



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 07:52 pm BST

PDB ID : 4V5Q  
Title : The crystal structure of EF-Tu and G24A-tRNA-Trp bound to a near- cognate codon on the 70S ribosome  
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.  
Deposited on : 2010-12-07  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

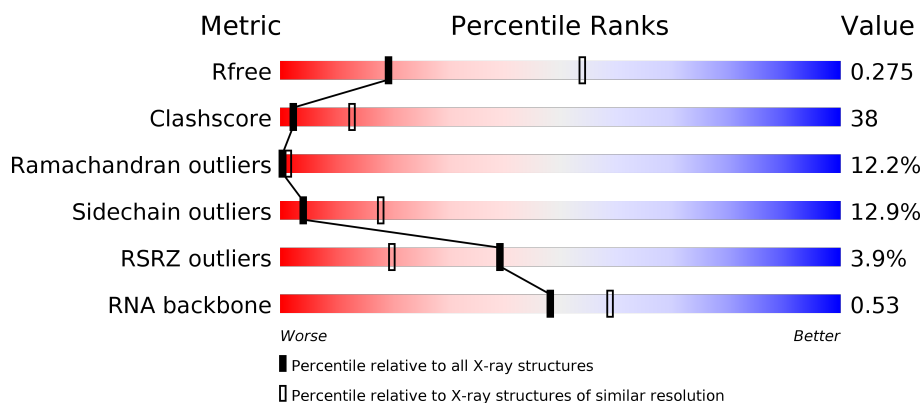
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>2%</div> <div>36% 47% 13% ..</div> </div>
1	CA	1522	<div> <div>2%</div> <div>28% 57% 12% ..</div> </div>
2	AB	256	<div> <div>%</div> <div>28% 45% 17% • 9%</div> </div>
2	CB	256	<div> <div>%</div> <div>19% 56% 16% • 9%</div> </div>



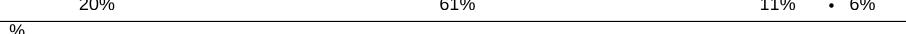
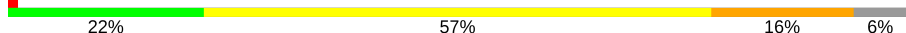
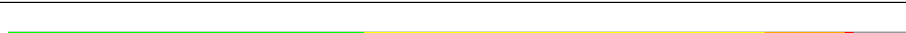
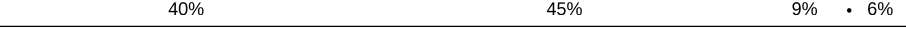

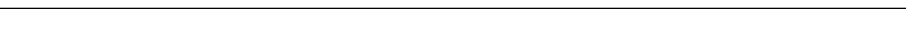
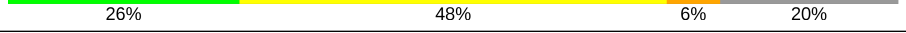
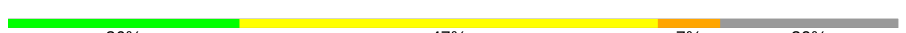
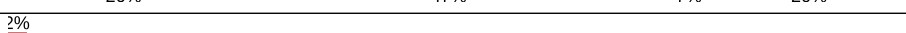


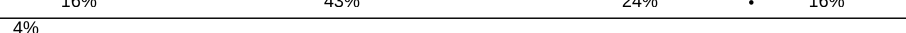
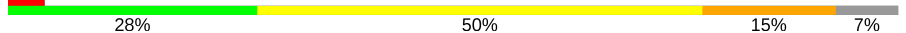




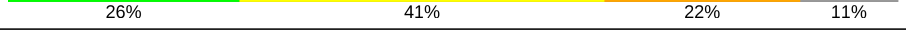

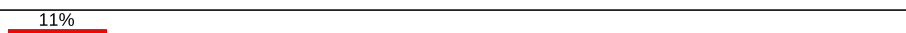
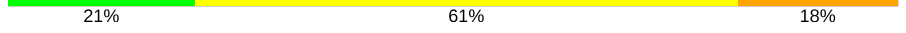


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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126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

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	AW	76	
22	CV	76	
22	CW	76	
23	AX	27	
23	CX	27	
24	AY	77	
24	CY	77	
25	AZ	405	
25	CZ	405	
26	B0	85	
26	D0	85	

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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
24	H2U	AY	16	-	-	-	X
24	H2U	CY	16	-	-	-	X
24	H2U	CY	17	-	-	-	X
59	ZN	AN	101	-	-	X	-
60	GDP	AZ	501	-	-	X	-
60	GDP	CZ	501	-	-	X	-
61	KIR	CZ	502	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 307194 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
2	CB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			
5	CE	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			
12	CL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	CP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			
19	CS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	24	Total	C	N	O	0	0	0
			208	128	50	30			
21	CU	24	Total	C	N	O	0	0	0
			208	128	50	30			

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

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

- Molecule 23 is a RNA chain called MRNA.

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

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

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

- Molecule 25 is a protein called ELONGATION FACTOR TU.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
26	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			
27	D1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			
29	D3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
33	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
34	D8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			
36	DA	2901	Total	C	N	O	P	0	0	0
			62477	27807	11683	20087	2900			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
40	DE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			
41	DF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			
43	DH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

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

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

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

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

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

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

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

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

*Continued on next page...*



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

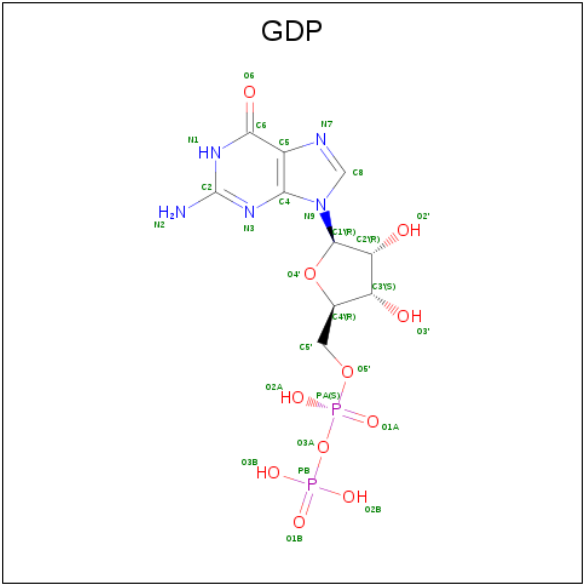
- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

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

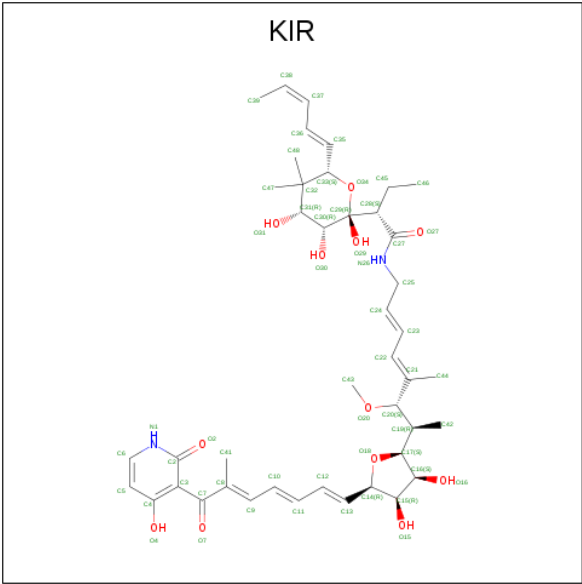
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

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



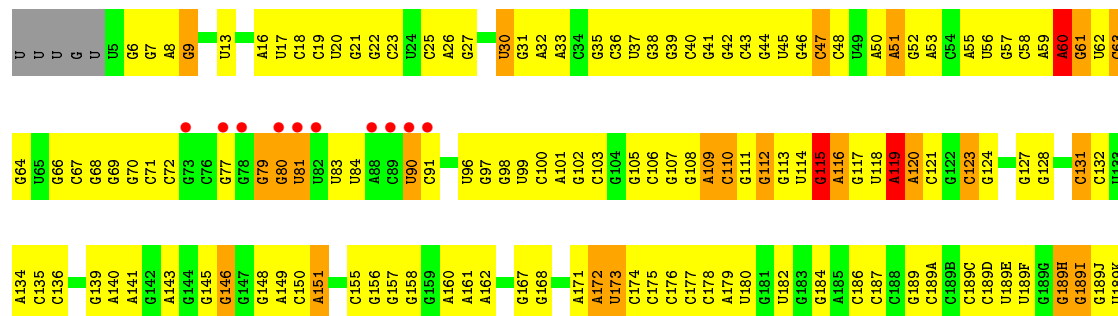
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
60	AZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
60	CZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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

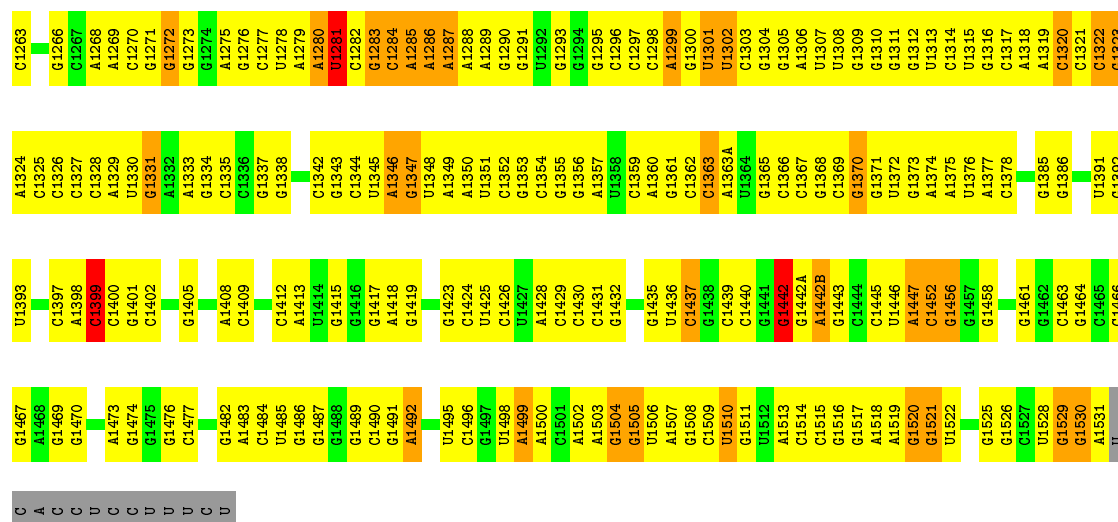


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AZ	1	Total	C	N	O		0	0
			57	43	2	12			
61	CZ	1	Total	C	N	O		0	0
			57	43	2	12			

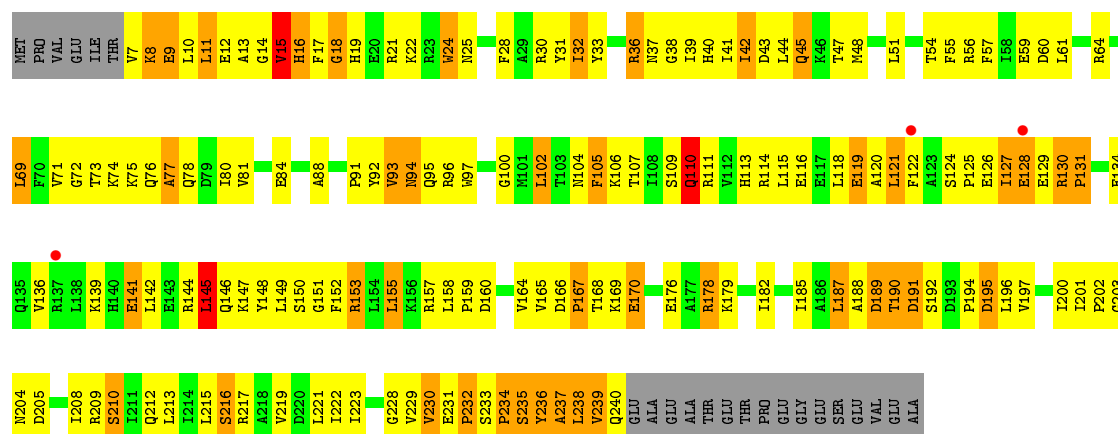




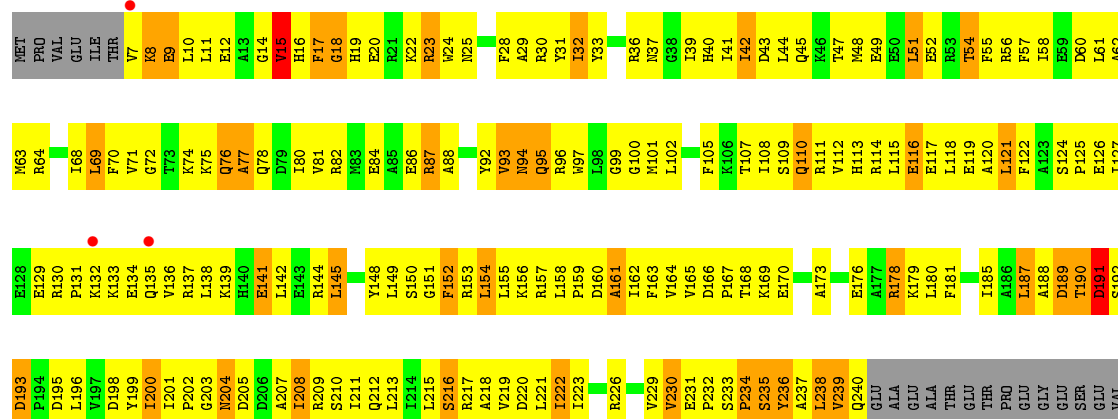
C1200	G1133	G1065	G1001A	G939	G854	G776	A704	U636	U561	A411	C341	C267	G189L
A1201	U1136	U1065	G1002	C940	G854	A777	U705	G637	C562	A412	C342	C268	U192
C1202	C1137	A1066	G1003	G941	G858	G778	A706	G638	G566	A413	U943	C269	C193
A1204	G1138	A1067	A1004	G942	A859	C779	C707	G639	G566	A414	A344	A270	C194
U1205	G1139	G1068	A1005	U943	A860	A780	C708	U640	A572	A415	C345	C271	A195
G1206	C1140	G1069	G1006	G944	G861	A781	G709	A641	A573	A416	G346	C272	A196
G1207	C1141	U1070	C1007	G945	G861	A782	G710	A642	A574	A417	G347	A273	A197
C1208	U1142	G1071	G1008	G946	A864	C783	G711	C643	A575	C418	G348	A274	G198
C1209	G1143	U1072	G1009	G947	A865	C784	A712	G644	A576	A349	G349	G275	G199
G1210	G1144	U1073	G1010	G948	C866	G789	G713	G645	G577	C422	G350	G276	G200
U1211	C1145	G1074	G1011	A949	G866	U788	G714	U646	G577	C423	G351	G277	G201
U1212	A1146	C1075	G1012	U950	G869	U789	G718	C647	G578	G426	C352	G278	U202
A1213	C1147	G1079	G1013	U951	U870	A790	C719	A648	G579	U427	A353	A279	U203
G1214	U1148	A1080	A1014	U952	G874	G791	C720	G649	U580	U428	G354	C280	U204
G1215	C1149	U1086	A1015	G953	A792	A792	G721	G650	G581	G428	C355	A281	G216
G1216	U1150	G1086	A1016	G954	C793	A793	G722	C651	U582	U429	A356	A282	C217
C1217	A1151	U1087	G1017	U955	G877	A794	A722	G652	A583	A430	G357	C283	C218
C1218	U1152	G1087	C1018	U956	C878	C795	U723	A653	G584	A431	U358	G284	C219
U1219	A1153	G1088	C1019	U957	C796	C796	G724	G656	G585	A432	U359	G285	G220
G1220	C1155	U1089	G1022	A958	C882	C797	G725	C656	U591	C433	A360	G286	G221
G1221	U1154	A959	G1023	U960	C883	G726	G727	G657	G592	U434	G361	G289	U222
G1222	G1155	G1024	G1024	U961	G885	G803	C732	G658	G592	C435	U367	C290	U223
C1223	A1157	U1095	G1025	G962	U884	G803	A733	G659	G597	C436	U371	C291	C224
G1224	C1158	C1096	G1026	G963	G885	G803	C736	G660	G597	U437	U368	C292	G226
A1225	U1159	C1097	G1026	A964	U891	C808	A733	A663	G597	C444	C374	U229	G227
C1226	U1160	C1098	G1030	A965	A892	C811	C736	G664	C599	C445	A374	U294	A228
A1227	G1161	G1099	C1030A	G966	A892	C811	A737	A665	C600	G446	C601	C294	G228
C1228	C1162	C1100	A1030B	G967	G895	A814	C738	G666	A602	G447	U375	U299	G230
A1229	G1163	A1101	G1030C	A968	C897	A815	C739	G667	G603	G448	U376	G301	G231
C1230	C1163	A1102	A1030D	G970	C898	A816	U740	G673	U531	G449	G377	A300	G232
G1231	A1168	G1103	G1031	G971	C899	C817	G741	G674	U532	U448	G378	C308	C234
U1234	A1169	G1104	G1032	G972	A900	G818	C744	A675	U533	A450	C381	G309	C235
C1236	G1171	A1106	G1033	G973	A901	A819	C745	A676	U534	A451	A382	G310	C241
C1237	C1172	G1107	G1036	A974	G906	U820	C746	U677	A608	A452	A383	C312	C242
A1238	G1175	G1108	C1037	A975	A907	G821	A746	U678	A609	A453	A384	C314	A244
U1240	A1176	A1111	C1038	G976	A908	C822	C747	C679	G610	C458	G385	A315	A245
G1241	G1177	C1112	U1040	A977	A909	C822	C748	C680	C613	C460	C386	A316	A246
C1242	C1178	C1113	A1041	A978	A913	G825	C749	G683	C614	G471	U387	G319	G247
G1243	C1179	C1114	G1044	C980	A914	C826	G755	A684	C615	A472	G388	C320	A250
C1244	A1180	C1115	A1045	U981	A915	U827	C756	G685	G616	G473	A389	A321	G251
A1245	G1181	G1117	A1046	U982	G916	G828	U757	U686	G617	G474	C390	C322	G252
C1246	G1184	C1118	G1047	A983	G917	G830	U758	A687	C620	G475	G391	U323	U253
U1247	G1185	C1119	U1048	C984	A918	U831	G760	G688	A621	G476	G392	G324	G254
A1250	G1186	G1120	A986	U990	U920	C832	G761	G690	A622	A477	A393	G325	G255
C1251	G1187	U1121	G1049	G987	U920	G836	C764	G691	C623	C479	G394	C326	U256
A1252	A1188	U1122	C1051	G988	C924	G837	G765	U692	C624	U480	A397	A328	U257
G1255	C1189	A1123	U1052	C989	G925	G838	A766	G693	G625	G484	C398	C330	G258
A1256	G1190	G1124	G1053	U991	G926	U839	A767	A694	U626	G485	G402	G331	G259
C1257	A1191	U1125	C1054	G992	G927	C840	A768	A695	G627	U486	C403	G332	G260
G1258	C1192	A1055	U1056	U992	U927	U841	G769	A696	G628	A487	U404	G333	U261
U1259	G1195	G1057	G993	G993	G933	C848	C770	U697	G629	U488	C403	C336	A262
C1260	C1196	U1058	G1058	C995	A935	U850	U772	G698	A632	C488	U405	C337	A263
A1261	U1197	C1059	G1059	A996	C936	G851	G773	C701	G633	C489	G406	A338	U264
C1262	U1199	C1132	G1061	A1001	A938	G853	G775	G703	G635	G490	G410	C339	G265



• Molecule 2: 30S RIBOSOMAL PROTEIN S2



• Molecule 2: 30S RIBOSOMAL PROTEIN S2

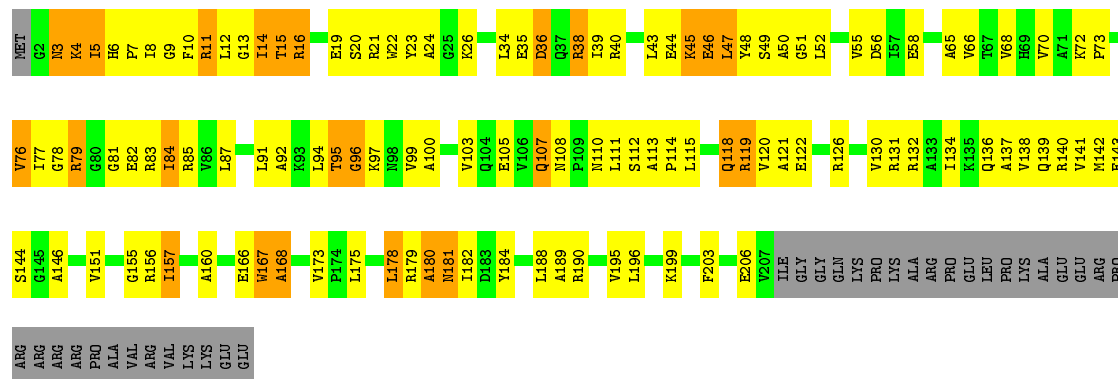




GLU  
ALA

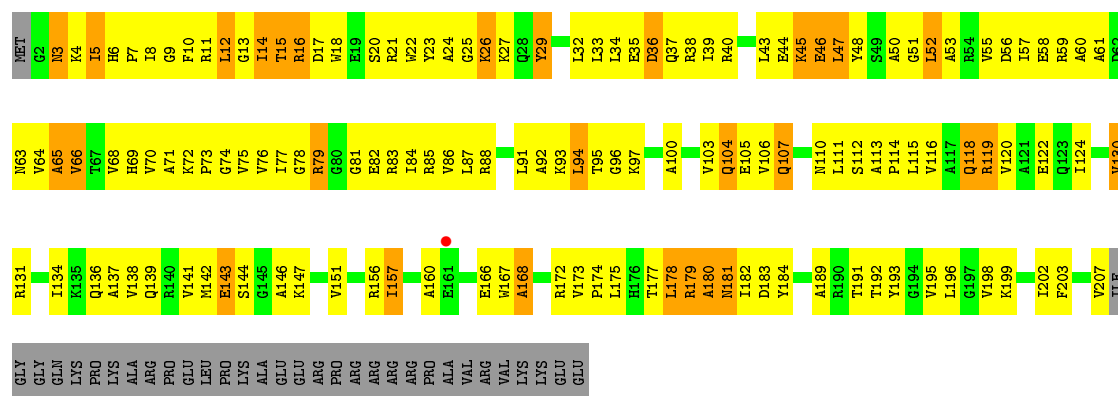
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC: 37% 38% 11% 14%



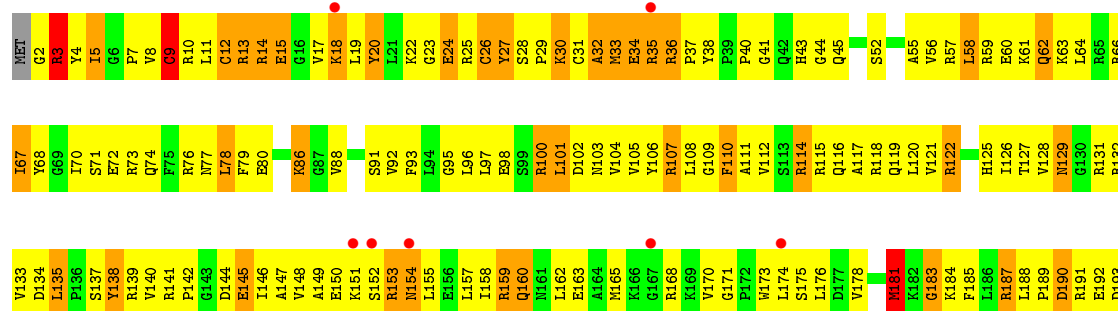
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC: 26% 48% 12% 14%

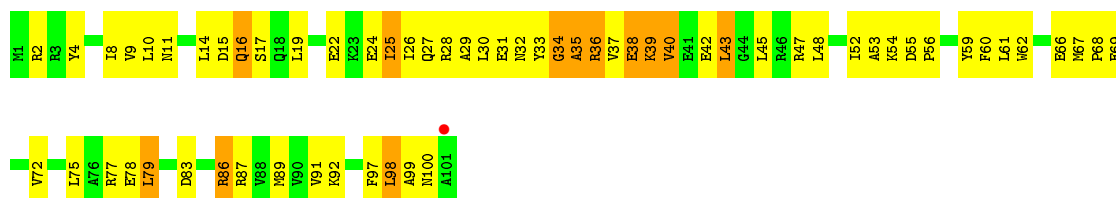


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

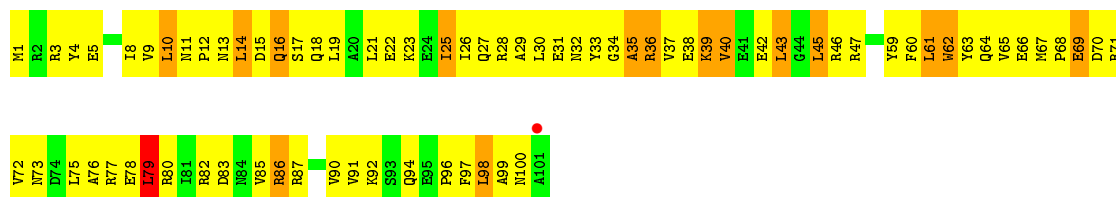
Chain AD: 4% 25% 55% 19%



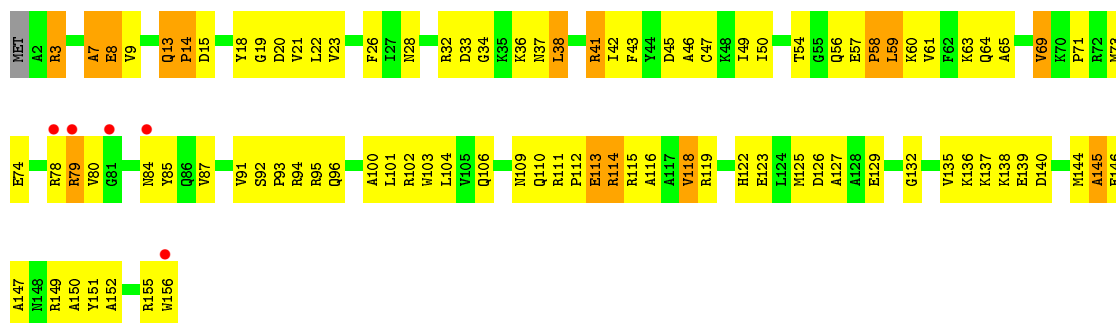
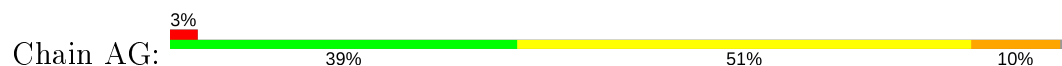




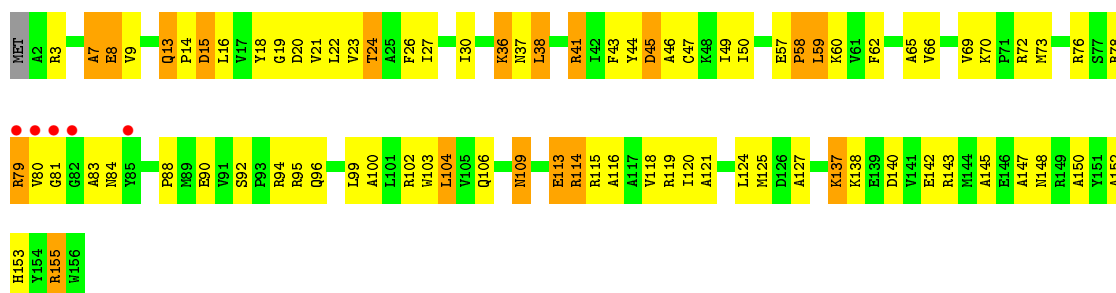
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



• Molecule 7: 30S RIBOSOMAL PROTEIN S7



• Molecule 7: 30S RIBOSOMAL PROTEIN S7



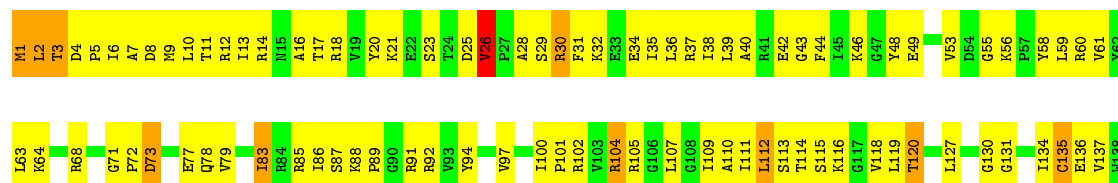
• Molecule 8: 30S RIBOSOMAL PROTEIN S8





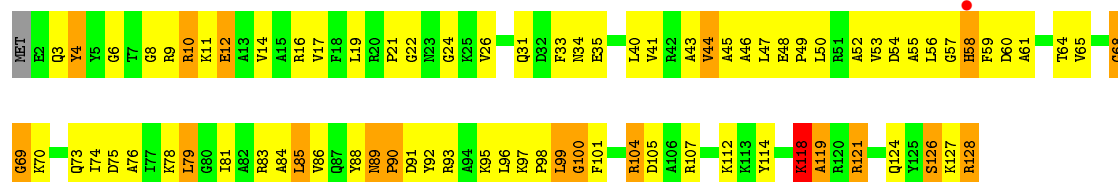
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH: 35% 57% 7%



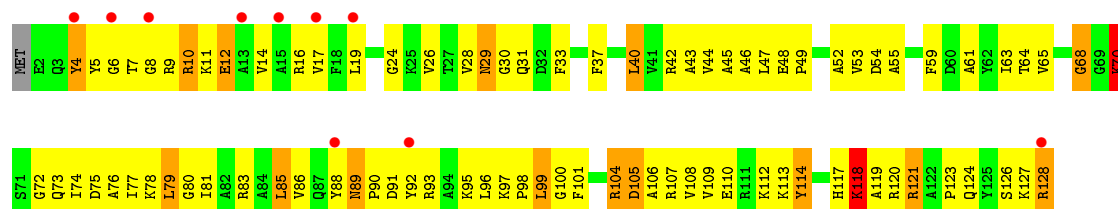
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI: 36% 48% 14%



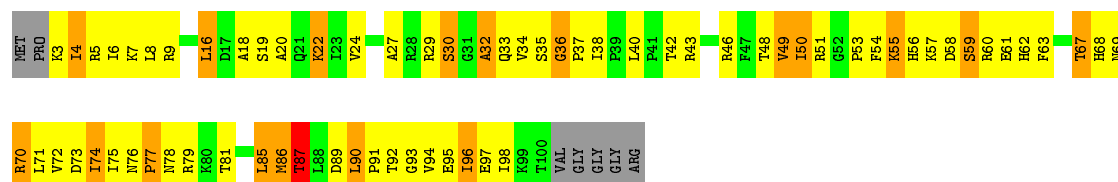
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI: 8% 31% 55% 12%



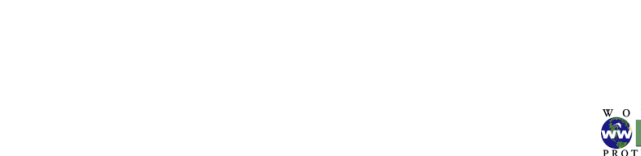
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

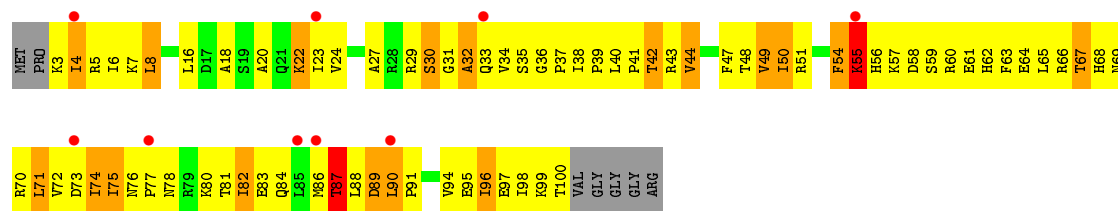
Chain AJ: 28% 48% 17% 7%



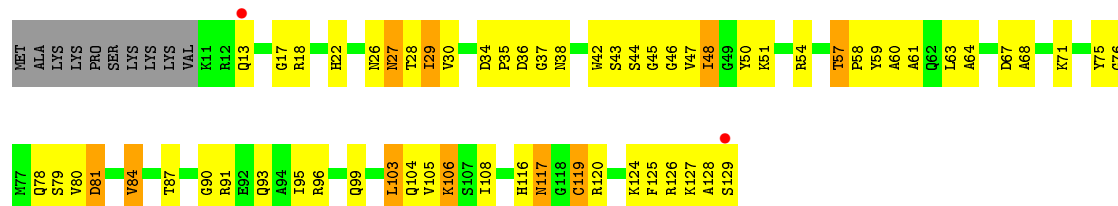
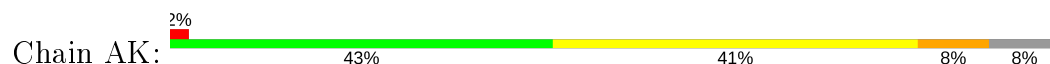
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ: 9% 20% 54% 17% 7%

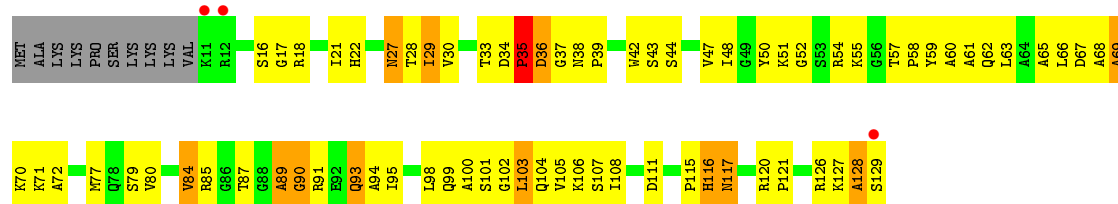




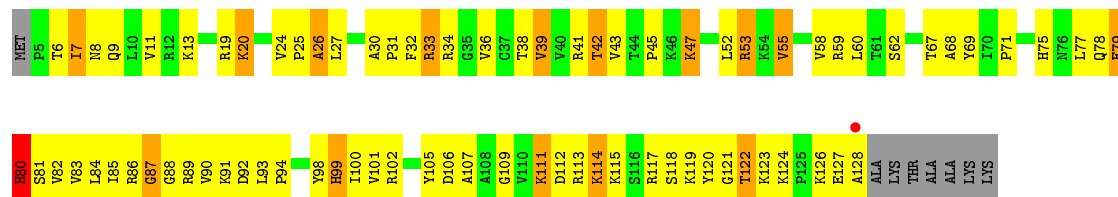
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



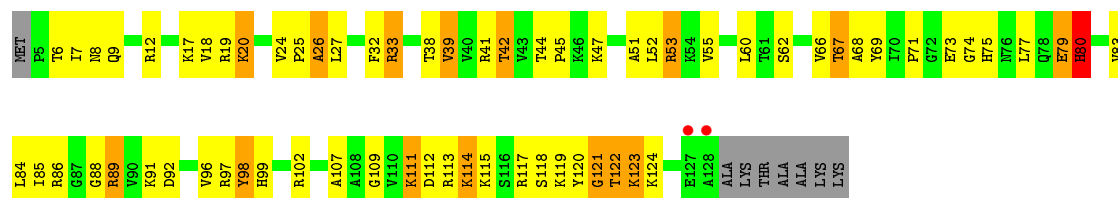
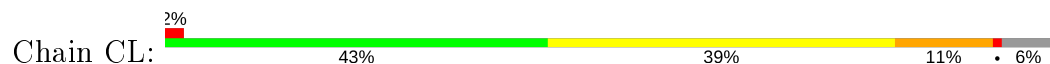
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



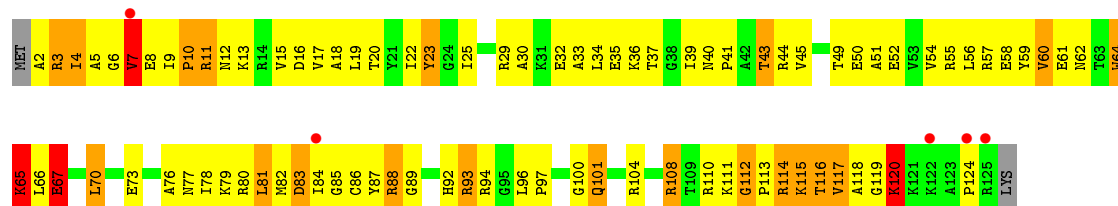
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



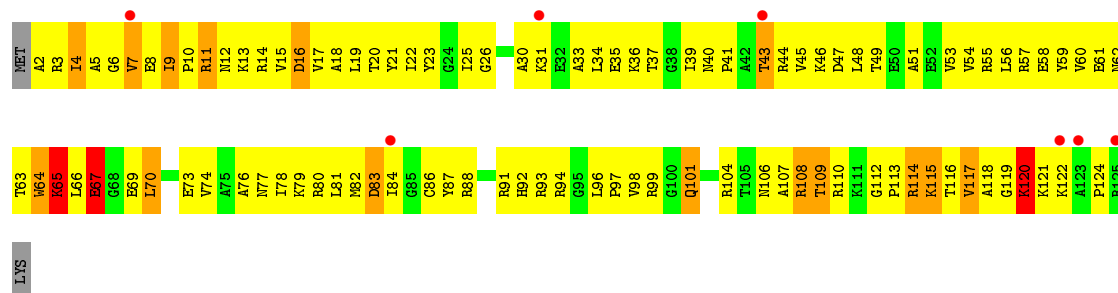
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



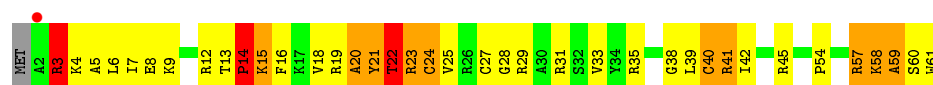
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



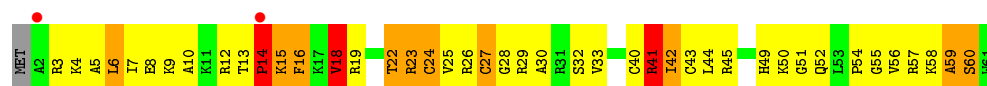
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



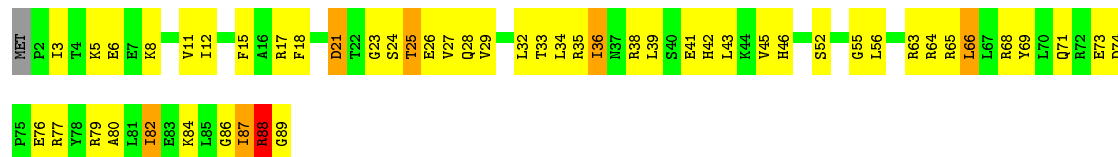
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



• Molecule 14: 30S RIBOSOMAL PROTEIN S14



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

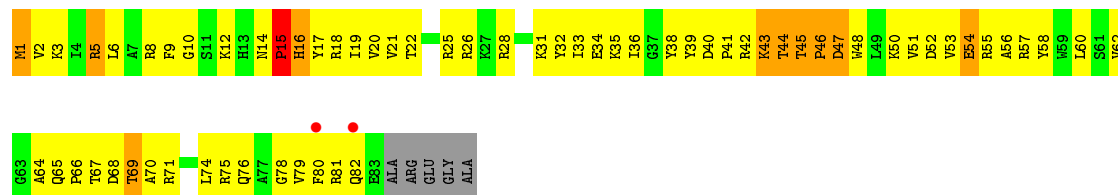


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

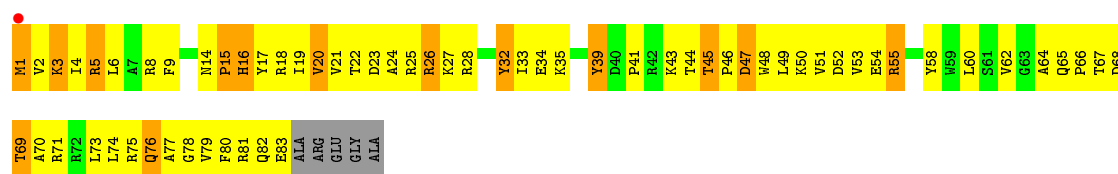




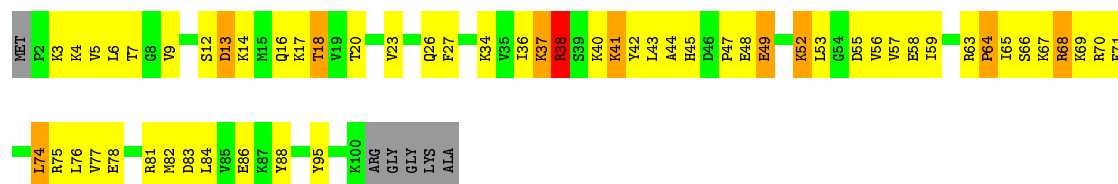
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



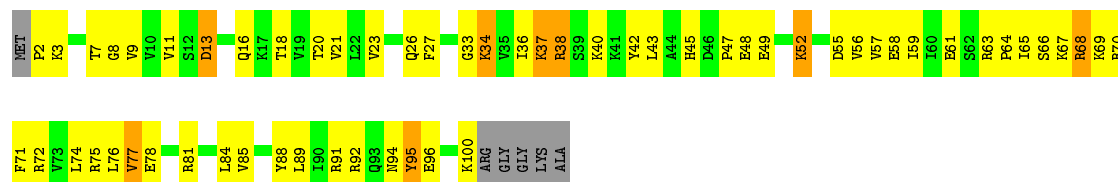
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



• Molecule 17: 30S RIBOSOMAL PROTEIN S17



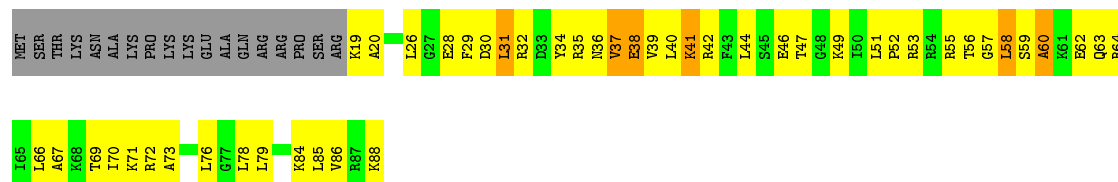
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



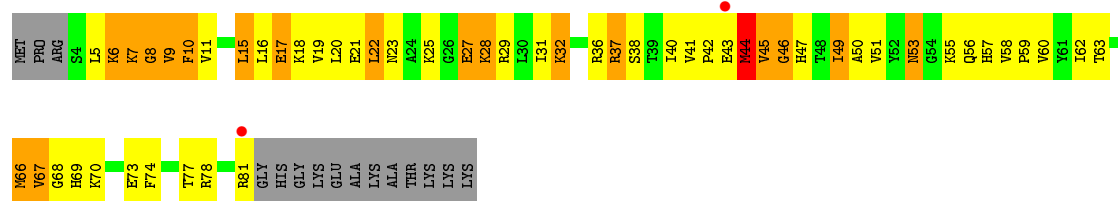
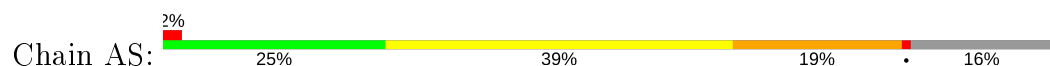
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



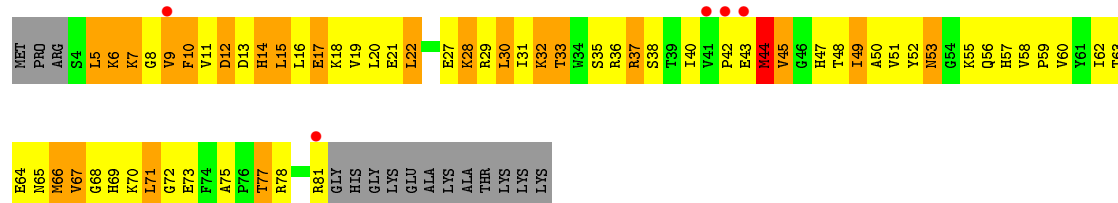
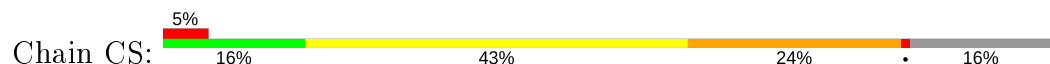
● Molecule 18: 30S RIBOSOMAL PROTEIN S18



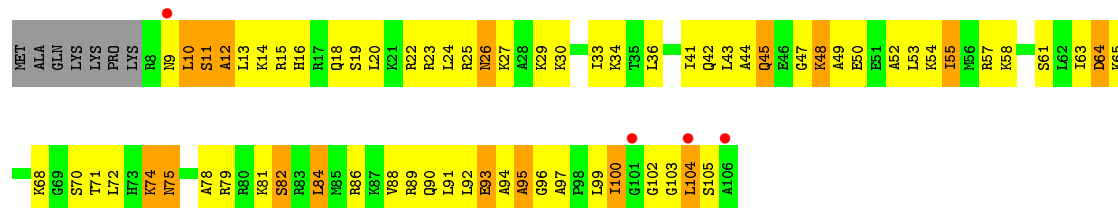
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



● Molecule 19: 30S RIBOSOMAL PROTEIN S19

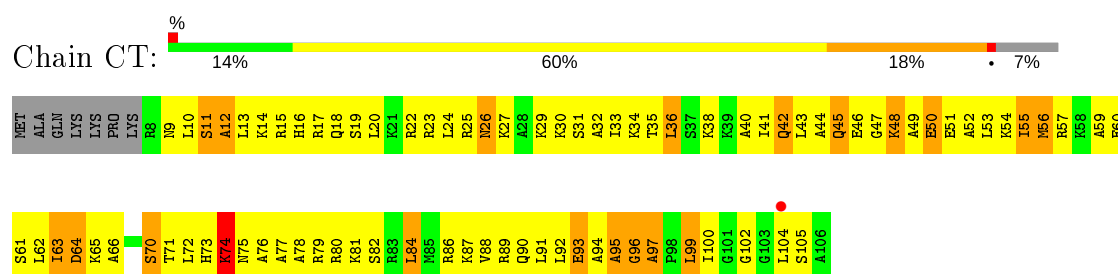


● Molecule 20: 30S RIBOSOMAL PROTEIN S20

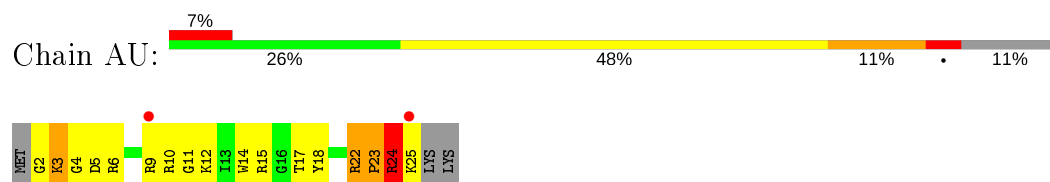


● Molecule 20: 30S RIBOSOMAL PROTEIN S20

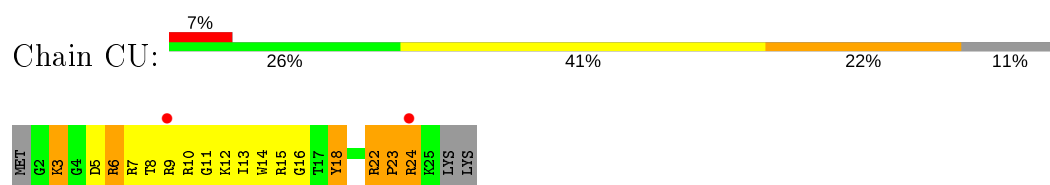




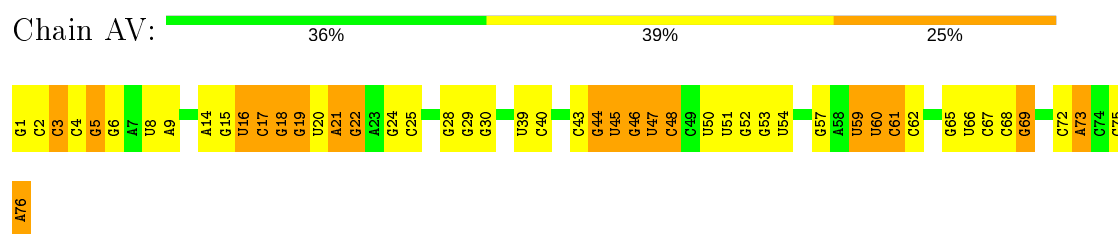
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



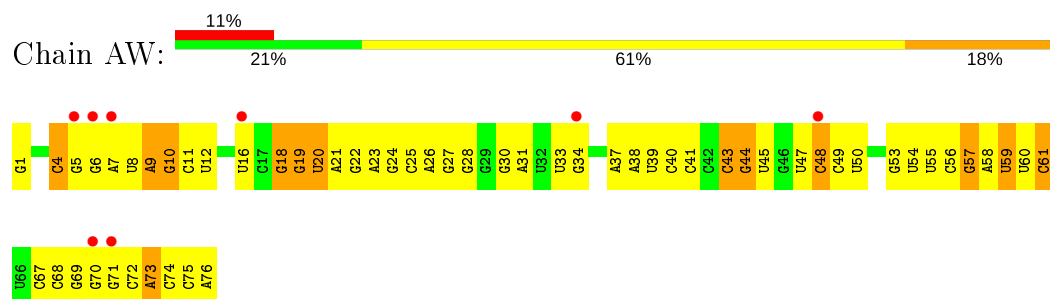
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



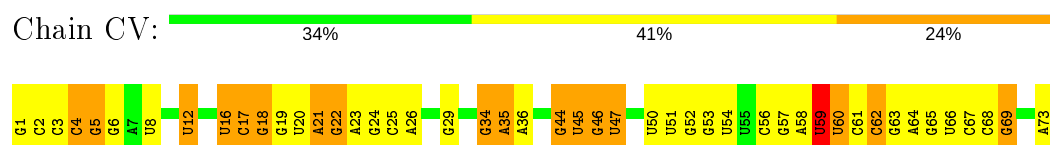
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



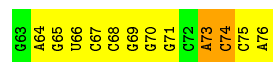
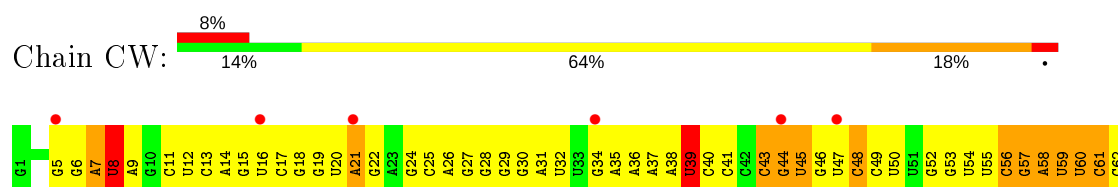
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



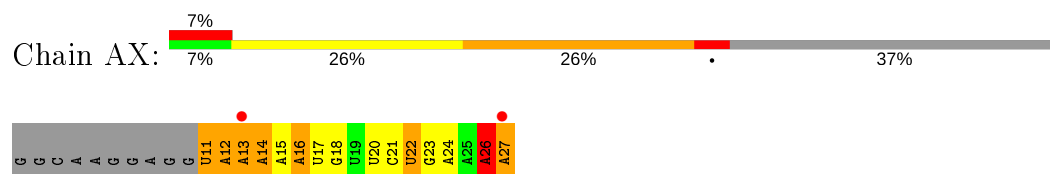
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



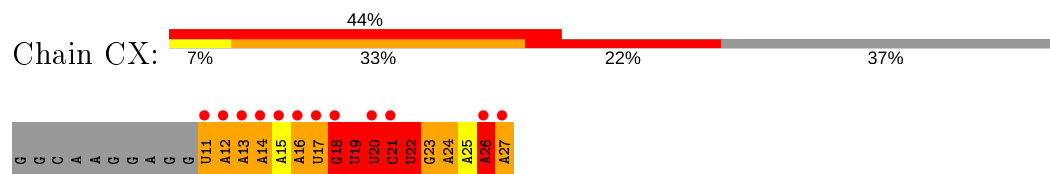
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



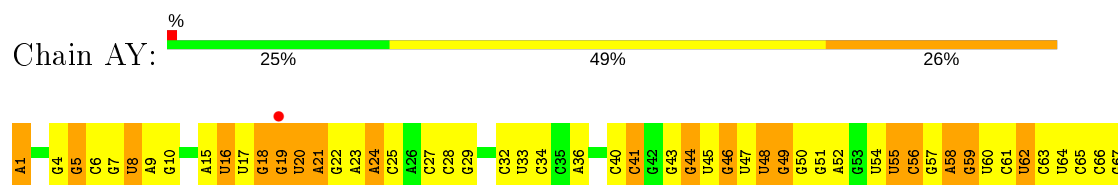
• Molecule 23: MRNA



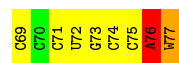
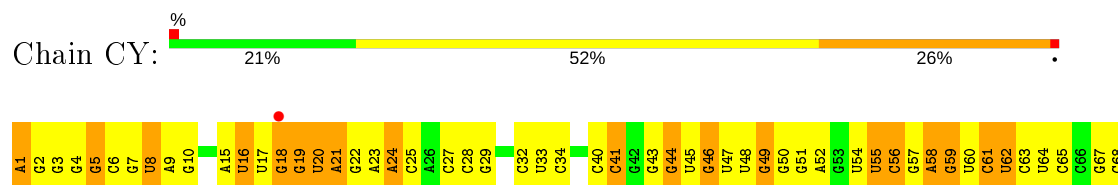
• Molecule 23: MRNA



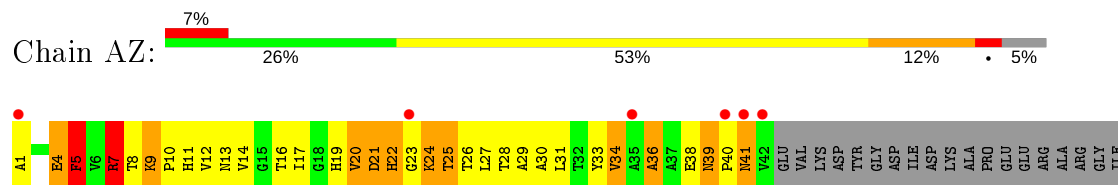
• Molecule 24: A-SITE TRNA G24A TRP-TRNA TRP

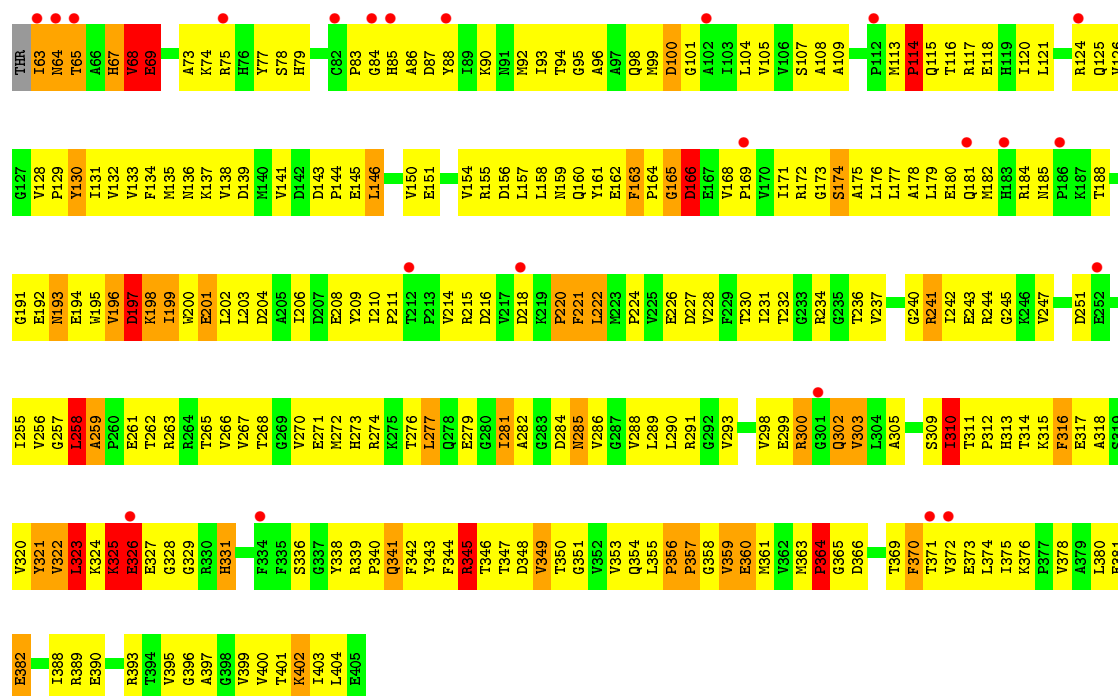


• Molecule 24: A-SITE TRNA G24A TRP-TRNA TRP

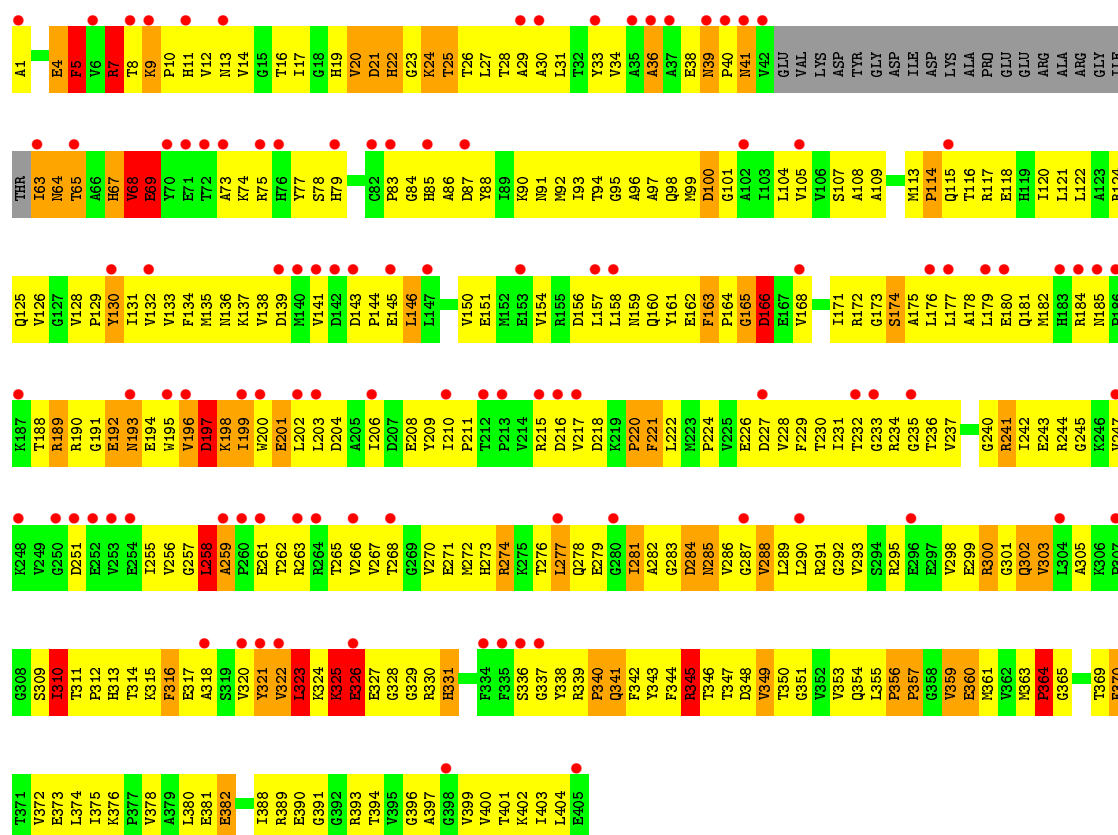


• Molecule 25: ELONGATION FACTOR TU





• Molecule 25: ELONGATION FACTOR TU



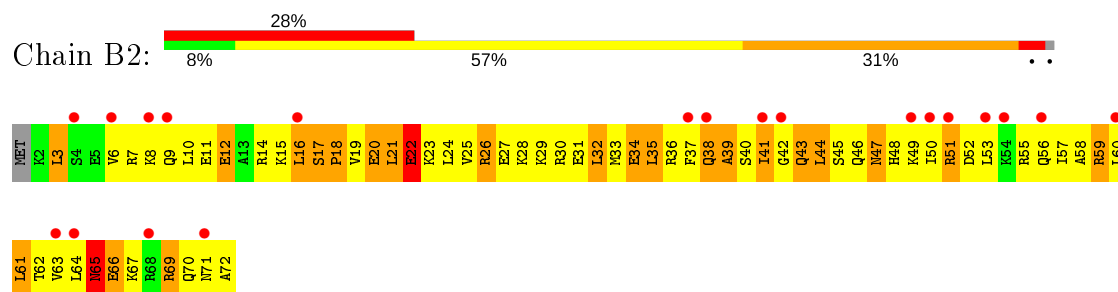
• Molecule 26: 50S RIBOSOMAL PROTEIN L27

● Molecule 26: 50S RIBOSOMAL PROTEIN L27

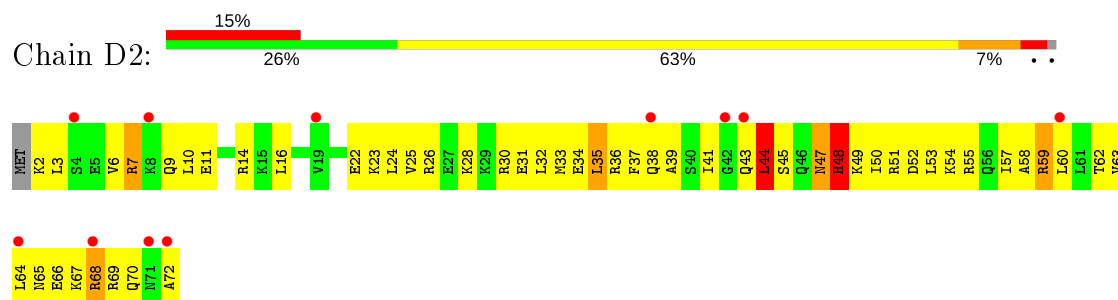
- Molecule 27: 50S RIBOSOMAL PROTEIN L28

- Molecule 27: 50S RIBOSOMAL PROTEIN L28

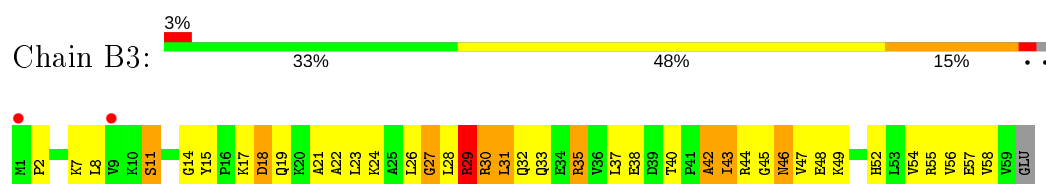
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



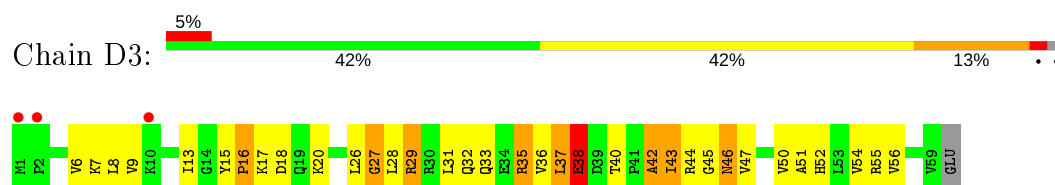
## ● Molecule 28: 50S RIBOSOMAL PROTEIN L29



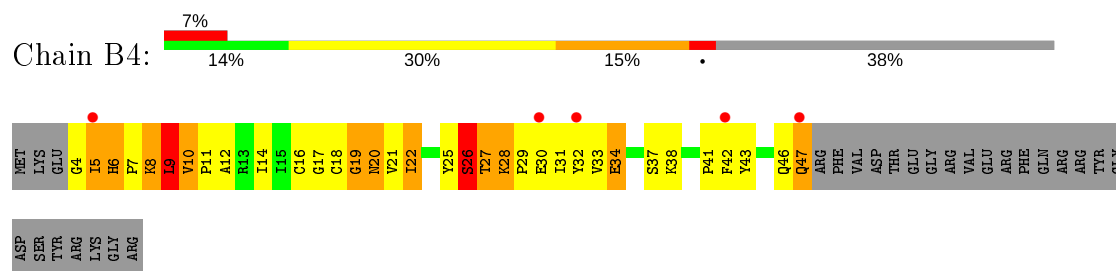
## ● Molecule 29: 50S RIBOSOMAL PROTEIN L30



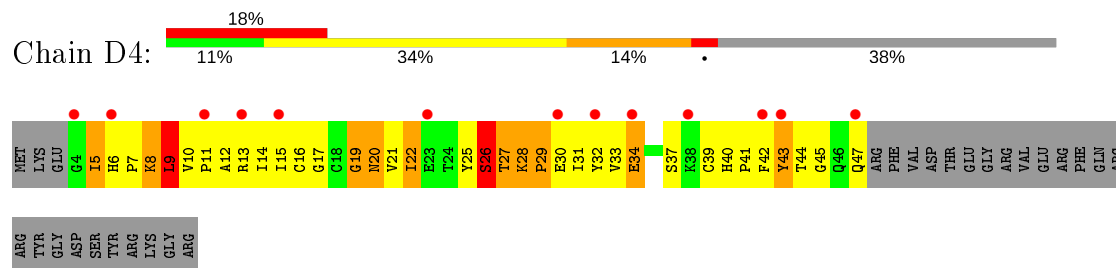
## ● Molecule 29: 50S RIBOSOMAL PROTEIN L30



## ● Molecule 30: 50S RIBOSOMAL PROTEIN L31

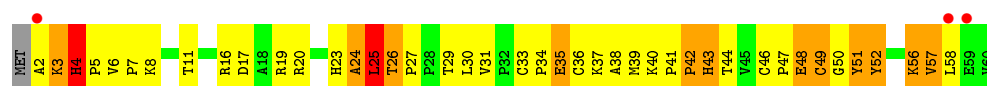


## ● Molecule 30: 50S RIBOSOMAL PROTEIN L31

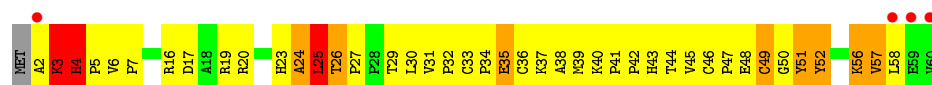


## ● Molecule 31: 50S RIBOSOMAL PROTEIN L32





• Molecule 31: 50S RIBOSOMAL PROTEIN L32



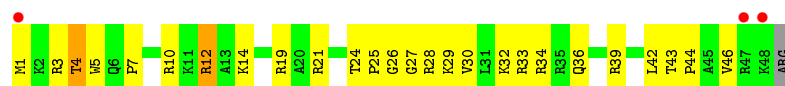
• Molecule 32: 50S RIBOSOMAL PROTEIN L33



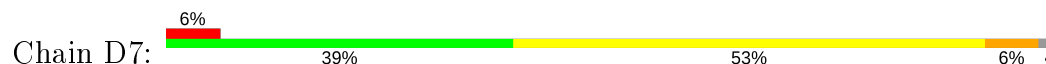
• Molecule 32: 50S RIBOSOMAL PROTEIN L33



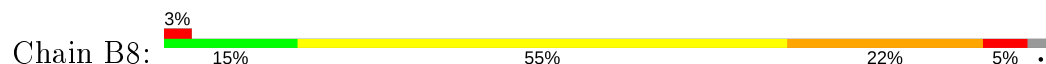
• Molecule 33: 50S RIBOSOMAL PROTEIN L34



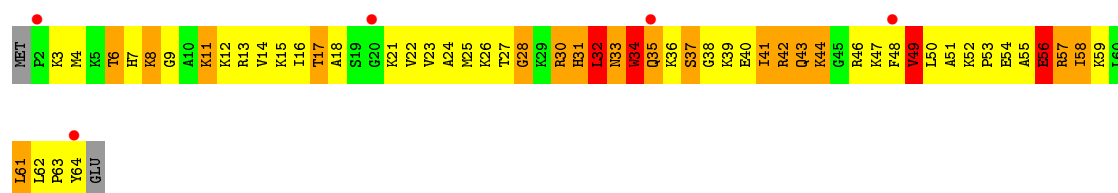
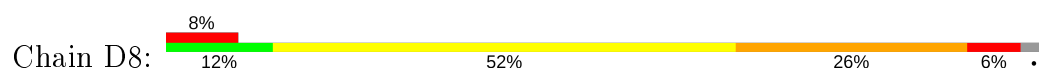
• Molecule 33: 50S RIBOSOMAL PROTEIN L34



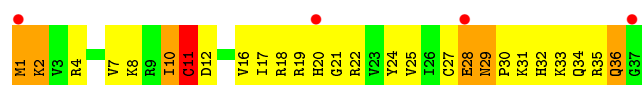
• Molecule 34: 50S RIBOSOMAL PROTEIN L35



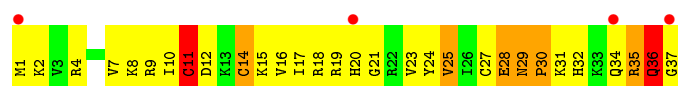
• Molecule 34: 50S RIBOSOMAL PROTEIN L35



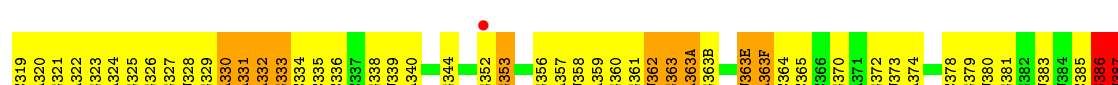
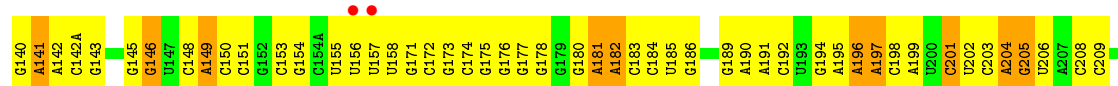
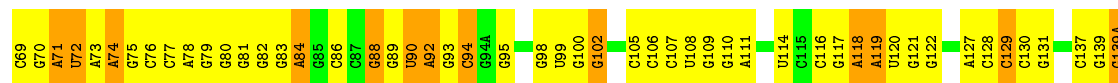
• Molecule 35: 50S RIBOSOMAL PROTEIN L36



• Molecule 35: 50S RIBOSOMAL PROTEIN L36



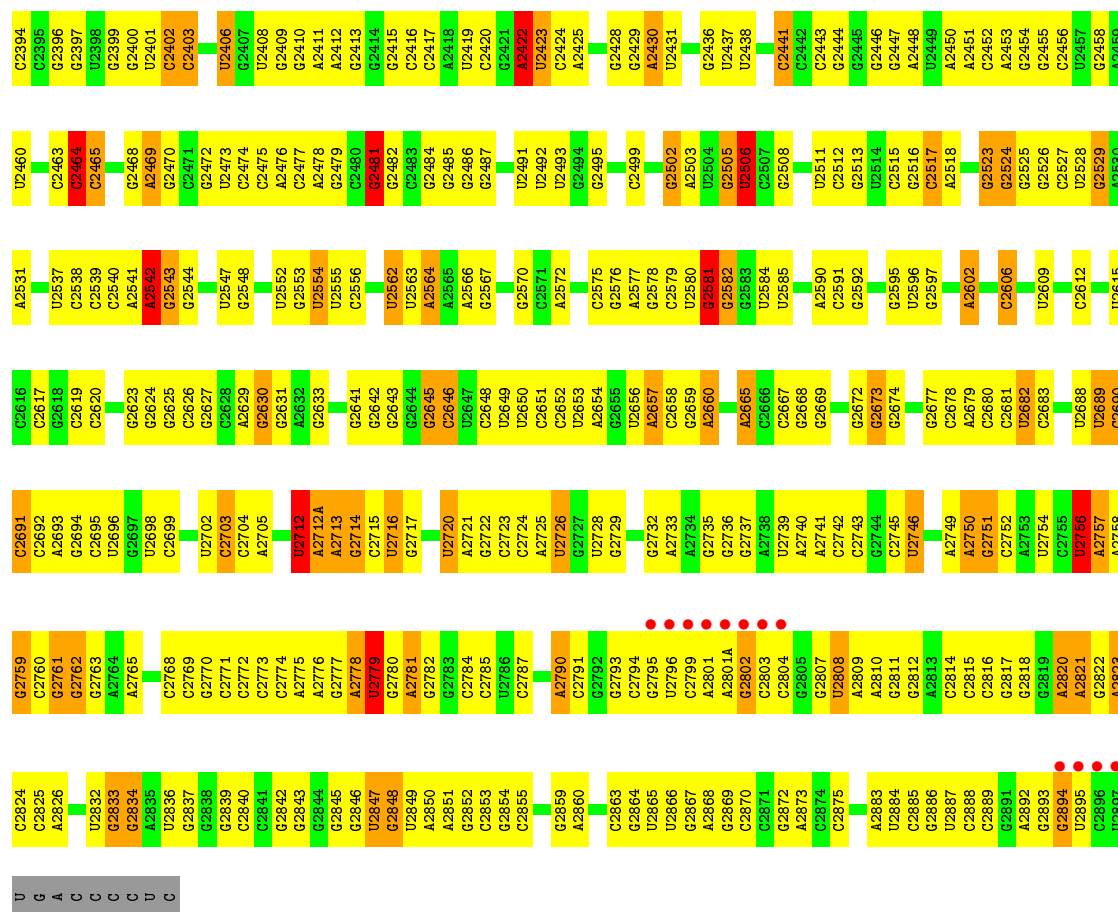
• Molecule 36: 23S RIBOSOMAL RNA



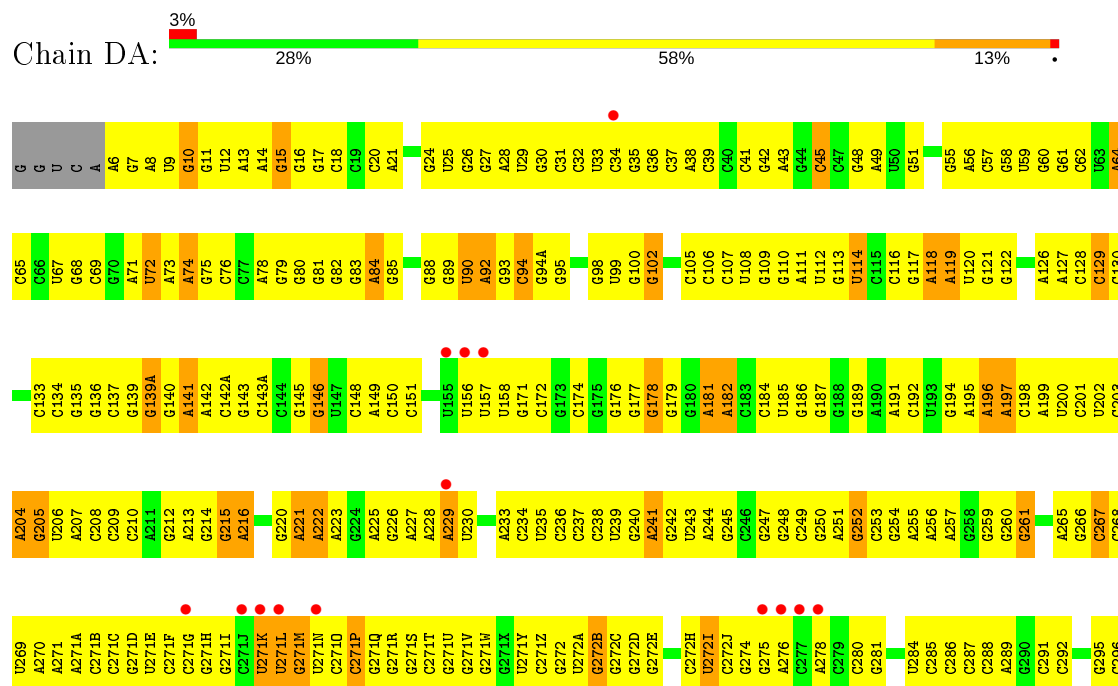
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G1256	G1193	G1124	U1060	C992	A918	U947	A781	U709	G654D	G596	A526	U459	G389
C1257	G1196	G1125	G1061	G993	G919	A849	A783	G710	G654E	U597	C527	A460	A390
G1259	G1197	G1126	G1062	C995	G920	A849	A784	G717	G654F	C461	A528	C461	G391
G1260	U1198	G1131	G1063	A996	C925	U851	A785	A718	G654G	A603	G529	G462	C392
C1261	U1199	A1132	U1065	G997	A926	G852	G766	C719	G654H	G604	U644	U464	G396
A1262	C1200	U1133	U1066	C998	G927	G853	U787	G719	G654I	C505	C531	G465	G396
U1263	G1201	U1135	U999	C998	G928	C856	A788	A722	G654J	U607	G533	A466	A402
G1264	C1202	A1136	A1067	U999	G928	C856	A789	G723	G654K	G608	U534	G467	U403
A1265	G1203	G1137	A1068	A1000	U930	C856	A790	U724	G654L	A609	C535	G468	C404
	U1204	G1138	A1069	A1001	G931	U858	C791	G725	G654M	G610	A536	G469	U405
	A1205	G1139	G932	U859	G932	U859	G792	G726	G654N	G611	C537	A470	G406
A1268	U1206	G1140	A933	U860	A933	U860	A793	G726	G654O	C612	G538	A471	G407
A1269	G1207	U1141	G940	U861	G940	U861	A794	G729	G654P	G613	G539	A472	G408
G1270	C1207	U1142	A941	A861	G941	A861	C795	G730	G654Q	U614	C540	A473	C409
A1271	U1208	A1143	G942	G862	G942	A862	C796	G731	G654R	U614A	C543	A474	G410
A1272	G1209	A1142A	G943	A863	U943	G875	C797	G732	G654S	A614C	A547	A475	G411
U1273	C1210	A1143	U943	C864	G943	C876	C798	G733	G654T	G615	A548	A476	C412
A1274	U1211	G1144	A944	C865	G944	U877	G798	G733	G654U	G616	A549	A477	C413
A1275	G1212	G1145	A945	A866	A945	U877	G799	A734	G654V	G618	A547	A478	C414
	A1213	U1146	G946	G873	G946	G873	A800	G738	A655	G619	A548	A479	A415
	G1214	G1149	G947	G874	G947	G874	A801	G739	G656	G620	A549	A480	C416
	G1215	G1150	G948	G875	G948	G875	A802	G739	U657	G621	A550	A481	C417
	G1216	G1151	C949	G876	C949	C876	U803	U740	G657	G622	U554	A482	C418
	C1217	C1152	G950	C877	G950	U877	A804	G741	C658	G623	U555	A483	C419
	G1218	C1153	C951	C878	C951	U877	G805	G742	C659	G624	U556	C484	C420
		G1154	G952	A878	G952	U877	C806	G743	G660	G625	U557	C485	U421
	C1221	G1155	A953	G879	A953	G879	U807	G744	C661	G626	U558	C486	A422
	C1221A	A1156	G954	C880	G954	G880	A808	G745	G662	U626	U562	C487	A423
	C1222	A1156	G955	C881	G955	C881	G809	G746	G663	G627	U563	G424	G425
	G1223	U1159	G956	G882	G956	C882	U810	G747	G664	G628	U564	G426	C426
	C1224	G1162	A957	C883	A957	C883	U811	G748	G665	G629	U565	G427	C427
	G1225	G1163	U958	C884	U958	C884	U812	G749	G666	G630	U566	G428	U427
	C1226	G1164	A959	C885	A959	C885	U813	G750	G667	A631	U567	A429	A428
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	G1228	U1166	G961	C887	G961	C887	C815	A752	C671	G633	U569	U432	U430
		G1167	G962	C888	G962	C888	C816	G753	C672	G634	U570	U433	A431
		U1167	U963	C889	U963	C889	C817	C754	C673	C635	G573	U434	A432
		G1168	C964	C890	C964	C890	C818	G755	G674	G636	C574	U435	C433
	G1231	G1169	G965	A890	G965	A890	A819	U757	A675	G637	U576	C436	G437
	G1232	G1170	C968	C893	C968	C893	A820	G758	A676	G638	C577	G505	G437
	C1233	U1171	U969	C894	U969	C894	U821	G759	G684	G639	U577	G506	G442
	U1234	G1172	C970	U995	C970	U995	U822	G760	G685	G640	C580	G507	A443
	G1235	A1173	C971	C897	C971	C897	U826	G761	G686	C641	C581	G508	C444
	A1236	U1174	G974	A901	G974	A901	U827	G762	G687	C642	C582	C509	C445
	U1237	U1175	C975	C902	C975	C902	U828	G763	G688	C643	C583	G510	C446
	G1238	U1176	G976	C903	G976	C903	G830	G764	G689	C644	C584	U511	G447
	G1239	A1177	G977	C906	G977	C906	G831	G765	G690	C645	C585	G512	A448
	U1241	G1178	G978	G907	G978	G907	G832	G766	C691	G646	C586	U449	U448
	A1242	C1179	G979	U907	G979	U907	G833	G767	C692	G647	C587	A513	U449
	G1243	G1182	A983	C908	A983	C908	U834	G768	G696	G648	C588	A514	A449
	G1244	G1183	A984	C909	A984	C909	U839	U773	C697	G649	C589	A515	G450
	U1246	C1184	G985	A910	G985	A910	C840	A774	G700	C650	U588	C451	C451
	G1249	U1185	C986	A911	C986	A911	A841	G775	G700	G651	C589	G452	G452
	C1250	G1186	G987	C912	G987	C912	G842	G776	U703	C652	A590	C453	C453
	U1251	U1187	G988	C913	G988	C913	G843	A777	U704	A653	C591	A454	A454
	G1252	G1188	G989	C914	G989	C914	G844	G778	G704	A654	G592	C455	C455
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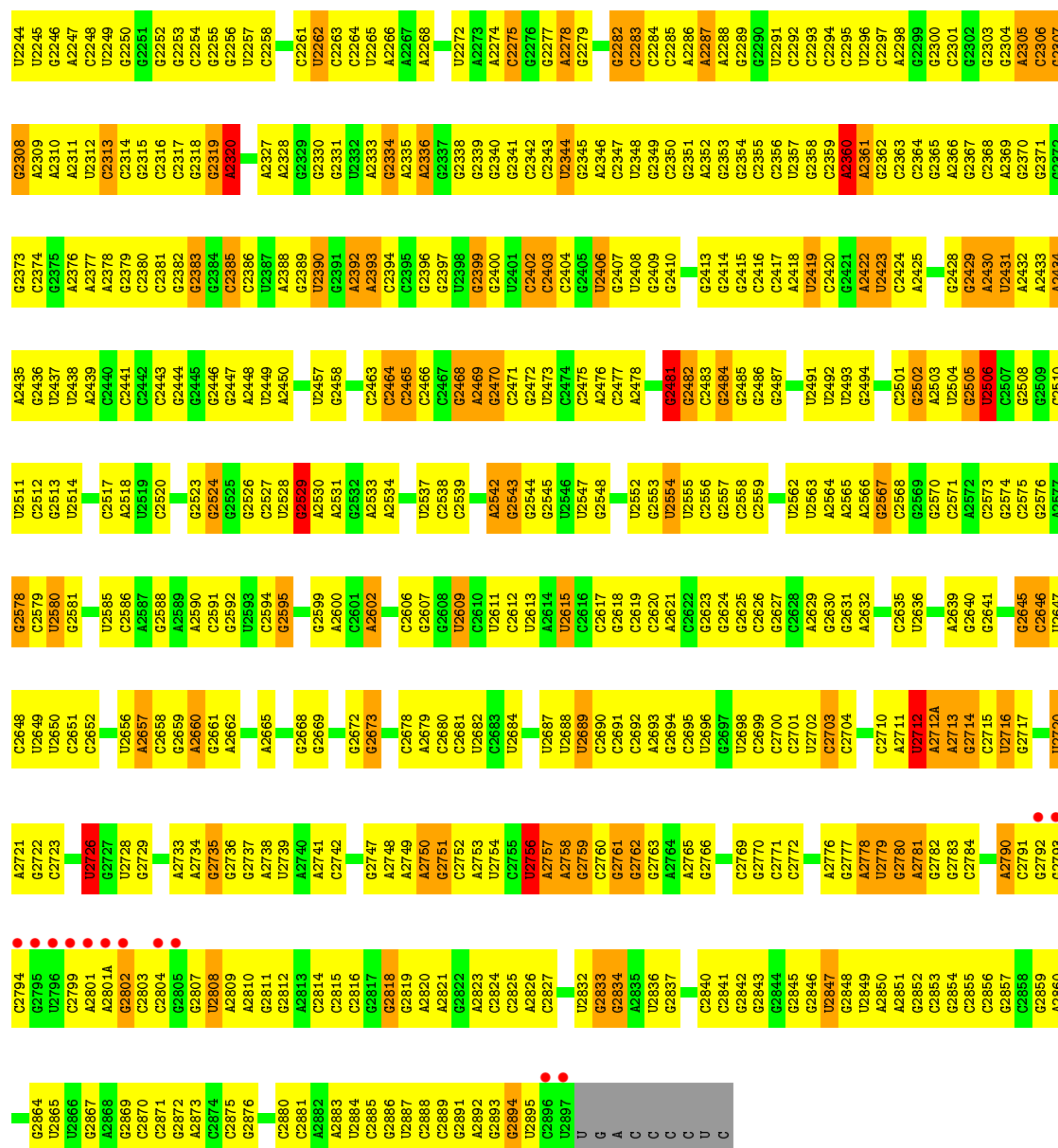


• Molecule 36: 23S RIBOSOMAL RNA



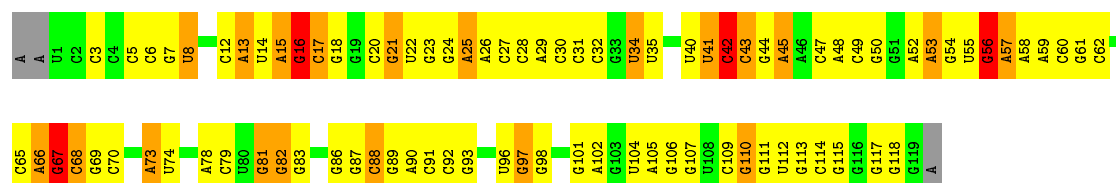


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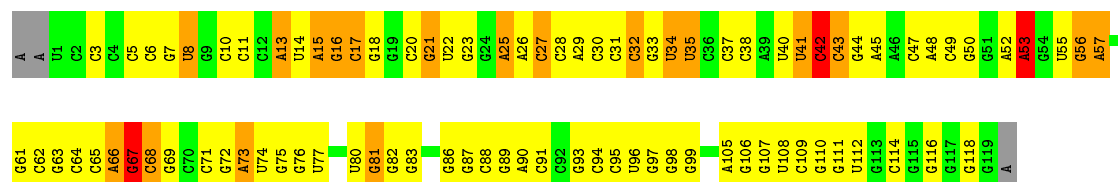
● Molecule 37: 5S RIBOSOMAL RNA

Chain BB: 26% 52% 16%

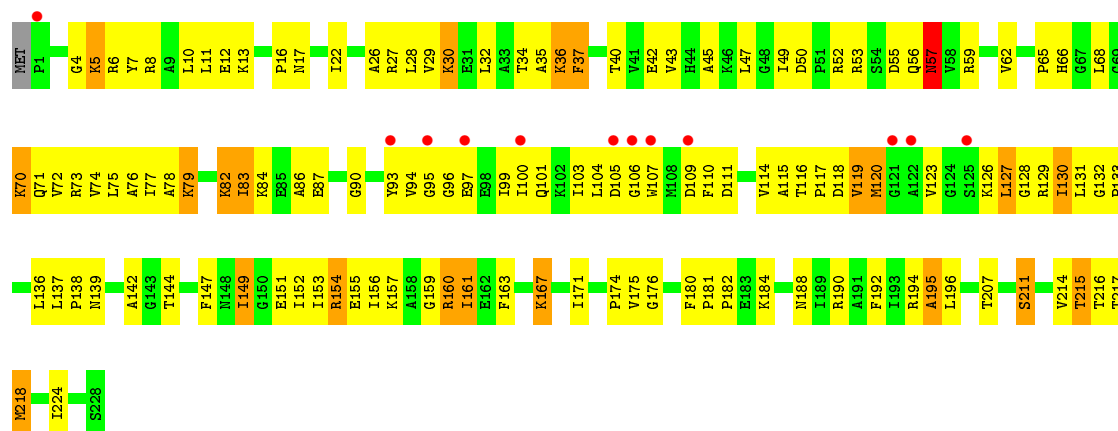
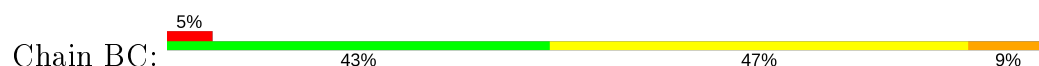


● Molecule 37: 5S RIBOSOMAL RNA

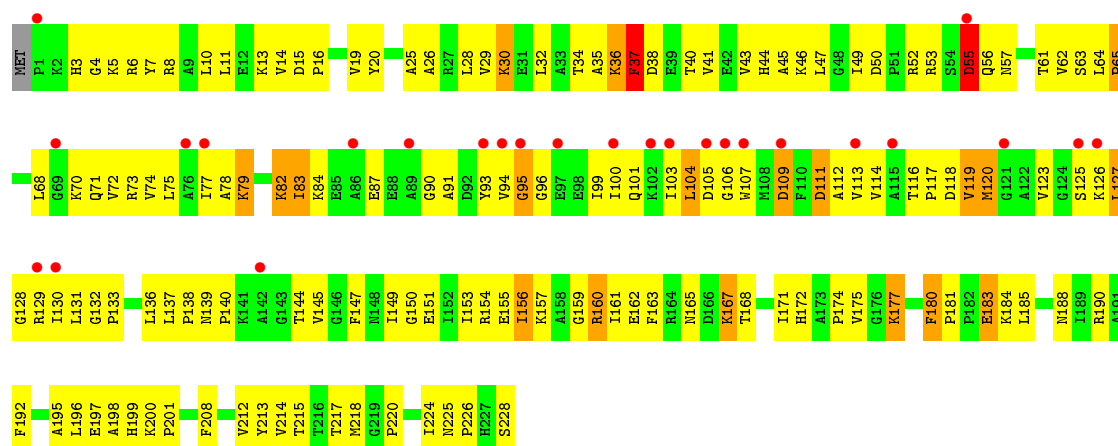
Chain DB: 25% 55% 16%



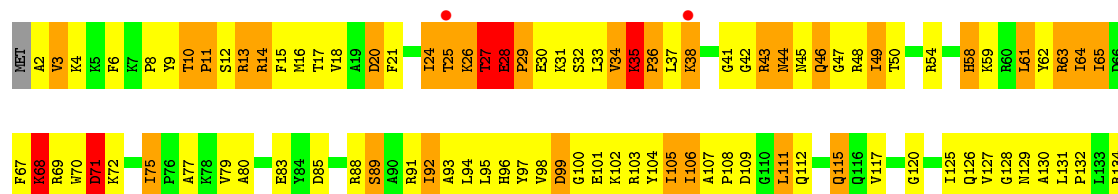
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

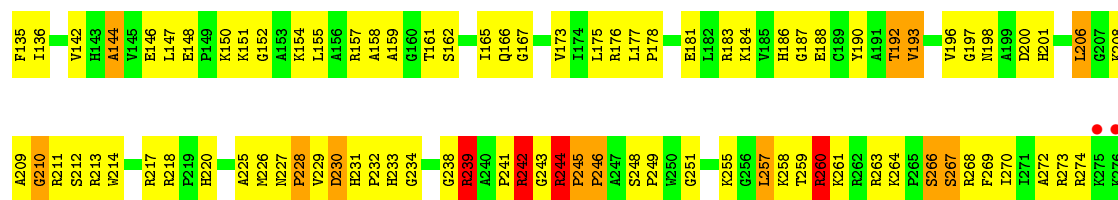


• Molecule 38: 50S RIBOSOMAL PROTEIN L1

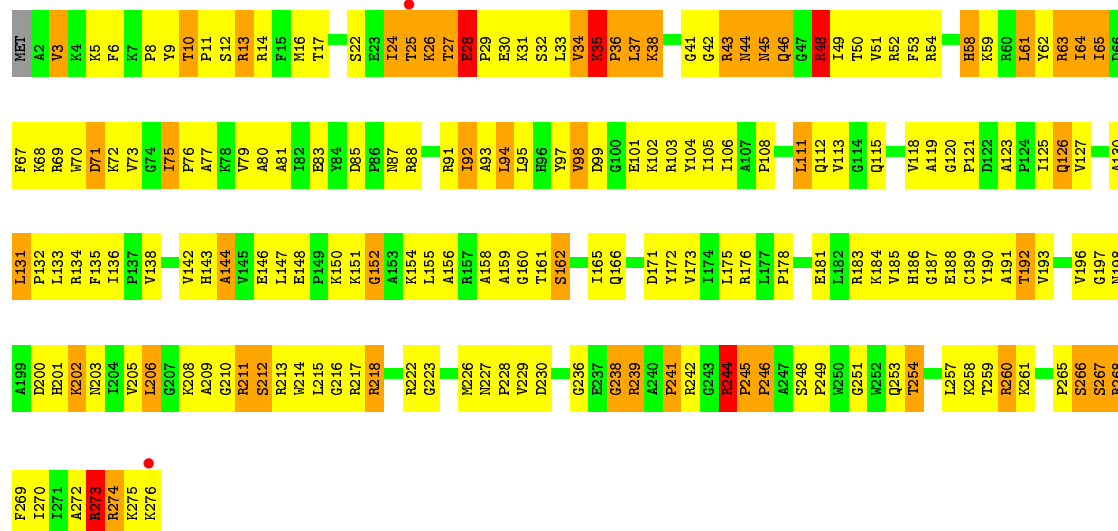


• Molecule 39: 50S RIBOSOMAL PROTEIN L2

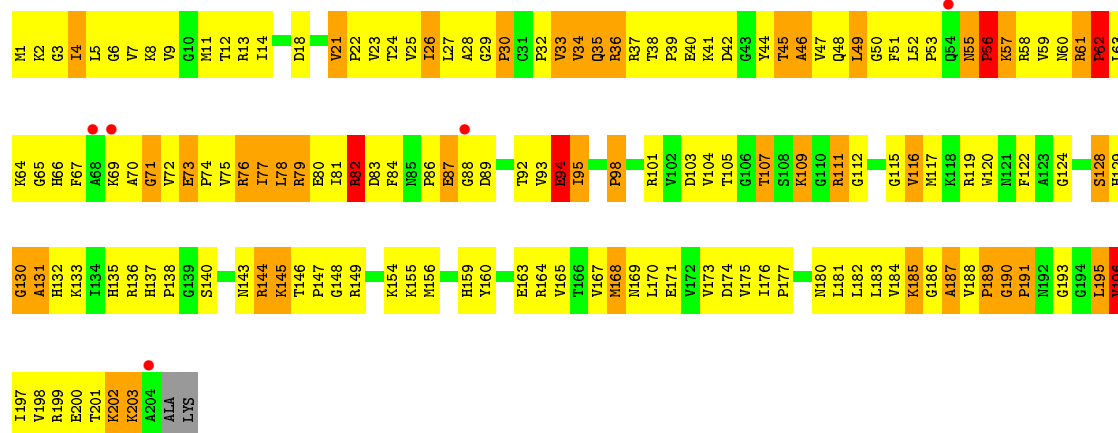




• Molecule 39: 50S RIBOSOMAL PROTEIN L2

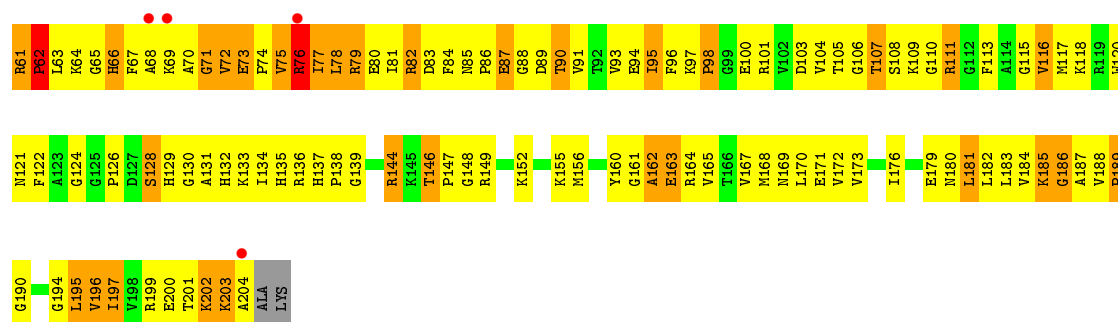


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

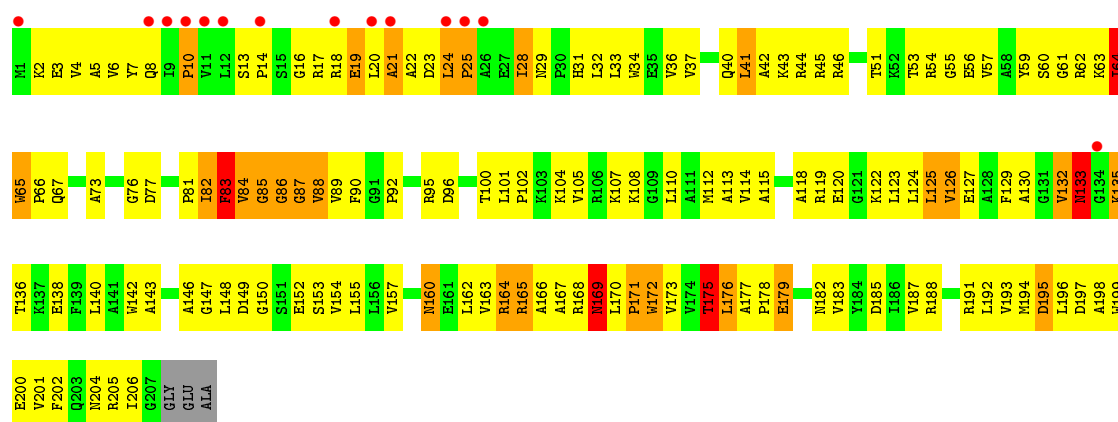


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

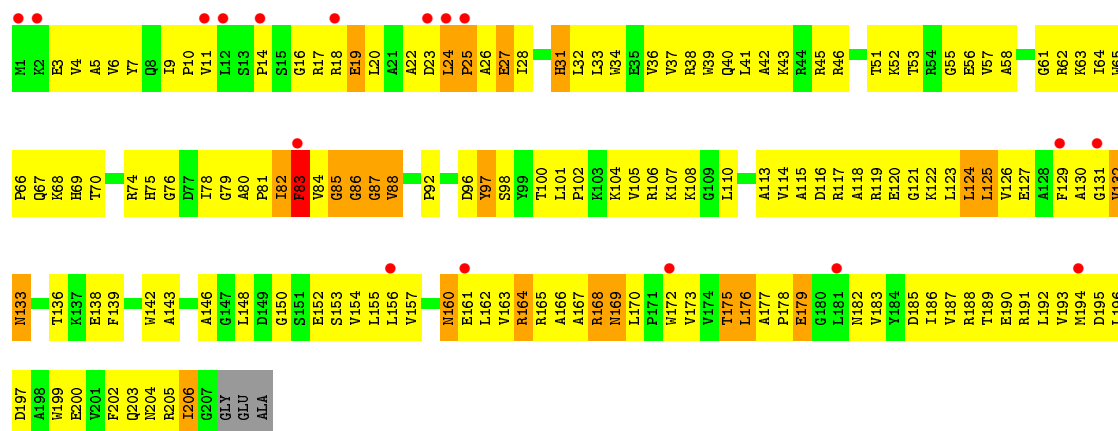




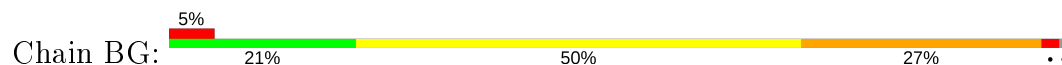
• Molecule 41: 50S RIBOSOMAL PROTEIN L4



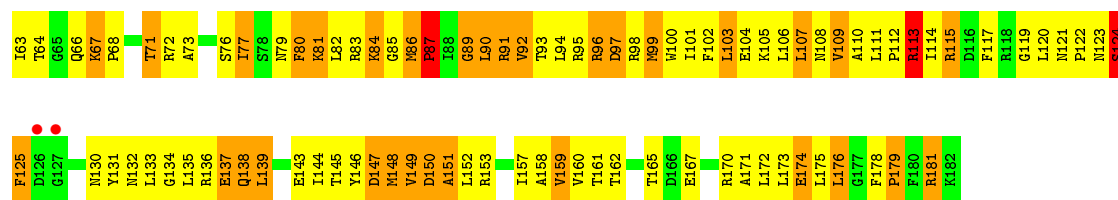
• Molecule 41: 50S RIBOSOMAL PROTEIN L4



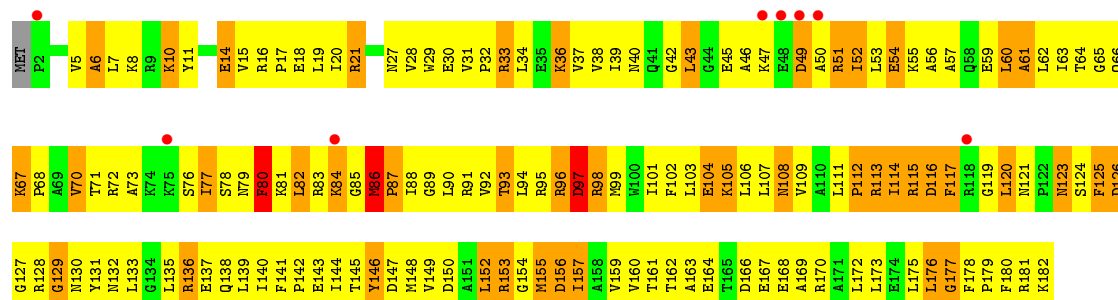
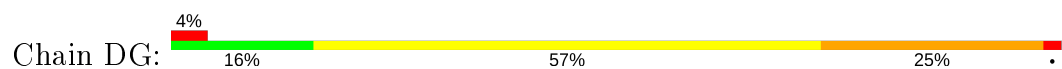
• Molecule 42: 50S RIBOSOMAL PROTEIN L5



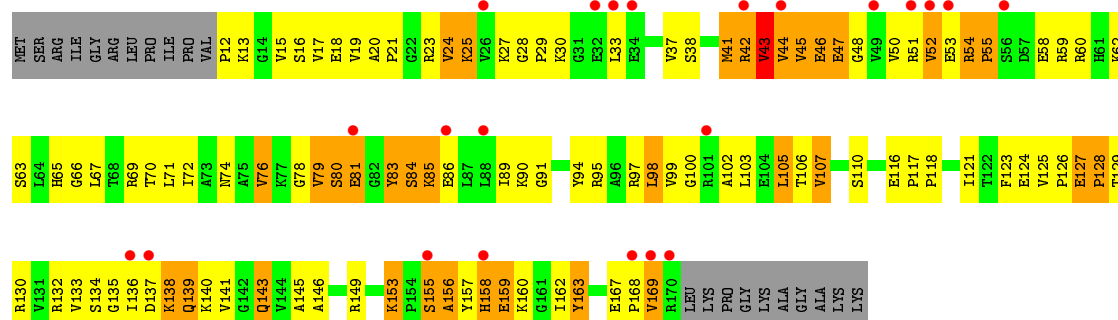




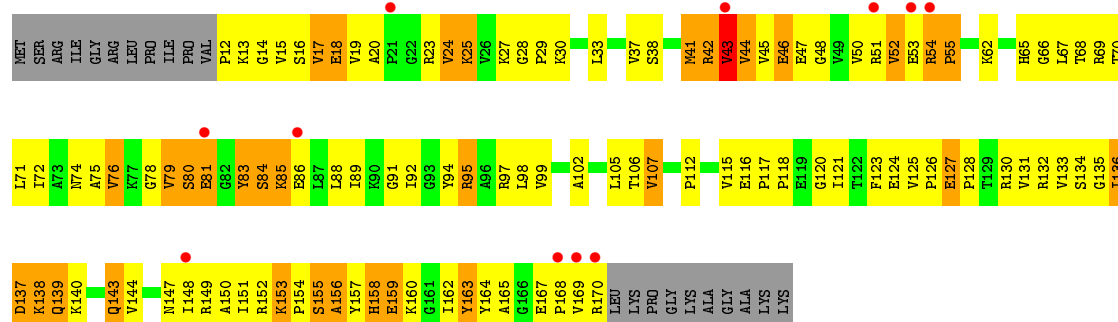
• Molecule 42: 50S RIBOSOMAL PROTEIN L5



• Molecule 43: 50S RIBOSOMAL PROTEIN L6

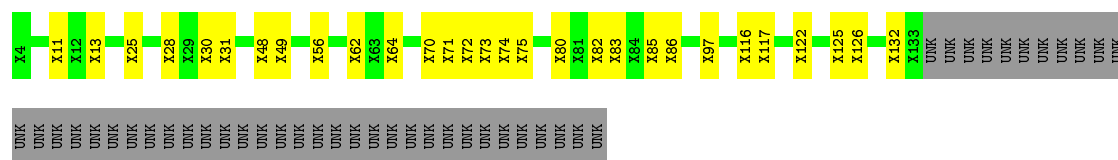


• Molecule 43: 50S RIBOSOMAL PROTEIN L6



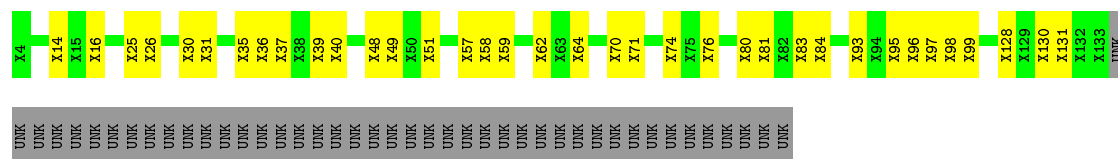
• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ: 




• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain DJ: 




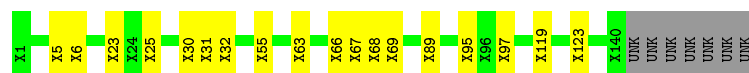
• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK: 



• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain DK: 



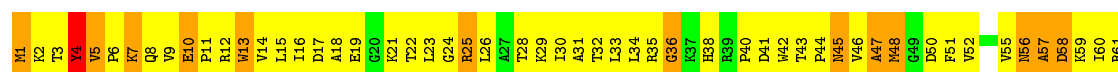
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

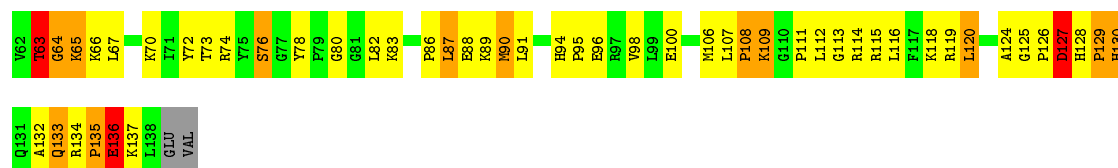
Chain BN: 



• Molecule 46: 50S RIBOSOMAL PROTEIN L13

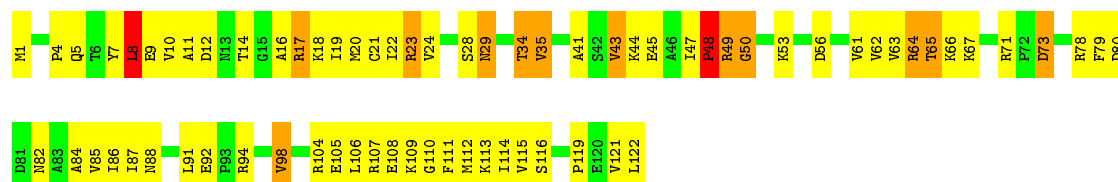
Chain DN: 





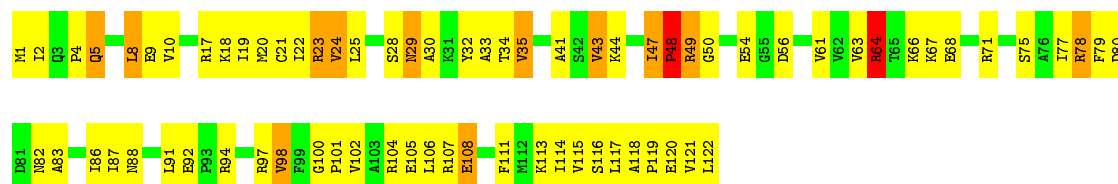
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO: 42% 47% 10% .



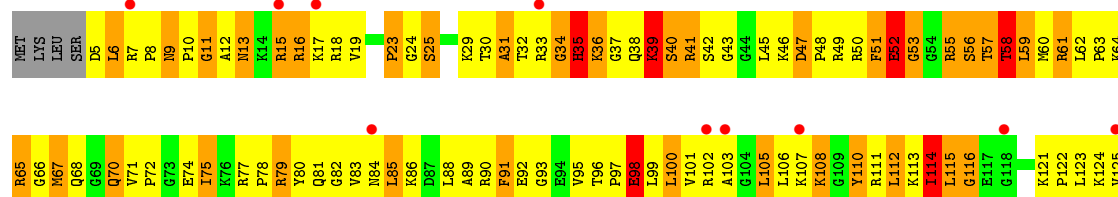
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO: 40% 48% 10% .



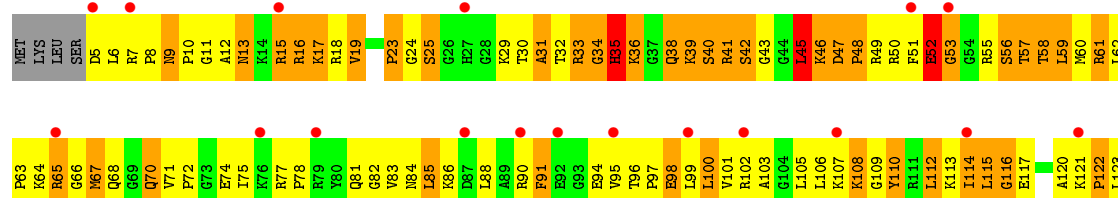
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

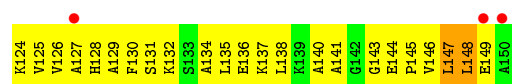
Chain BP: 9% 17% 51% 25% . .



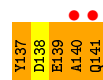
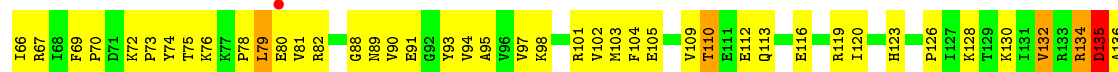
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP: 14% 18% 49% 28% . . .

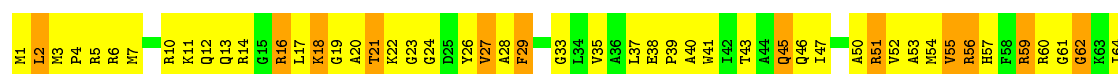




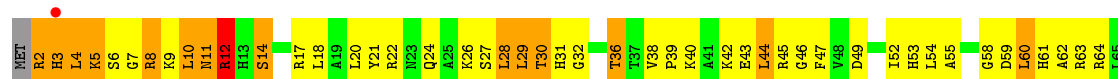
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



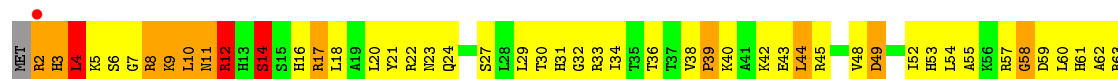
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



• Molecule 50: 50S RIBOSOMAL PROTEIN L17

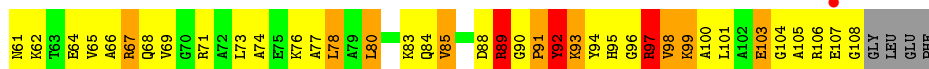
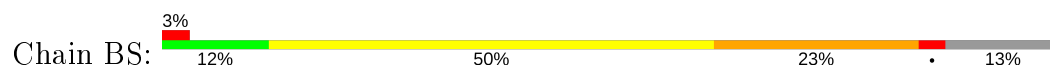


• Molecule 50: 50S RIBOSOMAL PROTEIN L17

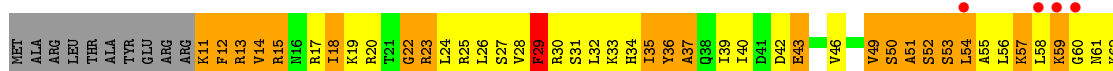




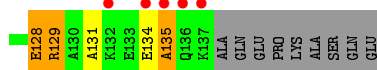
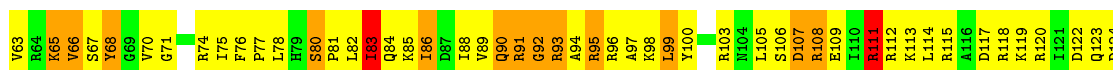
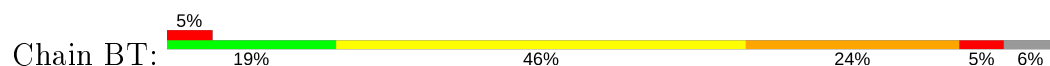
• Molecule 51: 50S RIBOSOMAL PROTEIN L18



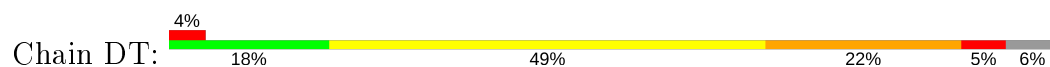
• Molecule 51: 50S RIBOSOMAL PROTEIN L18



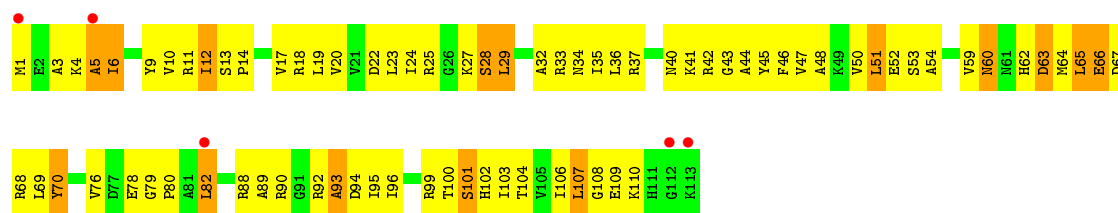
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



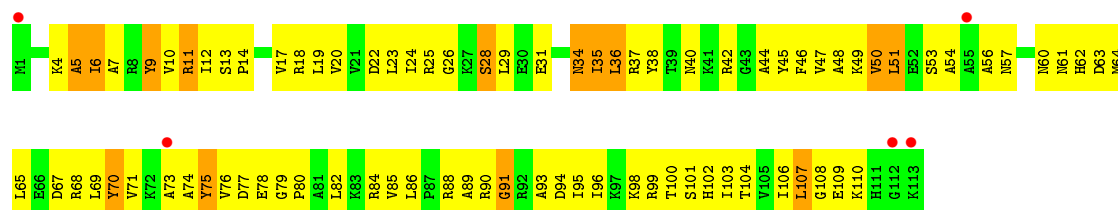
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



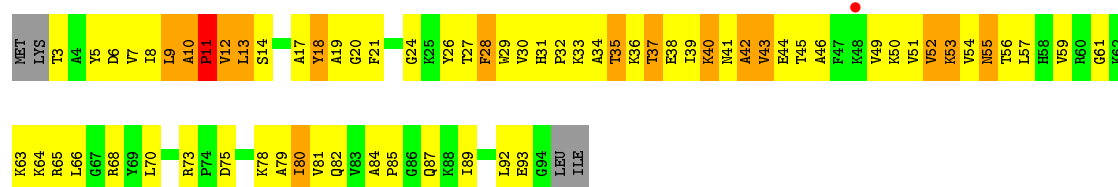




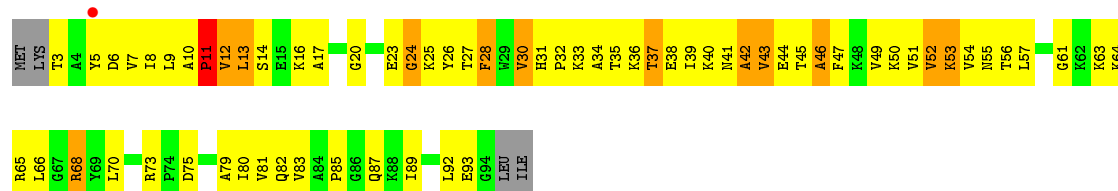
● Molecule 55: 50S RIBOSOMAL PROTEIN L22



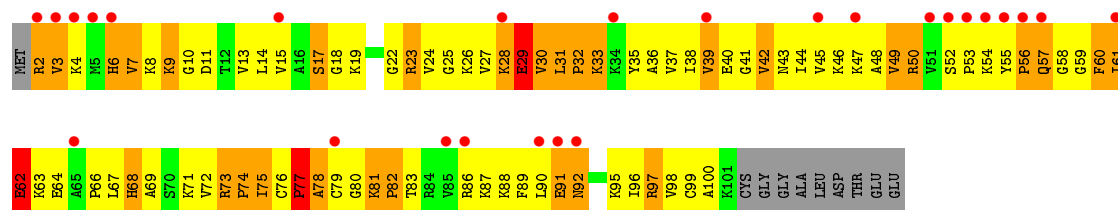
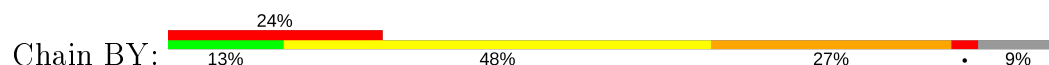
● Molecule 56: 50S RIBOSOMAL PROTEIN L23



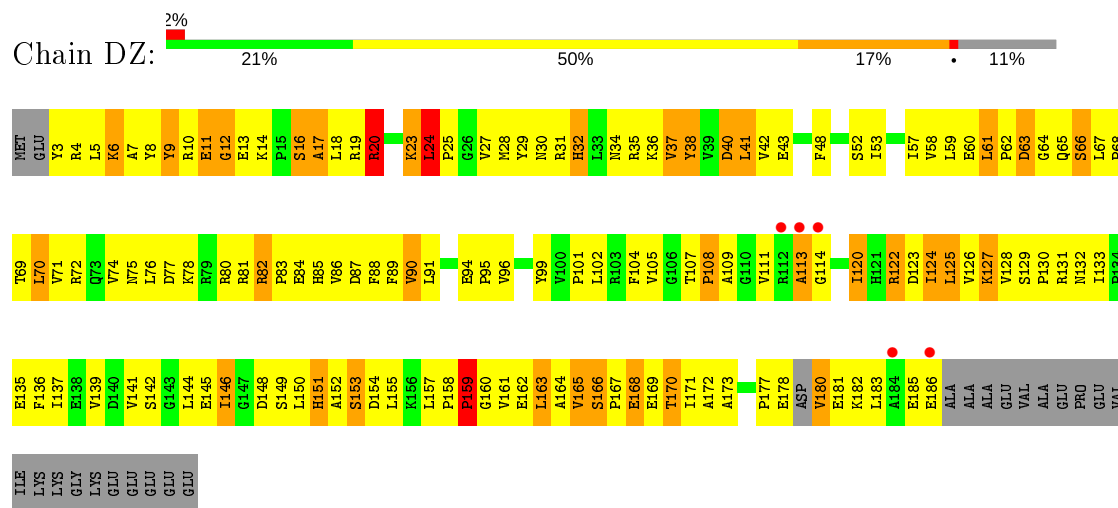
● Molecule 56: 50S RIBOSOMAL PROTEIN L23



● Molecule 57: 50S RIBOSOMAL PROTEIN L24



● Molecule 57: 50S RIBOSOMAL PROTEIN L24





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	289.90Å 269.40Å 404.50Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-3.10) 91.8 (49.22-2.80)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.238 , 0.275 0.238 , 0.275	Depositor DCC
$R_{free}$ test set	69565 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 74.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	307194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, GDP, ZN, H2U, KIR, MIA, 4SU, 7MG, 5MU, PSU

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

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

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	1	90
1	CA	2	54
5	AE	0	1
22	AV	0	1
22	CV	0	2
22	CW	0	2
23	AX	0	2
23	CX	0	6
24	CY	0	1
25	AZ	0	2
25	CZ	0	2
36	BA	2	87
36	DA	0	79
37	BB	0	4
37	DB	0	3
39	BD	0	1
46	BN	0	1
All	All	5	338

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

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

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

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

All (5) chirality outliers are listed below:

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

5 of 338 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	108	G	Sidechain
1	AA	123	C	Sidechain
1	AA	13	U	Sidechain
1	AA	189(G)	G	Sidechain
1	AA	20	U	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1034	0
1	CA	32329	0	16318	1280	0
2	AB	1900	0	1951	204	0
2	CB	1900	0	1951	237	0
3	AC	1612	0	1677	145	0
3	CC	1612	0	1677	183	0
4	AD	1703	0	1763	229	0
4	CD	1703	0	1763	265	0
5	AE	1146	0	1207	75	0
5	CE	1146	0	1207	108	0
6	AF	843	0	857	71	0
6	CF	843	0	857	94	0
7	AG	1257	0	1296	88	0
7	CG	1257	0	1296	87	0
8	AH	1116	0	1177	64	0
8	CH	1116	0	1177	92	0
9	AI	1010	0	1037	111	0
9	CI	1010	0	1037	117	0
10	AJ	794	0	840	126	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	D4	340	0	335	55	0
31	B5	459	0	480	82	0
31	D5	459	0	480	86	0
32	B6	433	0	461	143	0
32	D6	433	0	461	147	0
33	B7	418	0	467	35	0
33	D7	418	0	467	40	0
34	B8	507	0	576	118	0
34	D8	507	0	576	134	0
35	B9	307	0	335	35	0
35	D9	307	0	336	49	0
36	BA	62477	0	31497	2270	0
36	DA	62477	0	31497	2492	0
37	BB	2551	0	1295	108	0
37	DB	2551	0	1295	108	0
38	BC	1742	0	1800	152	0
38	DC	1742	0	1800	181	0
39	BD	2145	0	2234	297	0
39	DD	2145	0	2234	321	0
40	BE	1563	0	1629	227	0
40	DE	1563	0	1629	256	0
41	BF	1623	0	1677	197	0
41	DF	1623	0	1677	209	0
42	BG	1474	0	1535	241	0
42	DG	1474	0	1535	275	0
43	BH	1222	0	1282	171	0
43	DH	1222	0	1282	159	0
44	BJ	651	0	170	19	0
44	DJ	651	0	162	25	0
45	BK	700	0	175	15	0
45	DK	700	0	171	13	0
46	BN	1104	0	1180	160	0
46	DN	1104	0	1180	159	0
47	BO	933	0	996	92	0
47	DO	933	0	996	100	0
48	BP	1114	0	1187	291	0
48	DP	1114	0	1187	301	0
49	BQ	1122	0	1179	141	0
49	DQ	1122	0	1179	138	0
50	BR	960	0	1021	131	0
50	DR	960	0	1021	136	0
51	BS	770	0	832	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	DS	770	0	832	159	0
52	BT	1141	0	1202	234	0
52	DT	1141	0	1202	211	0
53	BU	958	0	1015	141	0
53	DU	958	0	1015	152	0
54	BV	779	0	852	135	0
54	DV	779	0	852	124	0
55	BW	896	0	953	100	0
55	DW	896	0	953	97	0
56	BX	725	0	778	98	0
56	DX	725	0	778	107	0
57	BY	775	0	870	176	0
57	DY	775	0	870	164	0
58	BZ	1459	0	1488	216	0
58	DZ	1459	0	1488	206	0
59	AD	1	0	0	0	0
59	AN	1	0	0	2	0
59	B4	1	0	0	0	0
59	B9	1	0	0	0	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D9	1	0	0	1	0
60	AZ	28	0	12	12	0
60	CZ	28	0	12	13	0
61	AZ	57	0	59	11	0
61	CZ	57	0	59	14	0
All	All	307194	0	208701	19681	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

The worst 5 of 19681 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CZ:69:GLU:CG	25:CZ:69:GLU:CB	1.85	1.54
25:AZ:69:GLU:CB	25:AZ:69:GLU:CG	1.83	1.52
25:CZ:68:VAL:CA	25:CZ:68:VAL:C	1.82	1.46
25:AZ:68:VAL:C	25:AZ:68:VAL:CA	1.85	1.45
25:CZ:198:LYS:HE3	25:CZ:201:GLU:OE1	1.33	1.29

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	232/256 (91%)	168 (72%)	35 (15%)	29 (12%)	0	1
2	CB	232/256 (91%)	154 (66%)	50 (22%)	28 (12%)	0	1
3	AC	204/239 (85%)	161 (79%)	29 (14%)	14 (7%)	1	7
3	CC	204/239 (85%)	147 (72%)	40 (20%)	17 (8%)	1	5
4	AD	206/209 (99%)	139 (68%)	44 (21%)	23 (11%)	0	2
4	CD	206/209 (99%)	128 (62%)	44 (21%)	34 (16%)	0	0
5	AE	148/162 (91%)	138 (93%)	8 (5%)	2 (1%)	11	40
5	CE	148/162 (91%)	122 (82%)	25 (17%)	1 (1%)	22	57
6	AF	99/101 (98%)	78 (79%)	15 (15%)	6 (6%)	1	9
6	CF	99/101 (98%)	75 (76%)	13 (13%)	11 (11%)	0	2
7	AG	153/156 (98%)	121 (79%)	20 (13%)	12 (8%)	1	5
7	CG	153/156 (98%)	121 (79%)	24 (16%)	8 (5%)	2	12
8	AH	136/138 (99%)	124 (91%)	8 (6%)	4 (3%)	4	24
8	CH	136/138 (99%)	117 (86%)	12 (9%)	7 (5%)	2	13
9	AI	125/128 (98%)	85 (68%)	26 (21%)	14 (11%)	0	2
9	CI	125/128 (98%)	79 (63%)	31 (25%)	15 (12%)	0	1
10	AJ	96/105 (91%)	72 (75%)	15 (16%)	9 (9%)	0	3
10	CJ	96/105 (91%)	71 (74%)	16 (17%)	9 (9%)	0	3
11	AK	117/129 (91%)	103 (88%)	13 (11%)	1 (1%)	17	52
11	CK	117/129 (91%)	88 (75%)	23 (20%)	6 (5%)	2	13
12	AL	122/132 (92%)	97 (80%)	15 (12%)	10 (8%)	1	5
12	CL	122/132 (92%)	92 (75%)	22 (18%)	8 (7%)	1	7

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BS	96/112 (86%)	44 (46%)	29 (30%)	23 (24%)	0	0
51	DS	96/112 (86%)	44 (46%)	22 (23%)	30 (31%)	0	0
52	BT	135/146 (92%)	76 (56%)	28 (21%)	31 (23%)	0	0
52	DT	135/146 (92%)	71 (53%)	35 (26%)	29 (22%)	0	0
53	BU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	5
53	DU	115/118 (98%)	74 (64%)	34 (30%)	7 (6%)	1	9
54	BV	99/101 (98%)	65 (66%)	21 (21%)	13 (13%)	0	1
54	DV	99/101 (98%)	67 (68%)	19 (19%)	13 (13%)	0	1
55	BW	111/113 (98%)	78 (70%)	17 (15%)	16 (14%)	0	1
55	DW	111/113 (98%)	72 (65%)	23 (21%)	16 (14%)	0	1
56	BX	90/96 (94%)	63 (70%)	15 (17%)	12 (13%)	0	1
56	DX	90/96 (94%)	58 (64%)	22 (24%)	10 (11%)	0	2
57	BY	98/110 (89%)	43 (44%)	28 (29%)	27 (28%)	0	0
57	DY	98/110 (89%)	43 (44%)	26 (26%)	29 (30%)	0	0
58	BZ	181/206 (88%)	117 (65%)	38 (21%)	26 (14%)	0	1
58	DZ	181/206 (88%)	114 (63%)	42 (23%)	25 (14%)	0	1
All	All	12270/13100 (94%)	8441 (69%)	2326 (19%)	1503 (12%)	0	1

5 of 1503 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	178 (88%)	24 (12%)	5	20
2	CB	202/220 (92%)	177 (88%)	25 (12%)	4	19
3	AC	160/188 (85%)	142 (89%)	18 (11%)	6	23
3	CC	160/188 (85%)	144 (90%)	16 (10%)	7	28
4	AD	180/181 (99%)	151 (84%)	29 (16%)	2	10
4	CD	180/181 (99%)	153 (85%)	27 (15%)	3	12
5	AE	115/123 (94%)	106 (92%)	9 (8%)	12	40
5	CE	115/123 (94%)	105 (91%)	10 (9%)	10	36
6	AF	90/90 (100%)	79 (88%)	11 (12%)	5	19
6	CF	90/90 (100%)	77 (86%)	13 (14%)	3	14
7	AG	126/127 (99%)	113 (90%)	13 (10%)	7	27
7	CG	126/127 (99%)	116 (92%)	10 (8%)	12	40
8	AH	119/119 (100%)	108 (91%)	11 (9%)	9	33
8	CH	119/119 (100%)	112 (94%)	7 (6%)	19	50
9	AI	98/99 (99%)	89 (91%)	9 (9%)	9	33
9	CI	98/99 (99%)	88 (90%)	10 (10%)	7	27
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	4	18
10	CJ	88/92 (96%)	74 (84%)	14 (16%)	2	11
11	AK	90/99 (91%)	77 (86%)	13 (14%)	3	14
11	CK	90/99 (91%)	77 (86%)	13 (14%)	3	14
12	AL	104/109 (95%)	91 (88%)	13 (12%)	4	18
12	CL	104/109 (95%)	93 (89%)	11 (11%)	6	26
13	AM	99/101 (98%)	85 (86%)	14 (14%)	3	15
13	CM	99/101 (98%)	85 (86%)	14 (14%)	3	15
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3	14
14	CN	49/50 (98%)	43 (88%)	6 (12%)	5	19
15	AO	79/80 (99%)	69 (87%)	10 (13%)	4	18
15	CO	79/80 (99%)	69 (87%)	10 (13%)	4	18
16	AP	72/74 (97%)	68 (94%)	4 (6%)	21	52
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	30
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13	42
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	53	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	61/77 (79%)	54 (88%)	7 (12%)	5	22
18	CR	61/77 (79%)	54 (88%)	7 (12%)	5	22
19	AS	69/80 (86%)	58 (84%)	11 (16%)	2	11
19	CS	69/80 (86%)	54 (78%)	15 (22%)	1	4
20	AT	76/82 (93%)	66 (87%)	10 (13%)	4	17
20	CT	76/82 (93%)	67 (88%)	9 (12%)	5	21
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	26
21	CU	19/22 (86%)	16 (84%)	3 (16%)	2	11
25	AZ	322/338 (95%)	282 (88%)	40 (12%)	4	19
25	CZ	322/338 (95%)	281 (87%)	41 (13%)	4	18
26	B0	66/67 (98%)	53 (80%)	13 (20%)	1	6
26	D0	66/67 (98%)	55 (83%)	11 (17%)	2	9
27	B1	78/83 (94%)	68 (87%)	10 (13%)	4	18
27	D1	78/83 (94%)	70 (90%)	8 (10%)	7	27
28	B2	66/67 (98%)	55 (83%)	11 (17%)	2	9
28	D2	66/67 (98%)	60 (91%)	6 (9%)	9	33
29	B3	51/52 (98%)	44 (86%)	7 (14%)	3	16
29	D3	51/52 (98%)	45 (88%)	6 (12%)	5	21
30	B4	39/63 (62%)	28 (72%)	11 (28%)	0	1
30	D4	39/63 (62%)	29 (74%)	10 (26%)	0	1
31	B5	51/52 (98%)	44 (86%)	7 (14%)	3	16
31	D5	51/52 (98%)	45 (88%)	6 (12%)	5	21
32	B6	49/52 (94%)	32 (65%)	17 (35%)	0	0
32	D6	49/52 (94%)	36 (74%)	13 (26%)	0	1
33	B7	41/42 (98%)	37 (90%)	4 (10%)	8	29
33	D7	41/42 (98%)	35 (85%)	6 (15%)	3	13
34	B8	53/55 (96%)	43 (81%)	10 (19%)	1	6
34	D8	53/55 (96%)	43 (81%)	10 (19%)	1	6
35	B9	34/34 (100%)	28 (82%)	6 (18%)	2	8
35	D9	34/34 (100%)	29 (85%)	5 (15%)	3	13
38	BC	180/181 (99%)	168 (93%)	12 (7%)	16	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DC	180/181 (99%)	165 (92%)	15 (8%)	11	38
39	BD	217/218 (100%)	176 (81%)	41 (19%)	1	6
39	DD	217/218 (100%)	185 (85%)	32 (15%)	3	13
40	BE	165/166 (99%)	137 (83%)	28 (17%)	2	9
40	DE	165/166 (99%)	137 (83%)	28 (17%)	2	9
41	BF	165/166 (99%)	147 (89%)	18 (11%)	6	25
41	DF	165/166 (99%)	152 (92%)	13 (8%)	12	40
42	BG	155/156 (99%)	130 (84%)	25 (16%)	2	10
42	DG	155/156 (99%)	127 (82%)	28 (18%)	1	7
43	BH	132/148 (89%)	122 (92%)	10 (8%)	13	41
43	DH	132/148 (89%)	123 (93%)	9 (7%)	16	45
46	BN	117/119 (98%)	102 (87%)	15 (13%)	4	18
46	DN	117/119 (98%)	99 (85%)	18 (15%)	2	11
47	BO	100/100 (100%)	92 (92%)	8 (8%)	12	40
47	DO	100/100 (100%)	90 (90%)	10 (10%)	7	28
48	BP	112/116 (97%)	89 (80%)	23 (20%)	1	5
48	DP	112/116 (97%)	92 (82%)	20 (18%)	2	8
49	BQ	111/111 (100%)	94 (85%)	17 (15%)	2	12
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	4	18
50	BR	100/101 (99%)	88 (88%)	12 (12%)	5	20
50	DR	100/101 (99%)	89 (89%)	11 (11%)	6	25
51	BS	77/88 (88%)	65 (84%)	12 (16%)	2	11
51	DS	77/88 (88%)	61 (79%)	16 (21%)	1	5
52	BT	120/127 (94%)	101 (84%)	19 (16%)	2	11
52	DT	120/127 (94%)	102 (85%)	18 (15%)	3	12
53	BU	92/94 (98%)	84 (91%)	8 (9%)	10	36
53	DU	92/94 (98%)	85 (92%)	7 (8%)	13	41
54	BV	82/82 (100%)	69 (84%)	13 (16%)	2	11
54	DV	82/82 (100%)	66 (80%)	16 (20%)	1	6
55	BW	91/92 (99%)	85 (93%)	6 (7%)	16	47
55	DW	91/92 (99%)	85 (93%)	6 (7%)	16	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	BX	74/78 (95%)	65 (88%)	9 (12%)	5	19
56	DX	74/78 (95%)	68 (92%)	6 (8%)	11	39
57	BY	84/91 (92%)	72 (86%)	12 (14%)	3	14
57	DY	84/91 (92%)	73 (87%)	11 (13%)	4	17
58	BZ	161/179 (90%)	134 (83%)	27 (17%)	2	9
58	DZ	161/179 (90%)	138 (86%)	23 (14%)	3	14
All	All	10350/10856 (95%)	9014 (87%)	1336 (13%)	4	18

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

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

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

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

### 5.3.3 RNA ⓘ

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

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

5 of 1679 RNA backbone outliers are listed below:

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

5 of 198 RNA pucker outliers are listed below:

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	MIA	AY	37	24	24,31,32	1.31	2 (8%)	26,44,47	1.83	4 (15%)
24	H2U	AY	16	24	18,21,22	0.80	0	21,30,33	1.75	4 (19%)
24	H2U	CY	20	24	18,21,22	0.84	0	21,30,33	1.98	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	4SU	CY	8	24	14,21,22	1.98	3 (21%)	15,30,33	2.64	2 (13%)
24	PSU	AY	55	24	17,21,22	1.19	2 (11%)	20,30,33	3.24	6 (30%)
24	H2U	AY	20	24	18,21,22	0.86	1 (5%)	21,30,33	1.92	5 (23%)
24	MIA	CY	37	24	24,31,32	1.47	3 (12%)	26,44,47	1.50	4 (15%)
24	OMC	CY	32	24	15,22,23	0.92	0	17,31,34	1.04	1 (5%)
24	5MU	CY	54	24	15,22,23	1.19	2 (13%)	16,32,35	3.72	1 (6%)
24	7MG	AY	46	24	22,26,27	1.27	2 (9%)	28,39,42	2.27	5 (17%)
24	7MG	CY	46	24	22,26,27	1.19	2 (9%)	28,39,42	2.28	5 (17%)
24	5MU	AY	54	24	15,22,23	1.14	2 (13%)	16,32,35	3.73	2 (12%)
24	4SU	AY	8	24	14,21,22	1.94	3 (21%)	15,30,33	2.64	3 (20%)
24	H2U	CY	16	24	18,21,22	0.89	0	21,30,33	1.77	4 (19%)
24	OMC	AY	32	24	15,22,23	0.92	0	17,31,34	1.02	1 (5%)
24	PSU	CY	55	24	17,21,22	1.23	2 (11%)	20,30,33	3.37	6 (30%)
24	H2U	AY	17	24	18,21,22	0.78	0	21,30,33	1.78	5 (23%)
24	H2U	CY	17	24	18,21,22	0.87	0	21,30,33	1.85	5 (23%)

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	MIA	AY	37	24	-	1/11/33/34	0/3/3/3
24	H2U	AY	16	24	-	2/7/38/39	0/2/2/2
24	H2U	CY	20	24	-	5/7/38/39	0/2/2/2
24	4SU	CY	8	24	-	1/5/25/26	0/2/2/2
24	PSU	AY	55	24	-	1/7/25/26	0/2/2/2
24	H2U	AY	20	24	-	5/7/38/39	0/2/2/2
24	MIA	CY	37	24	-	1/11/33/34	0/3/3/3
24	OMC	CY	32	24	-	0/7/27/28	0/2/2/2
24	5MU	CY	54	24	-	1/5/25/26	0/2/2/2
24	7MG	AY	46	24	-	5/7/37/38	0/3/3/3
24	7MG	CY	46	24	-	5/7/37/38	0/3/3/3
24	5MU	AY	54	24	-	1/5/25/26	0/2/2/2
24	4SU	AY	8	24	-	1/5/25/26	0/2/2/2
24	H2U	CY	16	24	-	2/7/38/39	0/2/2/2
24	OMC	AY	32	24	-	0/7/27/28	0/2/2/2
24	PSU	CY	55	24	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	H2U	AY	17	24	-	5/7/38/39	0/2/2/2
24	H2U	CY	17	24	-	5/7/38/39	0/2/2/2

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	37	MIA	C2-S10	5.33	1.80	1.75
24	CY	8	4SU	C5-C4	5.16	1.44	1.38
24	AY	8	4SU	C5-C4	4.91	1.44	1.38
24	AY	37	MIA	C2-S10	4.54	1.79	1.75
24	AY	46	7MG	C6-N1	3.94	1.39	1.33

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	54	5MU	C4-N3-C2	14.56	127.44	115.14
24	CY	54	5MU	C4-N3-C2	14.55	127.43	115.14
24	CY	55	PSU	N1-C2-N3	-10.53	120.06	128.43
24	AY	55	PSU	N1-C2-N3	-10.13	120.38	128.43
24	AY	8	4SU	C2-N3-C4	7.34	125.79	115.15

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	37	MIA	N6-C12-C13-C14
24	AY	55	PSU	C4'-C5'-O5'-P
24	AY	20	H2U	O4'-C1'-N1-C6
24	CY	37	MIA	N6-C12-C13-C14
24	CY	55	PSU	C4'-C5'-O5'-P

There are no ring outliers.

14 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	16	H2U	1	0
24	CY	20	H2U	3	0
24	CY	8	4SU	3	0
24	AY	55	PSU	2	0
24	AY	20	H2U	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CY	32	OMC	1	0
24	CY	54	5MU	3	0
24	AY	46	7MG	1	0
24	CY	46	7MG	1	0
24	AY	54	5MU	3	0
24	AY	8	4SU	3	0
24	CY	16	H2U	1	0
24	AY	32	OMC	1	0
24	CY	55	PSU	2	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	-	24,30,30	1.30	3 (12%)	31,47,47	2.12	10 (32%)
61	KIR	AZ	502	-	56,59,59	3.56	22 (39%)	62,84,84	1.67	13 (20%)
60	GDP	CZ	501	-	24,30,30	1.29	2 (8%)	31,47,47	2.12	10 (32%)
61	KIR	CZ	502	-	56,59,59	3.66	24 (42%)	62,84,84	1.66	12 (19%)

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	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	KIR	AZ	502	-	-	8/54/98/98	0/3/3/3
60	GDP	CZ	501	-	-	1/12/32/32	0/3/3/3
61	KIR	CZ	502	-	-	8/54/98/98	0/3/3/3

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	502	KIR	O18-C17	-14.95	1.22	1.44
61	CZ	502	KIR	O18-C17	-14.23	1.23	1.44
61	CZ	502	KIR	O30-C30	-12.29	1.18	1.42
61	AZ	502	KIR	O30-C30	-12.09	1.18	1.42
61	CZ	502	KIR	C32-C31	6.53	1.63	1.54

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CZ	501	GDP	C2-N3-C4	5.36	121.48	115.36
60	CZ	501	GDP	N3-C2-N1	-5.09	120.44	127.22
60	AZ	501	GDP	C2-N3-C4	5.07	121.14	115.36
60	AZ	501	GDP	N3-C2-N1	-4.91	120.67	127.22
60	AZ	501	GDP	PA-O3A-PB	-4.73	116.58	132.83

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

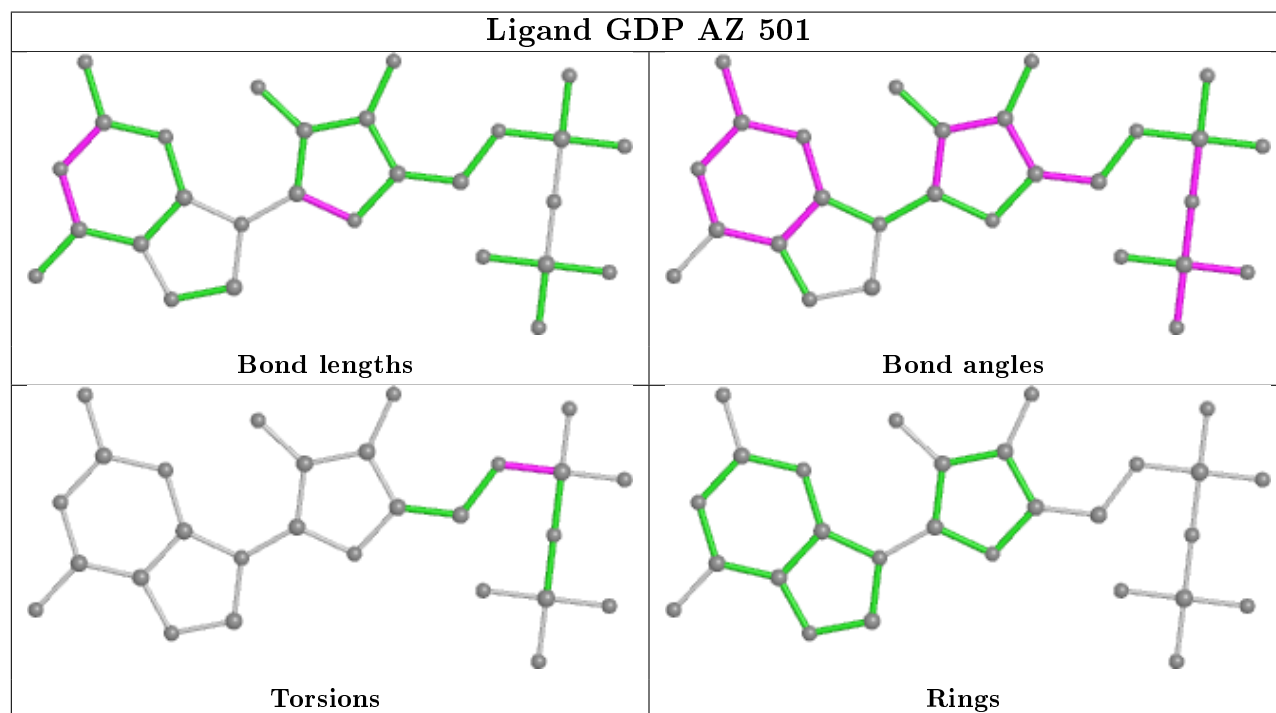
Mol	Chain	Res	Type	Atoms
60	AZ	501	GDP	C5'-O5'-PA-O1A
61	CZ	502	KIR	O18-C17-C19-C42
61	AZ	502	KIR	O18-C17-C19-C42
60	CZ	501	GDP	C5'-O5'-PA-O1A
61	AZ	502	KIR	C11-C10-C9-C8

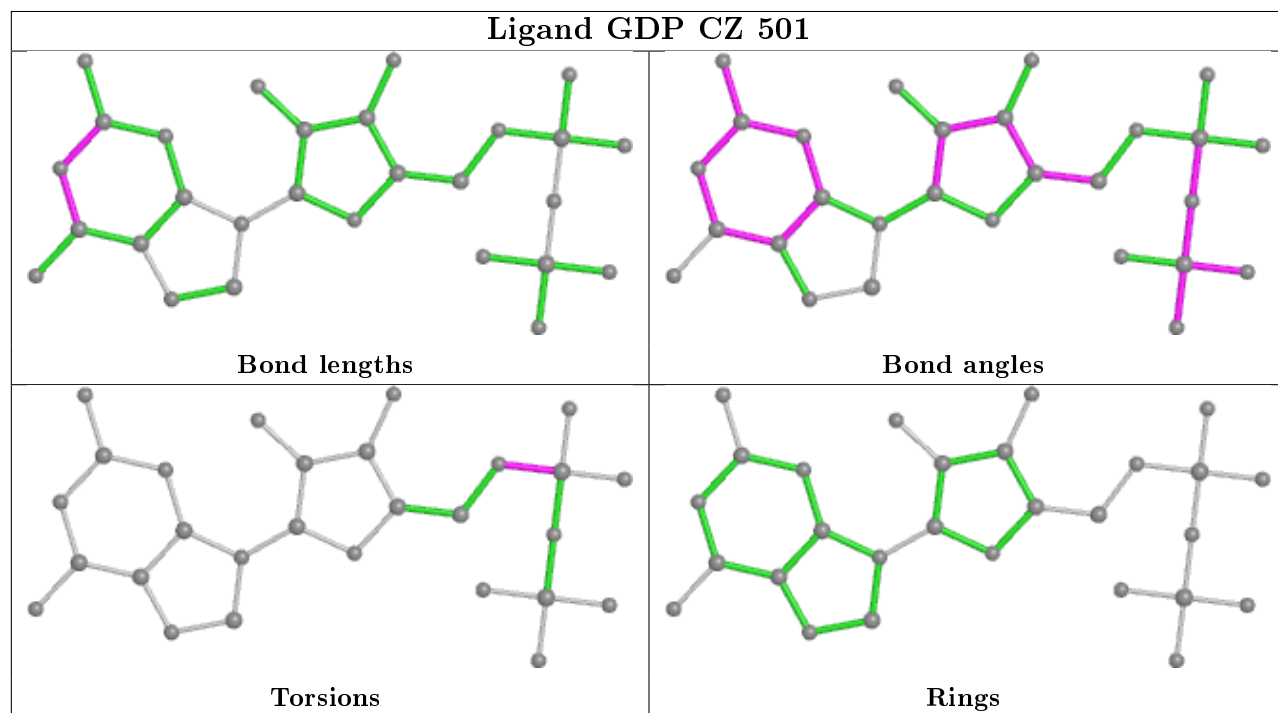
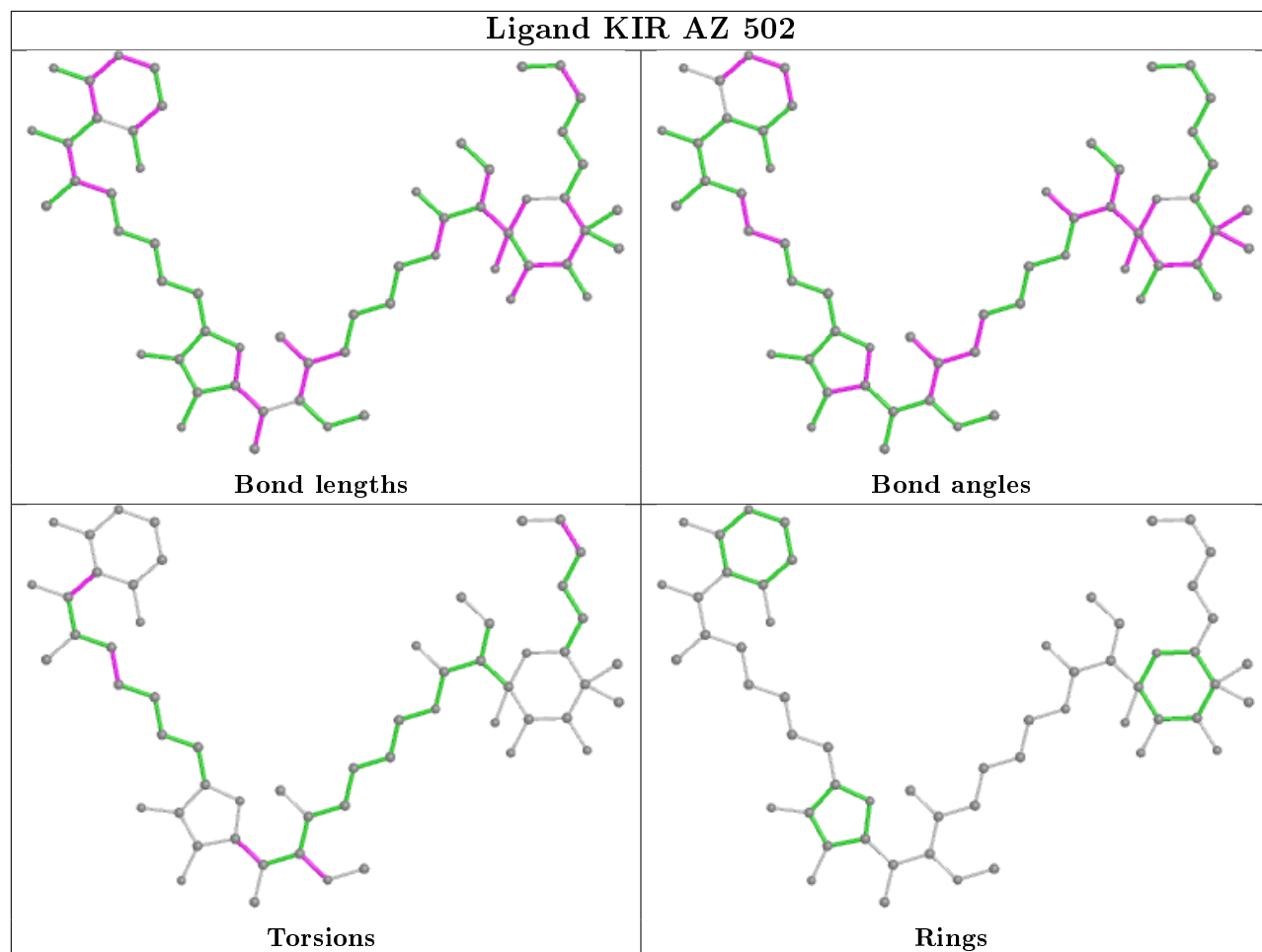
There are no ring outliers.

4 monomers are involved in 50 short contacts:

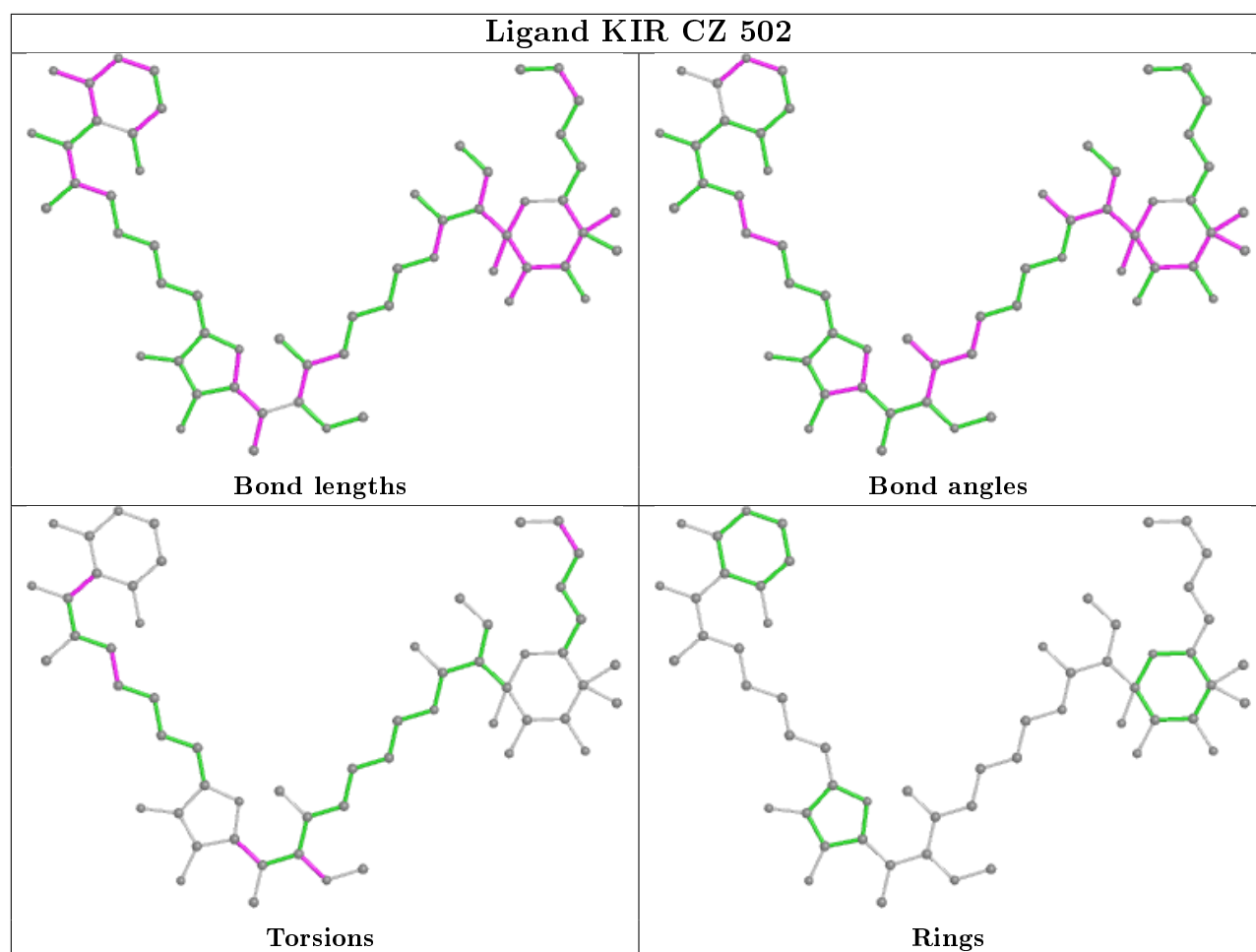
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	AZ	501	GDP	12	0
61	AZ	502	KIR	11	0
60	CZ	501	GDP	13	0
61	CZ	502	KIR	14	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1504/1522 (98%)	-0.27	28 (1%) 66 46	22, 58, 151, 200	0
1	CA	1504/1522 (98%)	-0.24	23 (1%) 73 54	39, 79, 157, 200	0
2	AB	234/256 (91%)	-0.32	3 (1%) 77 59	33, 66, 135, 154	0
2	CB	234/256 (91%)	-0.27	3 (1%) 77 59	50, 89, 142, 150	0
3	AC	206/239 (86%)	-0.59	0 100 100	25, 49, 78, 88	0
3	CC	206/239 (86%)	-0.44	1 (0%) 91 81	53, 80, 106, 113	0
4	AD	208/209 (99%)	0.07	8 (3%) 40 20	59, 88, 122, 126	0
4	CD	208/209 (99%)	0.15	9 (4%) 35 17	79, 105, 125, 135	0
5	AE	150/162 (92%)	-0.62	0 100 100	30, 45, 71, 97	0
5	CE	150/162 (92%)	-0.47	0 100 100	48, 63, 85, 102	0
6	AF	101/101 (100%)	-0.50	1 (0%) 82 67	48, 74, 94, 105	0
6	CF	101/101 (100%)	-0.14	1 (0%) 82 67	79, 98, 111, 119	0
7	AG	155/156 (99%)	-0.37	5 (3%) 47 25	39, 65, 96, 117	0
7	CG	155/156 (99%)	-0.08	5 (3%) 47 25	71, 95, 115, 127	0
8	AH	138/138 (100%)	-0.55	0 100 100	32, 49, 69, 74	0
8	CH	138/138 (100%)	-0.44	0 100 100	46, 64, 80, 87	0
9	AI	127/128 (99%)	-0.20	1 (0%) 86 72	32, 68, 111, 124	0
9	CI	127/128 (99%)	0.41	10 (7%) 12 5	66, 106, 132, 139	0
10	AJ	98/105 (93%)	-0.10	0 100 100	33, 70, 112, 125	0
10	CJ	98/105 (93%)	0.43	9 (9%) 9 3	66, 109, 144, 148	0
11	AK	119/129 (92%)	-0.43	2 (1%) 70 49	32, 50, 92, 118	0
11	CK	119/129 (92%)	-0.23	3 (2%) 57 34	52, 76, 100, 120	0
12	AL	124/132 (93%)	-0.28	1 (0%) 86 72	33, 61, 85, 124	0
12	CL	124/132 (93%)	-0.17	2 (1%) 72 51	47, 72, 99, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	124/126 (98%)	-0.09	5 (4%) 38 19	43, 72, 103, 131	0
13	CM	124/126 (98%)	0.04	7 (5%) 24 11	76, 99, 122, 142	0
14	AN	60/61 (98%)	-0.29	1 (1%) 70 49	30, 53, 78, 84	0
14	CN	60/61 (98%)	0.05	2 (3%) 46 24	65, 83, 102, 105	0
15	AO	88/89 (98%)	-0.51	0 100 100	36, 54, 82, 88	0
15	CO	88/89 (98%)	-0.31	0 100 100	44, 68, 90, 98	0
16	AP	83/88 (94%)	-0.02	2 (2%) 59 37	61, 74, 98, 133	0
16	CP	83/88 (94%)	0.16	1 (1%) 79 61	74, 90, 110, 132	0
17	AQ	99/105 (94%)	-0.37	0 100 100	40, 60, 79, 89	0
17	CQ	99/105 (94%)	-0.22	0 100 100	53, 71, 91, 102	0
18	AR	70/88 (79%)	-0.43	0 100 100	39, 60, 90, 99	0
18	CR	70/88 (79%)	-0.26	0 100 100	56, 81, 108, 118	0
19	AS	78/93 (83%)	-0.05	2 (2%) 56 33	52, 73, 117, 127	0
19	CS	78/93 (83%)	0.14	5 (6%) 19 8	81, 97, 126, 132	0
20	AT	99/106 (93%)	0.13	4 (4%) 38 19	55, 80, 126, 130	0
20	CT	99/106 (93%)	0.09	1 (1%) 82 67	74, 90, 120, 122	0
21	AU	24/27 (88%)	-0.02	2 (8%) 11 4	41, 55, 79, 99	0
21	CU	24/27 (88%)	0.60	2 (8%) 11 4	74, 92, 105, 113	0
22	AV	76/76 (100%)	-0.46	0 100 100	35, 72, 107, 124	0
22	AW	76/76 (100%)	0.37	8 (10%) 6 2	64, 140, 185, 199	0
22	CV	76/76 (100%)	-0.29	0 100 100	51, 86, 120, 137	0
22	CW	76/76 (100%)	0.42	6 (7%) 12 5	94, 170, 191, 200	0
23	AX	17/27 (62%)	0.45	2 (11%) 4 2	31, 91, 142, 143	0
23	CX	17/27 (62%)	2.24	12 (70%) 0 0	69, 122, 155, 157	0
24	AY	68/77 (88%)	0.24	1 (1%) 73 54	57, 140, 177, 197	0
24	CY	68/77 (88%)	0.36	1 (1%) 73 54	73, 142, 175, 198	0
25	AZ	385/405 (95%)	0.63	29 (7%) 14 5	87, 124, 151, 169	0
25	CZ	385/405 (95%)	1.37	104 (27%) 0 0	111, 133, 156, 170	0
26	B0	84/85 (98%)	0.15	6 (7%) 16 6	58, 73, 107, 122	0
26	D0	84/85 (98%)	0.48	9 (10%) 6 2	69, 86, 113, 123	0
27	B1	93/98 (94%)	0.02	4 (4%) 35 17	45, 69, 129, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	D1	93/98 (94%)	0.15	1 (1%) 80 64	59, 86, 133, 139	0
28	B2	71/72 (98%)	1.37	20 (28%) 0 0	130, 143, 155, 158	0
28	D2	71/72 (98%)	0.49	11 (15%) 2 1	100, 122, 136, 143	0
29	B3	59/60 (98%)	0.20	2 (3%) 45 24	65, 81, 106, 122	0
29	D3	59/60 (98%)	0.30	3 (5%) 28 13	60, 93, 106, 126	0
30	B4	44/71 (61%)	0.67	5 (11%) 5 2	111, 140, 167, 173	0
30	D4	44/71 (61%)	1.16	13 (29%) 0 0	136, 163, 184, 186	0
31	B5	59/60 (98%)	0.15	3 (5%) 28 13	62, 87, 148, 163	0
31	D5	59/60 (98%)	0.24	4 (6%) 17 7	63, 92, 145, 154	0
32	B6	50/54 (92%)	0.50	4 (8%) 12 5	57, 84, 103, 110	0
32	D6	50/54 (92%)	0.93	9 (18%) 1 0	73, 97, 116, 122	0
33	B7	48/49 (97%)	0.14	3 (6%) 20 8	51, 64, 101, 121	0
33	D7	48/49 (97%)	0.08	3 (6%) 20 8	64, 73, 104, 125	0
34	B8	63/65 (96%)	0.23	2 (3%) 47 25	56, 73, 91, 115	0
34	D8	63/65 (96%)	0.39	5 (7%) 12 5	72, 85, 101, 120	0
35	B9	37/37 (100%)	0.57	4 (10%) 5 2	73, 85, 103, 104	0
35	D9	37/37 (100%)	1.12	4 (10%) 5 2	67, 96, 107, 120	0
36	BA	2901/2915 (99%)	-0.15	76 (2%) 56 33	26, 77, 181, 200	0
36	DA	2901/2915 (99%)	-0.10	77 (2%) 54 31	37, 87, 180, 200	0
37	BB	119/122 (97%)	-0.48	0 100 100	59, 85, 112, 132	0
37	DB	119/122 (97%)	-0.44	0 100 100	69, 101, 126, 132	0
38	BC	228/229 (99%)	0.01	12 (5%) 26 12	50, 79, 160, 173	0
38	DC	228/229 (99%)	0.47	26 (11%) 5 2	68, 103, 170, 180	0
39	BD	275/276 (99%)	-0.41	4 (1%) 73 54	30, 49, 83, 105	0
39	DD	275/276 (99%)	-0.32	2 (0%) 87 75	42, 61, 91, 111	0
40	BE	204/206 (99%)	-0.02	5 (2%) 57 34	50, 79, 128, 140	0
40	DE	204/206 (99%)	0.00	6 (2%) 51 28	47, 84, 133, 138	0
41	BF	207/210 (98%)	0.32	14 (6%) 17 7	53, 112, 162, 170	0
41	DF	207/210 (98%)	0.43	17 (8%) 11 4	62, 118, 161, 170	0
42	BG	181/182 (99%)	-0.04	9 (4%) 28 13	63, 86, 117, 130	0
42	DG	181/182 (99%)	0.05	8 (4%) 34 17	89, 108, 136, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
43	BH	159/180 (88%)	0.74	22 (13%)	2 1	93, 134, 152, 156	0
43	DH	159/180 (88%)	0.53	11 (6%)	16 7	87, 129, 146, 154	0
44	BJ	0/173	-	-	-	-	-
44	DJ	0/173	-	-	-	-	-
45	BK	0/147	-	-	-	-	-
45	DK	0/147	-	-	-	-	-
46	BN	138/140 (98%)	-0.08	0	100 100	63, 89, 125, 134	0
46	DN	138/140 (98%)	-0.18	0	100 100	69, 90, 125, 133	0
47	BO	122/122 (100%)	-0.44	0	100 100	46, 63, 77, 85	0
47	DO	122/122 (100%)	-0.38	0	100 100	47, 67, 83, 89	0
48	BP	146/150 (97%)	0.52	13 (8%)	9 3	55, 103, 133, 150	0
48	DP	146/150 (97%)	0.72	21 (14%)	2 1	64, 115, 137, 153	0
49	BQ	141/141 (100%)	-0.22	3 (2%)	63 43	46, 64, 86, 128	0
49	DQ	141/141 (100%)	-0.22	2 (1%)	75 56	51, 66, 90, 126	0
50	BR	117/118 (99%)	0.06	2 (1%)	70 49	60, 85, 107, 126	0
50	DR	117/118 (99%)	0.06	1 (0%)	84 69	57, 90, 105, 123	0
51	BS	98/112 (87%)	0.13	3 (3%)	49 26	63, 90, 116, 126	0
51	DS	98/112 (87%)	0.44	8 (8%)	11 4	77, 102, 126, 128	0
52	BT	137/146 (93%)	-0.02	8 (5%)	23 10	58, 84, 142, 167	0
52	DT	137/146 (93%)	-0.03	6 (4%)	34 17	63, 90, 147, 169	0
53	BU	117/118 (99%)	-0.05	1 (0%)	84 69	64, 79, 111, 128	0
53	DU	117/118 (99%)	-0.03	1 (0%)	84 69	63, 86, 110, 124	0
54	BV	101/101 (100%)	0.28	3 (2%)	50 27	62, 116, 129, 136	0
54	DV	101/101 (100%)	0.38	5 (4%)	28 13	71, 115, 134, 136	0
55	BW	113/113 (100%)	0.10	5 (4%)	34 17	65, 90, 116, 141	0
55	DW	113/113 (100%)	0.31	5 (4%)	34 17	73, 93, 123, 145	0
56	BX	92/96 (95%)	0.22	1 (1%)	80 64	75, 95, 110, 118	0
56	DX	92/96 (95%)	0.20	1 (1%)	80 64	82, 100, 116, 120	0
57	BY	100/110 (90%)	1.25	26 (26%)	0 0	108, 134, 162, 168	0
57	DY	100/110 (90%)	1.13	20 (20%)	1 0	107, 136, 160, 169	0
58	BZ	183/206 (88%)	-0.13	4 (2%)	62 41	56, 83, 120, 132	0
58	DZ	183/206 (88%)	-0.05	5 (2%)	54 31	62, 88, 120, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	21996/23370 (94%)	-0.02	860 (3%) 39 20	22, 84, 151, 200	0

The worst 5 of 860 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	CZ	183	HIS	12.4
41	BF	24	LEU	11.5
25	AZ	85	HIS	10.9
49	BQ	141	GLN	10.5
36	BA	1077	A	9.4

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	H2U	CY	16	20/21	0.60	0.45	194,198,199,199	0
24	H2U	AY	16	20/21	0.61	0.47	196,198,199,200	0
24	H2U	CY	17	20/21	0.62	0.57	199,199,200,200	0
24	H2U	AY	17	20/21	0.68	0.36	199,199,200,200	0
24	PSU	CY	55	20/21	0.69	0.29	158,161,162,162	0
24	PSU	AY	55	20/21	0.77	0.25	156,161,162,162	0
24	4SU	AY	8	20/21	0.77	0.21	142,144,146,146	0
24	H2U	CY	20	20/21	0.79	0.38	188,191,192,192	0
24	5MU	AY	54	21/22	0.81	0.20	139,150,152,154	0
24	4SU	CY	8	20/21	0.81	0.27	143,145,147,148	0
24	H2U	AY	20	20/21	0.83	0.43	186,189,193,193	0
24	5MU	CY	54	21/22	0.84	0.26	139,149,151,155	0
24	7MG	AY	46	24/25	0.84	0.27	145,150,151,151	0
24	7MG	CY	46	24/25	0.85	0.30	148,153,154,154	0
24	OMC	CY	32	21/22	0.87	0.29	108,114,121,121	0
24	OMC	AY	32	21/22	0.89	0.20	101,105,115,115	0
24	MIA	AY	37	29/30	0.91	0.25	64,78,89,98	0
24	MIA	CY	37	29/30	0.92	0.23	80,87,95,99	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

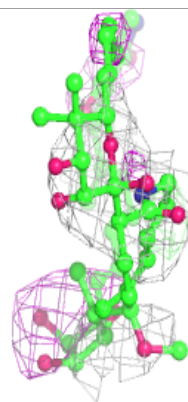
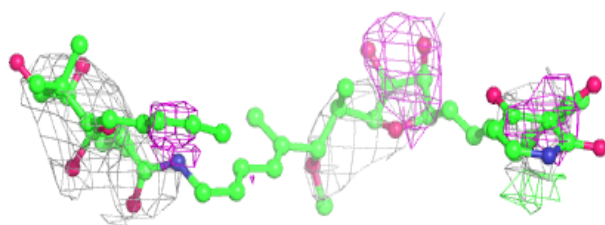
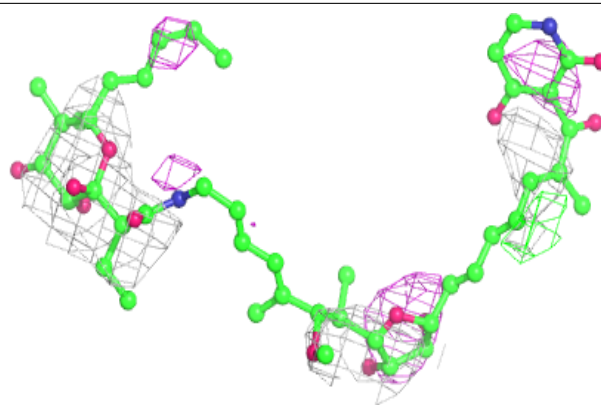
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
61	KIR	CZ	502	57/57	0.67	0.62	122,131,140,141	0
60	GDP	AZ	501	28/28	0.69	0.31	129,133,138,138	0
60	GDP	CZ	501	28/28	0.70	0.26	137,140,141,141	0
61	KIR	AZ	502	57/57	0.81	0.36	115,122,129,130	0
59	ZN	D4	101	1/1	0.85	0.12	196,196,196,196	0
59	ZN	D9	101	1/1	0.90	0.17	141,141,141,141	0
59	ZN	B9	101	1/1	0.92	0.12	113,113,113,113	0
59	ZN	B4	101	1/1	0.95	0.13	112,112,112,112	0
59	ZN	AN	101	1/1	0.98	0.18	48,48,48,48	0
59	ZN	CD	301	1/1	0.99	0.28	79,79,79,79	0
59	ZN	CN	101	1/1	0.99	0.17	77,77,77,77	0
59	ZN	AD	301	1/1	0.99	0.27	74,74,74,74	0

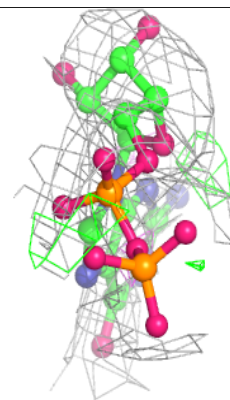
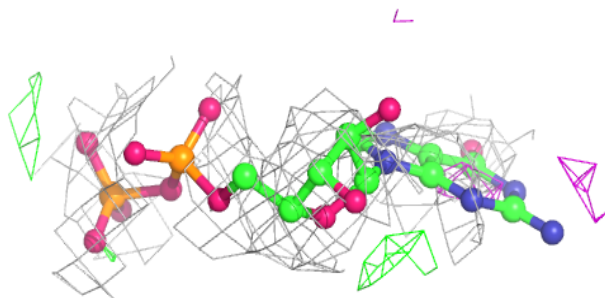
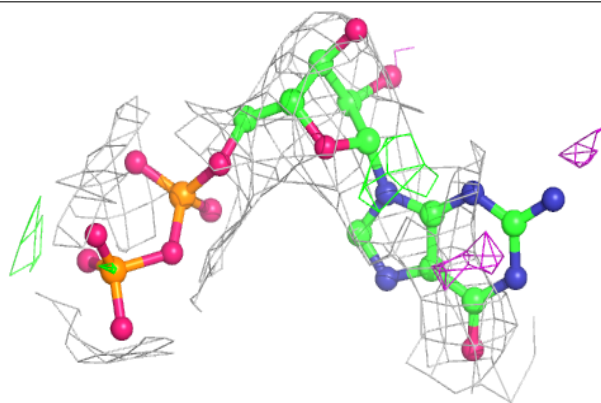
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around KIR CZ 502:**

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

**Electron density around GDP AZ 501:**

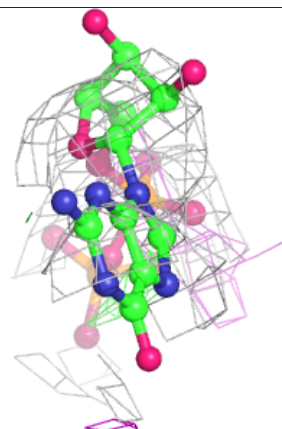
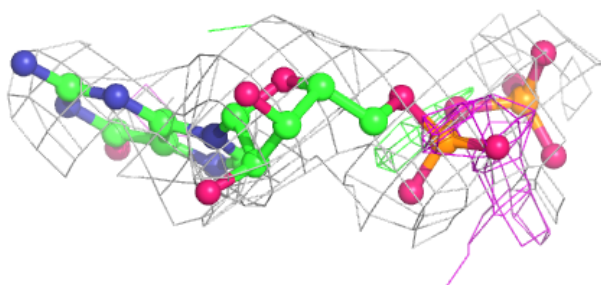
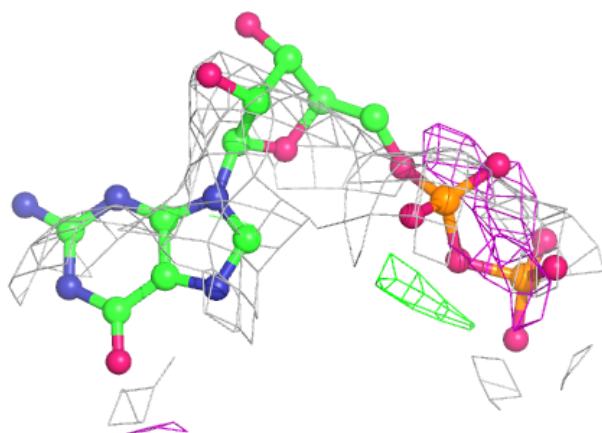
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



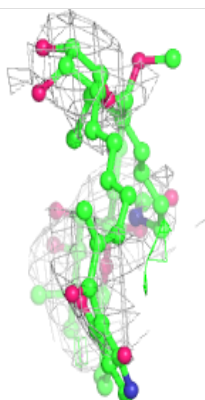
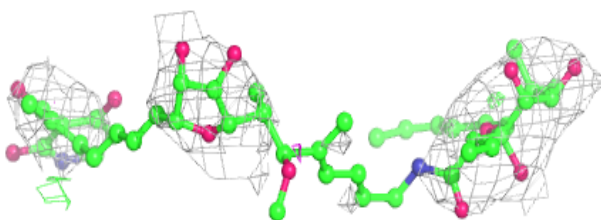
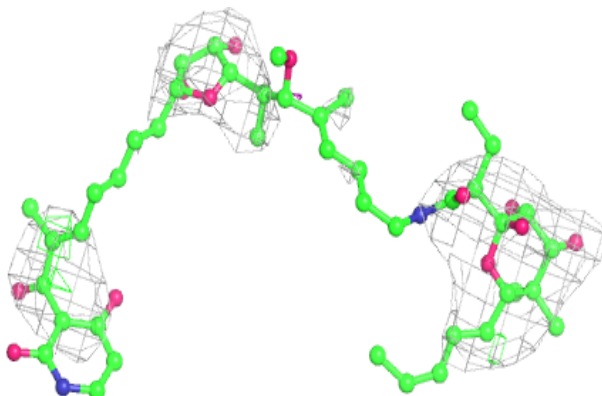


**Electron density around GDP CZ 501:**

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

**Electron density around KIR AZ 502:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.