100	52, 74, 100, 108	0
54	BV	101/101 (100%)	0.29	6 (5%) 26 11	61, 102, 117, 121	0
54	DV	101/101 (100%)	0.25	2 (1%) 68 46	50, 102, 117, 119	0
55	BW	113/113 (100%)	0.08	4 (3%) 48 23	60, 83, 111, 140	0
55	DW	113/113 (100%)	0.08	2 (1%) 71 50	59, 76, 112, 143	0
56	BX	92/96 (95%)	0.28	2 (2%) 65 42	69, 86, 109, 120	0
56	DX	92/96 (95%)	0.21	2 (2%) 65 42	60, 88, 108, 121	0
57	BY	100/110 (90%)	1.27	20 (20%) 1 0	103, 121, 153, 159	0
57	DY	100/110 (90%)	1.19	20 (20%) 1 0	99, 119, 153, 162	0
58	BZ	183/206 (88%)	0.13	13 (7%) 19 7	53, 85, 129, 139	0
58	DZ	183/206 (88%)	0.16	7 (3%) 44 21	59, 85, 124, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	21996/23368 (94%)	0.03	840 (3%) 44 21	20, 77, 144, 200	0

The worst 5 of 840 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
38	BC	106	GLY	16.6
57	BY	2	ARG	12.4
28	B2	72	ALA	9.7
36	BA	654(C)	G	9.1
28	B2	42	GLY	8.7

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	7MG	CY	46	24/25	0.85	0.26	-	125,128,129,130	0
24	H2U	AY	17	20/21	0.72	0.43	-	186,190,190,191	0
24	7MG	AY	46	24/25	0.84	0.26	-	121,123,124,124	0
24	OMC	CY	32	21/22	0.93	0.22	-	78,83,93,94	0
24	4SU	CY	8	20/21	0.82	0.25	-	115,116,119,119	0
24	H2U	AY	16	20/21	0.68	0.61	-	172,183,184,185	0
24	H2U	CY	17	20/21	0.61	0.53	-	186,194,196,196	0
24	OMC	AY	32	21/22	0.93	0.18	-	61,66,79,80	0
24	MIA	CY	37	29/30	0.93	0.24	-	52,66,80,85	0
24	H2U	CY	16	20/21	0.68	0.39	-	171,181,183,185	0
24	H2U	AY	20	20/21	0.83	0.31	-	174,177,179,179	0
24	5MU	CY	54	21/22	0.85	0.22	-	113,125,126,129	0
24	PSU	AY	55	20/21	0.83	0.24	-	130,139,140,140	0
24	PSU	CY	55	20/21	0.80	0.21	-	131,134,135,136	0
24	H2U	CY	20	20/21	0.76	0.28	-	176,177,180,180	0
24	MIA	AY	37	29/30	0.95	0.21	-	42,52,67,76	0
24	4SU	AY	8	20/21	0.85	0.23	-	110,113,114,115	0
24	5MU	AY	54	21/22	0.91	0.15	-	108,122,123,127	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
61	KIR	CZ	502	57/57	0.76	0.51	2.45	115,117,122,122	0
61	KIR	AZ	502	57/57	0.86	0.32	1.07	100,107,118,119	0
59	ZN	AN	101	1/1	0.98	0.18	-0.05	42,42,42,42	0
60	GDP	CZ	501	28/28	0.81	0.27	-0.35	114,131,139,140	0
60	GDP	AZ	501	28/28	0.89	0.20	-0.45	114,118,123,123	0
59	ZN	AD	301	1/1	0.99	0.25	-0.65	61,61,61,61	0
59	ZN	CD	301	1/1	0.97	0.26	-0.67	75,75,75,75	0
59	ZN	D4	101	1/1	0.95	0.08	-0.82	103,103,103,103	0
59	ZN	B4	101	1/1	0.96	0.15	-1.05	91,91,91,91	0
59	ZN	CN	101	1/1	0.97	0.16	-1.37	69,69,69,69	0
59	ZN	B9	101	1/1	0.88	0.13	-1.37	103,103,103,103	0
59	ZN	D9	101	1/1	0.97	0.14	-1.51	87,87,87,87	0

6.5 Other polymers ⓘ

There are no such residues in this entry.