



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 12:55 pm BST

PDB ID : 4V5S  
Title : The crystal structure of EF-Tu and G24A-tRNA-Trp bound to a cognate codon on the 70S ribosome.  
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.  
Deposited on : 2010-12-07  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

The 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

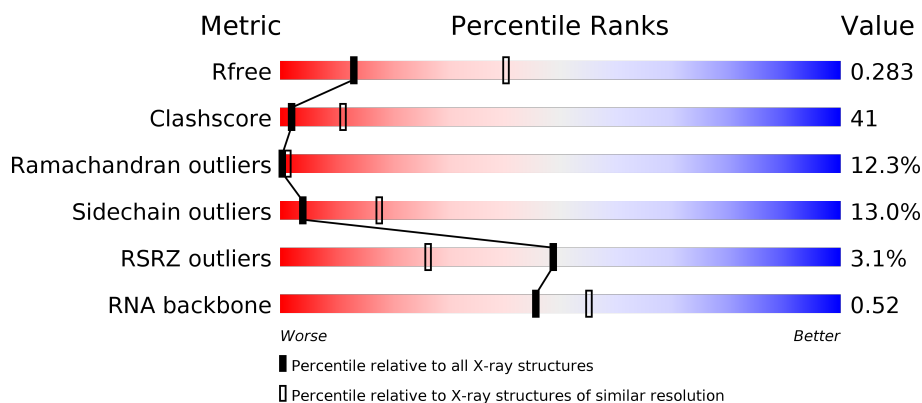
# 1 Overall quality at a glance

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>32% 52% 12% . .</div> </div>
1	CA	1522	<div> <div>2%</div> <div>26% 57% 13% . .</div> </div>
2	AB	256	<div> <div>2%</div> <div>21% 54% 15% . 9%</div> </div>
2	CB	256	<div> <div>2%</div> <div>24% 52% 15% . 9%</div> </div>




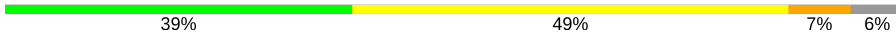
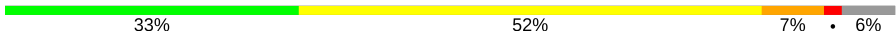
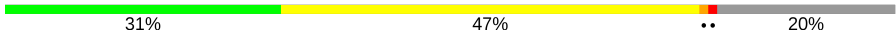
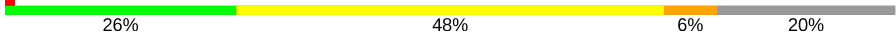
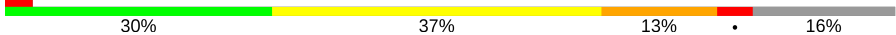
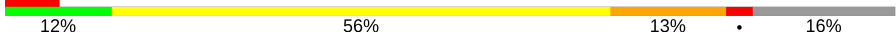
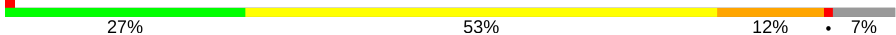

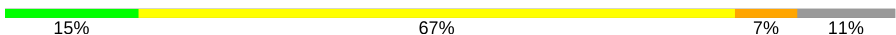
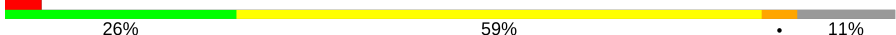
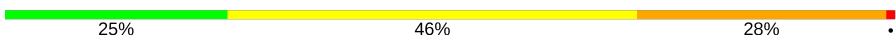
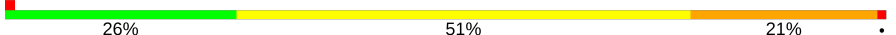






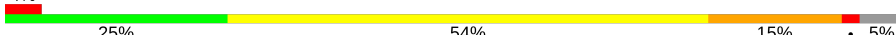
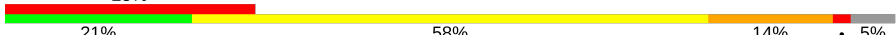


*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	131	
12	CL	131	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

*Continued on next page...*

Continued from previous page...

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	


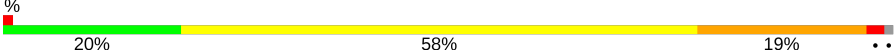
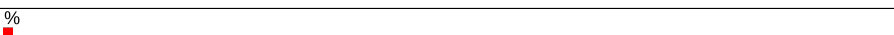
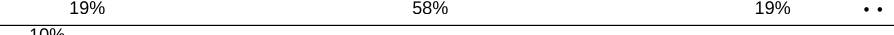
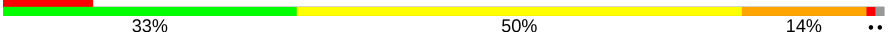

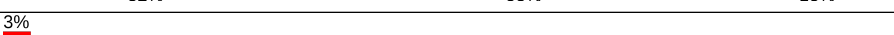
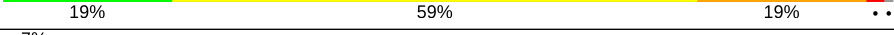


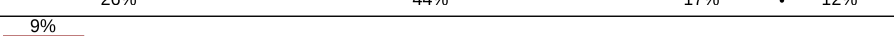
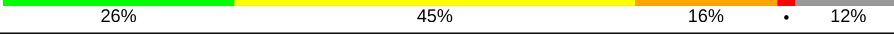

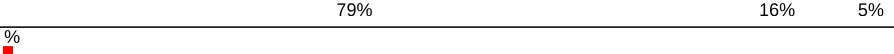
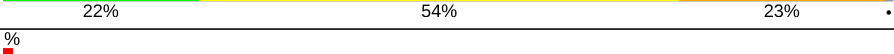
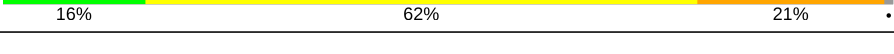


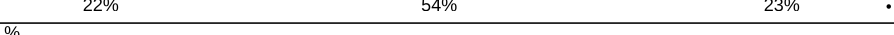
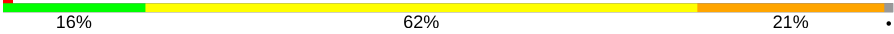

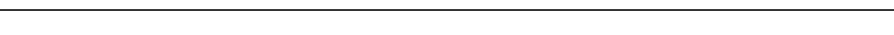

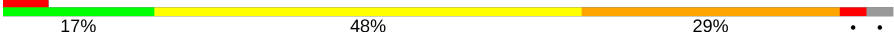

Continued on next page...

Continued from previous page...

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	

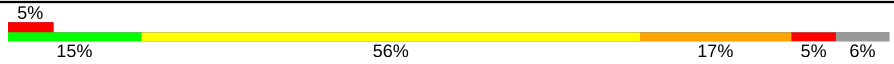

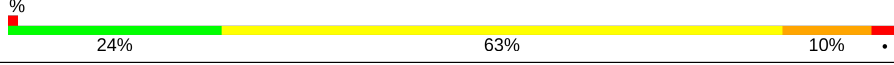
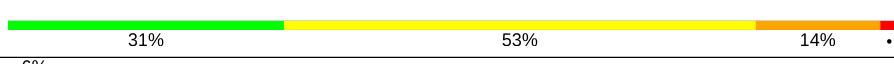
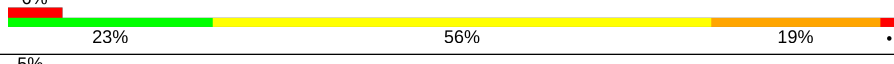
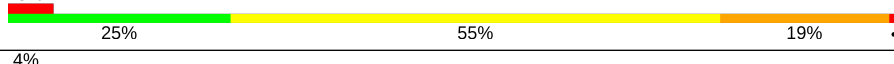
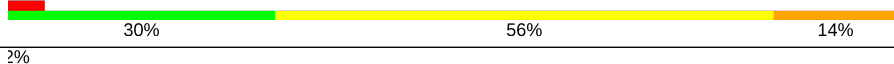

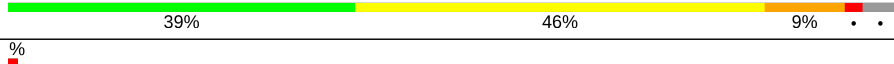
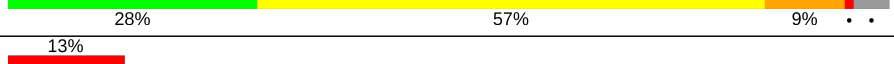

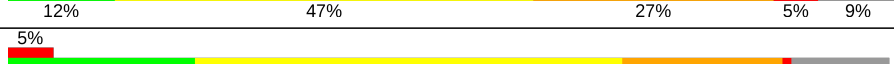
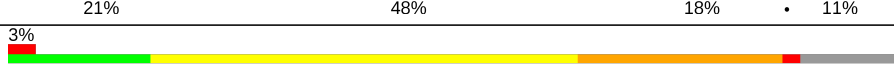

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	17	-	-	-	X
59	ZN	AD	301	-	-	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 307196 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	17	Total	C	N	O	P	0	0	0
			362	164	68	114	16			
23	CX	17	Total	C	N	O	P	0	0	0
			362	164	68	114	16			

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

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

- Molecule 25 is a protein called ELONGATION FACTOR TU.

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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...*



*Continued from previous page...*

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			

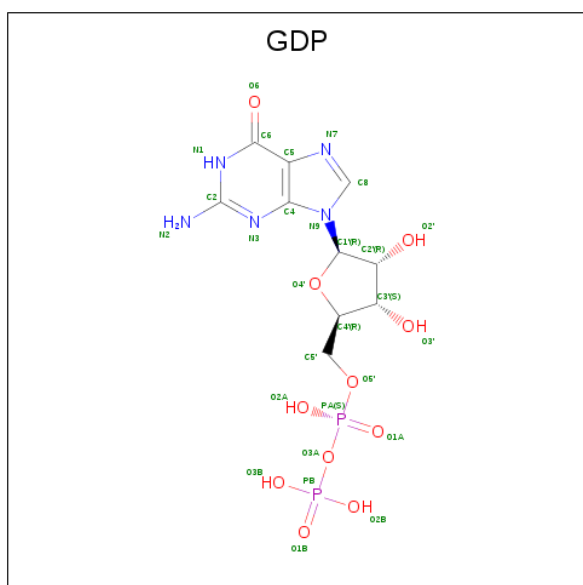
- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

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).

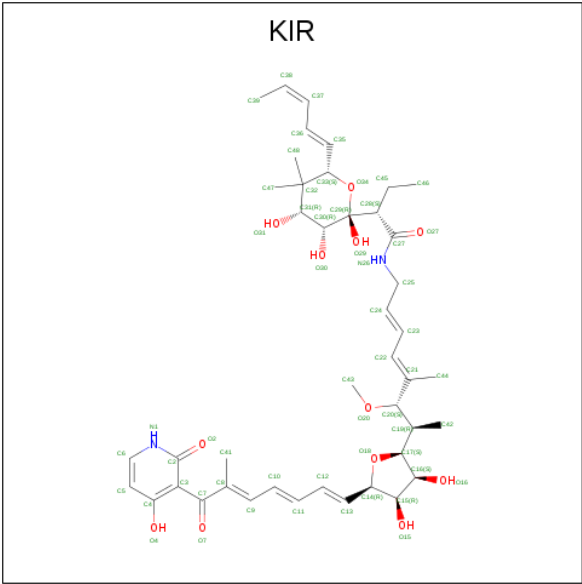
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		

- 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>).

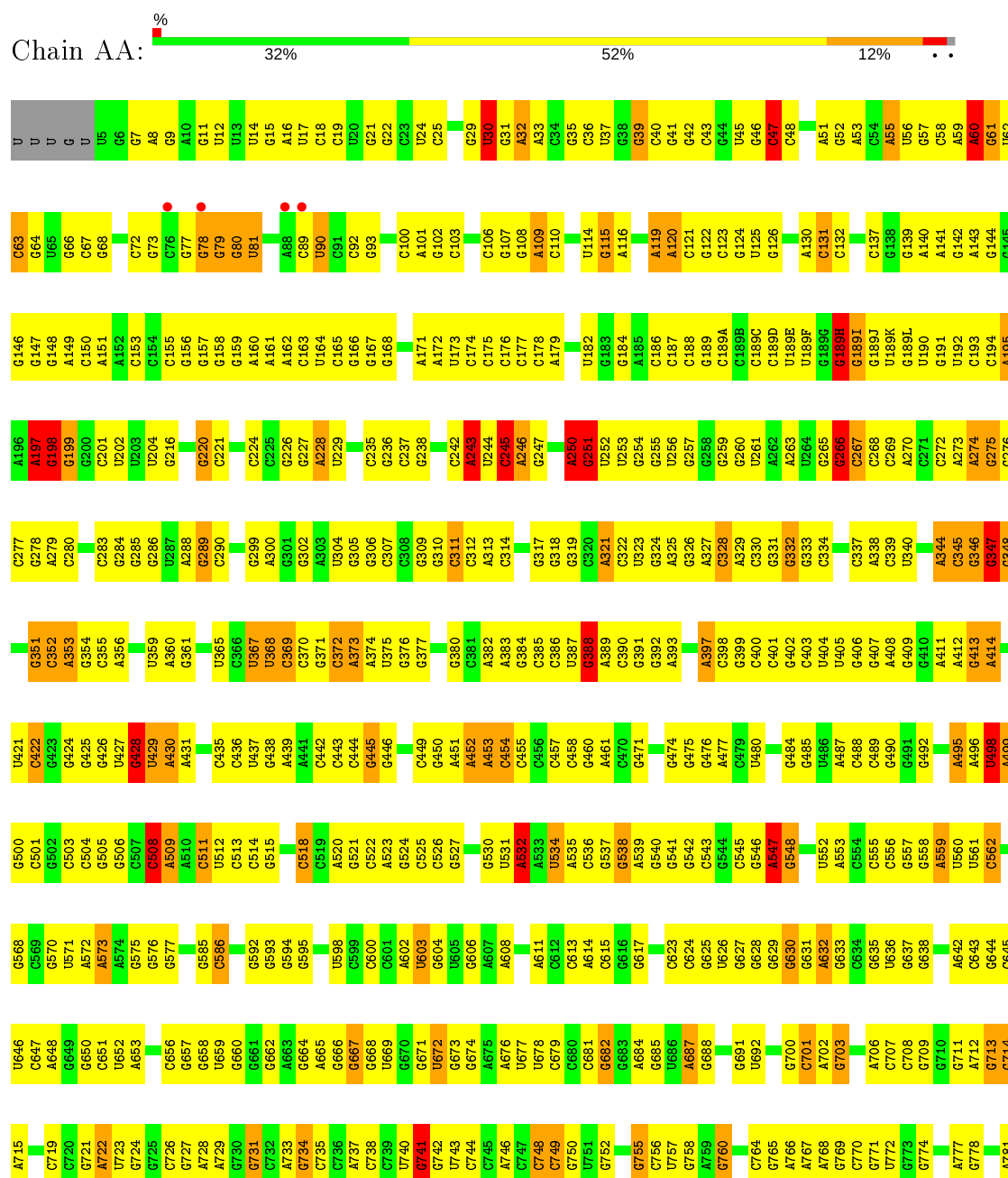


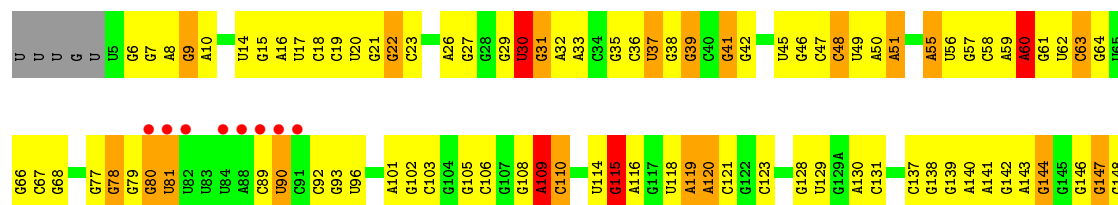
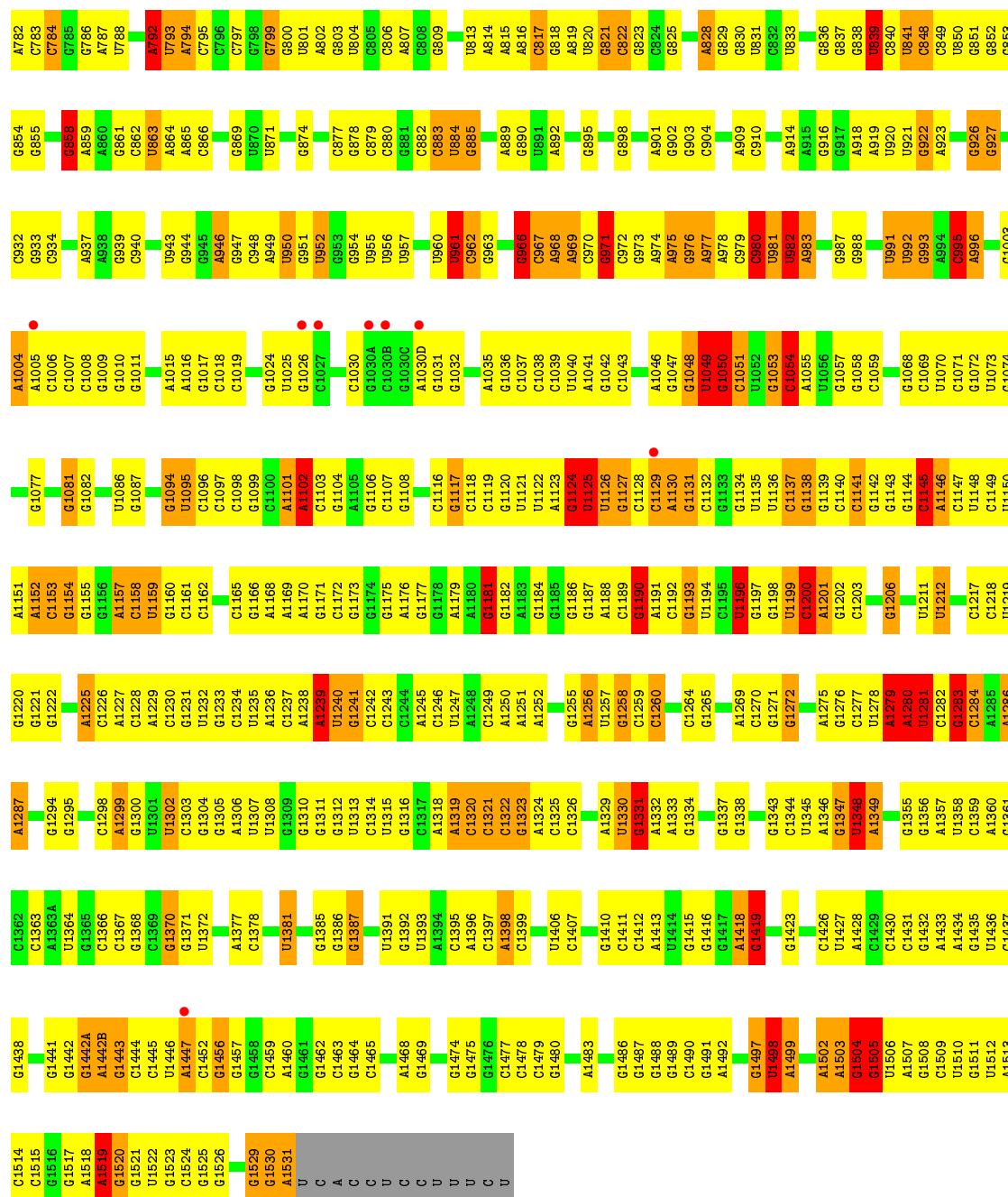
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AZ	1	Total	C	N	O		0	0
			57	43	2	12			
61	CZ	1	Total	C	N	O		0	0
			57	43	2	12			

### 3 Residue-property plots

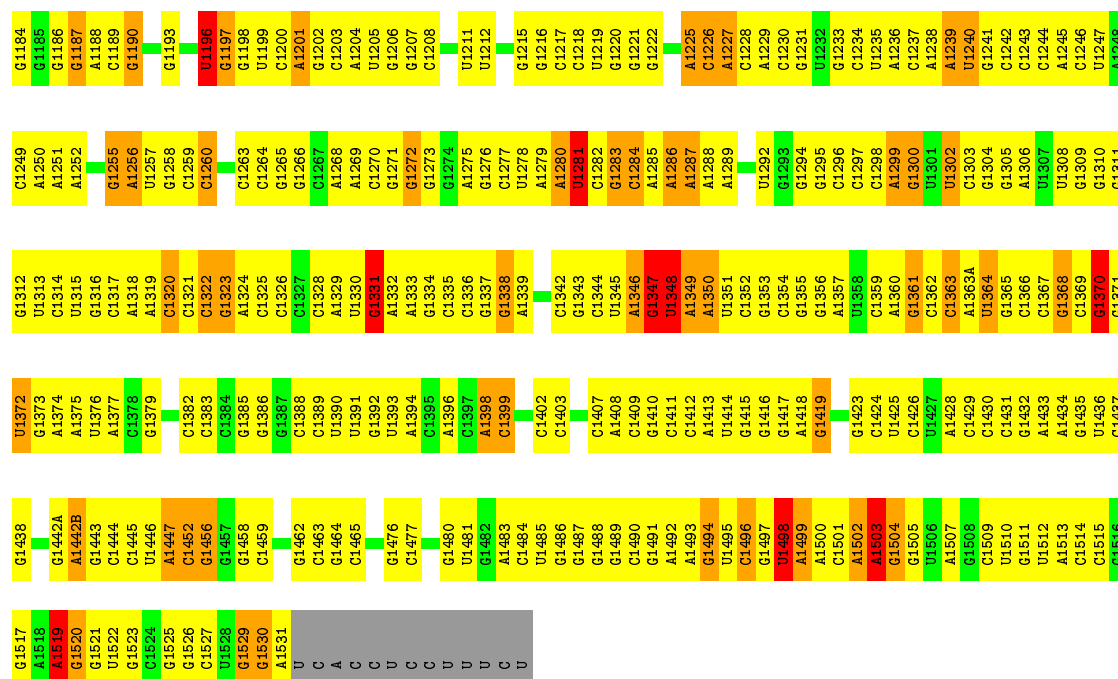
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 16S rRNA

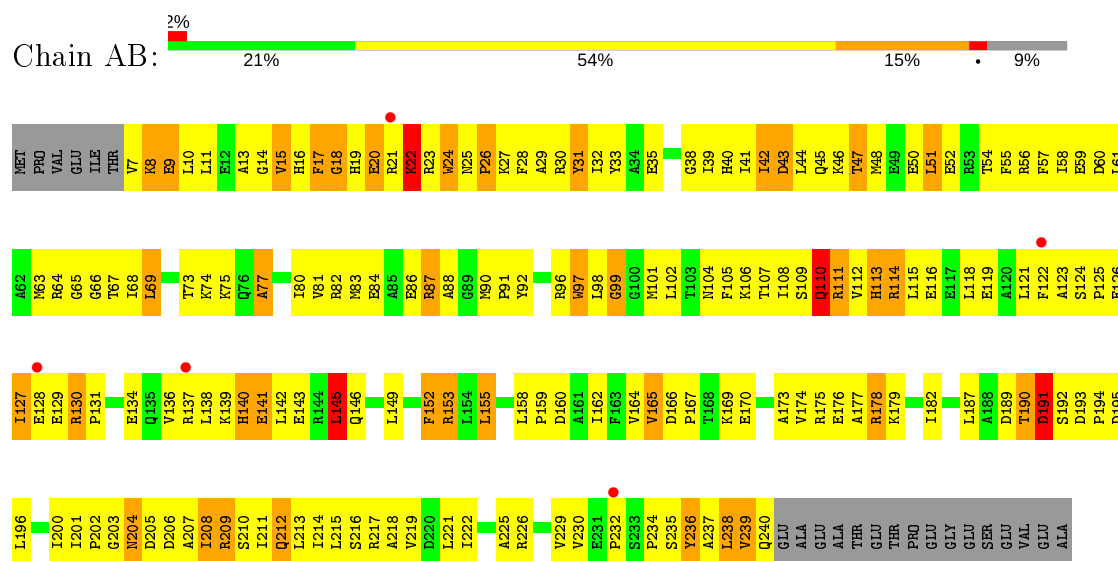




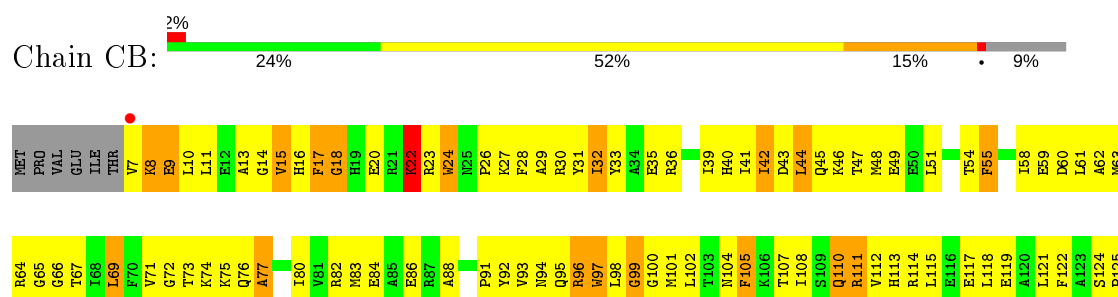
G1120	G1054	A923	U841	A777	C708	G638	G566	G492	C418	G351	G285	G220	A149
A1055	A1055	C924	C948	G778	G711	G643	G567	G493	C419	C352	G288	G221	A151
U1056	U1056	G925	C949	C779	A712	G644	G567	U494	U420	A353	A289	U222	
G1124	G1057	G926	G954	A780	G713	G645	G568	A495	G423	C355	C290	U223	G156
U1125	G1058	G927	G853	A781	G714	U646	A572	U498	G424	A356	C292	C224	G157
U1126	G1059	G928	G854	A782	A715	C647	A573	A499	G425	G357	G295	G225	G158
U1127	G1060	G929	G855	C783	A716		A574	G500	G426	U358	G296	G226	G159
C1128	U1061	C930	G856	G784	C717	G650	G575	C501	G428	U359	U294	G227	A160
G993	G993		A859	G785	G718	G651	G576	G502	U427	A360	U296	A228	A161
A994	A994	C934	A860	G786	G719	U652	G577	C503	G428	A361	U297	U229	A162
C995	C995	G935	G861	A787	C720	U653	G578	C504	U429	U365	A298	G230	
A996	A996	A935	G862	U788	G721	G654	G579	G505	A430	U366	G299	C234	G165
U997	U997	C936	U863	A790	A722	A655	G585	G506	A431	U367	A300	C235	G166
G1002	G1002	A937	A864	G791	U723	C656	C586	C507		U368	G302	G236	G167
A938	A938	G938	A865	A792	G724	G657	G592	C508	U434	C369	G302	C237	
G939	G939	C940	C966	U793	G725	G658	G593	A509	C435	C370	A303		A171
A1004	A1004	G941	G969	A794	G726	U659	G594	A510	C436	G371	U304	C242	A172
G940	G940	G942	U870	A795	G727	G660	G595	C511	U437	G372	G305	U243	U173
G942	G942	U943	C979	C796	G731	G661	C596		G438	A373		U244	C174
U943	U943	A944	G874	C797	G732	A663	U598	C518	A439	A374	G309	C245	C175
G945	G945	G946	C877	U801	A733	G664	C599	A520	A441	U375	G310	A246	C176
A946	A946	G947	G878	U804	G734	A665	C600	G521	C443	G376	C311	G247	C177
G947	G947	C948	C879	U804	G735	G666		G522	C444	G377	C312	C248	C178
C948	C948	A949	C882	U807	C736	G667	U603	A523	G445	G378	A313	U249	A179
A949	A949	U950	C883	A807	G737	G673	G604	G524	G446	C379	C314	A250	U180
U950	U950	G951	C884	C808	C738	G674	U605	C525	G447	G380	A315	G251	
G952	G952	U952	U884	A814	C739	G675	G606	C526	A448	C381	G319	G254	A185
G953	G953	G954	G885	C810	U740	G741	A607	G527	C449	A382	C320	G255	C186
U954	U954	U955	G886	C811	G741		A608		G450	A383	C321	U256	C187
U955	U955	U956	G887	C812	G742	U677	A609	G530	A451	G384	G322	G257	C188
U956	U956	U957	G888	U813	C744	U678	A610	U531	A452	C385	G323	G258	C189
U957	U957	A958	A889	A815	C745	C680	A611	A532	A453	C386	G324	G259	C189A
U958	U958	G959	G890	A816	C746	C681	C612	A533	C454	U387	A325	G260	C189B
A959	A959	U960	U891	A817	C747	G682	C613	U534	C455	G388	G326	U261	
U960	U960	U961	A892	C817	C748	G683	A614	A535	C456	A389	G327	A262	U189E
U961	U961	C962	C893	G818	C749	A684	C615	C536	C457	C390	A328	A263	G189H
C962	C962	G963	A900	A819	C750	G685	G616	G537	C458	G391	C329	U264	G189I
A963	A963	A964	A901	U820	U751	U686	C617	G538	C459	A392	G330	G265	G189J
G964	G964	A965	G902	G821	G754	A687	C618	A539	G471	A393	G331	C266	G189K
A965	A965	G966	G902	C822	C755	G688	U619	G540	A472	G394	G332	C267	G189L
G966	G966	C967	G906	G823	G756	C689	C620	G541	G473	A397	G333	C268	U190
C967	C967	A968	A907	C824	C757	G690	A621	G542	G474	C398	G334	C269	G191
A968	A968	A969	A908	G825	U757	G691	A622	G543	G475			C270	U192
G969	G969	C970	A909	C826	G758	U692	C623	G544	G476			C271	C193
C970	C970	C971	C910	U827	A759	G693	C624	C545		C403	C337	G272	C194
G971	G971	G972	C911	A828	G760	A694	G625	G546	U480	U404	A338	A273	A195
G972	G972	G973	U911	G829	G761	A695	U626	A547	G481	U405	C339	G274	
G973	G973	A974	C912	G830	G762	A696	G627	G548	A482	G406	U340	G275	G196
A974	A974	A975	A913	U831	G763	U697	G628	C549		G407	C341	G276	A197
G975	G975	G976	A914	C832	G764	G698	G629		C483	A408	C342	G277	G198
G976	G976	A977	A915	U833	G765	C699	G630	C555	C484	G409	U343	C278	G199
A977	A977	G978	G916	C834	A767	G700	G631	C556	G485	G410	A344	G279	G200
G978	G978	A979	G917	U835	G768	G701	A632	G557	U486	A411	C345	C280	C201
C979	C979	C980	A918	U836	C770	A702	G633	G558	A487	A412	G346	G281	U202
C980	C980	U981	A919	G837	G771	G703	C634	A559	C488	G413	G347	G282	U203
U981	U981	U982	U920	G838	G774	A706	G635	U560	C489	A414	C348	C283	U204
U982	U982	G983	U921	U839			U636	U561	G490	A415		G284	G216
G983	G983	G984	G922	C940			G637	C562	G491				



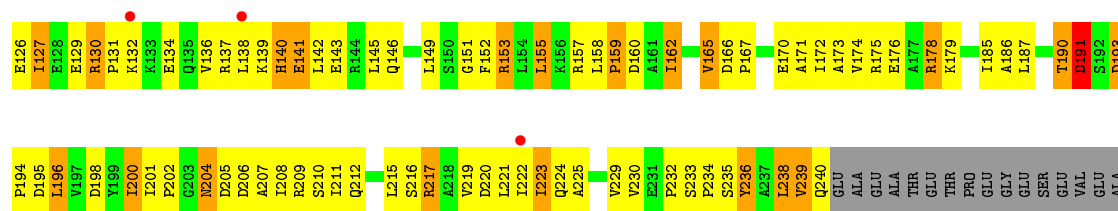
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



• Molecule 2: 30S RIBOSOMAL PROTEIN S2

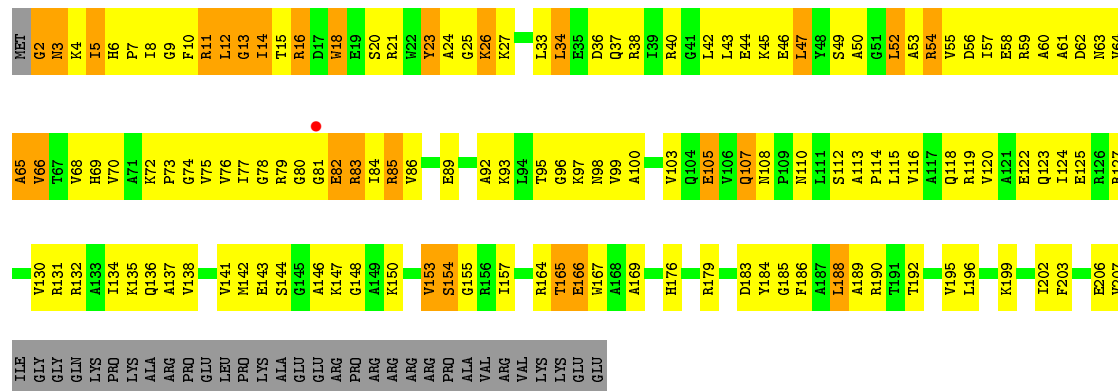






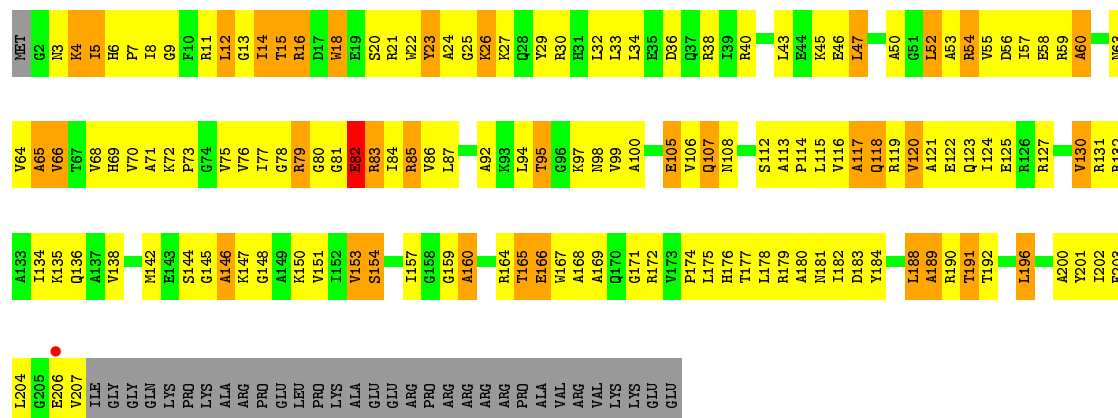
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC: 28% 47% 11% 14%



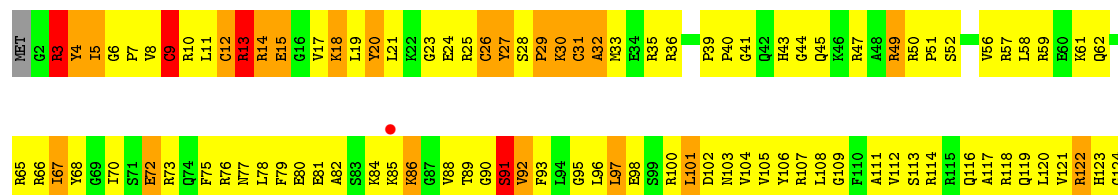
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3

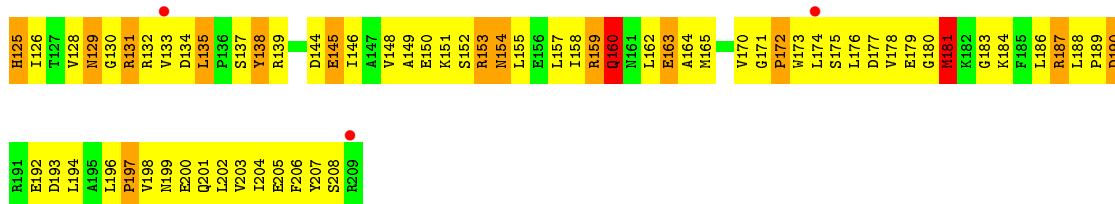
Chain CC: 26% 46% 15% 14%



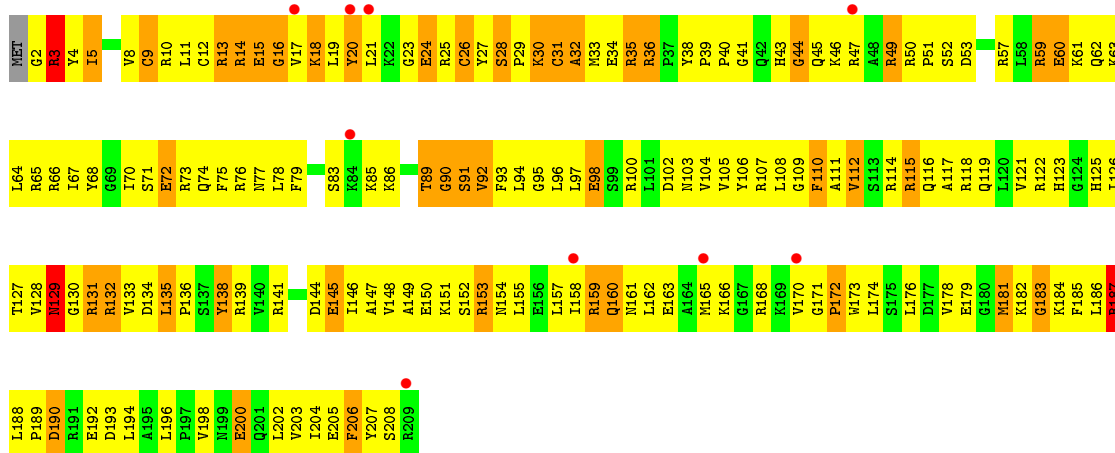
### • Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD: 20% 60% 17%

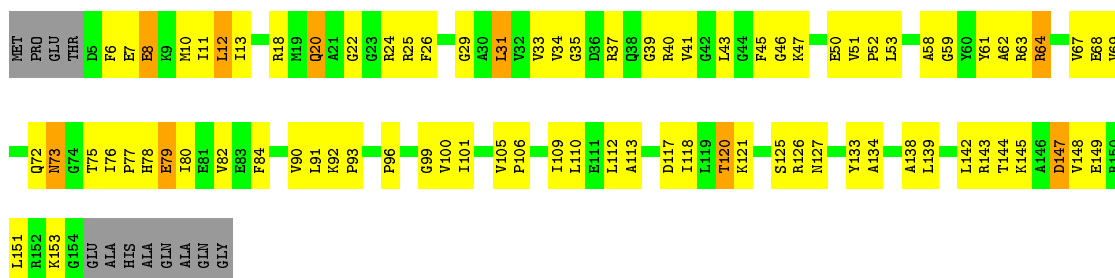




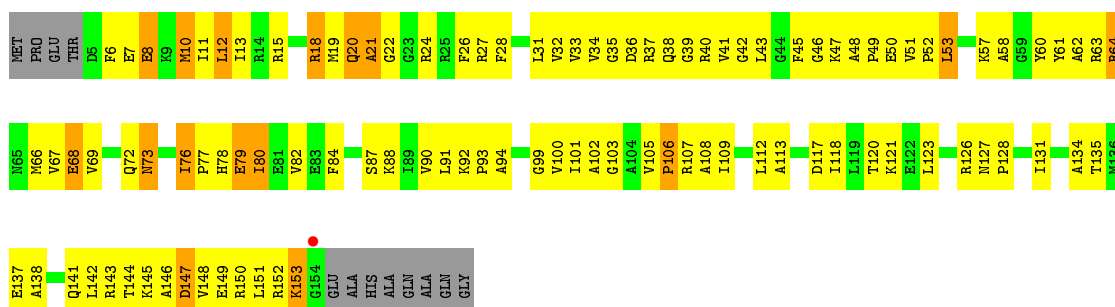
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



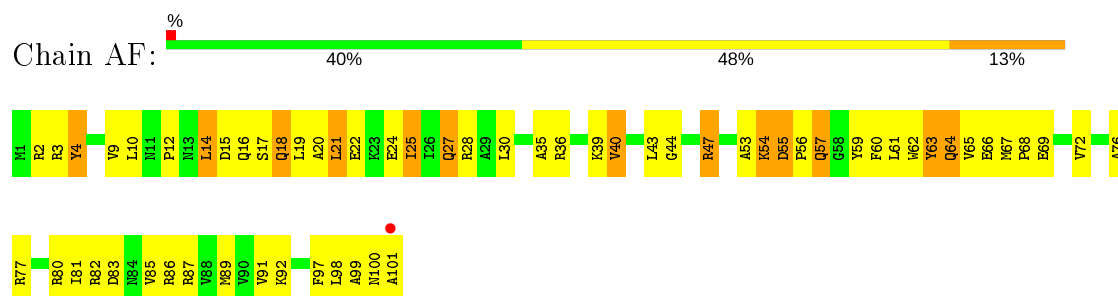
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



• Molecule 5: 30S RIBOSOMAL PROTEIN S5



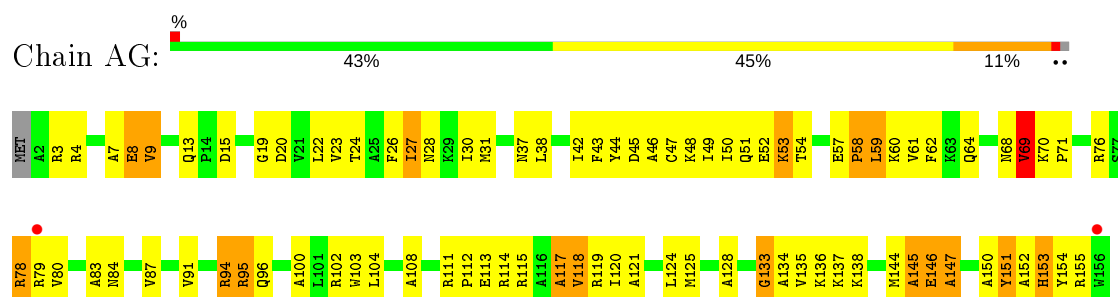
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



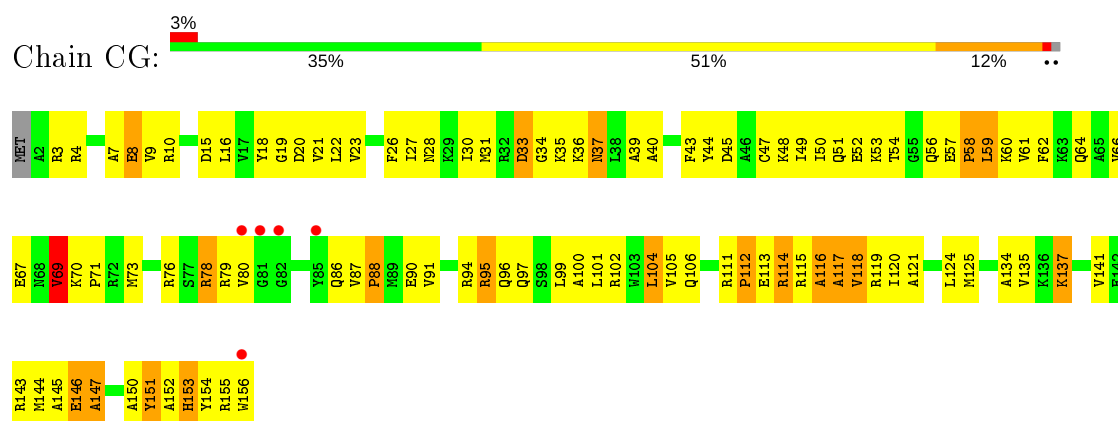
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



- Molecule 7: 30S RIBOSOMAL PROTEIN S7

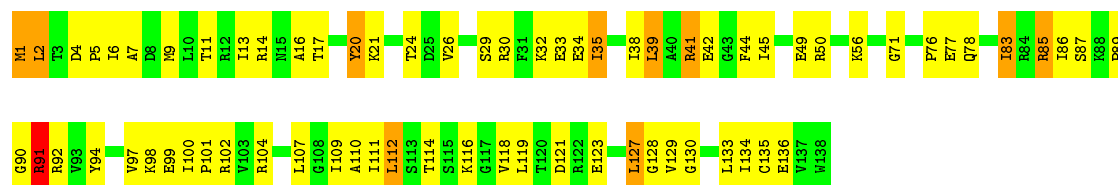


- Molecule 7: 30S RIBOSOMAL PROTEIN S7



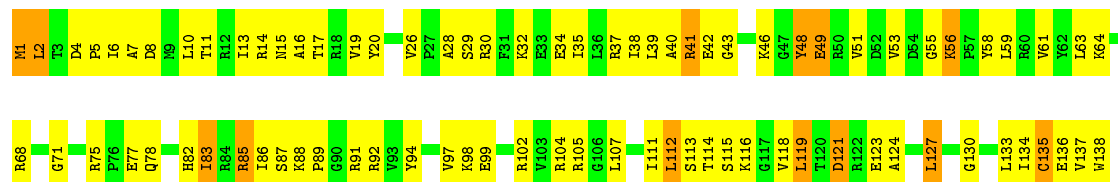
- Molecule 8: 30S RIBOSOMAL PROTEIN S8





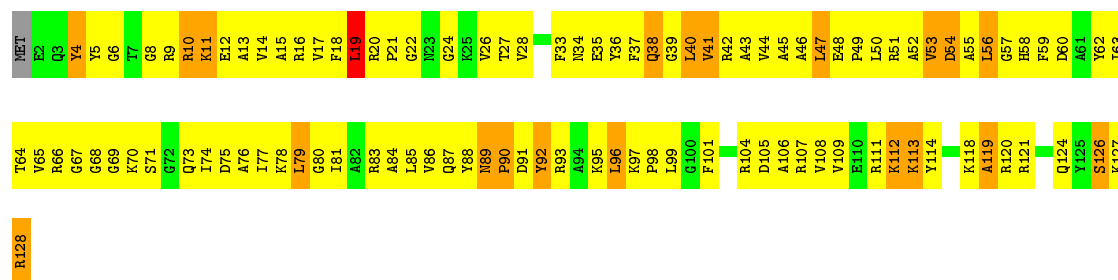
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH: 40% 51% 9%



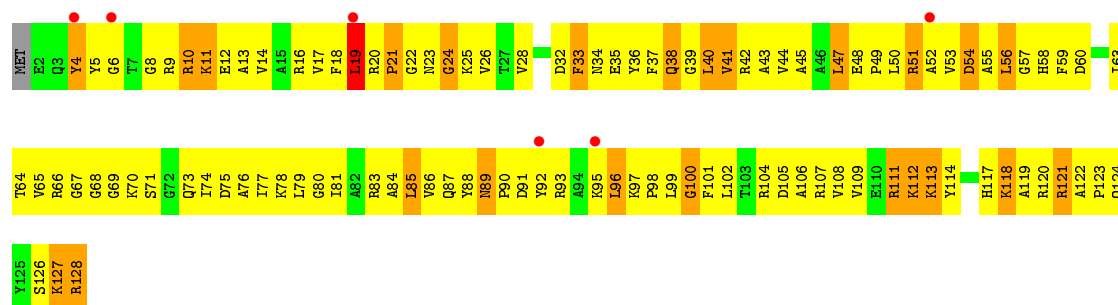
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI: 18% 65% 16% ..



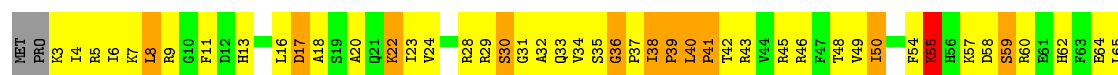
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

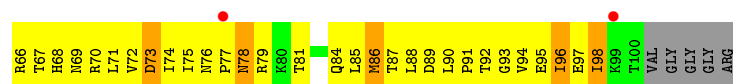
Chain CI: 5% 15% 65% 19% ..



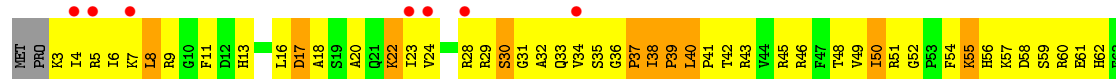
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ: 2% 21% 56% 15% • 7%





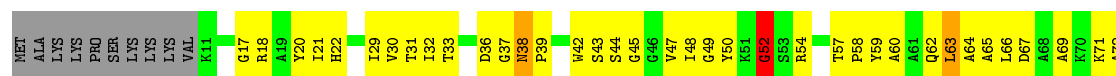
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

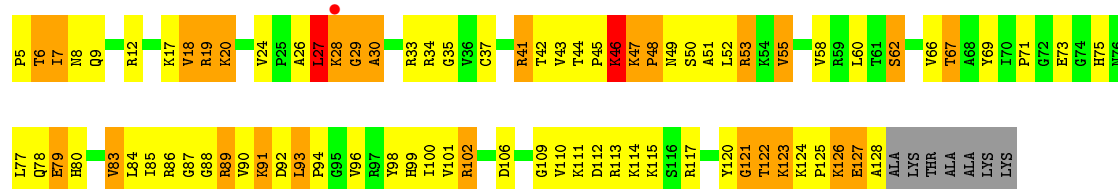


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

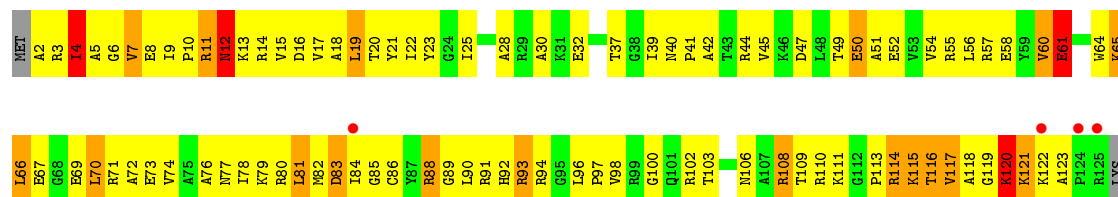


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

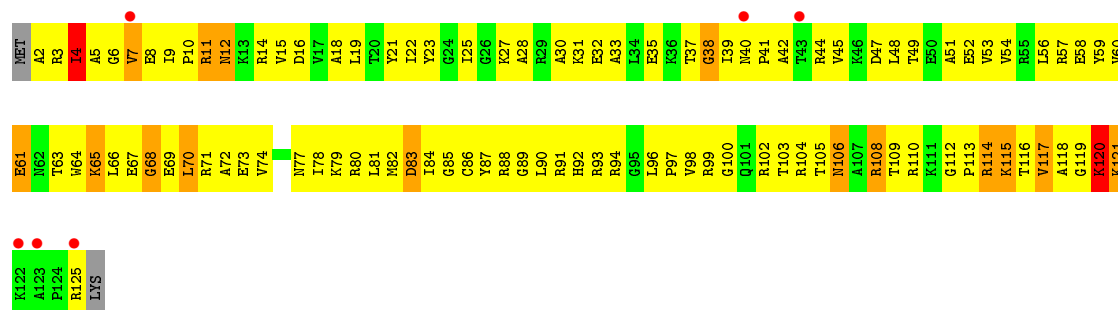




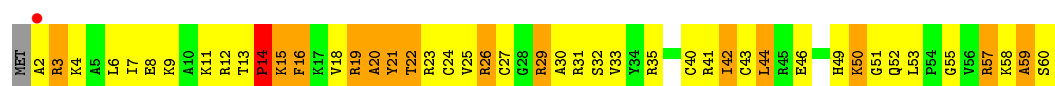
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



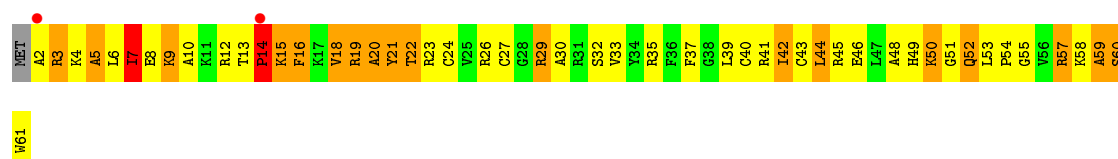
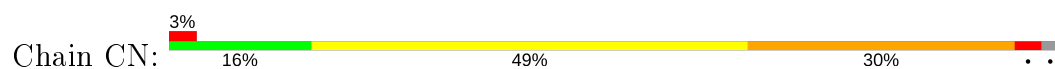
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



- Molecule 14: 30S RIBOSOMAL PROTEIN S14

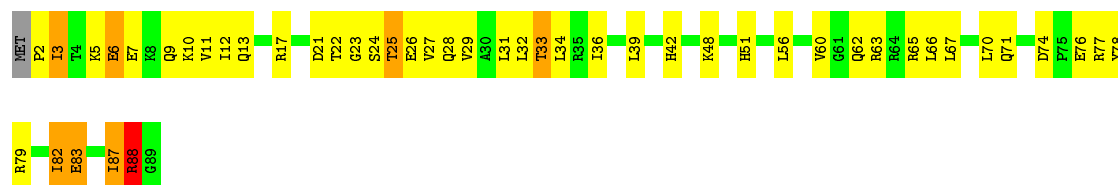


- Molecule 14: 30S RIBOSOMAL PROTEIN S14



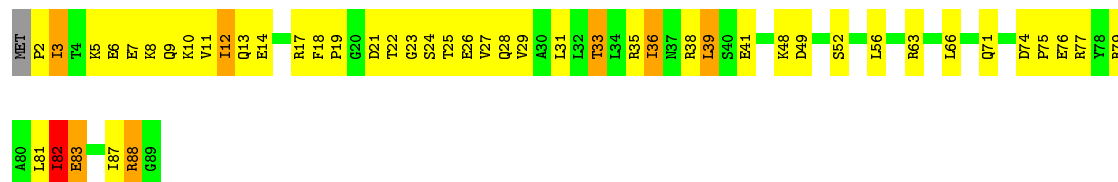
- Molecule 15: 30S RIBOSOMAL PROTEIN S15





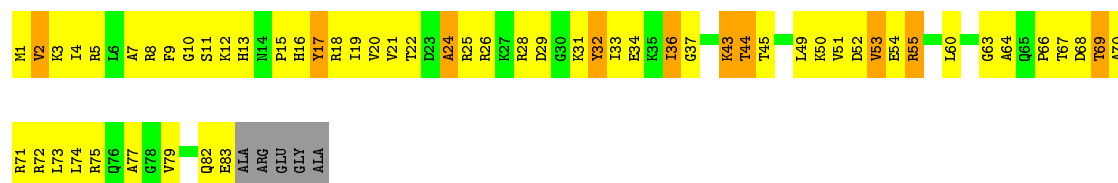
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO: 45% 45% 8% ..



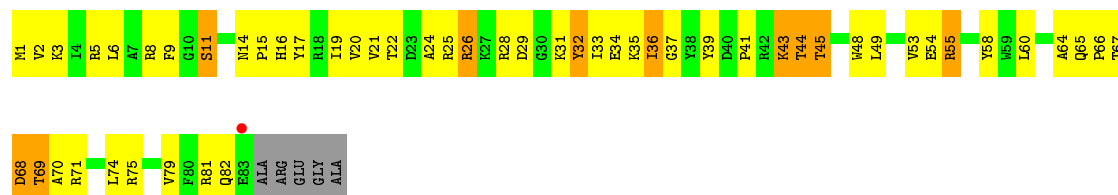
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP: 28% 55% 11% 6%



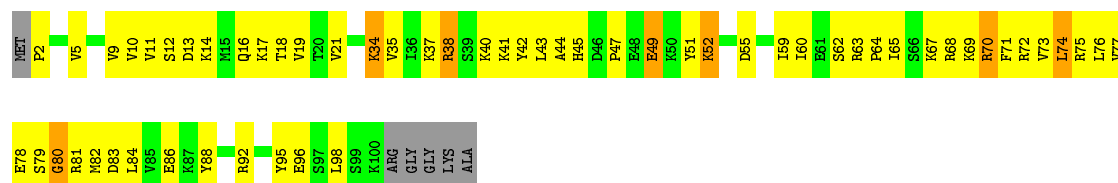
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP: 34% 49% 11% 6%



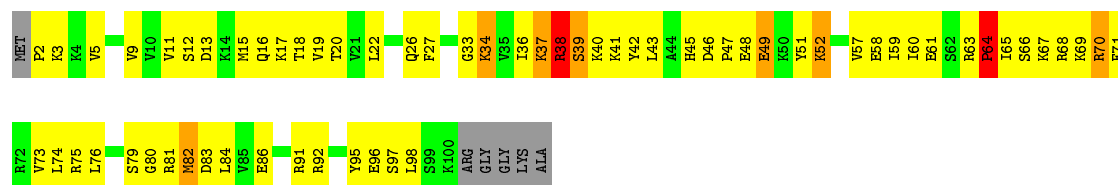
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ: 39% 49% 7% 6%

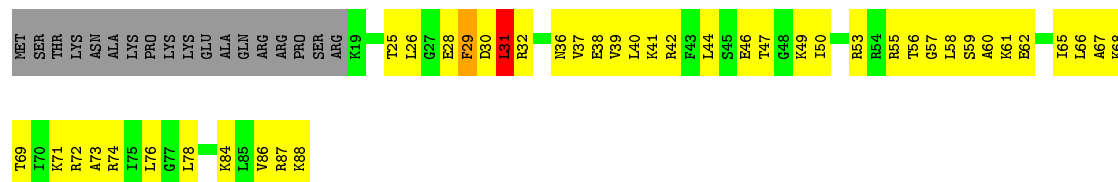


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

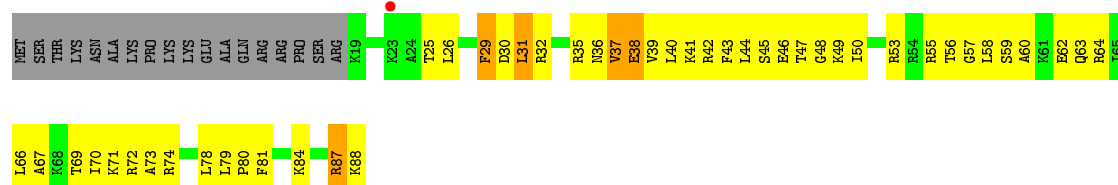
Chain CQ: 33% 52% 7% 6%



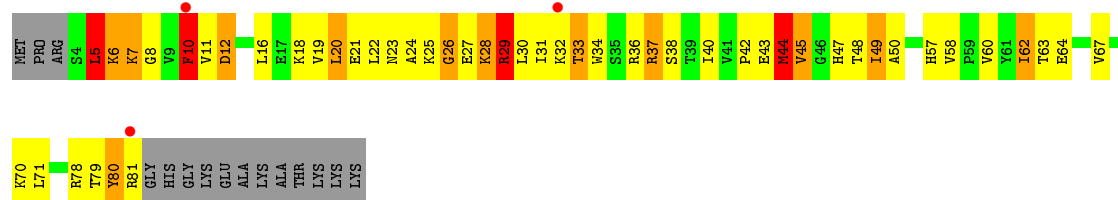
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



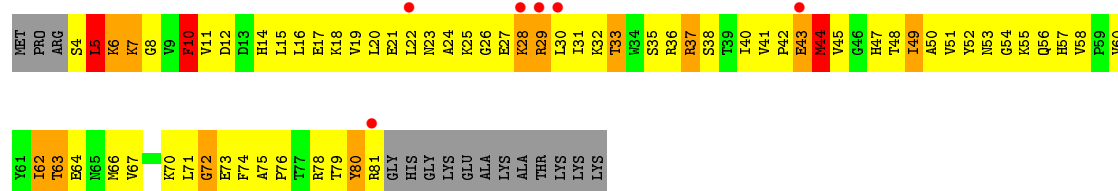
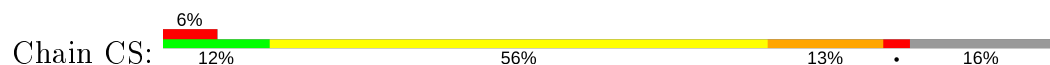
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

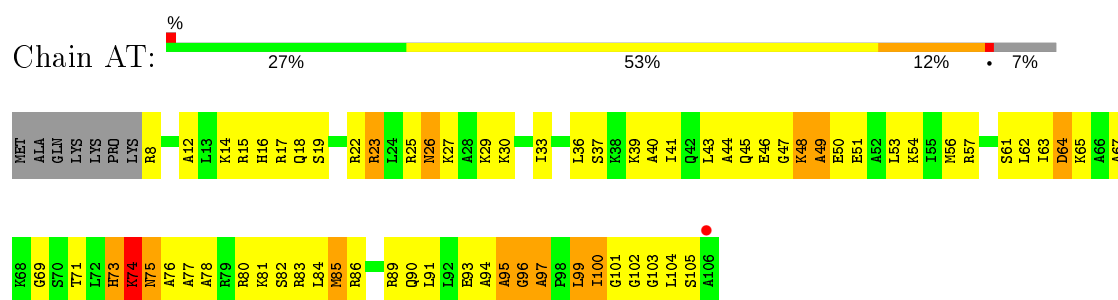


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

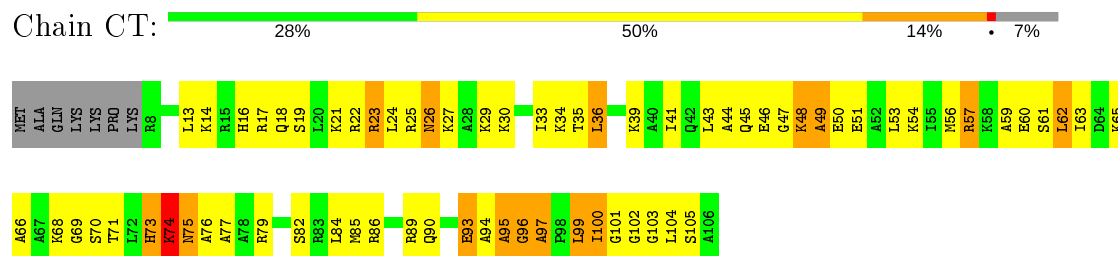


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

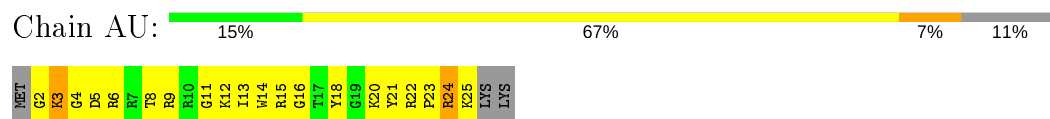




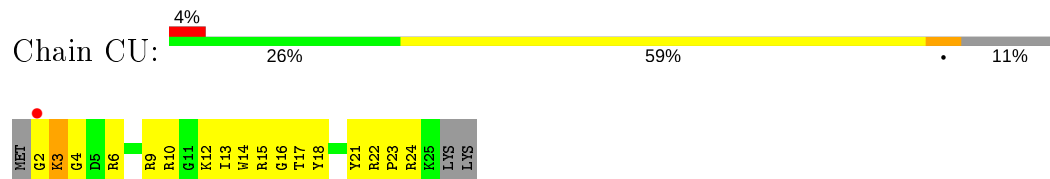
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



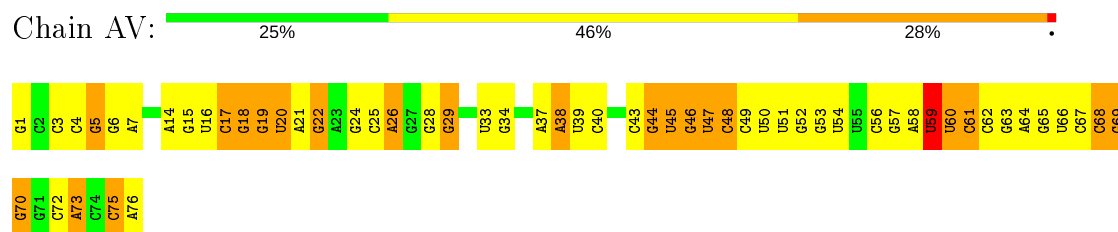
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



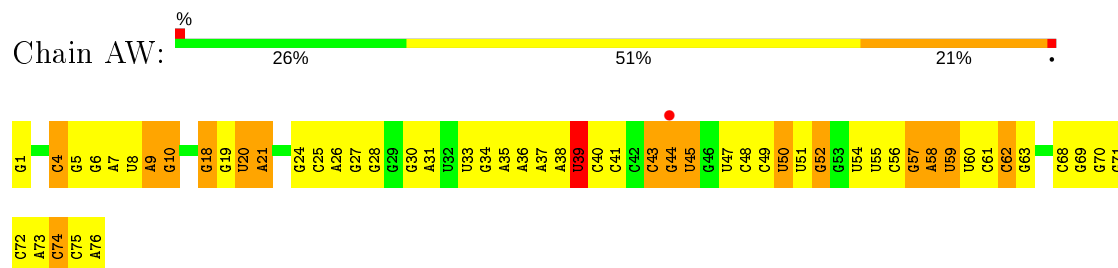
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



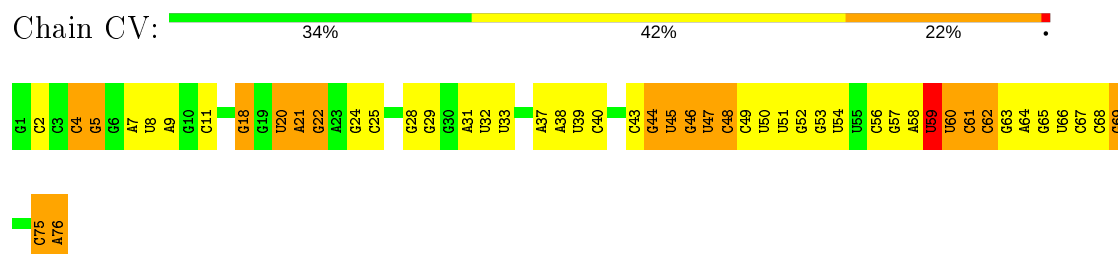
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



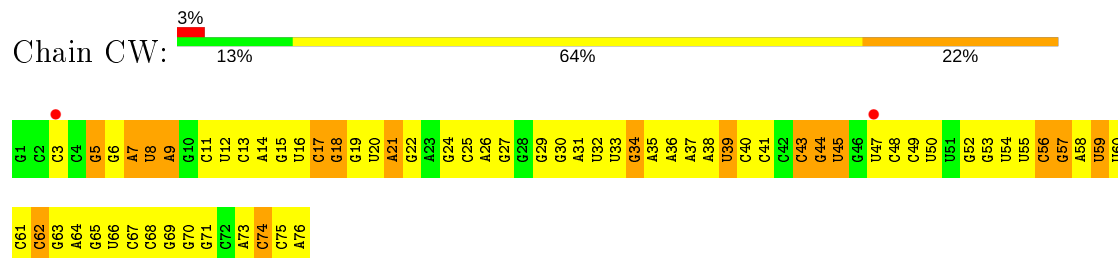
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



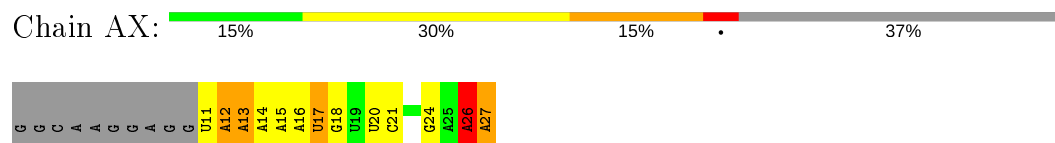
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



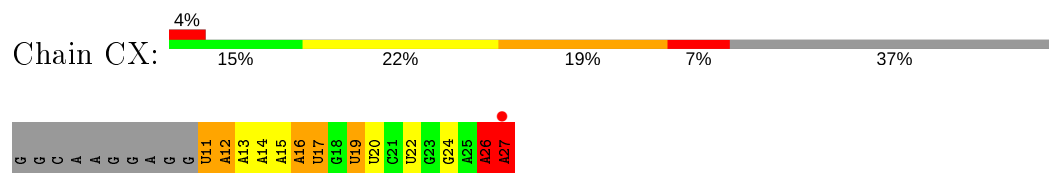
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



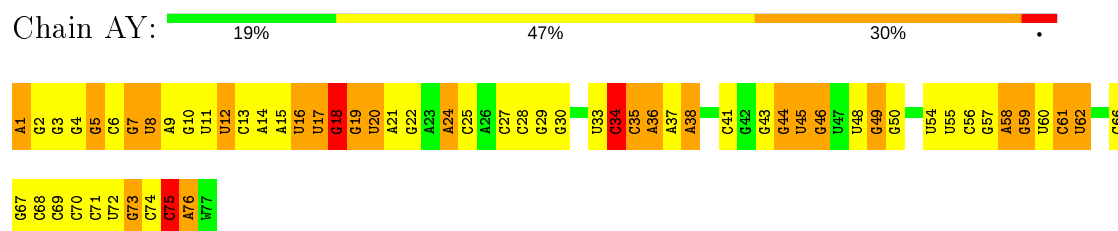
- Molecule 23: MRNA



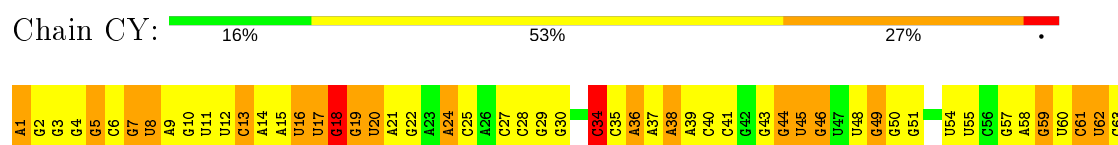
- Molecule 23: MRNA



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



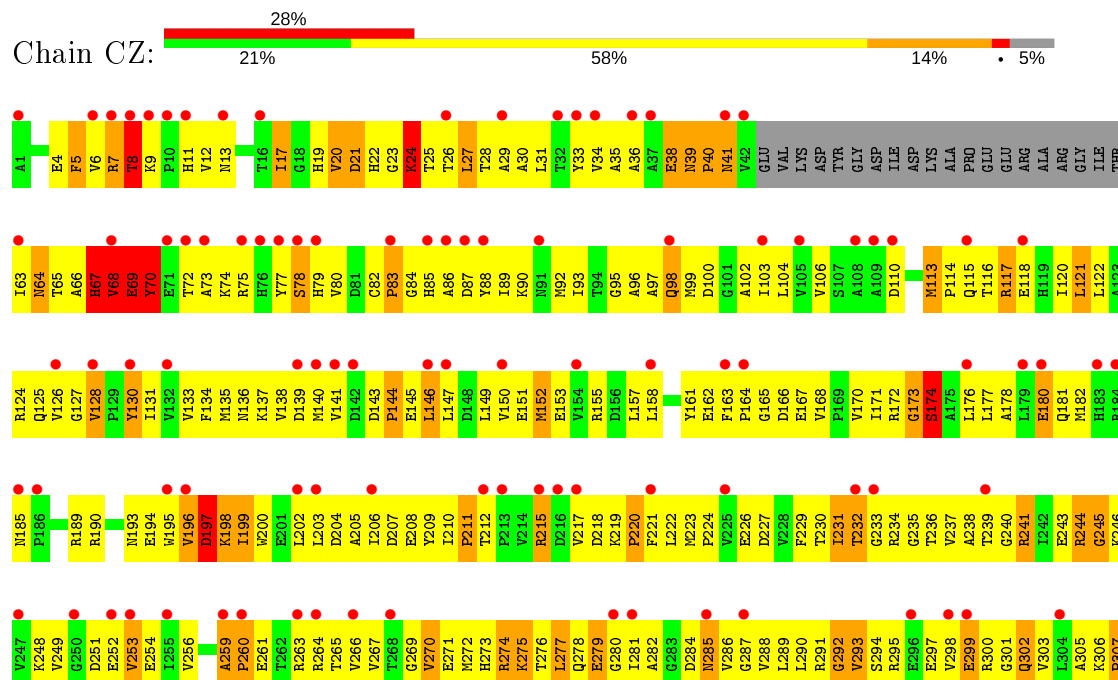
- Molecule 24: A-SITE TRNA G24A TRP-TRNA TRP

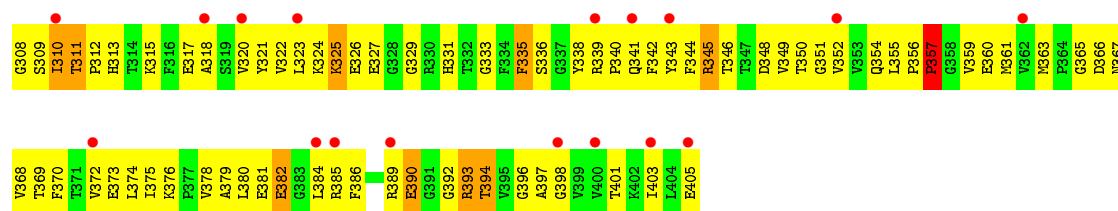


## Chain AZ:

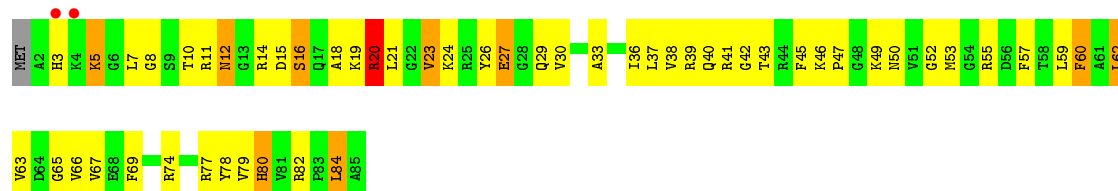


Chain CZ:

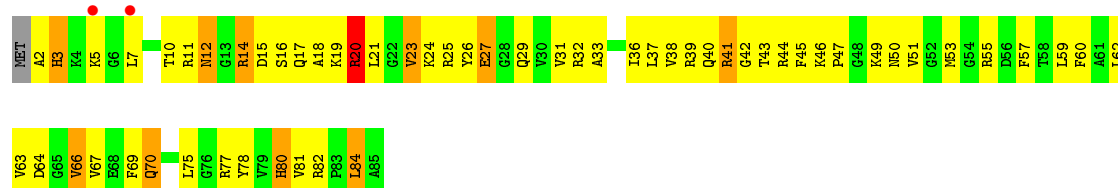




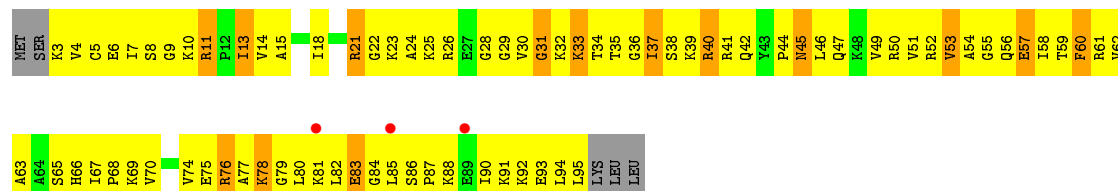
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



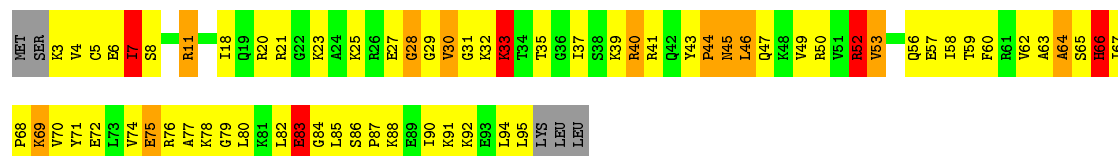
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



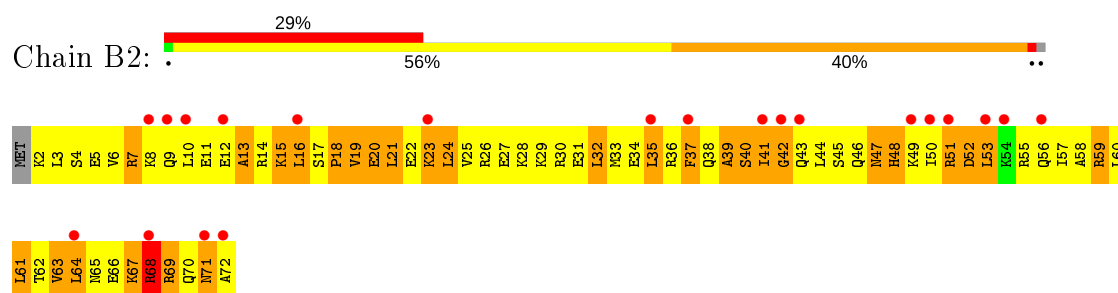
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



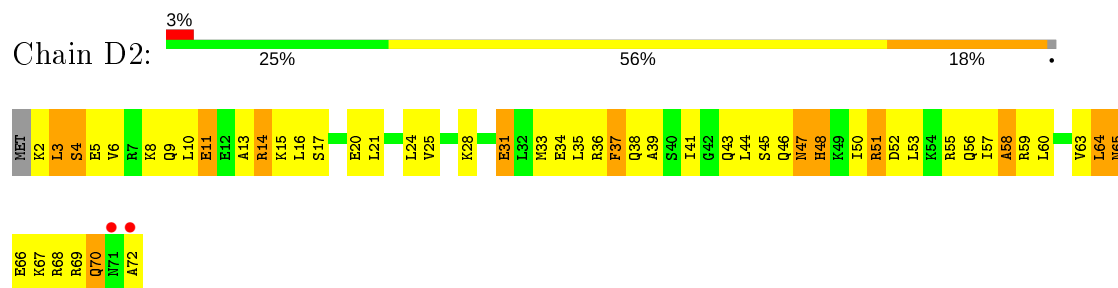
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



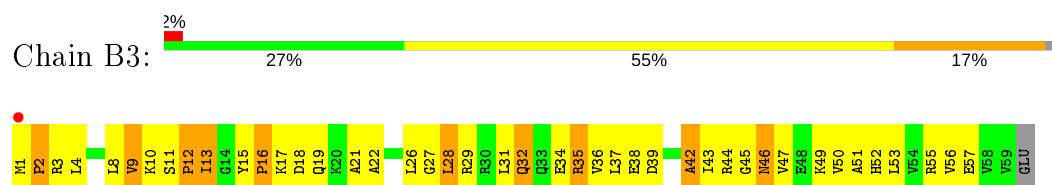
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



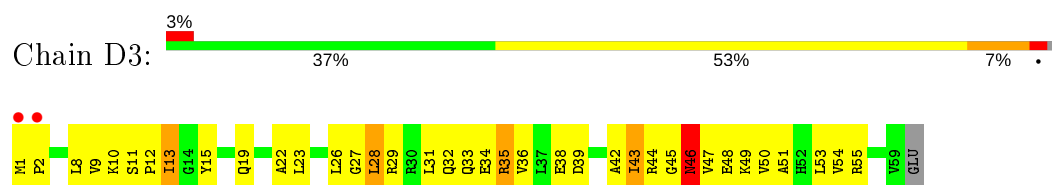
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



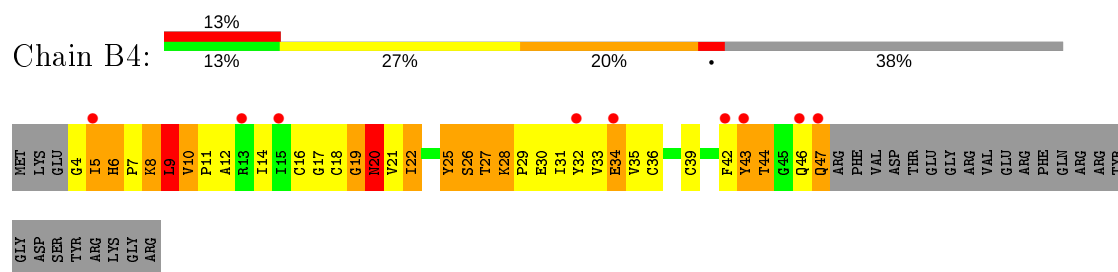
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



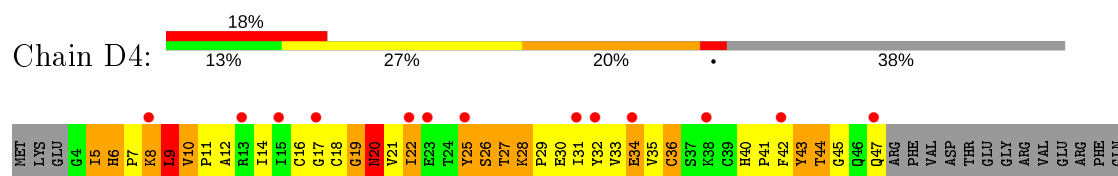
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



• Molecule 30: 50S RIBOSOMAL PROTEIN L31

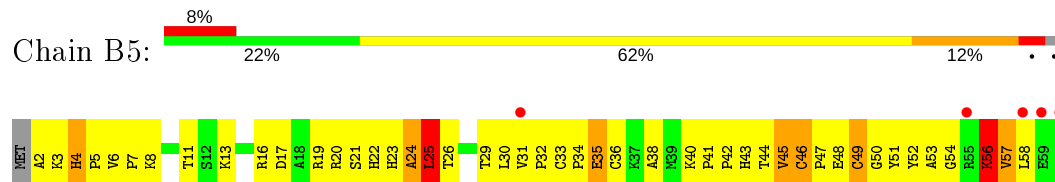


• Molecule 30: 50S RIBOSOMAL PROTEIN L31

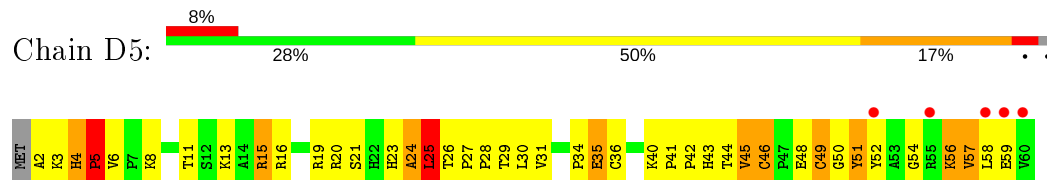


ARG  
ARG  
TYR  
GLY  
ASP  
SER  
TYR  
ARG  
LYS  
GLY  
ARG

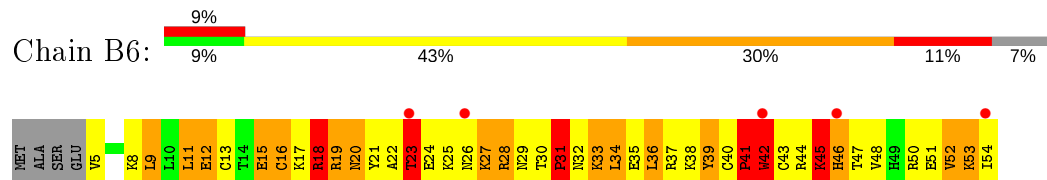
• Molecule 31: 50S RIBOSOMAL PROTEIN L32



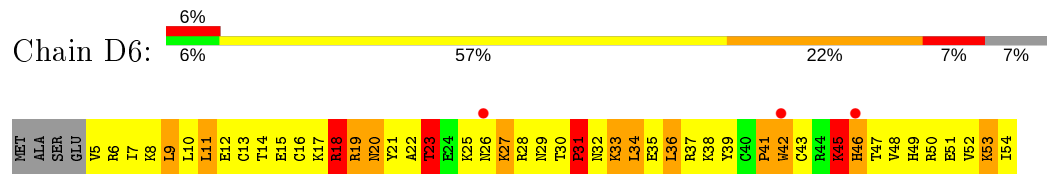
• Molecule 31: 50S RIBOSOMAL PROTEIN L32



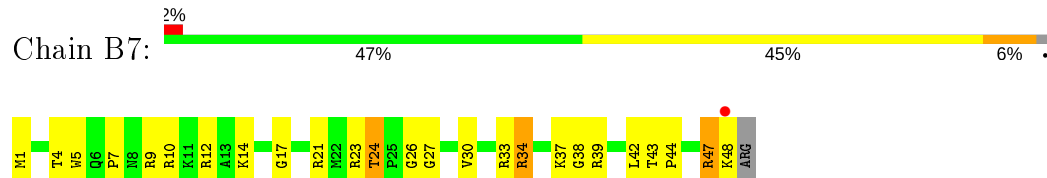
• Molecule 32: 50S RIBOSOMAL PROTEIN L33



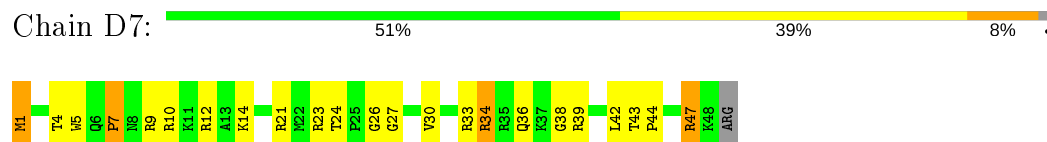
• Molecule 32: 50S RIBOSOMAL PROTEIN L33



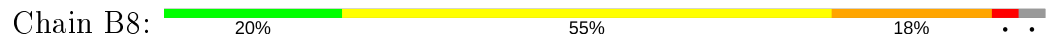
• Molecule 33: 50S RIBOSOMAL PROTEIN L34

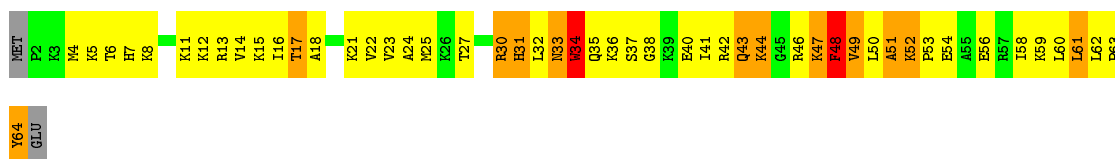


• Molecule 33: 50S RIBOSOMAL PROTEIN L34

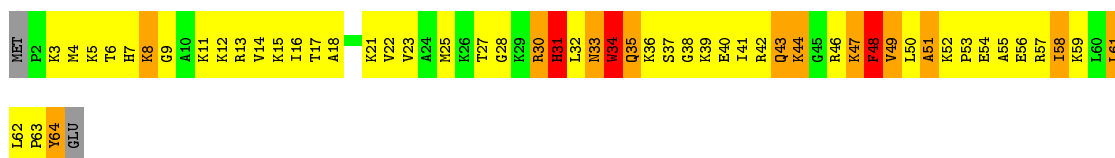
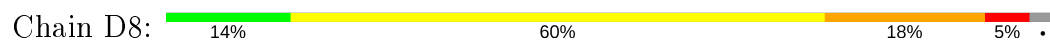


• Molecule 34: 50S RIBOSOMAL PROTEIN L35

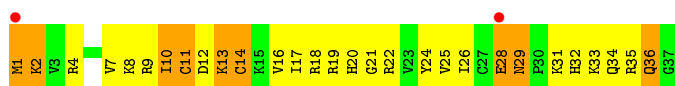




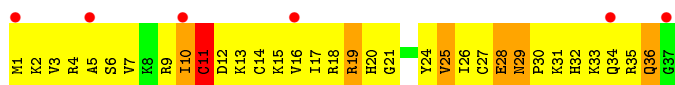
- Molecule 34: 50S RIBOSOMAL PROTEIN L35



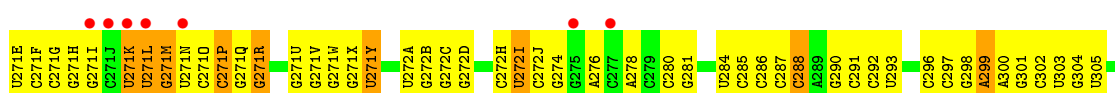
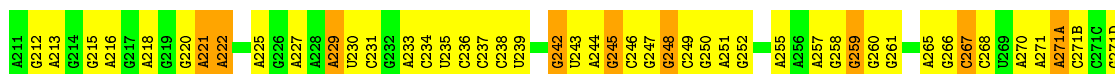
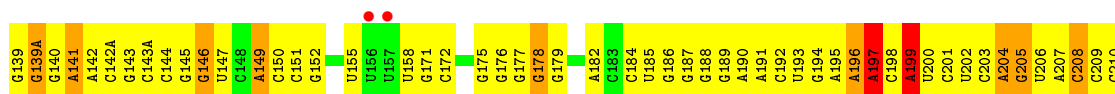
- Molecule 35: 50S RIBOSOMAL PROTEIN L36



- Molecule 35: 50S RIBOSOMAL PROTEIN L36



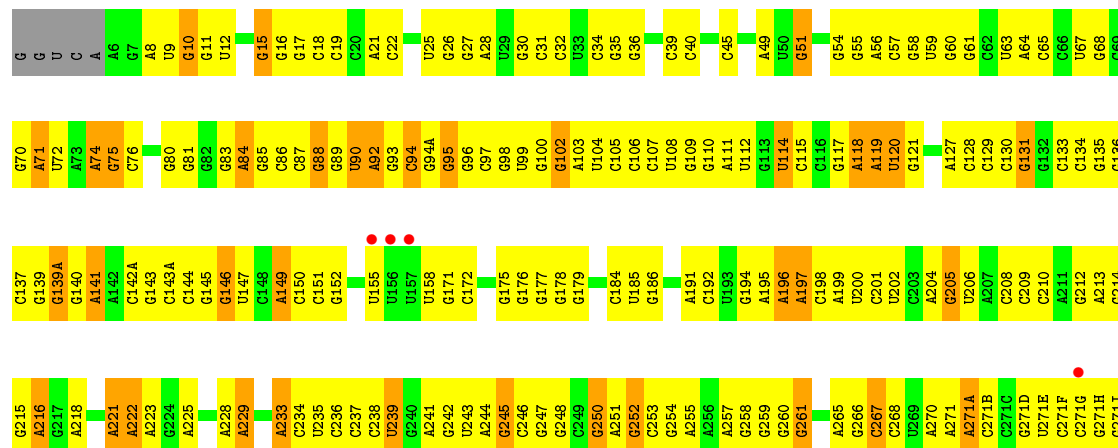
- Molecule 36: 23S RIBOSOMAL RNA





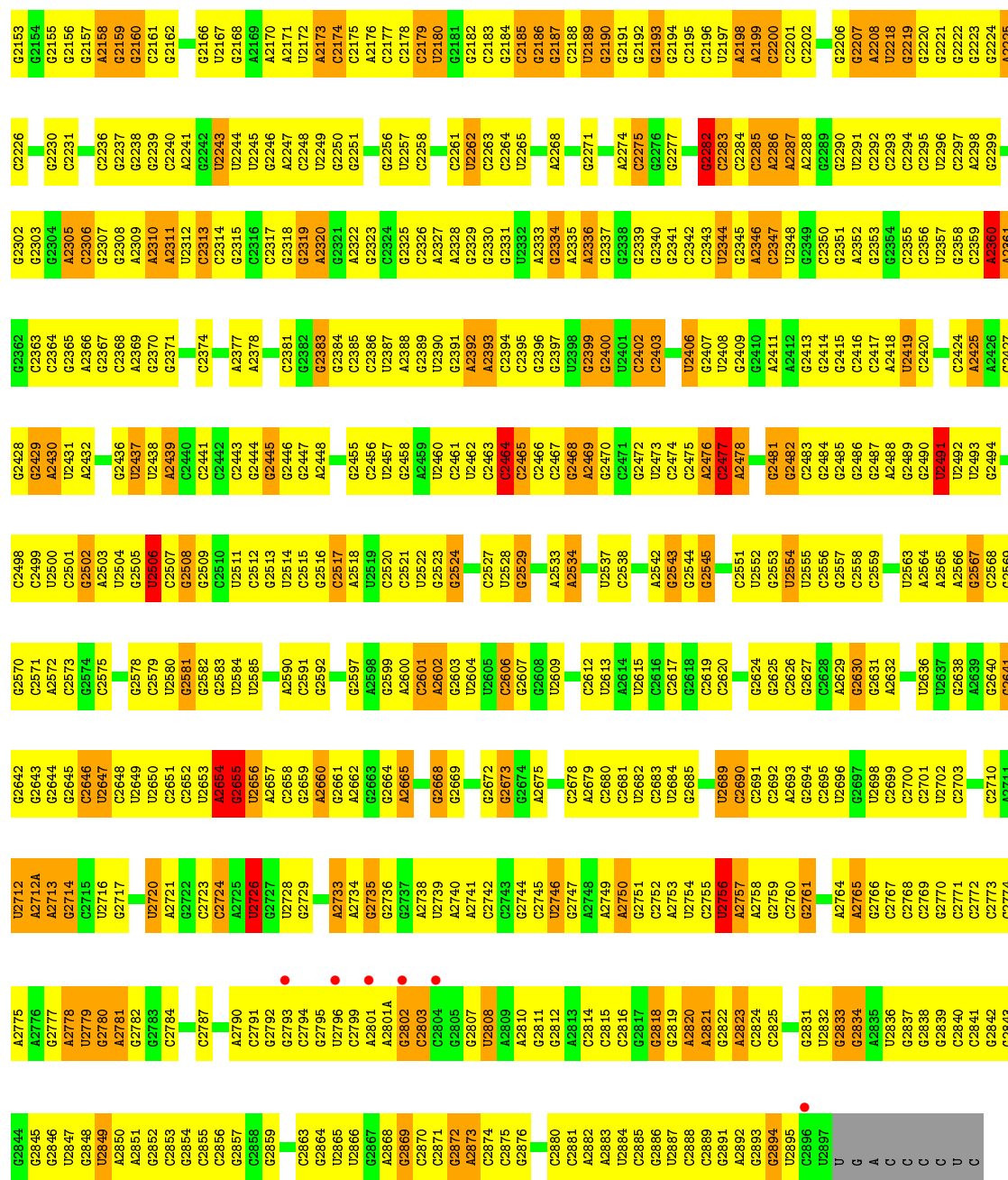






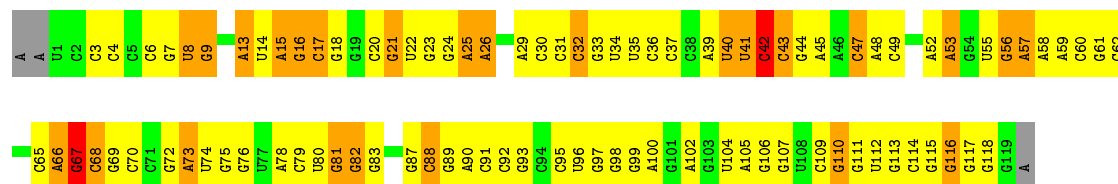
U1094	A1095	A1096	U1097	A1098	C970	C971	A896	C972	A973	C1038	G1039	C975	C1040	G975A	C902	C903	C976	G979	A980	A981	G982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	C1005	C1006	A1009	A1010	A1011	U1012	U1013	U1014	G1018	U1019	A1020	A1021	G1022	U1023	A957	A958	C1024	G1025	A959	A960	C1029	A1029	G1030	G1031	A1032	U1033	U1034	U1035	U1036	C1037	G1038	G1039	C975	G1041	A1045	A1046	A1047	A981	A1048	C1049	A982	A983	A1050	G1051	A984	C1052	C1053	A1054	G1055	A988	G989	A990	A991	G1057	G1058	U1059	U1060	G992	G993	C1061	C1062	C995	A996	G997	C1064	U1065	U1066	A1067	G1068	A1069	A1070	G1071	C1072	A1073	G1074	G1075	C1076	A1077	U1078	C1079	U1081	U1082	A1085	A1086	G1087	A1088	C1089	U1090	C1091	C1092	A1093	U1094	A1095	U1096	A1097	U1098	A1099	U1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	C1108	C1109	G1110	A1111	G1112	U1113	G1114	G1115	C1116	G1117	G1120	C1121	G1122	C1123	C1124	G1125	A1126	A1127	A1128	A1129	U1130	G1131	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	A1142A	A1143	G1144	C1145	C1146	C1147	G1148	A1149	G1150	A1088	G1151	C1152	G1153	C1154	A1155	C271J	U271K	U271L	U271M	U271N	U271O	C271P	U271Q	U271R	G271U	G271V	G271W	U271X	U271Y	U272A	U272B	G272C	G272D	G272E	C272H	U272I	C272J	G272K	G272L	G272M	C272N	C272O	C272P	U272Q	U272R	U272S	U272T	U272U	U272V	U272W	U272X	U272Y	U272Z	U273A	U273B	U273C	U273D	U273E	U273F	U273G	U273H	U273I	U273J	U273K	U273L	U273M	U273N	U273O	U273P	U273Q	U273R	U273S	U273T	U273U	U273V	U273W	U273X	U273Y	U273Z	U274A	U274B	U274C	U274D	U274E	U274F	U274G	U274H	U274I	U274J	U274K	U274L	U274M	U274N	U274O	U274P	U274Q	U274R	U274S	U274T	U274U	U274V	U274W	U274X	U274Y	U274Z	U275A	U275B	U275C	U275D	U275E	U275F	U275G	U275H	U275I	U275J	U275K	U275L	U275M	U275N	U275O	U275P	U275Q	U275R	U275S	U275T	U275U	U275V	U275W	U275X	U275Y	U275Z	U276A	U276B	U276C	U276D	U276E	U276F	U276G	U276H	U276I	U276J	U276K	U276L	U276M	U276N	U276O	U276P	U276Q	U276R	U276S	U276T	U276U	U276V	U276W	U276X	U276Y	U276Z	U277A	U277B	U277C	U277D	U277E	U277F	U277G	U277H	U277I	U277J	U277K	U277L	U277M	U277N	U277O	U277P	U277Q	U277R	U277S	U277T	U277U	U277V	U277W	U277X	U277Y	U277Z	U278A	U278B	U278C	U278D	U278E	U278F	U278G	U278H	U278I	U278J	U278K	U278L	U278M	U278N	U278O	U278P	U278Q	U278R	U278S	U278T	U278U	U278V	U278W	U278X	U278Y	U278Z	U279A	U279B	U279C	U279D	U279E	U279F	U279G	U279H	U279I	U279J	U279K	U279L	U279M	U279N	U279O	U279P	U279Q	U279R	U279S	U279T	U279U	U279V	U279W	U279X	U279Y	U279Z	U280A	U280B	U280C	U280D	U280E	U280F	U280G	U280H	U280I	U280J	U280K	U280L	U280M	U280N	U280O	U280P	U280Q	U280R	U280S	U280T	U280U	U280V	U280W	U280X	U280Y	U280Z	U281A	U281B	U281C	U281D	U281E	U281F	U281G	U281H	U281I	U281J	U281K	U281L	U281M	U281N	U281O	U281P	U281Q	U281R	U281S	U281T	U281U	U281V	U281W	U281X	U281Y	U281Z	U282A	U282B	U282C	U282D	U282E	U282F	U282G	U282H	U282I	U282J	U282K	U282L	U282M	U282N	U282O	U282P	U282Q	U282R	U282S	U282T	U282U	U282V	U282W	U282X	U282Y	U282Z	U283A	U283B	U283C	U283D	U283E	U283F	U283G	U283H	U283I	U283J	U283K	U283L	U283M	U283N	U283O	U283P	U283Q	U283R	U283S	U283T	U283U	U283V	U283W	U283X	U283Y	U283Z	U284A	U284B	U284C	U284D	U284E	U284F	U284G	U284H	U284I	U284J	U284K	U284L	U284M	U284N	U284O	U284P	U284Q	U284R	U284S	U284T	U284U	U284V	U284W	U284X	U284Y	U284Z	U285A	U285B	U285C	U285D	U285E	U285F	U285G	U285H	U285I	U285J	U285K	U285L	U285M	U285N	U285O	U285P	U285Q	U285R	U285S	U285T	U285U	U285V	U285W	U285X	U285Y	U285Z	U286A	U286B	U286C	U286D	U286E	U286F	U286G	U286H	U286I	U286J	U286K	U286L	U286M	U286N	U286O	U286P	U286Q	U286R	U286S	U286T	U286U	U286V	U286W	U286X	U286Y	U286Z	U287A	U287B	U287C	U287D	U287E	U287F	U287G	U287H	U287I	U287J	U287K	U287L	U287M	U287N	U287O	U287P	U287Q	U287R	U287S	U287T	U287U	U287V	U287W	U287X	U287Y	U287Z	U288A	U288B	U288C	U288D	U288E	U288F	U288G	U288H	U288I	U288J	U288K	U288L	U288M	U288N	U288O	U288P	U288Q	U288R	U288S	U288T	U288U	U288V	U288W	U288X	U288Y	U288Z	U289A	U289B	U289C	U289D	U289E	U289F	U289G	U289H	U289I	U289J	U289K	U289L	U289M	U289N	U289O	U289P	U289Q	U289R	U289S	U289T	U289U	U289V	U289W	U289X	U289Y	U289Z	U290A	U290B	U290C	U290D	U290E	U290F	U290G	U290H	U290I	U290J	U290K	U290L	U290M	U290N	U290O	U290P	U290Q	U290R	U290S	U290T	U290U	U290V	U290W	U290X	U290Y	U290Z	U291A	U291B	U291C	U291D	U291E	U291F	U291G	U291H	U291I	U291J	U291K	U291L	U291M	U291N	U291O	U291P	U291Q	U291R	U291S	U291T	U291U	U291V	U291W	U291X	U291Y	U291Z	U292A	U292B	U292C	U292D	U292E	U292F	U292G	U292H	U292I	U292J	U292K	U292L	U292M	U292N	U292O	U292P	U292Q	U292R	U292S	U292T	U292U	U292V	U292W	U292X	U292Y	U292Z	U293A	U293B	U293C	U293D	U293E	U293F	U293G	U293H	U293I	U293J	U293K	U293L	U293M	U293N	U293O	U293P	U293Q	U293R	U293S	U293T	U293U	U293V	U293W	U293X	U293Y	U293Z	U294A	U294B	U294C	U294D	U294E	U294F	U294G	U294H	U294I	U294J	U294K	U294L	U294M	U294N	U294O	U294P	U294Q	U294R	U294S	U294T	U294U	U294V	U294W	U294X	U294Y	U294Z	U295A	U295B	U295C	U295D	U295E	U295F	U295G	U295H	U295I	U295J	U295K	U295L	U295M	U295N	U295O	U295P	U295Q	U295R	U295S	U295T	U295U	U295V	U295W	U295X	U295Y	U295Z	U296A	U296B	U296C	U296D	U296E	U296F	U296G	U296H	U296I	U296J	U296K	U296L	U296M	U296N	U296O	U296P	U296Q	U296R	U296S	U296T	U296U	U296V	U296W	U296X	U296Y	U296Z	U297A	U297B	U297C	U297D	U297E	U297F	U297G	U297H	U297I	U297J	U297K	U297L	U297M	U297N	U297O	U297P	U297Q	U297R	U297S	U297T	U297U	U297V	U297W	U297X	U297Y	U297Z	U298A	U298B	U298C	U298D	U298E	U298F	U298G	U298H	U298I	U298J	U298K	U298L	U298M	U298N	U298O	U298P	U298Q	U298R	U298S	U298T	U298U	U298V	U298W	U298X	U298Y	U298Z	U299A	U299B	U299C	U299D	U299E	U299F	U299G	U299H	U299I	U299J	U299K	U299L	U299M	U299N	U299O	U299P	U299Q	U299R	U299S	U299T	U299U	U299V	U299W	U299X	U299Y	U299Z	U300A	U300B	U300C	U300D	U300E	U300F	U300G	U300H	U300I	U300J	U300K	U300L	U300M	U300N	U300O	U300P	U300Q	U300R	U300S	U300T	U300U	U300V	U300W	U300X	U300Y	U300Z	U301A	U301B	U301C	U301D	U301E	U301F	U301G	U301H	U301I	U301J	U301K	U301L	U301M	U301N	U301O	U301P	U301Q	U301R	U301S	U301T	U301U	U301V	U301W	U301X	U301Y	U301Z	U302A	U302B	U302C	U302D	U302E	U302F	U302G	U302H	U302I	U302J	U302K	U302L	U302M	U302N	U302O	U302P	U302Q	U302R	U302S	U302T	U302U	U302V	U302W	U302X	U302Y	U302Z	U303A	U303B	U303C	U303D	U303E	U303F	U303G	U303H	U303I	U303J	U303K	U303L	U303M	U303N	U303O	U303P	U303Q	U303R	U303S	U303T	U303U	U303V	U303W	U303X	U303Y	U303Z	U304A	U304B	U304C	U304D	U304E	U304F	U304G	U304H	U304I	U304J	U304K	U304L	U304M	U304N	U304O	U304P	U304Q	U304R	U304S	U304T	U304U	U304V	U304W	U304X	U304Y	U304Z	U305A	U305B	U305C	U305D	U305E	U305F	U305G	U305H	U305I	U305J	U305K	U305L	U305M	U305N	U305O	U305P	U305Q	U305R	U305S	U305T	U305U	U305V	U305W	U305X	U305Y	U305Z	U306A	U306B	U306C	U306D	U306E	U306F	U306G	U306H	U306I	U306J	U306K	U306L	U306M	U306N	U306O	U306P	U306Q	U306R	U306S	U306T	U306U	U306V	U306W	U306X	U306Y	U306Z	U307A	U307B	U307C	U307D	U307E	U307F	U307G	U307H	U307I	U307J	U307K	U307L	U307M	U307N	U307O	U307P	U307Q	U307R	U307S	U307T	U307U	U307V	U307W	U307X	U307Y	U307Z	U308A	U308B	U308C	U308D	U308E	U308F	U308G	U308H	U308I	U308J	U308K	U308L	U308M	U308N	U308O	U308P	U308Q	U308R	U308S	U308T	U308U	U308V	U308W	U308X	U308Y	U308Z	U309A	U309B	U309C	U309D	U309E	U309F	U309G	U309H	U309I	U309J	U309K	U309L	U309M	U309N	U309O	U309P	U309Q	U309R	U309S	U309T	U309U	U309V	U309W	U309X	U309Y	U309Z	U310A	U310B	U310C	U310D	U310E	U310F	U310G	U310H	U310I	U310J	U310K	U310L	U310M	U310N	U310O	U310P	U310Q	U310R	U310S	U310T	U310U	U310V	U310W	U310X	U310Y	U310Z	U311A	U311B	U311C	U311D	U311E	U311F	U311G	U311H	U311I	U311J	U311K	U311L	U311M	U311N	U311O	U311P	U311Q	U311R	U311S	U311T	U311U	U311V	U311W	U311X	U311Y	U311Z	U312A	U312B	U312C	U312D
-------	-------	-------	-------	-------	------	------	------	------	------	-------	-------	------	-------	-------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	------	------	-------	-------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	------	-------	-------	-------	-------	------	-------	-------	------	------	-------	-------	------	-------	-------	-------	-------	------	------	------	------	-------	-------	-------	-------	------	------	-------	-------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	--------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

U2016	G1863	G1792	U1639	A1569	C1505	U1431	C1363	G1222	A1156
U2017	U1864	C1793	C1640	A1570	C1506	C1432	G1364	G1223	U1159
G2018	C1865	C1794	A1641	A1571	C1509	U1433	A1385	U1226	G1163
A2019	C1866	C1795	G1642	A1572	A1509A	U1434	A1386	G1227	A1302
A2020	A1876	U1796	G1643	C1573	A1509B	G1441	A1367	G1231	G1164
G2021	C1877	C1797	C1644	C1574	G1510	G1442	G1368	G1232	U1165
U2022	G1878	U1798	U1645	U1575	C1511	G1443	G1369	G1233	U1166
G2023	C1879	U1799	G1647	U1576	U1511	G1444	G1374	U1237	U1167
G2024	C1880	C1800	C1648	A1577	G1515	G1445	G1375	A1242	G1170
G2025	C1881	G1801	G1649	A1580	G1516	U1445	C1376	G1243	G1173
C2026	C1882	A1802	G1650	G1581	G1517	C1445A	C1377	G1244	U1174
C2027	G1883	U1803	G1651	C1582	U1517	C1446	C1378	G1245	A1175
G2028	A1884	C1804	A1652	A1583	U1518	G1447	A1379	G1246	G1176
G2029	A1885	U1805	G1653	C1584	U1519	G1448	A1380	G1247	A1177
A2030	C1886	U1806	A1654	A1586	U1520	G1449	G1381	A1248	C1178
G2031	C1887	G1807	C1655	A1587	A1521	A1450	G1382	U1249	G1180
G2032	G1888	G1811	C1656	C1588	G1525	U1451	G1383	G1250	A1181
A2033	A1889	A1812	G1657	C1589	G1526	C1452	G1384	G1251	A1182
U2034	A1890	G1813	C1658	U1590	G1527	U1453	A1385	G1252	G1183
G2035	C1891	U1814	U1659	G1591	A1528	G1454	G1386	G1253	G1184
C2036	C1892	G1815	C1660	C1592	A1529	G1455	G1387	U1254	C1185
G2037	C1893	U1816	G1661	G1593	G1530	U1456	G1388	G1255	G1186
G2038	U1894	U1817	U1662	U1594	C1531	G1457	G1389	G1256	G1187
C2039	G1895	A1818	A1663	G1595	C1532	G1458	U1390	G1257	U1188
C2040	A1900	U1819	A1664	A1596	C1533	G1459	G1391	G1258	A1189
G2041	C1901	A1820	A1665	A1597	G1534	A1460	G1392	G1259	G1190
G2042	A1902	A1821	G1666	C1598	U1534	G1461	G1393	G1260	G1191
C2043	C1903	G1822	C1667	C1599	U1535	G1462	U1394	U1261	G1192
C2044	G1904	U1823	A1668	C1600	G1536	U1463	G1395	G1193	G1196
A2045	G1905	C1824	C1669	G1601	U1537	G1464	A1396	G1197	G1197
G2046	G1906	G1825	U1670	U1602	G1538	G1465	G1397	U1198	U1198
G2047	G1907	U1826	U1671	U1603	U1539	G1466	G1401	U1199	C1200
C2048	C1908	C1830	C1672	A1603	U1540	G1467	G1402	G1201	G1201
C2049	C1909	G1831	U1673	C1607	G1541	G1468	C1403	U1271	G1202
G2050	C1910	U1832	G1674	A1608	A1542	G1469	C1404	U1272	G1203
A2051	U1911	U1833	G1675	A1609	C1543	G1470	A1398	U1273	A1204
G2052	A1912	U1834	A1676	A1610	A1544	G1471	G1399	A1274	U1205
C2053	C1913	G1835	A1677	A1611	U1545	G1472	U1405	G1278	C1208
C2054	U1914	C1836	G1678	G1811	C1546	G1473	U1406	G1279	G1209
C2055	U1915	C1837	U1679	C1612	C1547	G1474	C1407	U1283	U1211
C2056	C1916	U1841	U1680	G1613	U1548	G1475	C1408	A1284	G1212
A2057	U1917	G1842	G1681	A1614	C1549	G1476	C1409	G1285	A1213
C2058	A1918	U1843	G1682	C1615	U1549	G1477	G1410	A1286	A1214
G2059	C1919	G1844	G1683	A1616	C1550	G1478	G1411	G1287	G1215
G2060	C1920	U1845	U1684	C1617	C1551	G1479	C1412	G1288	G1216
A2061	G1921	G1846	C1685	A1618	G1552	G1480	G1413	G1289	C1217
G2062	C1922	A1847	U1686	G1619	A1553	A1490	G1414	C1290	C1218
C2063	U1923	G1848	A1689	C1625	U1554	G1491	G1415	G1291	G1221
C2064	A1924	U1849	C1690	G1626	G1555	G1492	G1416	C1297	G1221A
C2065	G1925	U1851	U1692	G1627	C1556	G1493	G1417		
U2066	U1926	U1852	U1693	G1628	C1557	A1494	A1419		
G2067	G1927	C1853	U1694	U1629	A1558	A1495	U1420		
A2068	C1928	A1854	G1695	G1630	U1559	A1496	G1423		
G2069	U1929	U1855	G1696	C1631	G1560	U1497	G1424		
G2070	G1930	U1856	G1697	A1632	G1561	C1498	G1425		
A2071	U1931	G1857	A1698	G1633	U1562	C1499	G1426		
G2072	C1932	U1858	C1699	G1634	G1563	G1500	G1427		
C2073	G1933	G1859	G1700	G1635	U1564	C1501	A1428		
U2074	C1934	A1859	A1701	C1636	C1565	C1502	G1429		
G2075	U1935	U1860	G1702	G1637	G1566	U1503	G1430		
C2076	G1936	G1861		C1638	G1568	C1504			
C2077	A1937	U1862							
C2078	C1938	U1863							
G2079	U1939	G1864							
C2080	C1940	U1865							
A2081	G1941	U1866							
G2082	C1942	U1867							
C2083	U1943	U1868							
C2084	C1944	U1869							
A2085	G1945	U1870							
C2086	U1946	U1871							
G2087	C1947	U1872							
C2088	U1948	U1873							
G2089	C1949	U1874							
U2090	U1950	U1875							
U2091	C1951	U1876							
U2092	U1952	U1877							
U2093	C1953	U1878							
U2094	U1954	U1879							
U2095	C1955	U1880							
U2096	U1956	U1881							
U2097	C1957	U1882							
U2098	U1958	U1883							
U2099	C1959	U1884							
U2100	U1960	U1885							
U2101	C1961	U1886							
U2102	U1962	U1887							
U2103	C1963	U1888							
U2104	U1964	U1889							
U2105	C1965	U1890							
U2106	U1966	U1891							
U2107	C1967	U1892							
U2108	U1968	U1893							
U2109	C1969	U1894							
U2110	U1970	U1895							
U2111	C1971	U1896							
U2112	U1972	U1897							
U2113	C1973	U1898							
U2114	U1974	U1899							
U2115	C1975	U1900							
U2116	U1976	U1901							
U2117	C1977	U1902							
U2118	U1978	U1903							
U2119	C1979	U1904							
U2120	U1980	U1905							
U2121	C1981	U1906							
U2122	U1982	U1907							
U2123	C1983	U1908							
U2124	U1984	U1909							
U2125	C1985	U1910							
U2126	U1986	U1911							
U2127	C1987	U1912							
U2128	U1988	U1913							
U2129	C1989	U1914							
U2130	U1990	U1915							
U2131	C1991	U1916							
U2132	U1992	U1917							
U2133	C1993	U1918							
U2134	U1994	U1919							
U2135	C1995	U1920							
U2136	U1996	U1921							
U2137	C1997	U1922							
U2138	U1998	U1923							
U2139	C1999	U1924							
U2140	U2000	U1925							
U2141	C2001	U1926							
U2142	U2002	U1927							
U2143	C2003	U1928							
U2144	U2004	U1929							
U2145	C2005	U1930							
U2146	U2006	U1931							
U2147	C2007	U1932							
U2148	U2008	U1933							
U2149	C2009	U1934							
U2150	U2010	U1935							
U2151	C2011	U1936							
U2152	U2012	U1937							
U2153	C2013	U1938							
U2154	U2014	U1939							
U2155	C2015	U1940							
U2156	U2016	U1941							
U2157	C2017	U1942							
U2158	U2018	U1943							
U2159	C2019	U1944							
U2160	U2019	U1945							
U2161	C2020	U1946							
U2162	U2020	U1947							
U2163	C2021	U1948							
U2164	U2021	U1949							
U2165	C2022	U1950							
U2166	U2022	U1951							
U2167	C2023	U1952							
U2168	U2023	U1953							
U2169	C2024	U1954							
U2170	U2024	U1955							
U2171	C2025	U1956							
U2172	U2025	U1957							
U2173	C2026	U1958							
U2174	U2026	U1959							
U2175	C2027	U1960							
U2176	U2027	U1961							
U2177	C2028	U1962							
U2178	U2028	U1963							
U2179	C2029	U1964							
U2180	U2029	U1965							

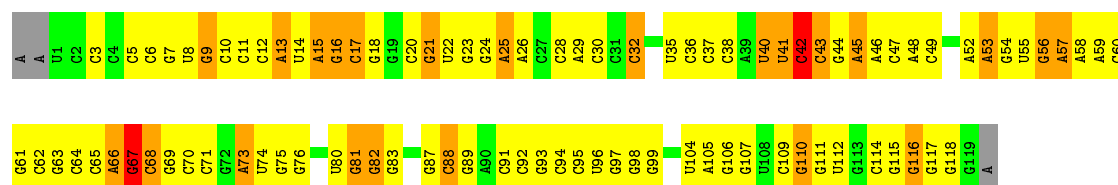


• Molecule 37: 5S RIBOSOMAL RNA

Chain BB:

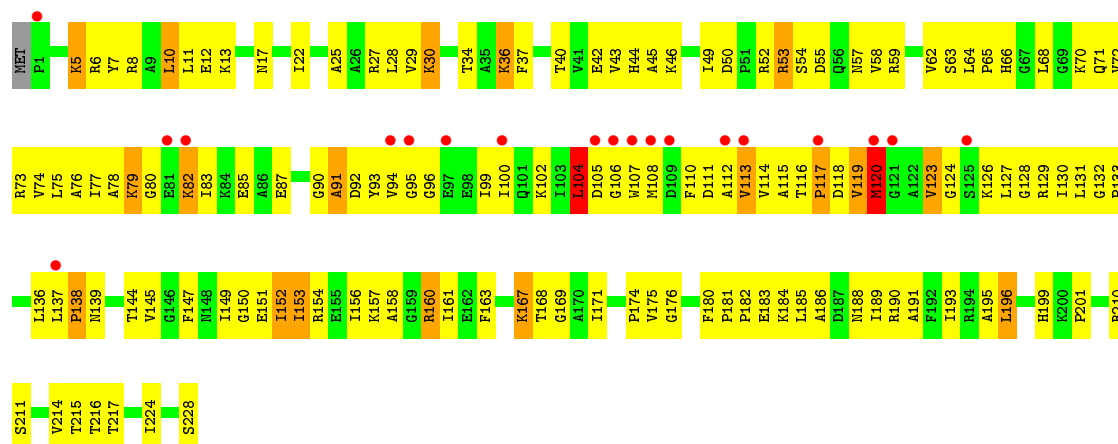


Chain DB: 



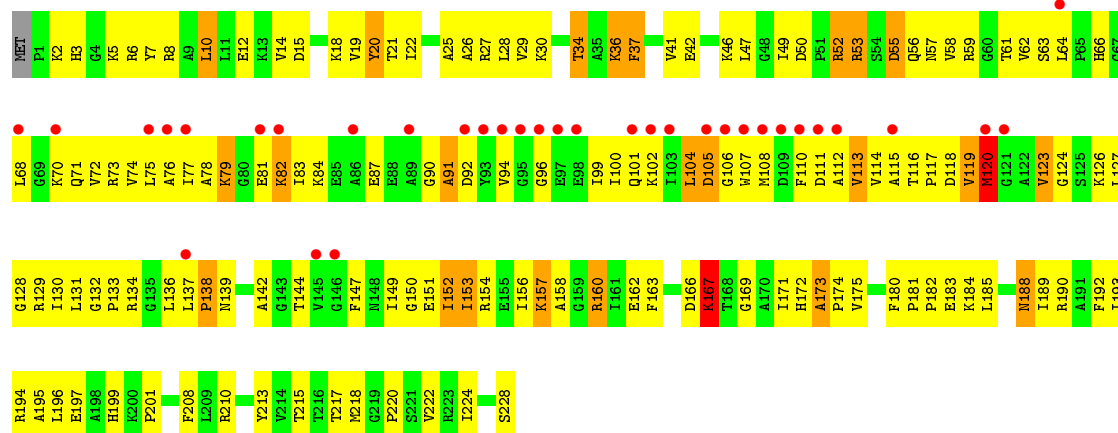
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

Chain BC: 

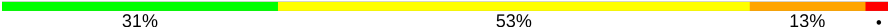


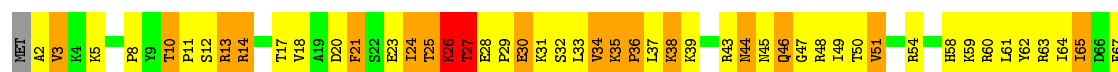
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

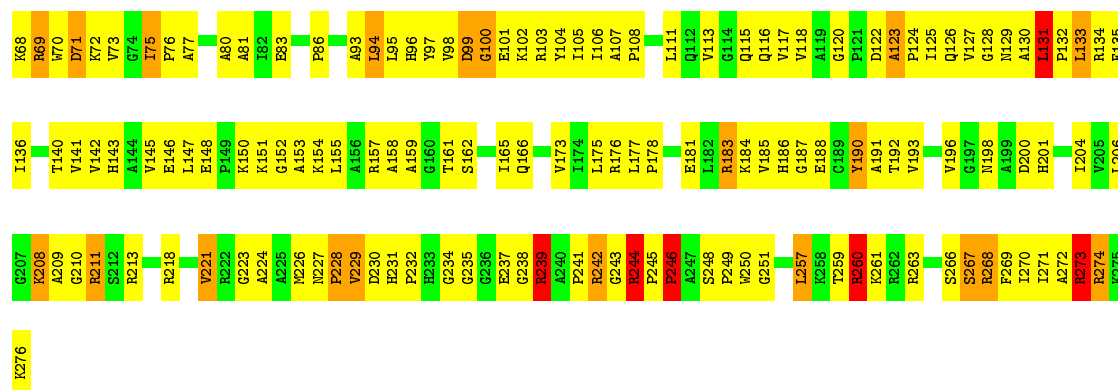
Chain DC: 



• Molecule 39: 50S RIBOSOMAL PROTEIN L2

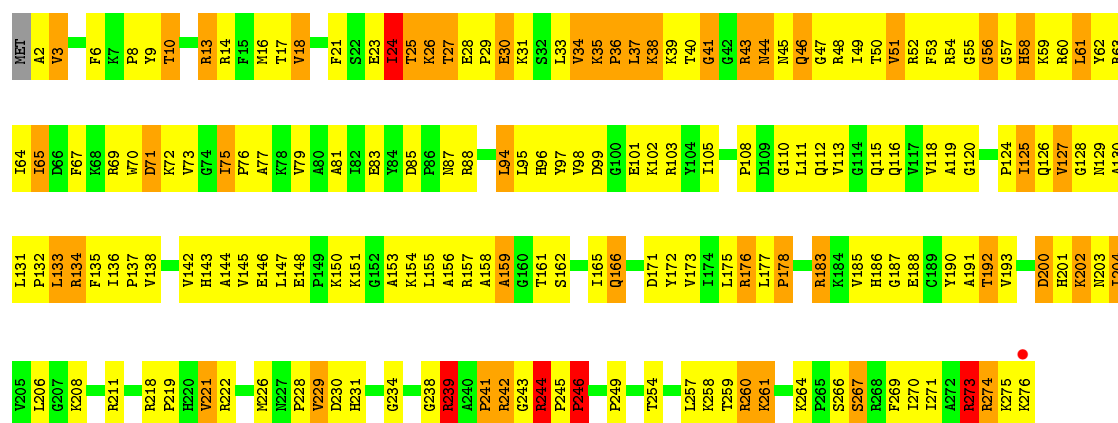
Chain BD: 





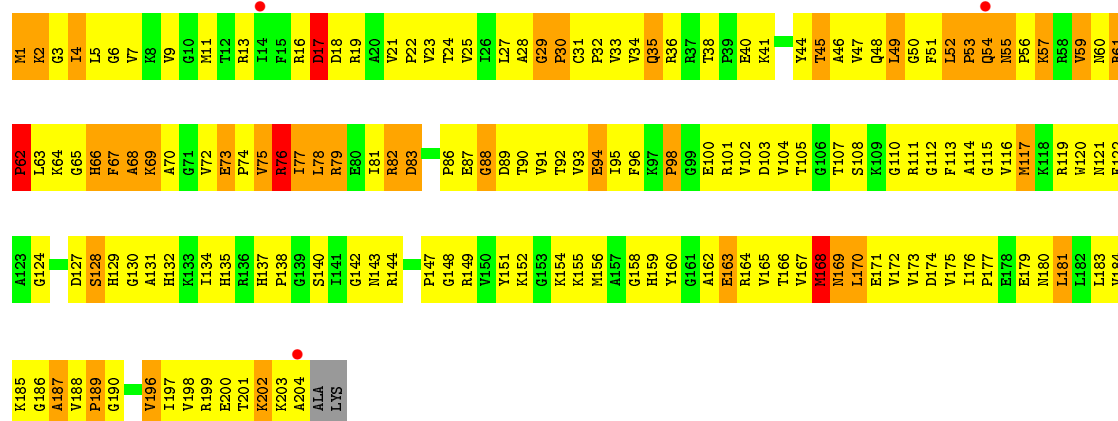
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

Chain DD: 34% 47% 17% .



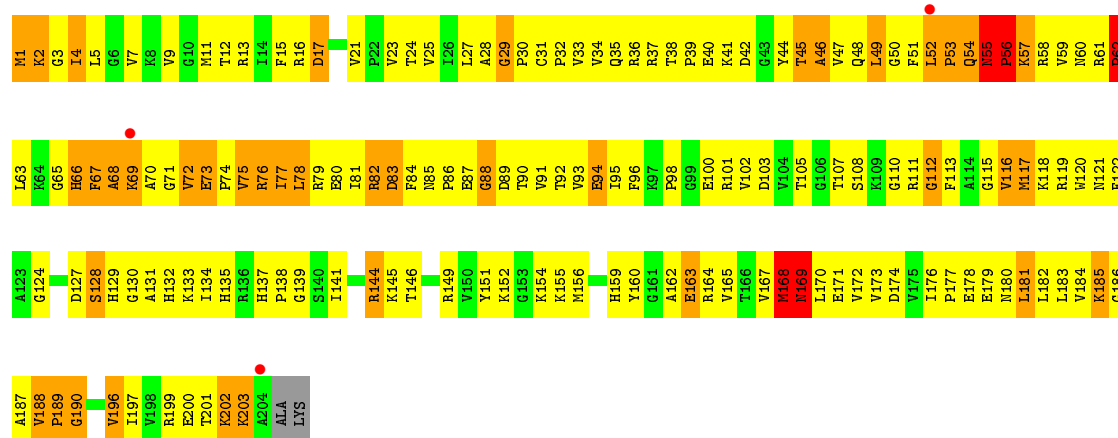
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain BE: 20% 58% 19% . .

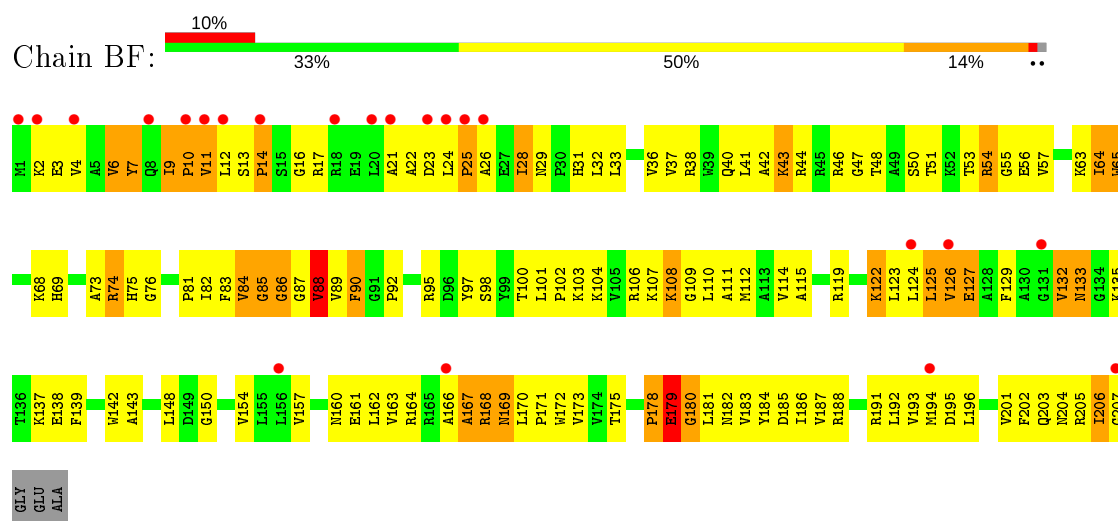


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

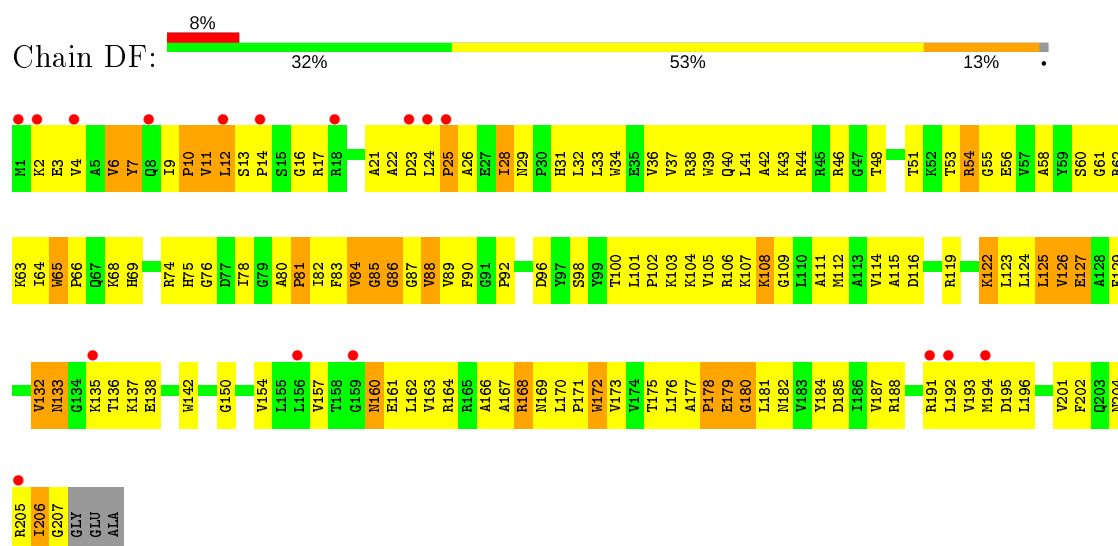
Chain DE: 19% 58% 19% . .



• Molecule 41: 50S RIBOSOMAL PROTEIN L4

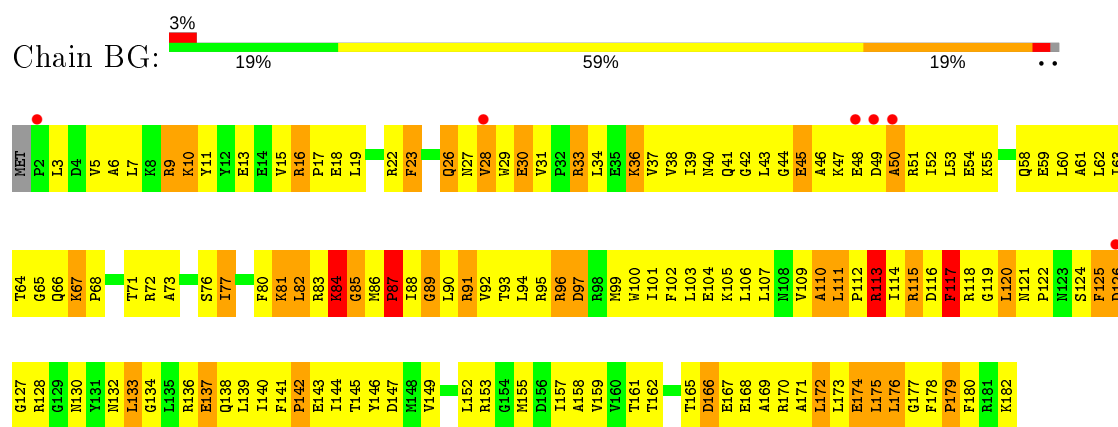


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

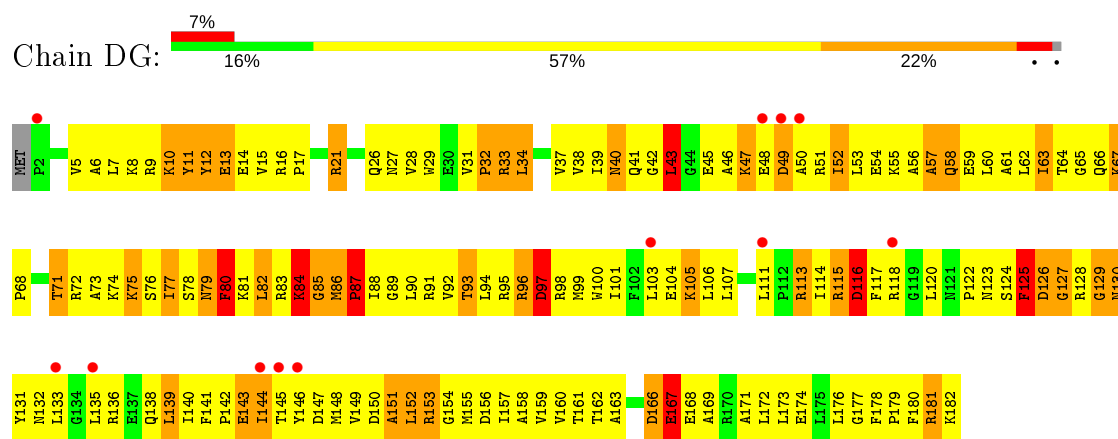


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

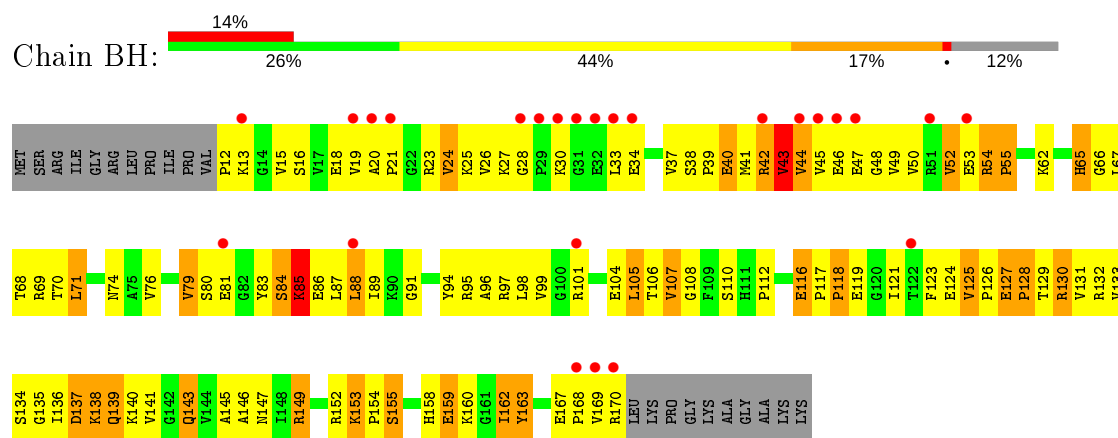




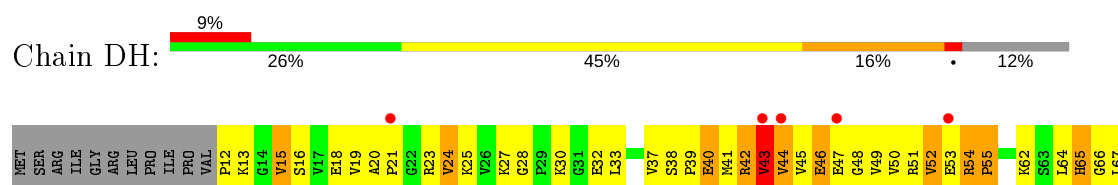
• Molecule 42: 50S RIBOSOMAL PROTEIN L5



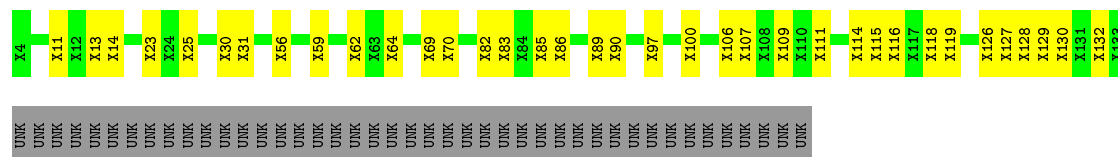
• Molecule 43: 50S RIBOSOMAL PROTEIN L6



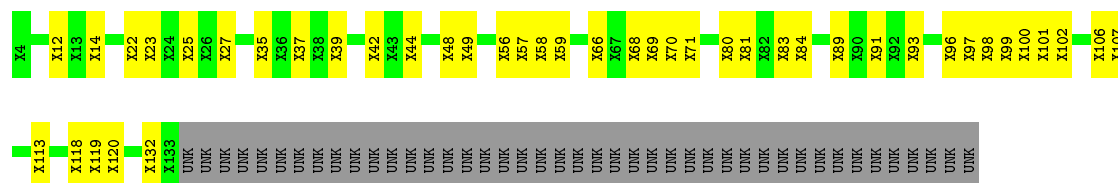
• Molecule 43: 50S RIBOSOMAL PROTEIN L6



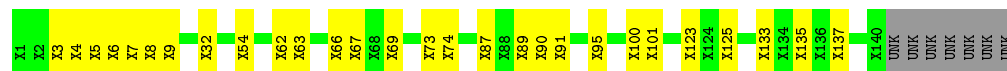
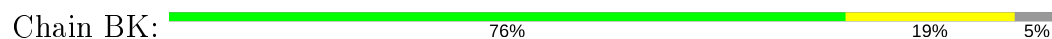
● Molecule 44: 50S RIBOSOMAL PROTEIN L10



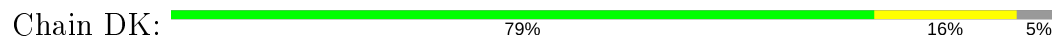
• Molecule 44: 50S RIBOSOMAL PROTEIN L10



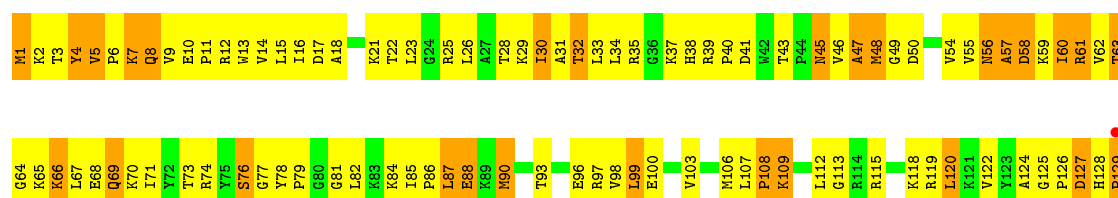
- Molecule 45: 50S RIBOSOMAL PROTEIN L11

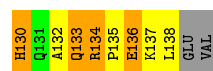


- Molecule 45: 50S RIBOSOMAL PROTEIN L11

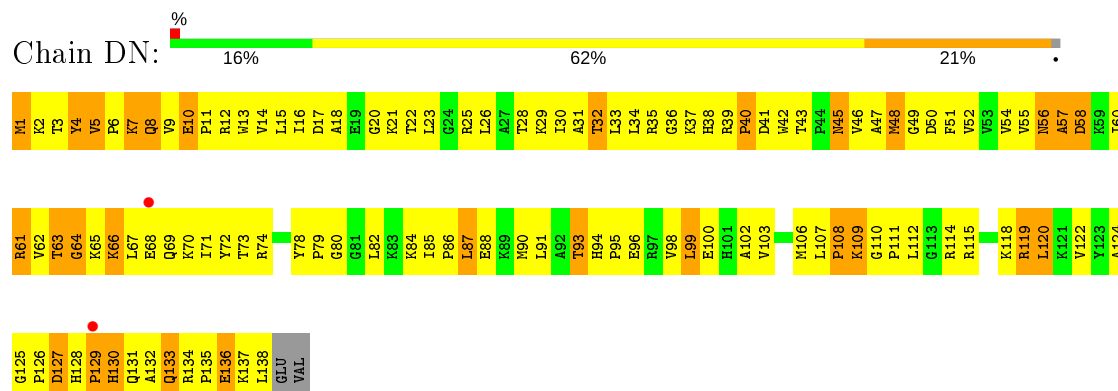


- Molecule 46: 50S RIBOSOMAL PROTEIN L13

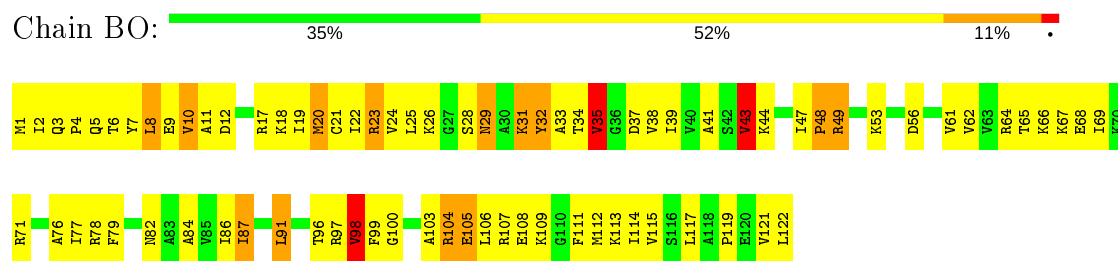




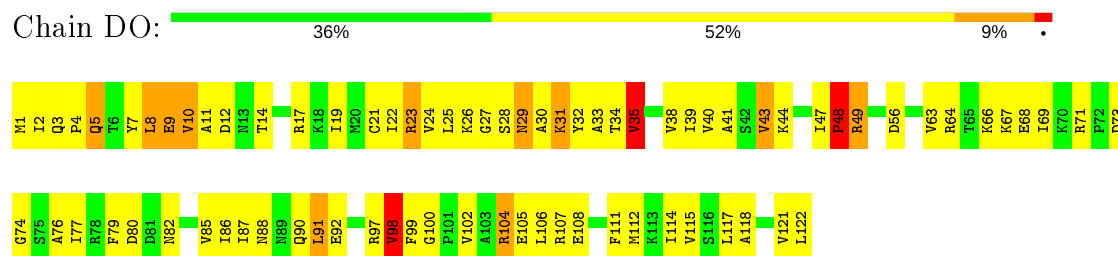
• Molecule 46: 50S RIBOSOMAL PROTEIN L13



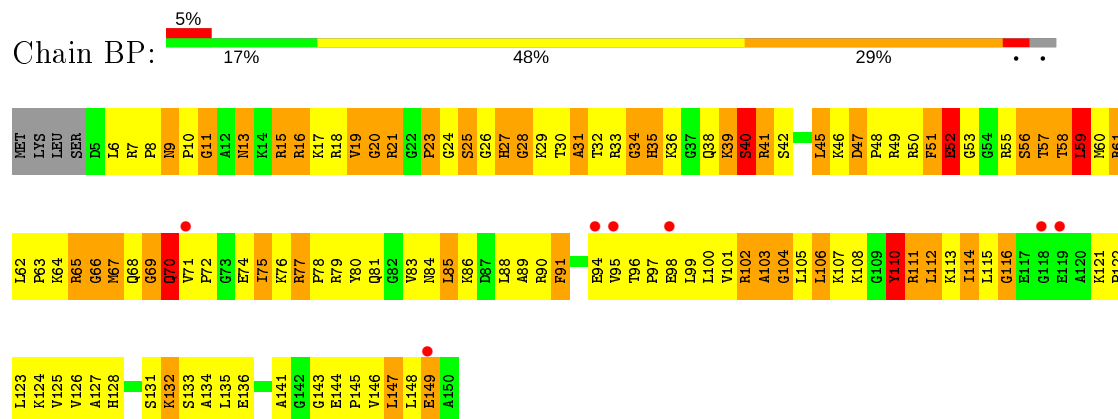
• Molecule 47: 50S RIBOSOMAL PROTEIN L14




• Molecule 47: 50S RIBOSOMAL PROTEIN L14

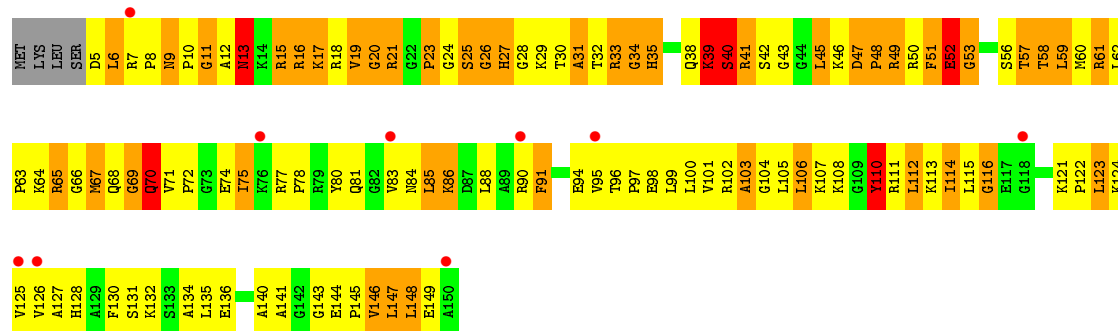


• Molecule 48: 50S RIBOSOMAL PROTEIN L15



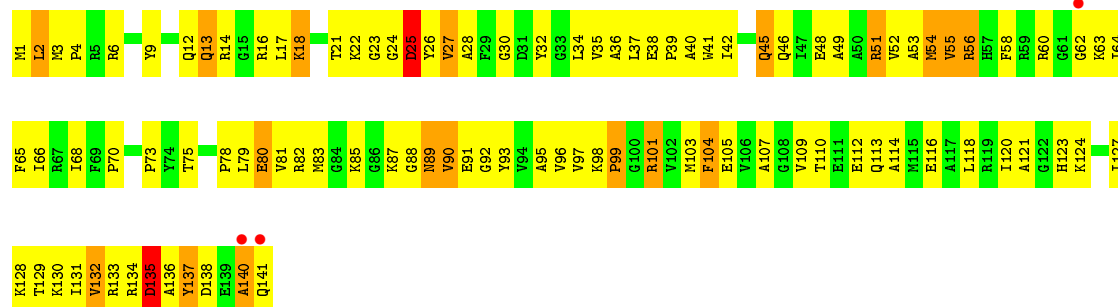
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP: 



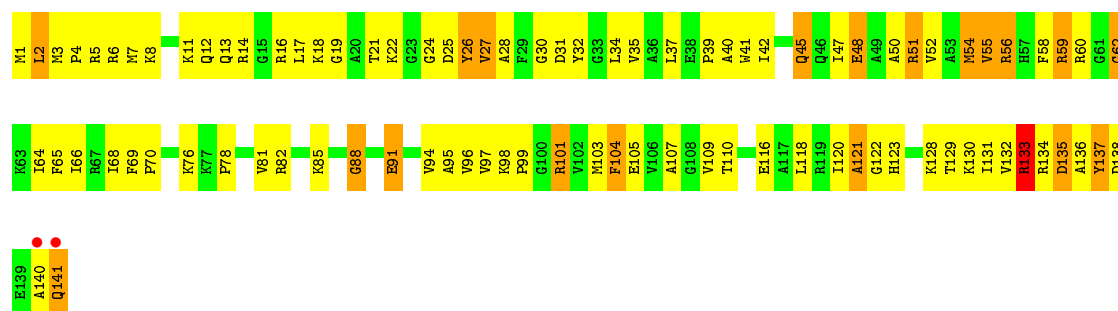
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ: 



• Molecule 49: 50S RIBOSOMAL PROTEIN L16

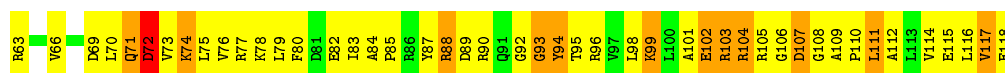
Chain DQ: 



• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain BR: 





• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain DR: 18% 55% 24%



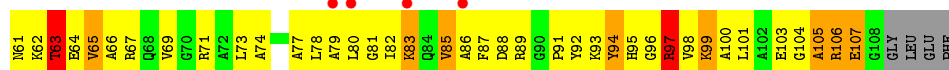
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS: 4% 13% 54% 19% 13%



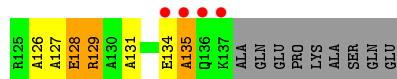
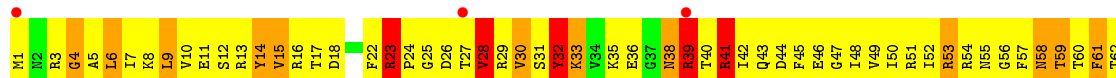
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain DS: 4% 13% 50% 22% 13%



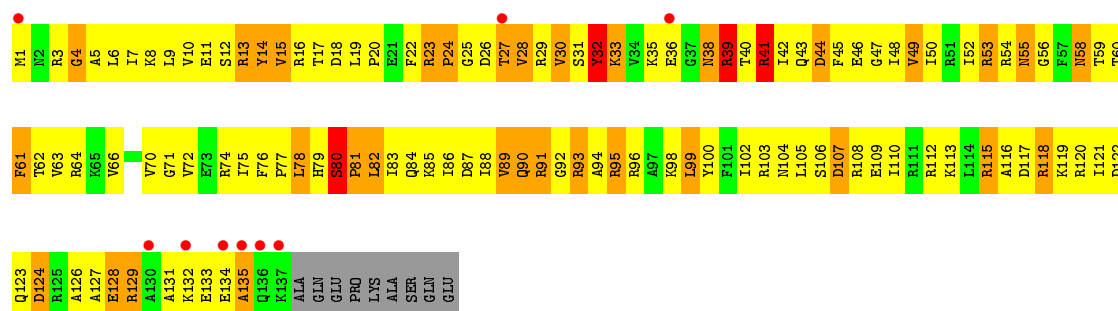
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain BT: 5% 15% 56% 17% 5% 6%

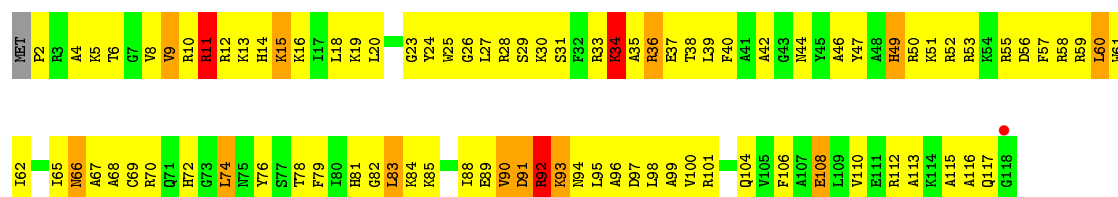


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

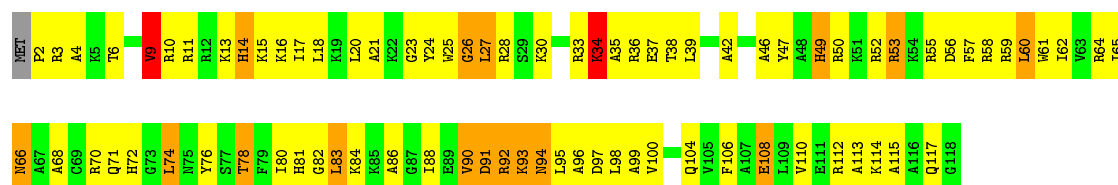
Chain DT: 6% 13% 55% 23% 6%



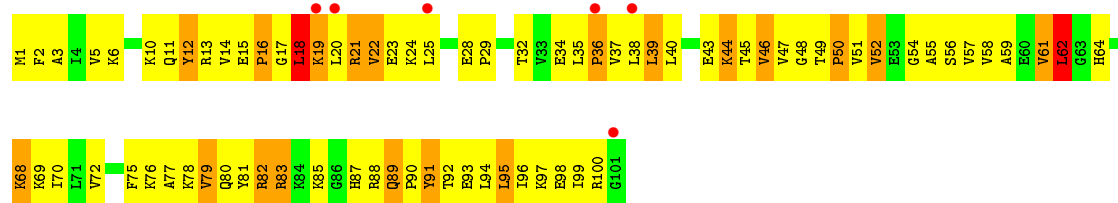
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



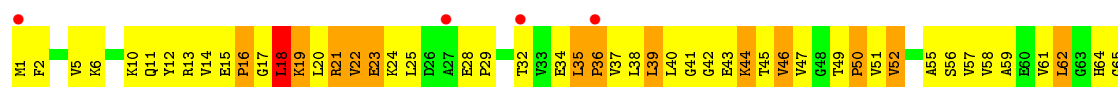
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

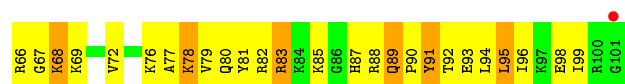


• Molecule 54: 50S RIBOSOMAL PROTEIN L21

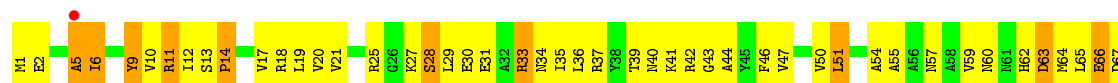


• Molecule 54: 50S RIBOSOMAL PROTEIN L21





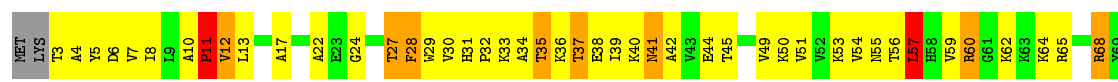
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



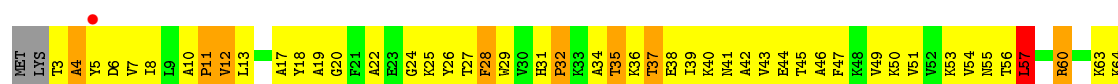
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



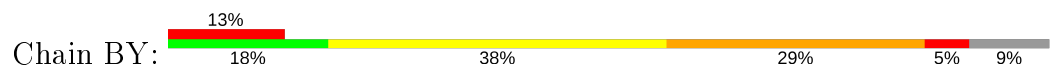
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

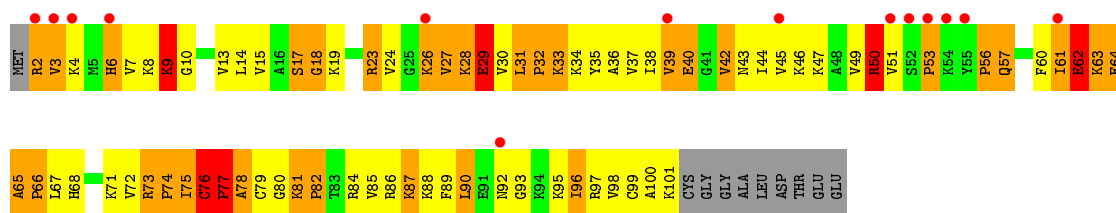


• Molecule 56: 50S RIBOSOMAL PROTEIN L23

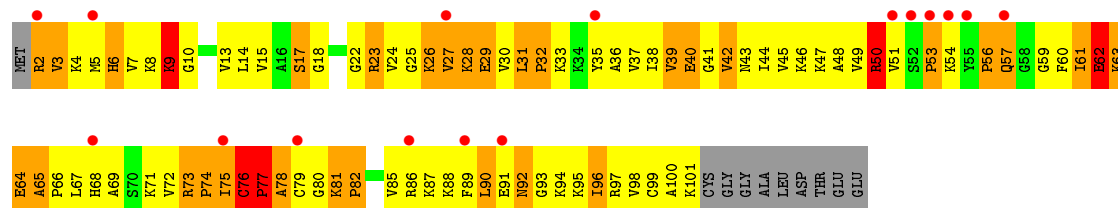
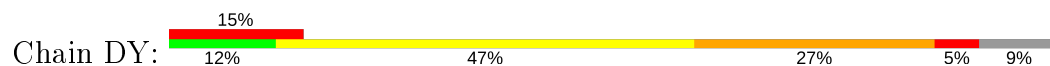


• Molecule 57: 50S RIBOSOMAL PROTEIN L24

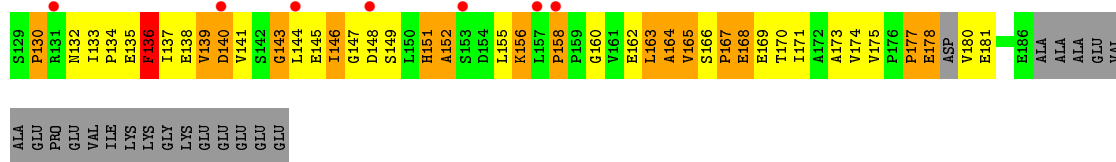
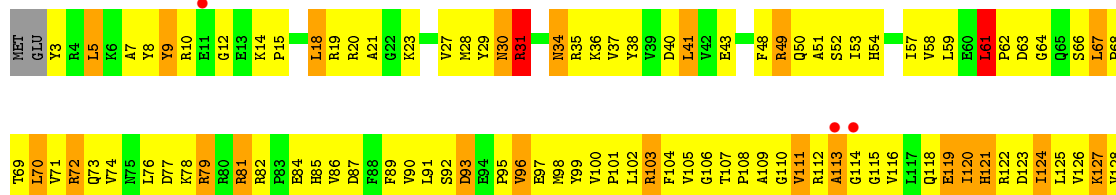
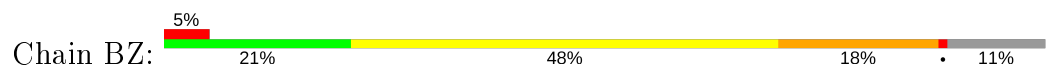




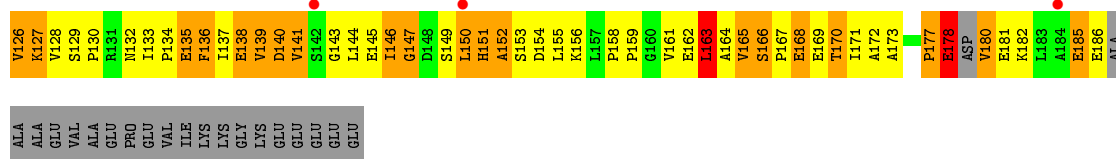
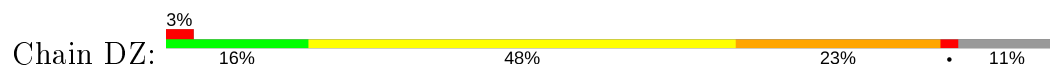
• Molecule 57: 50S RIBOSOMAL PROTEIN L24



• Molecule 58: 50S RIBOSOMAL PROTEIN L25



• Molecule 58: 50S RIBOSOMAL PROTEIN L25





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	289.80Å 269.10Å 403.90Å 90.00° 91.22° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.83 – 2.93	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-3.10) 89.6 (49.83-2.93)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.96Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.247 , 0.285 0.246 , 0.283	Depositor DCC
$R_{free}$ test set	58969 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.3	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	307196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

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

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

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

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

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

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

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

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

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

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

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

5 of 15 chirality outliers are listed below:

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

5 of 440 planarity outliers are listed below:

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

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1145	0
1	CA	32329	0	16317	1398	0
2	AB	1900	0	1951	238	3
2	CB	1900	0	1951	239	3
3	AC	1612	0	1677	194	0
3	CC	1612	0	1677	201	0
4	AD	1703	0	1765	251	0
4	CD	1703	0	1763	265	0
5	AE	1146	0	1207	111	0
5	CE	1146	0	1207	159	0
6	AF	843	0	857	75	0
6	CF	843	0	857	82	0
7	AG	1257	0	1296	81	0
7	CG	1257	0	1296	109	0
8	AH	1116	0	1177	72	0
8	CH	1116	0	1177	99	0
9	AI	1010	0	1037	145	0
9	CI	1010	0	1037	159	0

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B4	340	0	336	62	0
30	D4	340	0	337	55	0
31	B5	459	0	480	90	0
31	D5	459	0	480	73	0
32	B6	433	0	461	134	0
32	D6	433	0	461	134	0
33	B7	418	0	467	37	0
33	D7	418	0	467	31	0
34	B8	507	0	576	115	0
34	D8	507	0	576	130	0
35	B9	307	0	336	53	0
35	D9	307	0	338	83	0
36	BA	62477	0	31497	2434	0
36	DA	62477	0	31497	2526	0
37	BB	2551	0	1295	127	0
37	DB	2551	0	1295	122	0
38	BC	1742	0	1800	167	3
38	DC	1742	0	1800	184	3
39	BD	2145	0	2234	266	0
39	DD	2145	0	2234	290	0
40	BE	1563	0	1629	263	0
40	DE	1563	0	1629	276	0
41	BF	1623	0	1677	212	0
41	DF	1623	0	1677	226	0
42	BG	1474	0	1535	247	0
42	DG	1474	0	1535	278	0
43	BH	1222	0	1282	178	0
43	DH	1222	0	1282	193	0
44	BJ	651	0	170	25	0
44	DJ	651	0	157	32	0
45	BK	700	0	180	17	0
45	DK	700	0	176	16	0
46	BN	1104	0	1180	178	0
46	DN	1104	0	1180	205	0
47	BO	933	0	996	116	0
47	DO	933	0	996	108	0
48	BP	1114	0	1187	292	0
48	DP	1114	0	1187	290	0
49	BQ	1122	0	1179	166	0
49	DQ	1122	0	1179	165	0
50	BR	960	0	1021	150	0
50	DR	960	0	1021	154	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	BS	770	0	832	148	0
51	DS	770	0	832	140	0
52	BT	1141	0	1202	257	0
52	DT	1141	0	1202	227	0
53	BU	958	0	1015	165	0
53	DU	958	0	1015	154	0
54	BV	779	0	852	122	0
54	DV	779	0	852	122	0
55	BW	896	0	953	98	0
55	DW	896	0	953	93	0
56	BX	725	0	778	91	0
56	DX	725	0	778	108	0
57	BY	775	0	870	165	0
57	DY	775	0	870	168	0
58	BZ	1459	0	1488	216	0
58	DZ	1459	0	1488	254	0
59	AD	1	0	0	2	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B9	1	0	0	0	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D9	1	0	0	1	0
60	AZ	28	0	12	7	0
60	CZ	28	0	12	17	0
61	AZ	57	0	58	5	0
61	CZ	57	0	58	7	0
All	All	307196	0	208708	20879	6

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

The worst 5 of 20879 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AZ:357:PRO:CB	25:AZ:357:PRO:CG	1.77	1.43
38:DC:100:ILE:HG23	38:DC:127:LEU:CD1	1.68	1.23
4:CD:187:ARG:NH1	4:CD:187:ARG:HB3	1.52	1.22
15:AO:87:ILE:HG22	15:AO:88:ARG:H	1.08	1.18
24:CY:76:A:H1'	25:CZ:287:GLY:HA3	1.26	1.18

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

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	232/256 (91%)	163 (70%)	43 (18%)	26 (11%)	0	2
2	CB	232/256 (91%)	157 (68%)	52 (22%)	23 (10%)	0	3
3	AC	204/239 (85%)	148 (72%)	37 (18%)	19 (9%)	0	3
3	CC	204/239 (85%)	136 (67%)	43 (21%)	25 (12%)	0	1
4	AD	206/209 (99%)	130 (63%)	48 (23%)	28 (14%)	0	1
4	CD	206/209 (99%)	124 (60%)	53 (26%)	29 (14%)	0	1
5	AE	148/162 (91%)	131 (88%)	13 (9%)	4 (3%)	5	25
5	CE	148/162 (91%)	125 (84%)	18 (12%)	5 (3%)	3	21
6	AF	99/101 (98%)	79 (80%)	14 (14%)	6 (6%)	1	9
6	CF	99/101 (98%)	76 (77%)	16 (16%)	7 (7%)	1	6
7	AG	153/156 (98%)	113 (74%)	27 (18%)	13 (8%)	1	5
7	CG	153/156 (98%)	113 (74%)	23 (15%)	17 (11%)	0	2
8	AH	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	4	24
8	CH	136/138 (99%)	118 (87%)	13 (10%)	5 (4%)	3	19
9	AI	125/128 (98%)	79 (63%)	29 (23%)	17 (14%)	0	1
9	CI	125/128 (98%)	81 (65%)	25 (20%)	19 (15%)	0	0

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	D2	69/72 (96%)	43 (62%)	19 (28%)	7 (10%)	0	3
29	B3	57/60 (95%)	39 (68%)	10 (18%)	8 (14%)	0	1
29	D3	57/60 (95%)	43 (75%)	7 (12%)	7 (12%)	0	1
30	B4	42/71 (59%)	24 (57%)	10 (24%)	8 (19%)	0	0
30	D4	42/71 (59%)	19 (45%)	13 (31%)	10 (24%)	0	0
31	B5	57/60 (95%)	33 (58%)	14 (25%)	10 (18%)	0	0
31	D5	57/60 (95%)	35 (61%)	13 (23%)	9 (16%)	0	0
32	B6	48/54 (89%)	20 (42%)	11 (23%)	17 (35%)	0	0
32	D6	48/54 (89%)	23 (48%)	13 (27%)	12 (25%)	0	0
33	B7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	6	29
33	D7	46/49 (94%)	31 (67%)	14 (30%)	1 (2%)	6	29
34	B8	61/65 (94%)	39 (64%)	15 (25%)	7 (12%)	0	2
34	D8	61/65 (94%)	40 (66%)	12 (20%)	9 (15%)	0	0
35	B9	35/37 (95%)	18 (51%)	12 (34%)	5 (14%)	0	1
35	D9	35/37 (95%)	18 (51%)	10 (29%)	7 (20%)	0	0
38	BC	226/229 (99%)	159 (70%)	52 (23%)	15 (7%)	1	7
38	DC	226/229 (99%)	153 (68%)	54 (24%)	19 (8%)	1	5
39	BD	273/276 (99%)	194 (71%)	51 (19%)	28 (10%)	0	3
39	DD	273/276 (99%)	200 (73%)	47 (17%)	26 (10%)	0	3
40	BE	202/206 (98%)	133 (66%)	41 (20%)	28 (14%)	0	1
40	DE	202/206 (98%)	134 (66%)	37 (18%)	31 (15%)	0	0
41	BF	205/210 (98%)	137 (67%)	40 (20%)	28 (14%)	0	1
41	DF	205/210 (98%)	140 (68%)	37 (18%)	28 (14%)	0	1
42	BG	179/182 (98%)	109 (61%)	44 (25%)	26 (14%)	0	1
42	DG	179/182 (98%)	103 (58%)	40 (22%)	36 (20%)	0	0
43	BH	157/180 (87%)	94 (60%)	40 (26%)	23 (15%)	0	1
43	DH	157/180 (87%)	94 (60%)	39 (25%)	24 (15%)	0	0
46	BN	136/140 (97%)	85 (62%)	29 (21%)	22 (16%)	0	0
46	DN	136/140 (97%)	89 (65%)	27 (20%)	20 (15%)	0	0
47	BO	120/122 (98%)	102 (85%)	10 (8%)	8 (7%)	1	7
47	DO	120/122 (98%)	99 (82%)	14 (12%)	7 (6%)	1	10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	BP	144/150 (96%)	66 (46%)	39 (27%)	39 (27%)	0	0
48	DP	144/150 (96%)	68 (47%)	39 (27%)	37 (26%)	0	0
49	BQ	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	0	3
49	DQ	139/141 (99%)	102 (73%)	29 (21%)	8 (6%)	1	10
50	BR	115/118 (98%)	79 (69%)	17 (15%)	19 (16%)	0	0
50	DR	115/118 (98%)	69 (60%)	24 (21%)	22 (19%)	0	0
51	BS	96/112 (86%)	53 (55%)	24 (25%)	19 (20%)	0	0
51	DS	96/112 (86%)	52 (54%)	23 (24%)	21 (22%)	0	0
52	BT	135/146 (92%)	79 (58%)	32 (24%)	24 (18%)	0	0
52	DT	135/146 (92%)	77 (57%)	34 (25%)	24 (18%)	0	0
53	BU	115/118 (98%)	75 (65%)	27 (24%)	13 (11%)	0	2
53	DU	115/118 (98%)	76 (66%)	25 (22%)	14 (12%)	0	1
54	BV	99/101 (98%)	63 (64%)	23 (23%)	13 (13%)	0	1
54	DV	99/101 (98%)	61 (62%)	26 (26%)	12 (12%)	0	1
55	BW	111/113 (98%)	79 (71%)	21 (19%)	11 (10%)	0	3
55	DW	111/113 (98%)	81 (73%)	20 (18%)	10 (9%)	1	4
56	BX	90/96 (94%)	64 (71%)	21 (23%)	5 (6%)	2	11
56	DX	90/96 (94%)	64 (71%)	19 (21%)	7 (8%)	1	5
57	BY	98/110 (89%)	39 (40%)	27 (28%)	32 (33%)	0	0
57	DY	98/110 (89%)	43 (44%)	26 (26%)	29 (30%)	0	0
58	BZ	181/206 (88%)	114 (63%)	39 (22%)	28 (16%)	0	0
58	DZ	181/206 (88%)	106 (59%)	34 (19%)	41 (23%)	0	0
All	All	12270/13098 (94%)	8296 (68%)	2465 (20%)	1509 (12%)	0	1

5 of 1509 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	174 (86%)	28 (14%)	3	15
2	CB	202/220 (92%)	173 (86%)	29 (14%)	3	14
3	AC	160/188 (85%)	139 (87%)	21 (13%)	4	17
3	CC	160/188 (85%)	141 (88%)	19 (12%)	5	20
4	AD	180/181 (99%)	150 (83%)	30 (17%)	2	9
4	CD	180/181 (99%)	151 (84%)	29 (16%)	2	10
5	AE	115/123 (94%)	104 (90%)	11 (10%)	8	31
5	CE	115/123 (94%)	103 (90%)	12 (10%)	7	27
6	AF	90/90 (100%)	76 (84%)	14 (16%)	2	11
6	CF	90/90 (100%)	77 (86%)	13 (14%)	3	14
7	AG	126/127 (99%)	116 (92%)	10 (8%)	12	40
7	CG	126/127 (99%)	118 (94%)	8 (6%)	18	48
8	AH	119/119 (100%)	105 (88%)	14 (12%)	5	21
8	CH	119/119 (100%)	106 (89%)	13 (11%)	6	25
9	AI	98/99 (99%)	84 (86%)	14 (14%)	3	14
9	CI	98/99 (99%)	86 (88%)	12 (12%)	5	19
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	5	23
10	CJ	88/92 (96%)	79 (90%)	9 (10%)	7	27
11	AK	90/99 (91%)	84 (93%)	6 (7%)	16	46
11	CK	90/99 (91%)	81 (90%)	9 (10%)	7	28
12	AL	104/108 (96%)	84 (81%)	20 (19%)	1	6
12	CL	104/108 (96%)	84 (81%)	20 (19%)	1	6
13	AM	99/101 (98%)	85 (86%)	14 (14%)	3	15
13	CM	99/101 (98%)	90 (91%)	9 (9%)	9	33
14	AN	49/50 (98%)	41 (84%)	8 (16%)	2	10
14	CN	49/50 (98%)	40 (82%)	9 (18%)	1	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	79/80 (99%)	73 (92%)	6 (8%)	13	41
15	CO	79/80 (99%)	69 (87%)	10 (13%)	4	18
16	AP	72/74 (97%)	64 (89%)	8 (11%)	6	24
16	CP	72/74 (97%)	66 (92%)	6 (8%)	11	38
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	10	37
17	CQ	94/97 (97%)	85 (90%)	9 (10%)	8	31
18	AR	61/77 (79%)	55 (90%)	6 (10%)	8	29
18	CR	61/77 (79%)	54 (88%)	7 (12%)	5	22
19	AS	69/80 (86%)	56 (81%)	13 (19%)	1	6
19	CS	69/80 (86%)	57 (83%)	12 (17%)	2	9
20	AT	76/82 (93%)	70 (92%)	6 (8%)	12	40
20	CT	76/82 (93%)	69 (91%)	7 (9%)	9	33
21	AU	19/22 (86%)	18 (95%)	1 (5%)	22	54
21	CU	19/22 (86%)	17 (90%)	2 (10%)	7	26
25	AZ	322/338 (95%)	281 (87%)	41 (13%)	4	18
25	CZ	322/338 (95%)	284 (88%)	38 (12%)	5	21
26	B0	66/67 (98%)	57 (86%)	9 (14%)	3	16
26	D0	66/67 (98%)	56 (85%)	10 (15%)	3	12
27	B1	78/83 (94%)	67 (86%)	11 (14%)	3	15
27	D1	78/83 (94%)	64 (82%)	14 (18%)	2	8
28	B2	66/67 (98%)	54 (82%)	12 (18%)	1	7
28	D2	66/67 (98%)	60 (91%)	6 (9%)	9	33
29	B3	51/52 (98%)	46 (90%)	5 (10%)	8	29
29	D3	51/52 (98%)	47 (92%)	4 (8%)	12	40
30	B4	39/63 (62%)	28 (72%)	11 (28%)	0	1
30	D4	39/63 (62%)	28 (72%)	11 (28%)	0	1
31	B5	51/52 (98%)	48 (94%)	3 (6%)	19	50
31	D5	51/52 (98%)	45 (88%)	6 (12%)	5	21
32	B6	49/52 (94%)	38 (78%)	11 (22%)	1	3
32	D6	49/52 (94%)	40 (82%)	9 (18%)	1	7
33	B7	41/42 (98%)	34 (83%)	7 (17%)	2	9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	D7	41/42 (98%)	34 (83%)	7 (17%)	2	9
34	B8	53/55 (96%)	43 (81%)	10 (19%)	1	6
34	D8	53/55 (96%)	44 (83%)	9 (17%)	2	9
35	B9	34/34 (100%)	28 (82%)	6 (18%)	2	8
35	D9	34/34 (100%)	31 (91%)	3 (9%)	10	36
38	BC	180/181 (99%)	164 (91%)	16 (9%)	9	34
38	DC	180/181 (99%)	167 (93%)	13 (7%)	14	44
39	BD	217/218 (100%)	185 (85%)	32 (15%)	3	13
39	DD	217/218 (100%)	185 (85%)	32 (15%)	3	13
40	BE	165/166 (99%)	142 (86%)	23 (14%)	3	15
40	DE	165/166 (99%)	139 (84%)	26 (16%)	2	11
41	BF	165/166 (99%)	156 (94%)	9 (6%)	21	53
41	DF	165/166 (99%)	158 (96%)	7 (4%)	30	62
42	BG	155/156 (99%)	133 (86%)	22 (14%)	3	14
42	DG	155/156 (99%)	131 (84%)	24 (16%)	2	11
43	BH	132/148 (89%)	117 (89%)	15 (11%)	5	23
43	DH	132/148 (89%)	115 (87%)	17 (13%)	4	18
46	BN	117/119 (98%)	102 (87%)	15 (13%)	4	18
46	DN	117/119 (98%)	104 (89%)	13 (11%)	6	24
47	BO	100/100 (100%)	88 (88%)	12 (12%)	5	20
47	DO	100/100 (100%)	90 (90%)	10 (10%)	7	28
48	BP	112/116 (97%)	95 (85%)	17 (15%)	3	12
48	DP	112/116 (97%)	90 (80%)	22 (20%)	1	6
49	BQ	111/111 (100%)	97 (87%)	14 (13%)	4	18
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	4	18
50	BR	100/101 (99%)	86 (86%)	14 (14%)	3	15
50	DR	100/101 (99%)	86 (86%)	14 (14%)	3	15
51	BS	77/88 (88%)	66 (86%)	11 (14%)	3	14
51	DS	77/88 (88%)	66 (86%)	11 (14%)	3	14
52	BT	120/127 (94%)	98 (82%)	22 (18%)	1	7
52	DT	120/127 (94%)	99 (82%)	21 (18%)	2	8

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	BU	92/94 (98%)	82 (89%)	10 (11%)	6	25
53	DU	92/94 (98%)	83 (90%)	9 (10%)	8	29
54	BV	82/82 (100%)	66 (80%)	16 (20%)	1	6
54	DV	82/82 (100%)	69 (84%)	13 (16%)	2	11
55	BW	91/92 (99%)	80 (88%)	11 (12%)	5	20
55	DW	91/92 (99%)	81 (89%)	10 (11%)	6	25
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%)	71 (84%)	13 (16%)	2	11
57	DY	84/91 (92%)	71 (84%)	13 (16%)	2	11
58	BZ	161/179 (90%)	137 (85%)	24 (15%)	3	13
58	DZ	161/179 (90%)	133 (83%)	28 (17%)	2	9
All	All	10350/10854 (95%)	9007 (87%)	1343 (13%)	4	18

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

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

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

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

### 5.3.3 RNA ⓘ

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

Continued on next page...

*Continued from previous page...*

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

5 of 1715 RNA backbone outliers are listed below:

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

5 of 208 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2036	C
1	CA	266	G
36	DA	2033	A
36	BA	2131	G
37	BB	56	G

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	7MG	CY	46	24	22,26,27	1.17	2 (9%)	28,39,42	2.34	5 (17%)
24	H2U	AY	17	24	18,21,22	0.81	1 (5%)	21,30,33	1.83	4 (19%)
24	7MG	AY	46	24	22,26,27	1.20	2 (9%)	28,39,42	2.31	5 (17%)
24	OMC	CY	32	24	15,22,23	0.75	0	17,31,34	1.17	2 (11%)
24	4SU	CY	8	24	14,21,22	1.65	3 (21%)	15,30,33	2.64	2 (13%)
24	H2U	AY	16	24	18,21,22	0.83	0	21,30,33	1.85	4 (19%)
24	H2U	CY	17	24	18,21,22	0.89	1 (5%)	21,30,33	1.80	4 (19%)
24	OMC	AY	32	24	15,22,23	0.78	0	17,31,34	1.21	2 (11%)
24	MIA	CY	37	24	24,31,32	2.00	4 (16%)	26,44,47	2.06	4 (15%)
24	H2U	CY	16	24	18,21,22	0.86	0	21,30,33	1.80	4 (19%)
24	H2U	AY	20	24	18,21,22	0.91	1 (5%)	21,30,33	1.90	6 (28%)
24	5MU	CY	54	24	15,22,23	1.15	2 (13%)	16,32,35	3.70	1 (6%)
24	4SU	AY	8	24	14,21,22	1.60	4 (28%)	15,30,33	2.64	2 (13%)
24	PSU	CY	55	24	17,21,22	1.05	2 (11%)	20,30,33	3.37	8 (40%)
24	H2U	CY	20	24	18,21,22	0.96	1 (5%)	21,30,33	1.92	6 (28%)
24	MIA	AY	37	24	24,31,32	1.35	4 (16%)	26,44,47	2.24	4 (15%)
24	PSU	AY	55	24	17,21,22	1.23	3 (17%)	20,30,33	3.32	8 (40%)
24	5MU	AY	54	24	15,22,23	1.16	2 (13%)	16,32,35	3.70	2 (12%)

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	7MG	CY	46	24	-	3/7/37/38	0/3/3/3
24	H2U	AY	17	24	-	4/7/38/39	0/2/2/2
24	7MG	AY	46	24	-	3/7/37/38	0/3/3/3
24	OMC	CY	32	24	-	0/7/27/28	0/2/2/2
24	4SU	CY	8	24	-	1/5/25/26	0/2/2/2
24	H2U	AY	16	24	-	2/7/38/39	0/2/2/2
24	H2U	CY	17	24	-	4/7/38/39	0/2/2/2
24	OMC	AY	32	24	-	0/7/27/28	0/2/2/2
24	MIA	CY	37	24	-	3/11/33/34	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	H2U	CY	16	24	-	2/7/38/39	0/2/2/2
24	H2U	AY	20	24	-	4/7/38/39	0/2/2/2
24	5MU	CY	54	24	-	0/5/25/26	0/2/2/2
24	4SU	AY	8	24	-	1/5/25/26	0/2/2/2
24	PSU	CY	55	24	-	1/7/25/26	0/2/2/2
24	H2U	CY	20	24	-	4/7/38/39	0/2/2/2
24	MIA	AY	37	24	-	3/11/33/34	0/3/3/3
24	PSU	AY	55	24	-	0/7/25/26	0/2/2/2
24	5MU	AY	54	24	-	0/5/25/26	0/2/2/2

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	37	MIA	C2-S10	7.97	1.82	1.75
24	CY	8	4SU	C5-C4	4.60	1.43	1.38
24	AY	8	4SU	C5-C4	4.03	1.43	1.38
24	AY	37	MIA	C2-S10	3.96	1.79	1.75
24	AY	46	7MG	C6-N1	3.89	1.39	1.33

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CY	54	5MU	C4-N3-C2	14.50	127.39	115.14
24	AY	54	5MU	C4-N3-C2	14.45	127.34	115.14
24	CY	55	PSU	N1-C2-N3	-10.27	120.26	128.43
24	AY	55	PSU	N1-C2-N3	-9.92	120.55	128.43
24	AY	37	MIA	C11-S10-C2	8.90	108.91	102.27

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	17	H2U	O4'-C1'-N1-C6
24	CY	17	H2U	O4'-C1'-N1-C2
24	CY	17	H2U	O4'-C1'-N1-C6
24	CY	37	MIA	C5-C6-N6-C12
24	AY	20	H2U	O4'-C1'-N1-C2

There are no ring outliers.

16 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CY	46	7MG	4	0
24	AY	17	H2U	1	0
24	AY	46	7MG	3	0
24	CY	8	4SU	4	0
24	AY	16	H2U	1	0
24	CY	17	H2U	1	0
24	CY	37	MIA	1	0
24	CY	16	H2U	1	0
24	AY	20	H2U	3	0
24	CY	54	5MU	2	0
24	AY	8	4SU	5	0
24	CY	55	PSU	1	0
24	CY	20	H2U	3	0
24	AY	37	MIA	1	0
24	AY	55	PSU	1	0
24	AY	54	5MU	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
61	KIR	CZ	502	-	56,59,59	3.71	25 (44%)	62,84,84	1.64	14 (22%)
60	GDP	CZ	501	-	24,30,30	1.75	4 (16%)	31,47,47	2.11	8 (25%)
60	GDP	AZ	501	-	24,30,30	2.24	3 (12%)	31,47,47	2.53	9 (29%)
61	KIR	AZ	502	-	56,59,59	3.47	23 (41%)	62,84,84	1.65	11 (17%)

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
61	KIR	CZ	502	-	-	11/54/98/98	0/3/3/3
60	GDP	CZ	501	-	-	6/12/32/32	0/3/3/3
60	GDP	AZ	501	-	-	2/12/32/32	0/3/3/3
61	KIR	AZ	502	-	-	10/54/98/98	0/3/3/3

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CZ	502	KIR	O18-C17	-14.47	1.22	1.44
61	AZ	502	KIR	O18-C17	-14.29	1.23	1.44
61	CZ	502	KIR	O30-C30	-12.76	1.17	1.42
61	AZ	502	KIR	O30-C30	-12.71	1.17	1.42
60	AZ	501	GDP	C6-C5	-7.93	1.27	1.41

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AZ	501	GDP	C4-C5-N7	-6.34	102.80	109.40
60	CZ	501	GDP	C5-C6-N1	-6.22	114.93	123.43
60	AZ	501	GDP	N3-C2-N1	-5.90	119.35	127.22
61	CZ	502	KIR	O29-C29-O34	-5.24	101.42	110.21
60	CZ	501	GDP	N3-C2-N1	-5.12	120.39	127.22

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	AZ	502	KIR	C16-C17-C19-C20
61	AZ	502	KIR	C16-C17-C19-C42
61	AZ	502	KIR	O18-C17-C19-C20
61	AZ	502	KIR	O18-C17-C19-C42
61	CZ	502	KIR	C16-C17-C19-C20

There are no ring outliers.

4 monomers are involved in 36 short contacts:

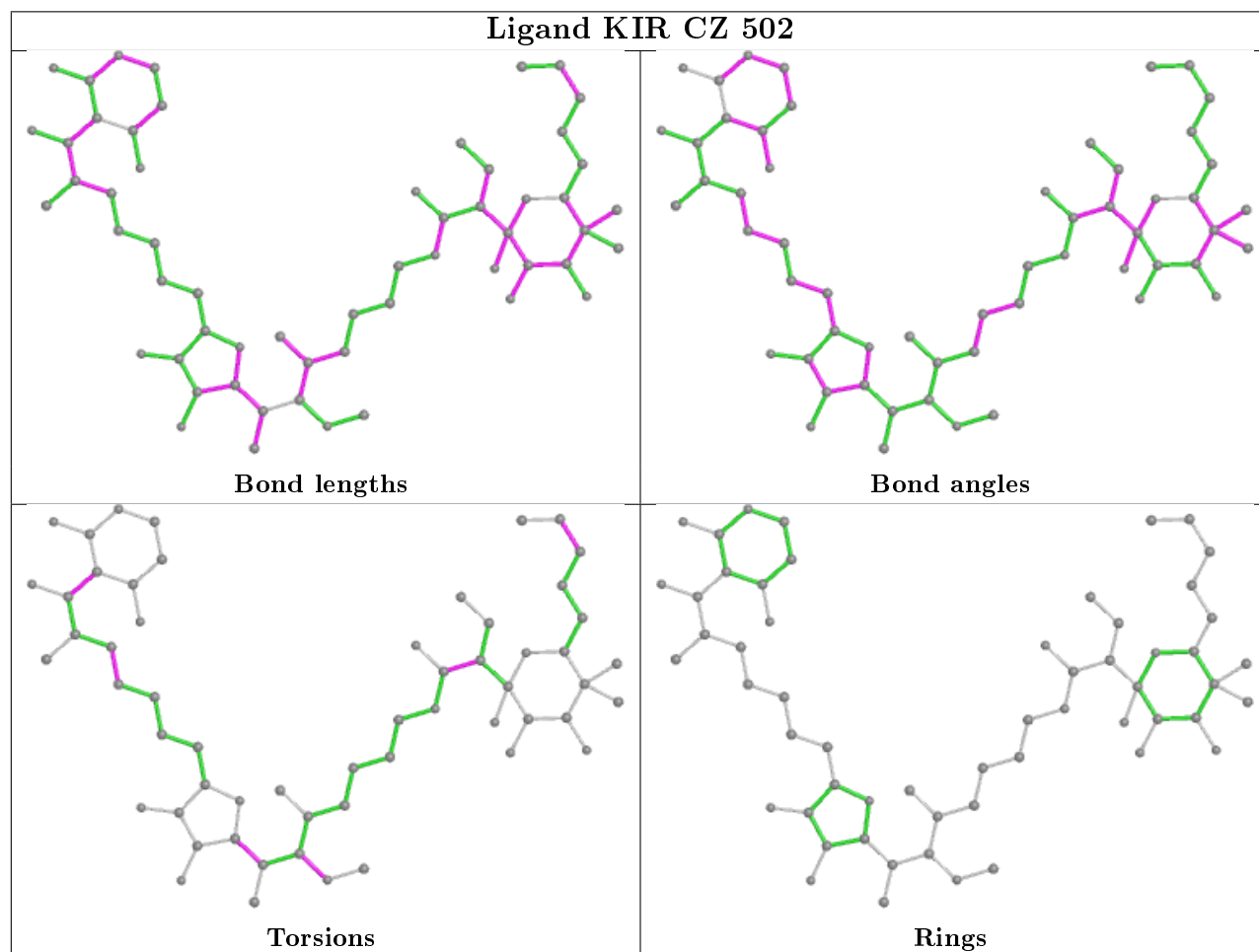
Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	CZ	502	KIR	7	0

*Continued on next page...*

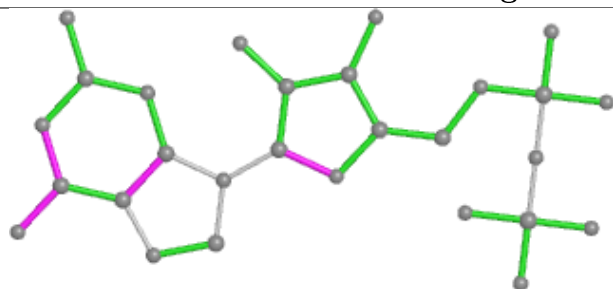
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	CZ	501	GDP	17	0
60	AZ	501	GDP	7	0
61	AZ	502	KIR	5	0

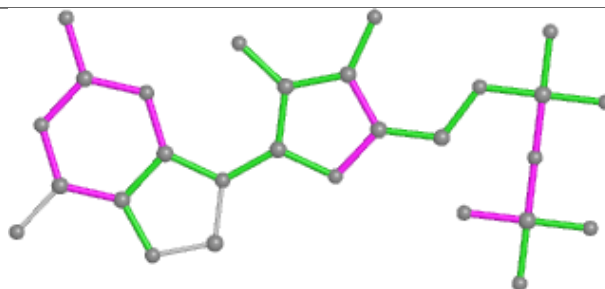
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



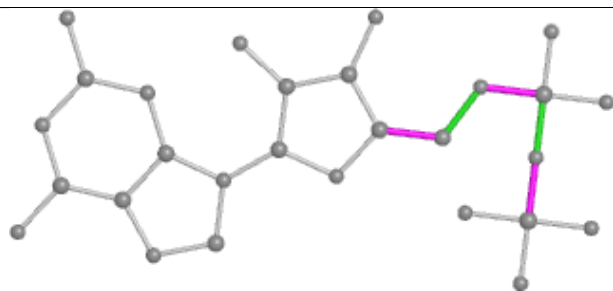
## Ligand GDP CZ 501



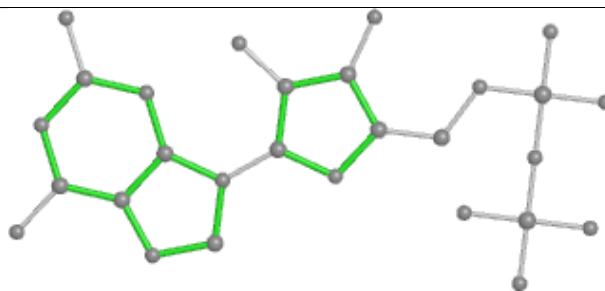
Bond lengths



Bond angles

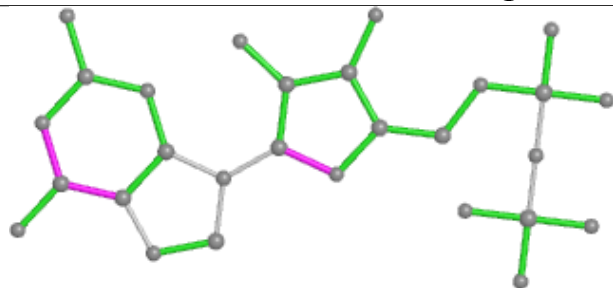


Torsions

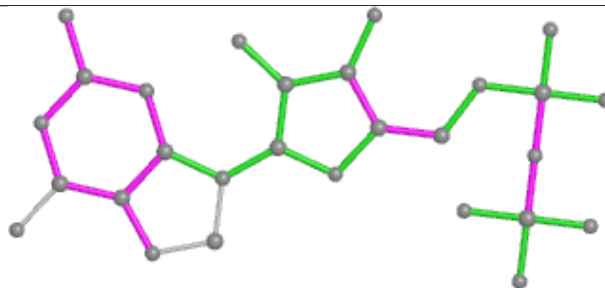


Rings

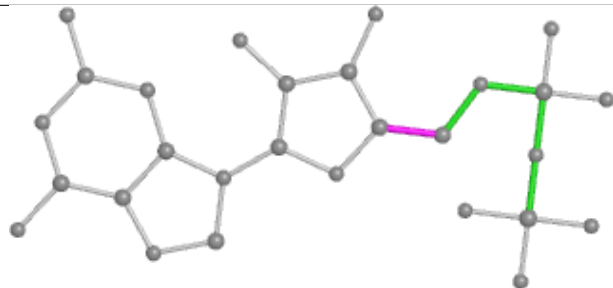
## Ligand GDP AZ 501



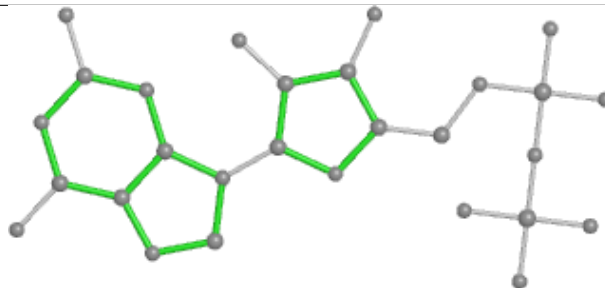
Bond lengths



Bond angles

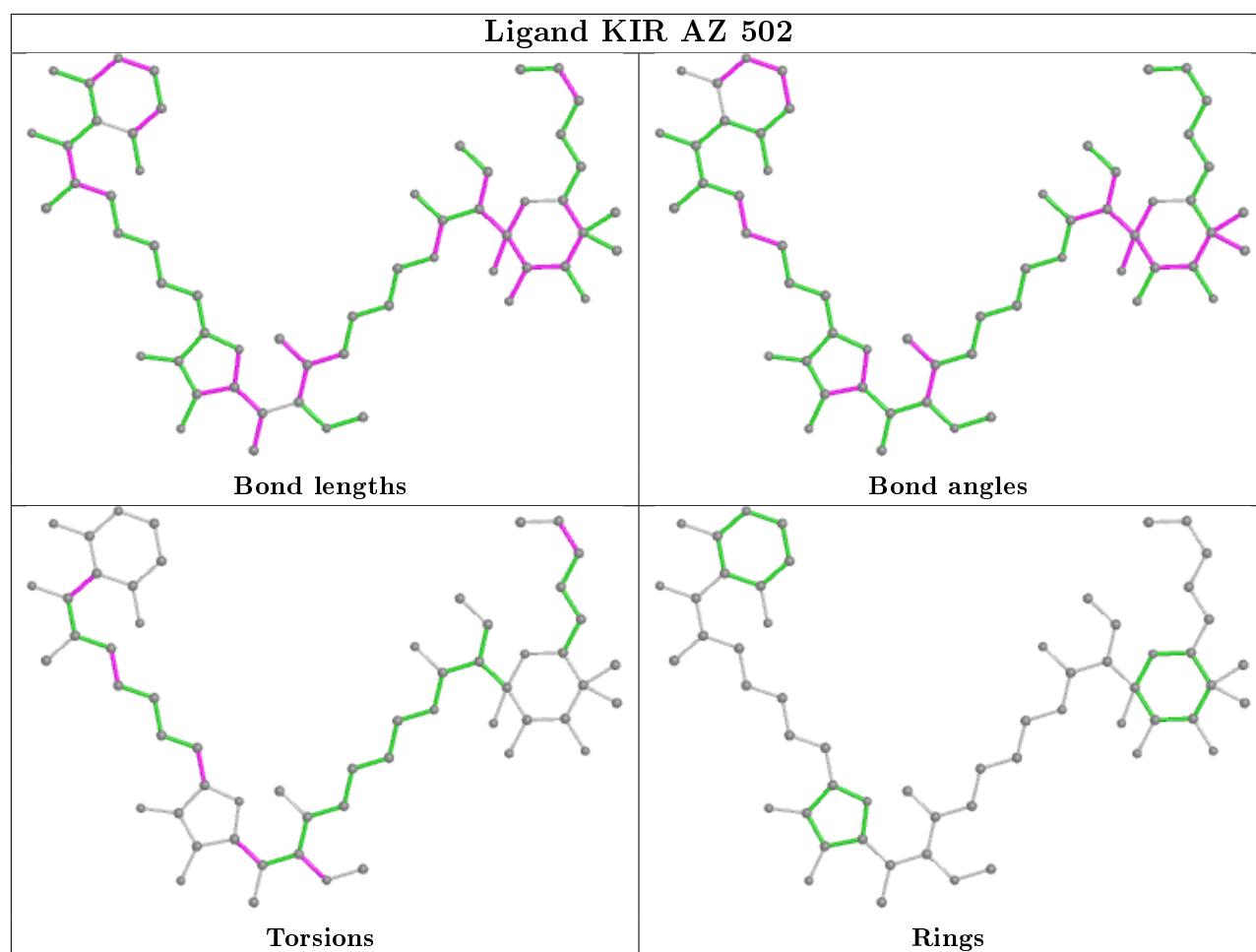


Torsions



Rings





## 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%)	-0.28	12 (0%) 86 72	21, 54, 143, 200	0
1	CA	1504/1522 (98%)	-0.37	10 (0%) 87 75	31, 70, 146, 200	0
2	AB	234/256 (91%)	-0.16	5 (2%) 63 43	31, 60, 136, 149	0
2	CB	234/256 (91%)	-0.10	4 (1%) 70 49	46, 81, 139, 148	0
3	AC	206/239 (86%)	-0.32	1 (0%) 91 81	20, 46, 78, 89	0
3	CC	206/239 (86%)	-0.16	1 (0%) 91 81	49, 74, 96, 100	0
4	AD	208/209 (99%)	0.08	4 (1%) 66 46	45, 83, 112, 119	0
4	CD	208/209 (99%)	0.23	9 (4%) 35 17	64, 95, 118, 126	0
5	AE	150/162 (92%)	-0.42	0 100 100	25, 42, 69, 86	0
5	CE	150/162 (92%)	-0.31	1 (0%) 87 75	43, 58, 82, 100	0
6	AF	101/101 (100%)	-0.17	1 (0%) 82 67	44, 70, 86, 94	0
6	CF	101/101 (100%)	-0.12	1 (0%) 82 67	64, 86, 97, 101	0
7	AG	155/156 (99%)	-0.26	2 (1%) 77 59	37, 66, 97, 113	0
7	CG	155/156 (99%)	0.02	5 (3%) 47 25	67, 87, 107, 122	0
8	AH	138/138 (100%)	-0.41	0 100 100	31, 47, 68, 75	0
8	CH	138/138 (100%)	-0.33	0 100 100	41, 61, 75, 84	0
9	AI	127/128 (99%)	-0.16	0 100 100	32, 72, 111, 123	0
9	CI	127/128 (99%)	0.21	6 (4%) 31 15	59, 97, 119, 124	0
10	AJ	98/105 (93%)	0.13	2 (2%) 65 44	30, 73, 126, 129	0
10	CJ	98/105 (93%)	0.73	19 (19%) 1 0	57, 102, 133, 137	0
11	AK	119/129 (92%)	-0.33	2 (1%) 70 49	29, 45, 78, 105	0
11	CK	119/129 (92%)	-0.27	0 100 100	43, 66, 91, 106	0
12	AL	124/131 (94%)	-0.41	1 (0%) 86 72	24, 49, 70, 103	0
12	CL	124/131 (94%)	-0.35	1 (0%) 86 72	38, 54, 78, 111	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	124/126 (98%)	-0.05	4 (3%)	47	25	46, 82, 106, 147	0
13	CM	124/126 (98%)	0.06	6 (4%)	30	14	67, 92, 114, 148	0
14	AN	60/61 (98%)	-0.26	1 (1%)	70	49	28, 51, 84, 90	0
14	CN	60/61 (98%)	0.13	2 (3%)	46	24	65, 78, 98, 105	0
15	AO	88/89 (98%)	-0.40	0	100	100	31, 51, 79, 85	0
15	CO	88/89 (98%)	-0.29	0	100	100	41, 63, 85, 92	0
16	AP	83/88 (94%)	-0.26	0	100	100	48, 67, 85, 123	0
16	CP	83/88 (94%)	-0.28	1 (1%)	79	61	62, 77, 92, 122	0
17	AQ	99/105 (94%)	-0.43	0	100	100	40, 58, 77, 85	0
17	CQ	99/105 (94%)	-0.36	0	100	100	44, 65, 85, 93	0
18	AR	70/88 (79%)	-0.33	0	100	100	35, 55, 88, 104	0
18	CR	70/88 (79%)	-0.19	1 (1%)	75	56	47, 73, 100, 113	0
19	AS	78/93 (83%)	-0.00	3 (3%)	40	20	48, 75, 119, 122	0
19	CS	78/93 (83%)	0.11	6 (7%)	13	5	71, 91, 120, 124	0
20	AT	99/106 (93%)	-0.15	1 (1%)	82	67	65, 83, 117, 119	0
20	CT	99/106 (93%)	-0.19	0	100	100	64, 84, 117, 118	0
21	AU	24/27 (88%)	-0.46	0	100	100	45, 61, 75, 90	0
21	CU	24/27 (88%)	-0.05	1 (4%)	36	18	67, 79, 92, 94	0
22	AV	76/76 (100%)	-0.39	0	100	100	35, 70, 102, 112	0
22	AW	76/76 (100%)	-0.09	1 (1%)	77	59	63, 136, 178, 190	0
22	CV	76/76 (100%)	-0.43	0	100	100	48, 76, 115, 128	0
22	CW	76/76 (100%)	-0.07	2 (2%)	56	33	71, 165, 186, 196	0
23	AX	17/27 (62%)	0.07	0	100	100	30, 82, 132, 133	0
23	CX	17/27 (62%)	0.28	1 (5%)	22	10	36, 99, 145, 145	0
24	AY	68/77 (88%)	-0.36	0	100	100	37, 108, 152, 185	0
24	CY	68/77 (88%)	-0.33	0	100	100	45, 111, 145, 185	0
25	AZ	385/405 (95%)	0.36	16 (4%)	36	18	63, 105, 134, 163	0
25	CZ	385/405 (95%)	1.40	115 (29%)	0	0	93, 117, 143, 169	0
26	B0	84/85 (98%)	-0.12	2 (2%)	59	37	62, 73, 100, 114	0
26	D0	84/85 (98%)	0.02	2 (2%)	59	37	66, 79, 101, 111	0
27	B1	93/98 (94%)	-0.14	3 (3%)	47	25	47, 63, 120, 125	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	D1	93/98 (94%)	-0.16	0 100 100	51, 74, 115, 120	0
28	B2	71/72 (98%)	1.41	21 (29%) 0 0	122, 140, 151, 153	0
28	D2	71/72 (98%)	0.18	2 (2%) 53 30	90, 106, 126, 139	0
29	B3	59/60 (98%)	-0.06	1 (1%) 70 49	59, 79, 101, 116	0
29	D3	59/60 (98%)	0.10	2 (3%) 45 24	58, 80, 97, 114	0
30	B4	44/71 (61%)	1.24	9 (20%) 1 0	102, 156, 180, 186	0
30	D4	44/71 (61%)	1.43	13 (29%) 0 0	113, 165, 186, 187	0
31	B5	59/60 (98%)	0.41	5 (8%) 10 4	52, 86, 150, 164	0
31	D5	59/60 (98%)	0.18	5 (8%) 10 4	55, 80, 148, 161	0
32	B6	50/54 (92%)	0.36	5 (10%) 7 2	55, 88, 106, 112	0
32	D6	50/54 (92%)	0.32	3 (6%) 21 10	57, 95, 107, 113	0
33	B7	48/49 (97%)	-0.18	1 (2%) 63 43	47, 61, 95, 116	0
33	D7	48/49 (97%)	-0.37	0 100 100	47, 61, 91, 109	0
34	B8	63/65 (96%)	-0.11	0 100 100	55, 72, 84, 112	0
34	D8	63/65 (96%)	-0.19	0 100 100	56, 73, 85, 109	0
35	B9	37/37 (100%)	0.47	2 (5%) 25 12	79, 98, 112, 116	0
35	D9	37/37 (100%)	1.02	6 (16%) 1 1	84, 104, 115, 119	0
36	BA	2901/2915 (99%)	-0.29	45 (1%) 72 51	25, 74, 176, 200	0
36	DA	2901/2915 (99%)	-0.31	38 (1%) 77 59	32, 76, 175, 200	0
37	BB	119/122 (97%)	-0.43	0 100 100	54, 97, 123, 144	0
37	DB	119/122 (97%)	-0.50	0 100 100	61, 104, 128, 140	0
38	BC	228/229 (99%)	0.32	19 (8%) 11 4	40, 73, 163, 176	0
38	DC	228/229 (99%)	0.60	34 (14%) 2 1	64, 87, 166, 174	0
39	BD	275/276 (99%)	-0.36	0 100 100	28, 48, 78, 93	0
39	DD	275/276 (99%)	-0.34	1 (0%) 92 84	28, 53, 80, 94	0
40	BE	204/206 (99%)	-0.10	3 (1%) 73 54	46, 73, 120, 129	0
40	DE	204/206 (99%)	-0.11	3 (1%) 73 54	39, 72, 122, 132	0
41	BF	207/210 (98%)	0.40	22 (10%) 6 2	42, 102, 155, 162	0
41	DF	207/210 (98%)	0.33	17 (8%) 11 4	47, 105, 155, 161	0
42	BG	181/182 (99%)	0.12	6 (3%) 46 24	66, 85, 120, 134	0
42	DG	181/182 (99%)	0.33	12 (6%) 18 7	89, 108, 130, 139	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BH	159/180 (88%)	0.82	25 (15%) 2 1	85, 123, 148, 152	0
43	DH	159/180 (88%)	0.53	16 (10%) 7 2	85, 123, 145, 150	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	138/140 (98%)	-0.07	1 (0%) 87 75	56, 86, 130, 138	0
46	DN	138/140 (98%)	-0.05	2 (1%) 75 56	61, 83, 132, 136	0
47	BO	122/122 (100%)	-0.33	0 100 100	43, 60, 73, 82	0
47	DO	122/122 (100%)	-0.35	0 100 100	40, 60, 73, 77	0
48	BP	146/150 (97%)	0.33	7 (4%) 30 14	49, 98, 124, 145	0
48	DP	146/150 (97%)	0.28	9 (6%) 20 9	47, 102, 126, 141	0
49	BQ	141/141 (100%)	-0.20	3 (2%) 63 43	47, 61, 84, 125	0
49	DQ	141/141 (100%)	-0.26	2 (1%) 75 56	43, 60, 87, 122	0
50	BR	117/118 (99%)	-0.05	1 (0%) 84 69	55, 84, 101, 108	0
50	DR	117/118 (99%)	-0.14	0 100 100	52, 79, 97, 106	0
51	BS	98/112 (87%)	0.23	5 (5%) 28 13	69, 101, 122, 126	0
51	DS	98/112 (87%)	0.48	5 (5%) 28 13	86, 106, 124, 126	0
52	BT	137/146 (93%)	0.13	7 (5%) 28 13	54, 84, 135, 163	0
52	DT	137/146 (93%)	0.12	9 (6%) 18 7	56, 81, 137, 160	0
53	BU	117/118 (99%)	-0.19	1 (0%) 84 69	60, 74, 102, 111	0
53	DU	117/118 (99%)	-0.27	0 100 100	52, 74, 100, 108	0
54	BV	101/101 (100%)	0.24	6 (5%) 22 10	61, 102, 117, 121	0
54	DV	101/101 (100%)	0.35	5 (4%) 28 13	50, 102, 117, 119	0
55	BW	113/113 (100%)	-0.01	4 (3%) 44 23	60, 83, 111, 140	0
55	DW	113/113 (100%)	-0.01	2 (1%) 68 47	59, 76, 112, 143	0
56	BX	92/96 (95%)	0.10	0 100 100	69, 86, 109, 120	0
56	DX	92/96 (95%)	0.04	1 (1%) 80 64	60, 88, 108, 121	0
57	BY	100/110 (90%)	0.78	14 (14%) 2 1	103, 121, 153, 159	0
57	DY	100/110 (90%)	0.80	16 (16%) 1 1	99, 119, 153, 162	0
58	BZ	183/206 (88%)	0.21	10 (5%) 25 11	53, 85, 129, 139	0
58	DZ	183/206 (88%)	0.22	6 (3%) 46 24	59, 85, 124, 132	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	21996/23368 (94%)	-0.09	687 (3%) 49 26	20, 77, 144, 200	0

The worst 5 of 687 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
38	BC	106	GLY	12.9
38	DC	97	GLU	12.1
28	B2	72	ALA	11.6
36	BA	654(K)	C	11.0
31	B5	60	VAL	10.8

## 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	17	20/21	0.60	0.43	186,194,196,196	0
24	H2U	CY	16	20/21	0.67	0.27	171,181,183,185	0
24	H2U	AY	16	20/21	0.70	0.49	172,183,184,185	0
24	H2U	CY	20	20/21	0.73	0.26	176,177,180,180	0
24	H2U	AY	17	20/21	0.77	0.34	186,190,190,191	0
24	H2U	AY	20	20/21	0.81	0.23	174,177,179,179	0
24	4SU	AY	8	20/21	0.84	0.17	110,113,114,115	0
24	5MU	CY	54	21/22	0.86	0.18	113,125,126,129	0
24	PSU	AY	55	20/21	0.86	0.17	130,139,140,140	0
24	7MG	CY	46	24/25	0.87	0.19	125,128,129,130	0
24	4SU	CY	8	20/21	0.88	0.18	115,116,119,119	0
24	PSU	CY	55	20/21	0.89	0.17	131,134,135,136	0
24	7MG	AY	46	24/25	0.90	0.19	121,123,124,124	0
24	5MU	AY	54	21/22	0.90	0.14	108,122,123,127	0
24	MIA	CY	37	29/30	0.93	0.23	52,66,80,85	0
24	OMC	AY	32	21/22	0.94	0.16	61,66,79,80	0
24	OMC	CY	32	21/22	0.94	0.17	78,83,93,94	0
24	MIA	AY	37	29/30	0.96	0.23	42,52,67,76	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

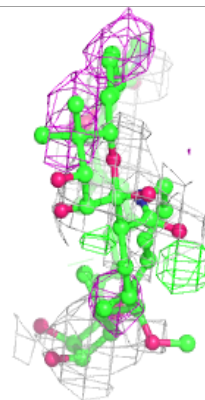
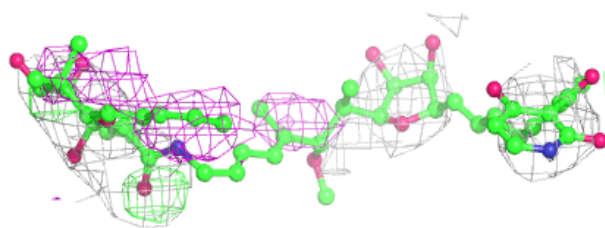
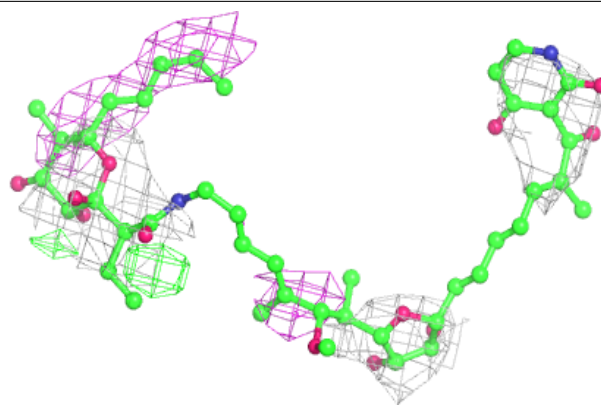
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	0.76	0.66	115,117,122,122	0
60	GDP	CZ	501	28/28	0.86	0.23	114,131,139,140	0
61	KIR	AZ	502	57/57	0.89	0.38	100,107,118,119	0
59	ZN	B9	101	1/1	0.91	0.16	103,103,103,103	0
60	GDP	AZ	501	28/28	0.92	0.18	114,118,123,123	0
59	ZN	D9	101	1/1	0.95	0.18	87,87,87,87	0
59	ZN	D4	101	1/1	0.96	0.12	103,103,103,103	0
59	ZN	B4	101	1/1	0.97	0.19	91,91,91,91	0
59	ZN	CD	301	1/1	0.97	0.29	75,75,75,75	0
59	ZN	AD	301	1/1	0.99	0.29	61,61,61,61	0
59	ZN	CN	101	1/1	0.99	0.18	69,69,69,69	0
59	ZN	AN	101	1/1	0.99	0.20	42,42,42,42	0

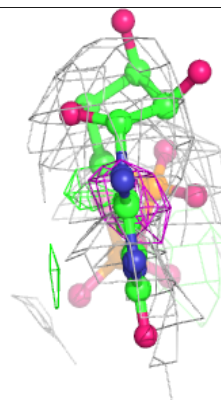
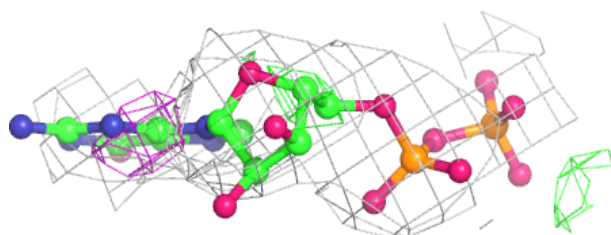
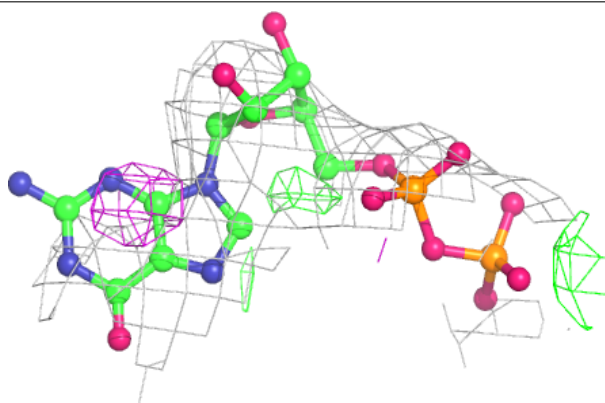
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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 CZ 501:**

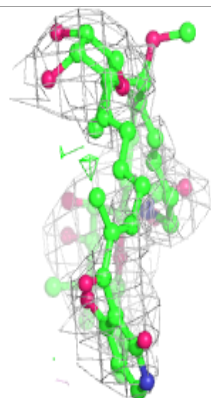
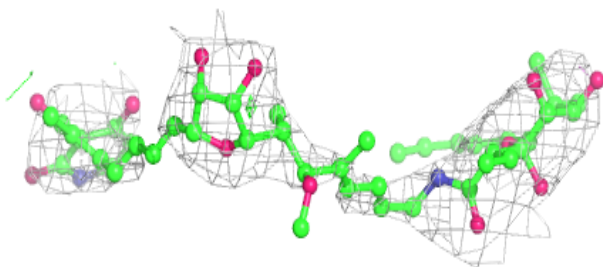
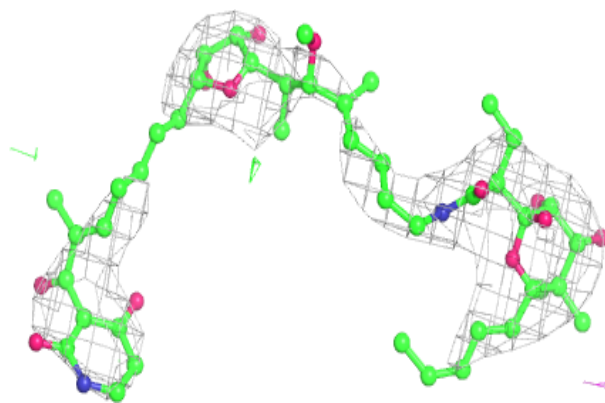
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



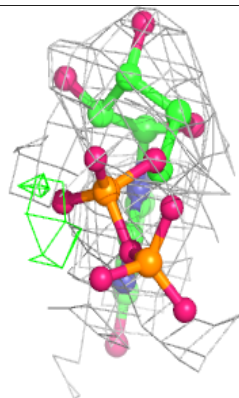
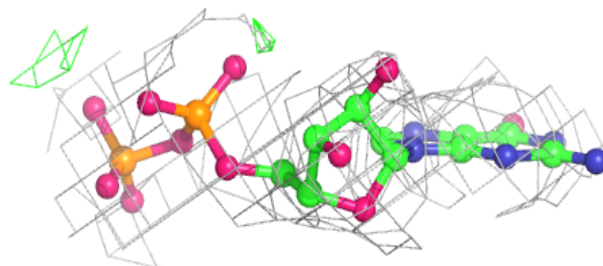
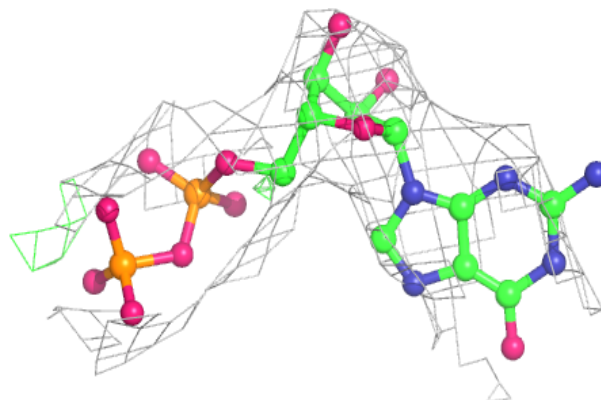


**Electron density around KIR AZ 502:**

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

**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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.