



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2018 – 11:15 PM EST

PDB ID : 4V5F  
Title : The structure of the ribosome with elongation factor G trapped in the post-translocational state  
Authors : Gao, Y.-G.; Selmer, M.; Dunham, C.M.; Weixlbaumer, A.; Kelley, A.C.; Ramakrishnan, V.  
Deposited on : 2009-09-01  
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

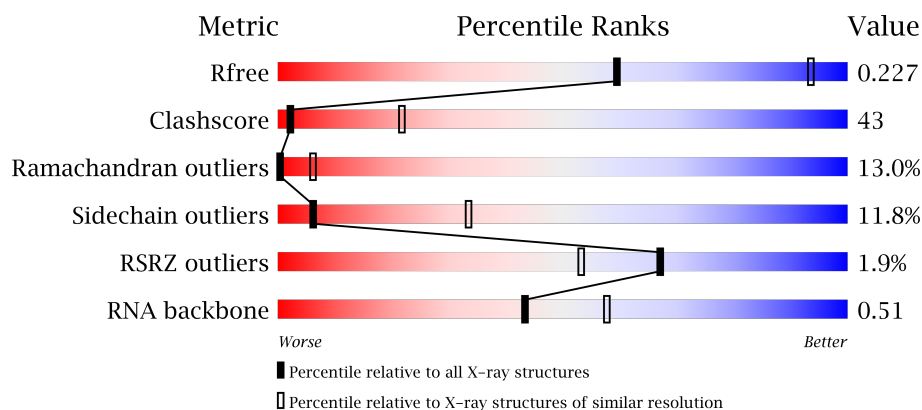
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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.



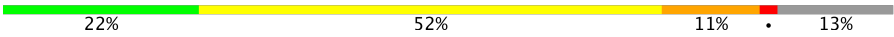
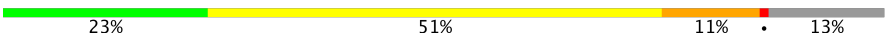



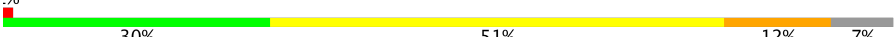
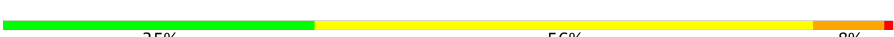
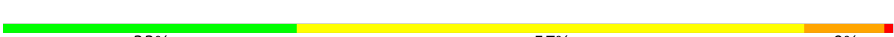
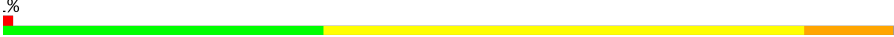

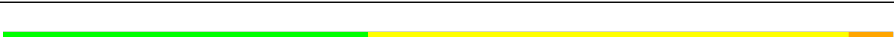
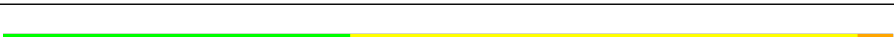

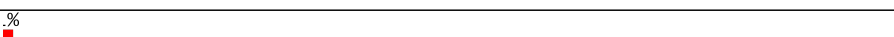
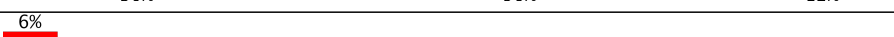
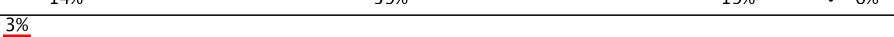



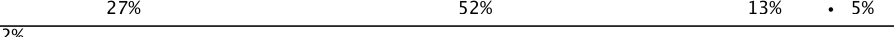
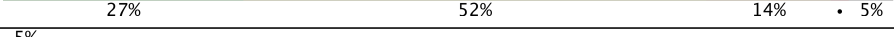
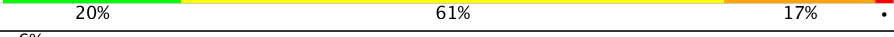
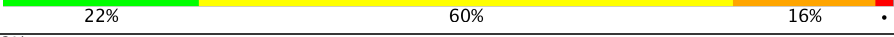


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)
RNA backbone	2435	1002 (4.30-2.90)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>28%</div> <div>55%</div> <div>13%</div> <div>..</div> </div>
1	CA	1522	<div> <div>27%</div> <div>57%</div> <div>14%</div> <div>..</div> </div>
2	AB	256	<div> <div>24%</div> <div>50%</div> <div>16%</div> <div>8%</div> </div>
2	CB	256	<div> <div>23%</div> <div>50%</div> <div>16%</div> <div>8%</div> </div>


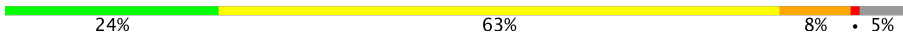
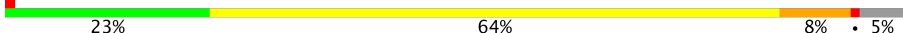


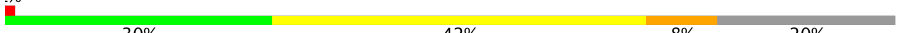
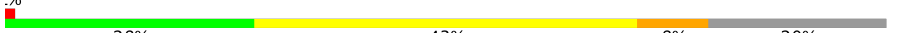




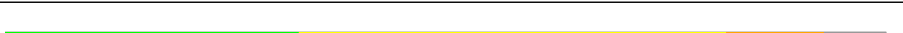





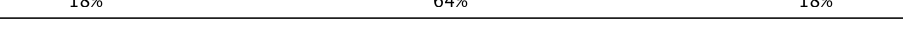


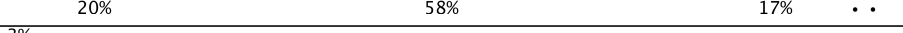
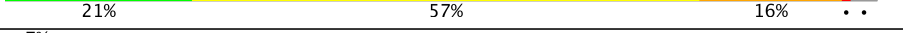


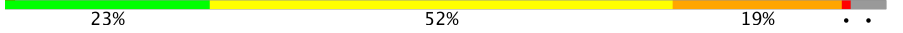
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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126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

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	AW	77	
22	CV	77	
22	CW	77	
23	AX	25	
23	CX	25	
24	AY	691	
24	CY	691	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	

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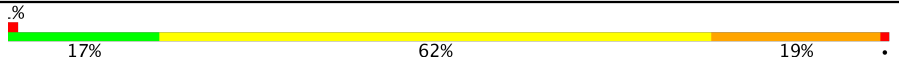
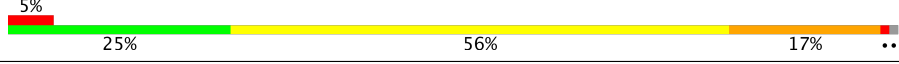
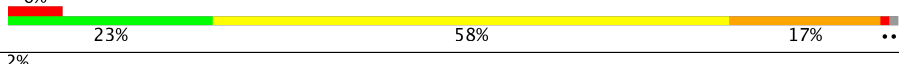
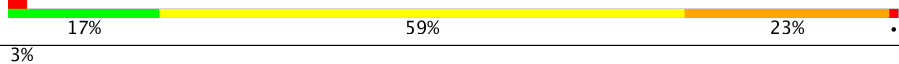
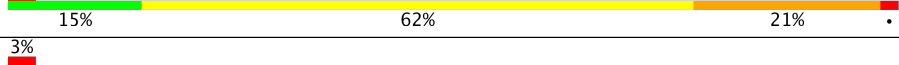
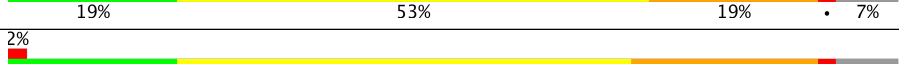
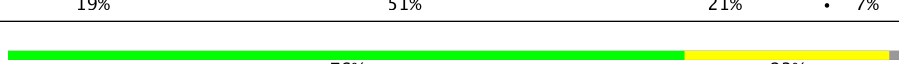
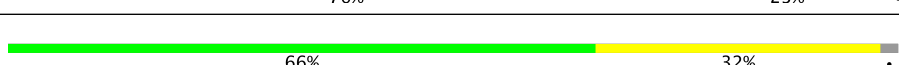
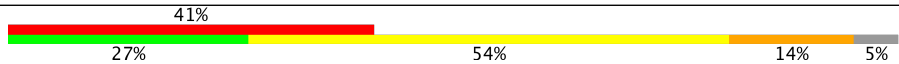






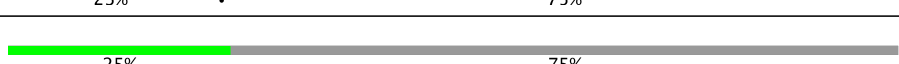
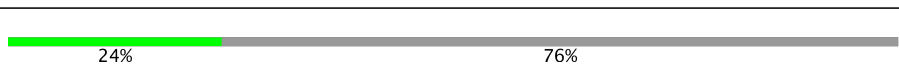
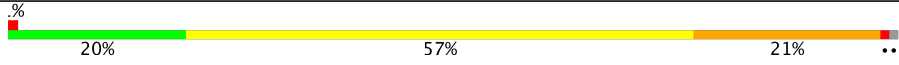
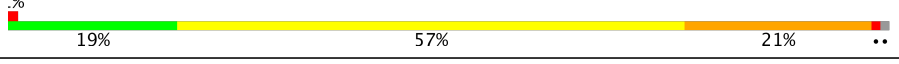








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Mol	Chain	Length	Quality of chain
27	B2	72	
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2915	
35	DA	2915	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	



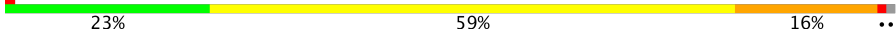
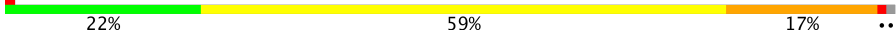
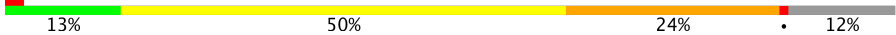
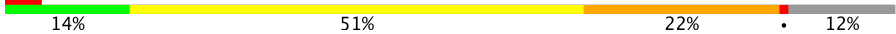
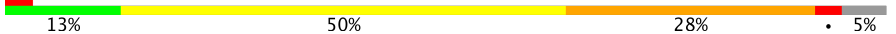
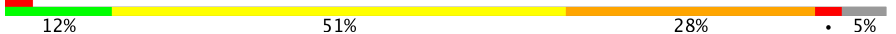
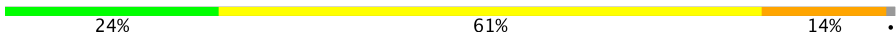
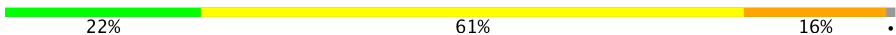
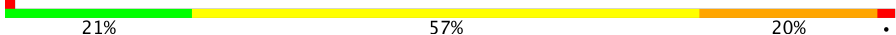

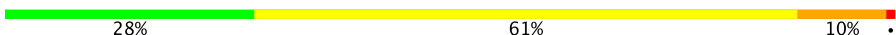







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Mol	Chain	Length	Quality of chain
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BJ	173	
43	DJ	173	
44	BK	147	
44	DK	147	
45	BL	125	
45	BM	125	
45	Bl	125	
45	Bm	125	
45	DL	125	
45	DM	125	
45	Dl	125	
45	Dm	125	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	

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Mol	Chain	Length	Quality of chain
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	
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
61	FUA	AY	702	-	-	-	X
61	FUA	CY	702	-	-	X	-

## 2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 311552 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called E-SITE TRNA FMET OR P-SITE TRNA FMET (UN-MODIFIED BASES EXCEPT FOR THYMINE 54).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	AW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	CV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	CW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	11	Total	C	N	O	P	0	0	0
			230	105	41	74	10			
23	CX	11	Total	C	N	O	P	0	0	0
			230	105	41	74	10			

- Molecule 24 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	667	Total	C	N	O	S	0	0	1
			5215	3316	893	988	18			
24	CY	667	Total	C	N	O	S	0	0	1
			5215	3316	893	988	18			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
26	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
28	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			
29	D4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
30	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
32	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
33	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			
35	DA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
39	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
40	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	167	Total	C	N	O	S	0	0	1
			1269	803	238	227	1			
42	DH	167	Total	C	N	O	S	0	0	1
			1269	803	238	227	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BJ	170	Total	C	N	O	S	0	0	0
			851	510	170	171				
43	DJ	170	Total	C	N	O	S	0	0	0
			851	510	170	171				

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BK	140	Total	C	N	O	S	0	0	1
			1026	653	182	186	5			
44	DK	140	Total	C	N	O	S	0	0	1
			1026	653	182	186	5			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BL	102	Total	C	N	O		0	0	1
			506	303	102	101				
45	BM	31	Total	C	N	O		0	0	1
			151	90	31	30				
45	Bl	31	Total	C	N	O		0	0	1
			151	90	31	30				
45	Bm	30	Total	C	N	O		0	0	1
			146	87	30	29				
45	DL	102	Total	C	N	O		0	0	1
			506	303	102	101				
45	DM	31	Total	C	N	O		0	0	1
			151	90	31	30				
45	Dl	31	Total	C	N	O		0	0	1
			151	90	31	30				
45	Dm	30	Total	C	N	O		0	0	1
			146	87	30	29				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
46	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	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			
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	99	Total	C	N	O		0	0	1
			771	486	155	130				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	DS	99	Total	C	N	O	0	0	1
			771	486	155	130			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	BT	138	Total	C	N	O	0	0	1
			1142	710	235	196			
52	DT	138	Total	C	N	O	0	0	1
			1142	710	235	196			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
56	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	107	Total	C	N	O	S	0	0	1
			811	520	155	131	5			
57	DY	107	Total	C	N	O	S	0	0	1
			811	520	155	131	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			
58	DZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			

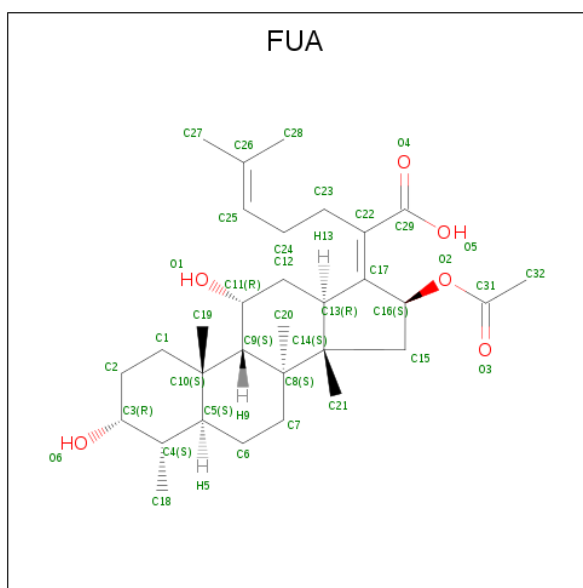
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

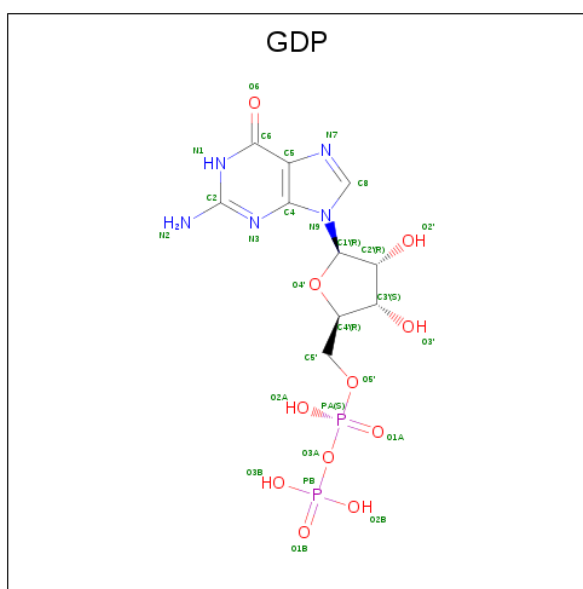
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AY	1	Total	Mg	0	0
			1	1		
60	CY	1	Total	Mg	0	0
			1	1		

- Molecule 61 is FUSIDIC ACID (three-letter code: FUA) (formula:  $C_{31}H_{48}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AY	1	Total	C	O	0	0
			37	31	6		
61	CY	1	Total	C	O	0	0
			37	31	6		

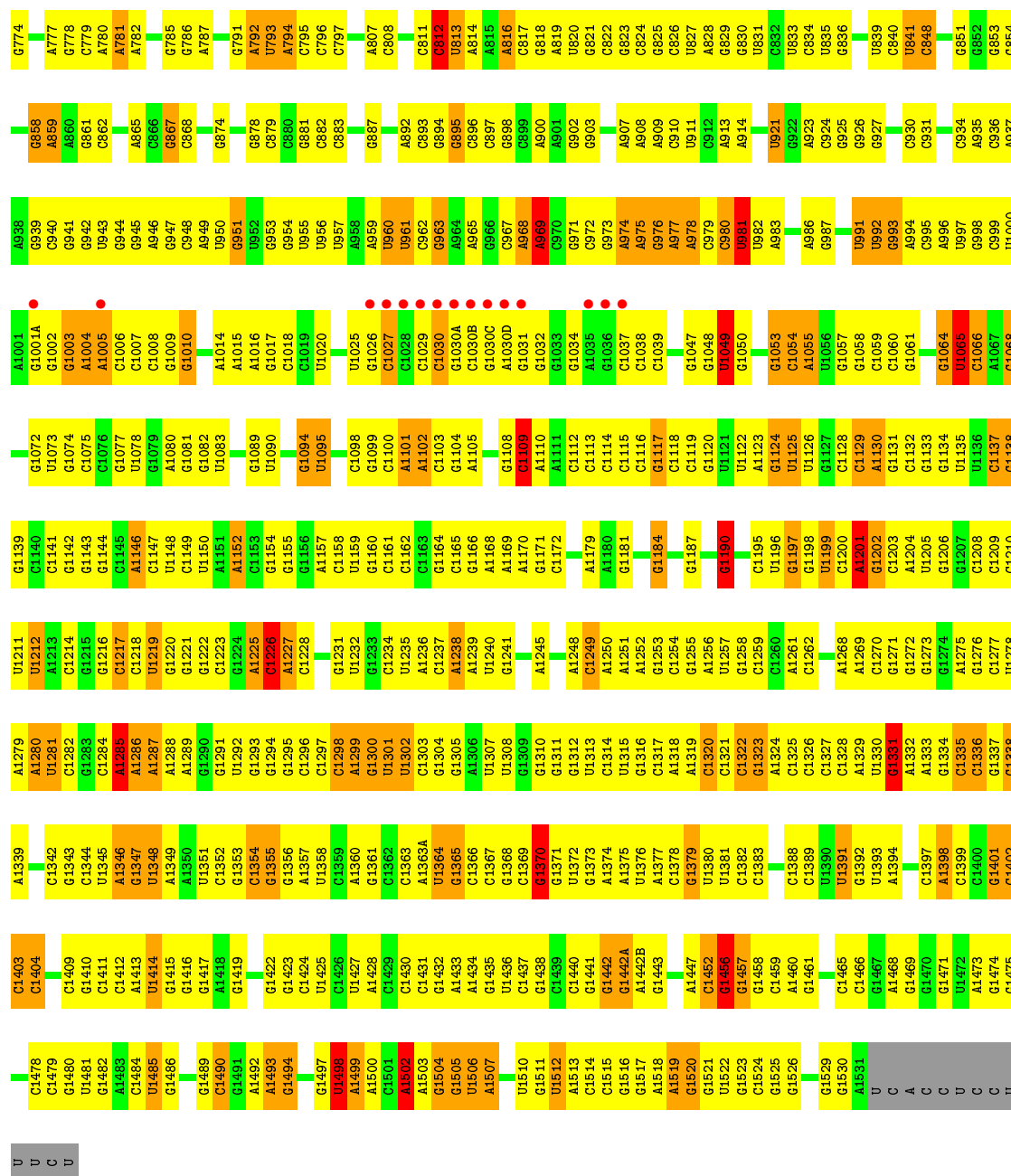
- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



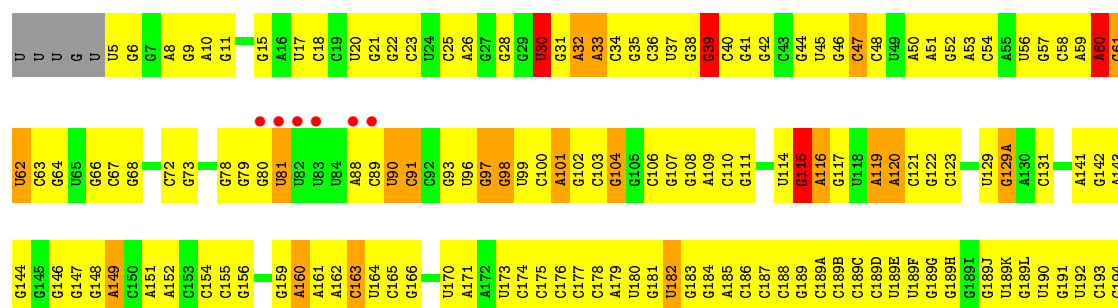


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
62	AY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
62	CY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

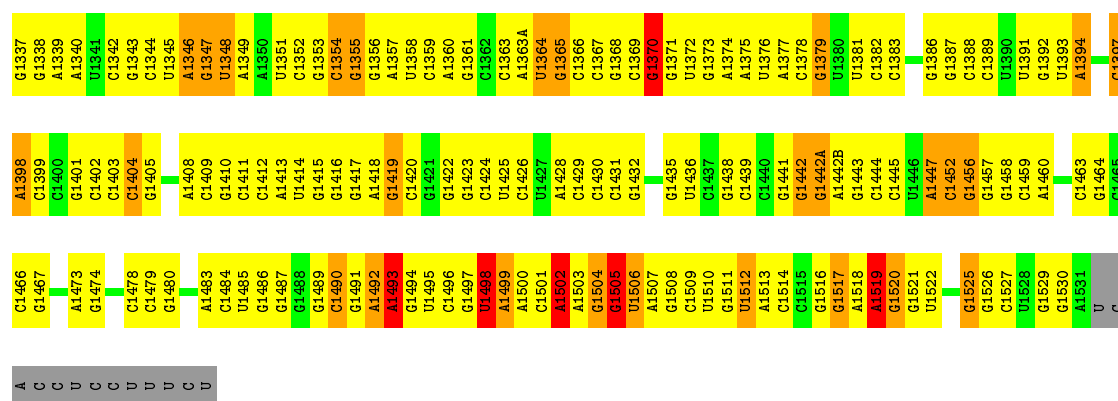




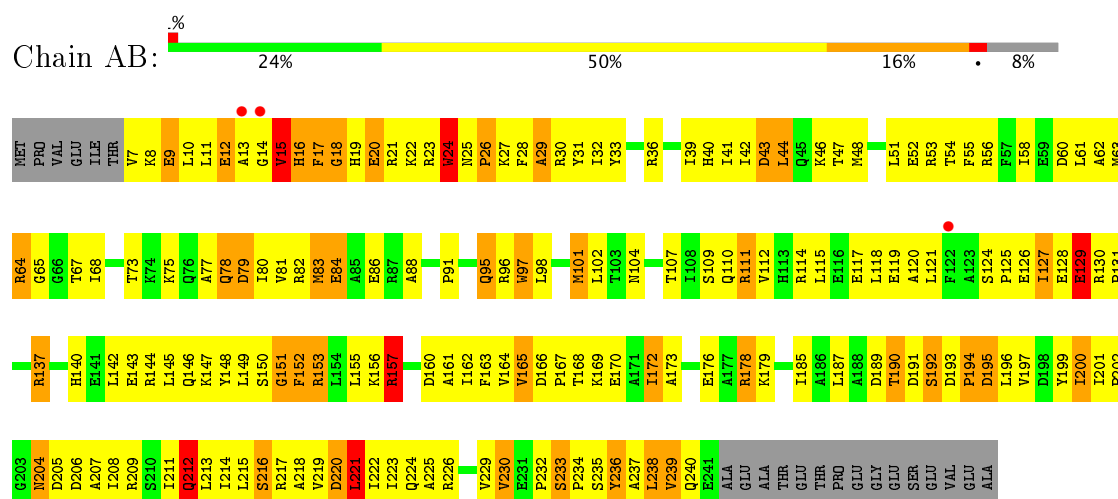
● Molecule 1: 16S ribosomal RNA



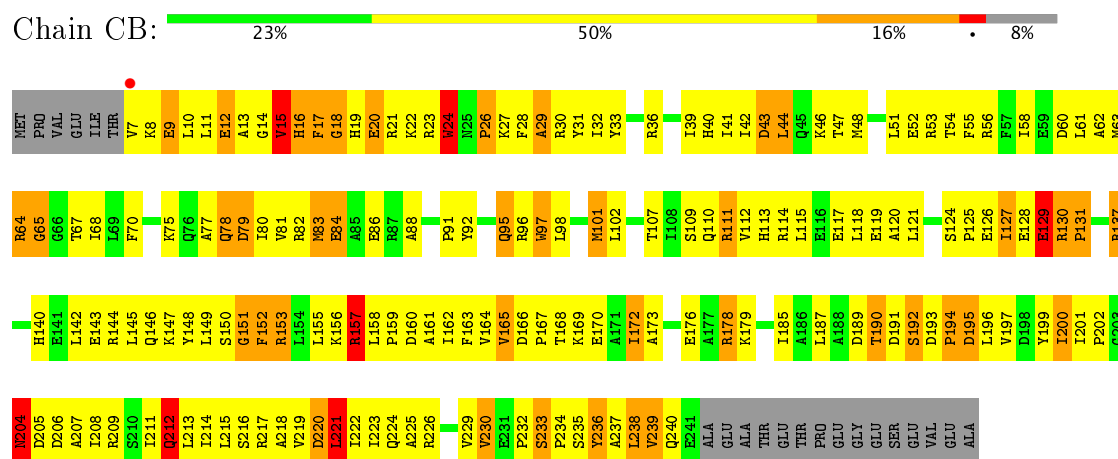
G1277	U1211	G1143	G1001A	G939	G854	G778	A712	G638	C556	U486	A408	A344	G278	A195
U1278	U1212	G1144	G1002	G940	G858	G779	G713	G641	G557	A487	G409	G345	G281	A196
A1279	A1213	C1145	G1003	G941	A780	A781	G714	U641	G558	C488	A412	G346	A281	A197
A1280	C1214	A1146	A1004	G942	A859	A782	G715	U646	U560	C489	A413	G347	C283	G198
U1281	G1215	C1147	A1005	G943	A860	A783	G716	U647	U561	G490	A414	A348	C284	C201
C1282	G1216	U1148	C1006	G944	G861	G783	G717	C547	C562	G491	A415	G350	G285	U202
G1283	G1217	C1149	C1007	G945	C862	G784	G718	G650	A572	G492	A416	G351	U203	U203
C1284	U1218	U1150	C1008	G946	A865	G785	G719	G651	U573	A495	G417	G352	G289	U204
A1285	U1219	A1151	G1009	G947	G866	G786	G720	C651	A574	A496	C418	A353	C290	G216
A1286	G1220	A1152	A1080	C948	G867	A787	A722	A653	U575	U498	C419	G354	C291	C217
A1287	G1221	C1153	G1081	A949	C868	G791	U723	G656	G576	A499	U420	C355	G292	C218
A1288	G1222	G1154	G1082	U950	C869	A792	G724	G657	G577	G500	C422	A356	G293	C219
G1290	C1223	G1155	U1083	G951	G874	U793	G725	G658	G578	G501	G423	G357	U294	G220
G1291	G1224	A1156	A1014	U952	G875	U794	G726	G659	C579	G502	G424	U358	C295	G221
G1292	A1225	A1157	A1015	G953	G876	A795	G727	U659	G579	U503	G425	U359	U296	U222
U1292	C1226	C1158	A1016	G954	G877	C796	A728	G660	G579	U504	G426	A360	C297	U223
G1293	A1227	U1159	C1019	U955	C879	C797	A729	G661	U582	G505	G428	G362	A298	U229
G1294	C1228	G1160	U1020	U956	G880	C798	G730	G662	A583	A509	U429	A363	G299	U230
G1295	A1229	C1161	U1095	U957	C881	A802	G731	A663	G584	A510	A430	A364	A300	U231
C1296	G1230	C1162	U1025	A958	C882	G803	C732	A664	G585	C511	A431	U365	G301	C235
C1297	G1231	C1163	G1026	A959	C883	G804	A733	A665	G586	C512	C433	U366	G302	
C1298	U1232	A1164	C1027	U960	C884	C805	C736	G666	C586	C513	U434	U368	G306	G238
A1299	G1233	C1165	C1028	U961	C885	A807	A737	U672	U588	C514	C435	U369	C307	U239
G1300	G1234	G1166	G1029	G962	G886	C808	C738	G673	G599	C515	C436	G370	G308	G240
U1301	U1235	A1168	C1030	G963	G887	C811	C739	G674	A602	C516	C437	G371	G309	C241
U1302	A1236	A1169	G1030A	A964	G888	C812	C740	A675	A603	G521	C438	G372	C311	A243
C1303	C1237	A1170	C1030B	A965	C889	C813	C741	A676	A604	C522	A439	C373	C312	U244
G1304	A1238	G1171	G1030C	G966	C890	C814	G742	A677	U603	C523	A441	A374	A313	C245
G1305	A1239	C1172	G1031	A967	C891	A815	U743	U678	G604	A523	C444	U375	C314	A246
A1306	U1240	G1173	G1032	A968	C892	A816	C744	U679	G605	U524	C445	G376	A315	G247
U1307	G1241	C1174	G1033	C970	C893	C817	C745	U680	A606	C525	G446	G377	G316	
U1308		C1175	G1034	G971	C894	G818	C746	C681	A607	C526	G447	G380	G317	A250
G1309	C1244	A1179	G1035	G972	A900	U820	C747	C682	U608	C527	G448	G381	G318	G251
G1310	A1245	A1180	G1036	G973	A901	U821	C748	G683	A609	C528	C449	G382	G319	U252
U1311	U1246	G1181	C1037	A974	A902	G822	C749	U684	U610	C529	C450	G383	C320	U253
U1312	A1248	C1182	G1038	C976	A903	G823	G750	G685	G611	C530	A451	G384	A321	G254
U1313	A1250	G1184	C1039	A977	A904	G824	C751	U686	G612	C531	C452	G385	U323	U255
U1314	A1251	C1185	G1047	A978	A905	C825	C752	A687	U613	C532	C453	C386	U324	G257
G1316	A1252	G1187	C1048	C979	A906	C826	C753	G688	U614	C533	G454	A387	G325	
C1317	G1253	A1188	U1049	C980	A907	U827	C754	C689	U615	C534	G455	A388	U326	
A1318	C1254	G1190	U1049A	U981	A908	U828	C755	G690	U616	C535	C456	A389	A325	
A1319	G1255	C1191	G1050	U982	A909	G829	C756	G691	A621	C536	G457	C390	G326	G260
C1320	A1256	U1194	C1051	U983	C910	G830	C757	U692	A622	C537	G458	G391	G327	U261
C1321	U1257	C1195	G1052	A983	G922	G831	C758	U693	A623	C538	G459	G392	A328	A262
C1322	G1258	U1196	C1053	A984	A923	U831	C759	G694	C623	C539	C470	A393	A329	A263
G1323	C1259	G1197	A1055	A986	C924	C832	C763	A694	C624	C540	G471	G394	C320	G264
A1324	C1260	G1198	U1056	G987	G925	U833	C764	A695	G625	C541	A472	C395	G330	U265
C1325	A1261	U1199	G1057	G988	G926	C834	C765	A696	U626	C542	G473	G396	G331	G265
C1326	C1262	C1200	G1058	U991	G927	U835	C766	U697	G627	C543	G474	A397	G332	G266
G1327		A1201	C1059	U992	G928	G836	C767	G698	G628	C544	G475	C398	G333	C267
C1328	A1268	G1202	C1060	G993	C930	U837	C768	A768	G629	C545	G476	G399	C334	C268
A1329	A1269	C1203	U1061	A994	C931	U838	C769	G769	G630	C546	A477	C400	C335	C269
U1330	C1270	A1204	U1062	C995	C932	U839	C770	A704	G631	C547	C478	C401	C336	A270
G1331	G1271	U1205	C1063	A996	G933	U841	C771	G707	A632	C548	U480	G402	C337	C271
A1332	G1272	G1206	G1064	U997	G934	C848	C772	C708	G633	C549	G481	C403	A338	C272
A1333	G1273	G1207	U1065	G998	A935	C849	C773	G709	C634	C550	A482	U404	C341	G275
G1334	C1274	C1208	U1066	G999	C936	G851	C774	G710	G635	C551	C483	U405	C342	G276
C1335	A1275	U1209	A1067	U1000	A937	G852	C775	G711	U636	C552	G484	G406	C343	G277
C1336	G1276	C1210	G1068	A1001	A938	G853	C776		G637	C553	G485	G407	U343	



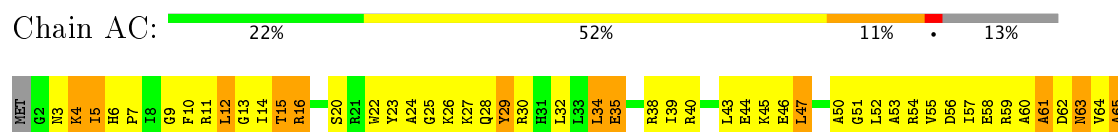
### • Molecule 2: 30S RIBOSOMAL PROTEIN S2



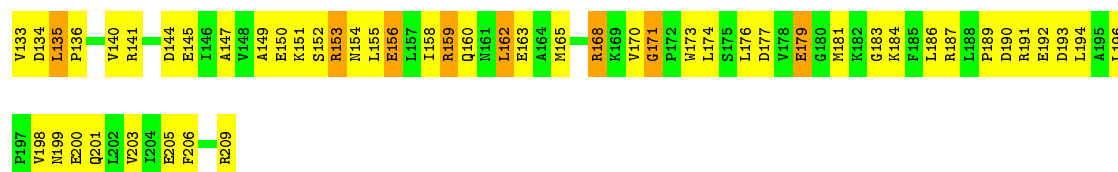
### • Molecule 2: 30S RIBOSOMAL PROTEIN S2



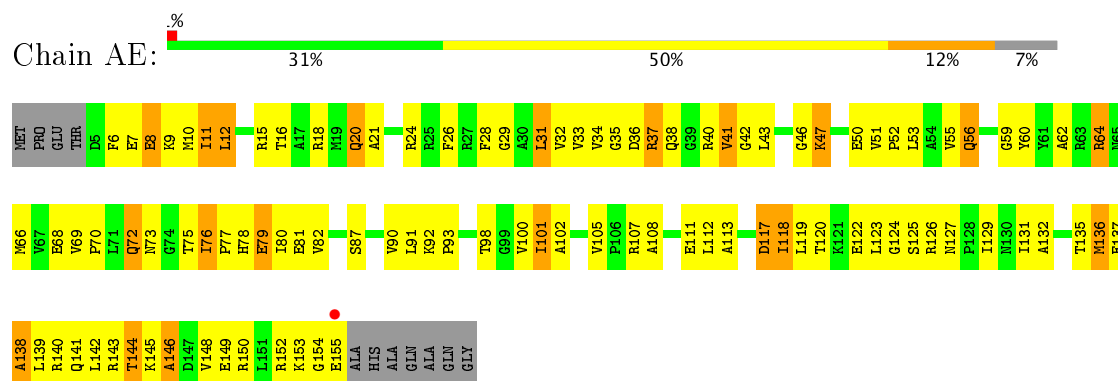
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3



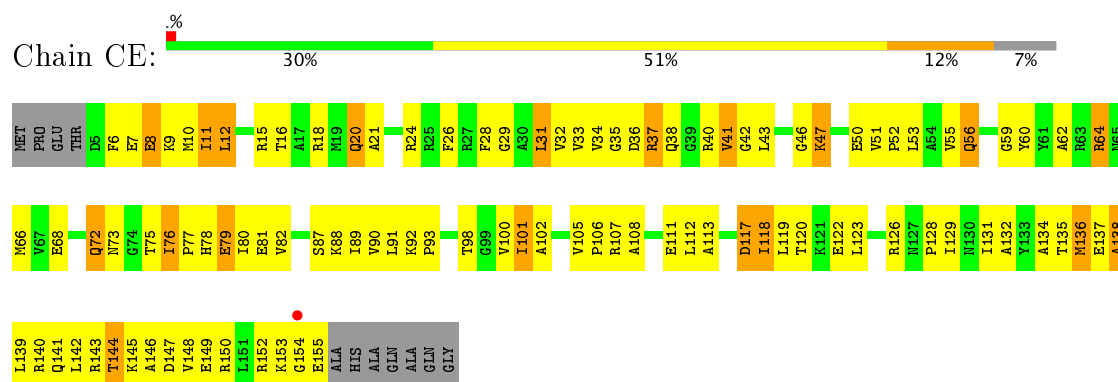




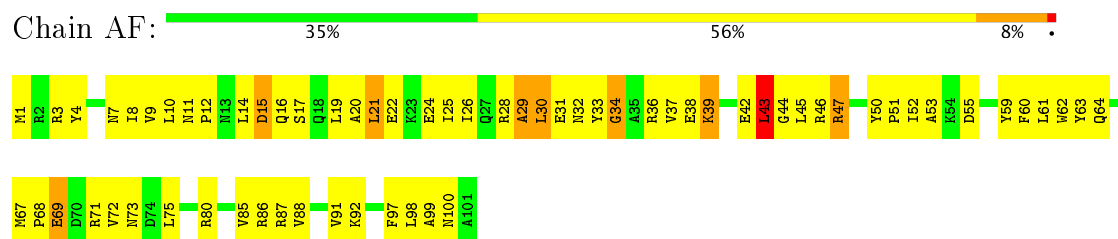
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



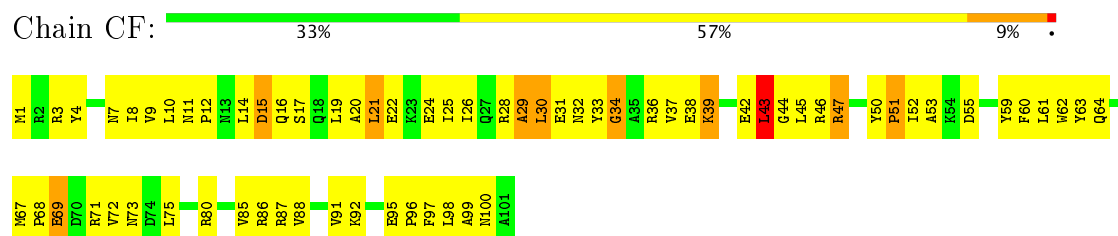
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



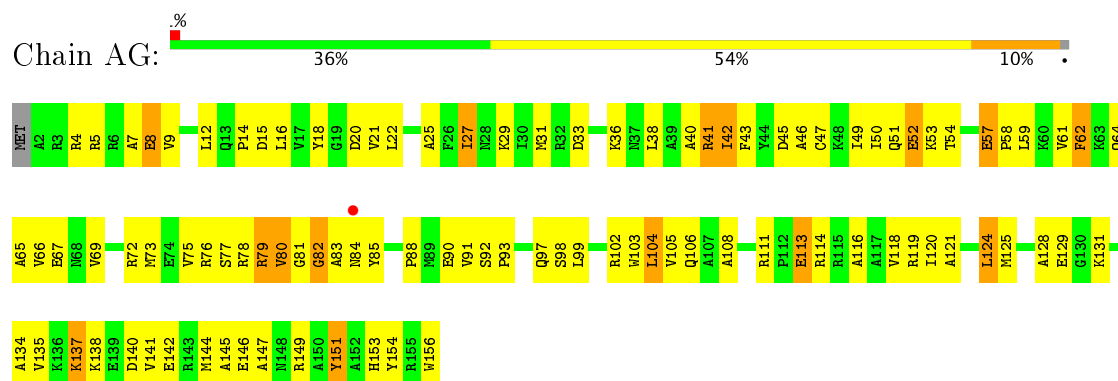
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



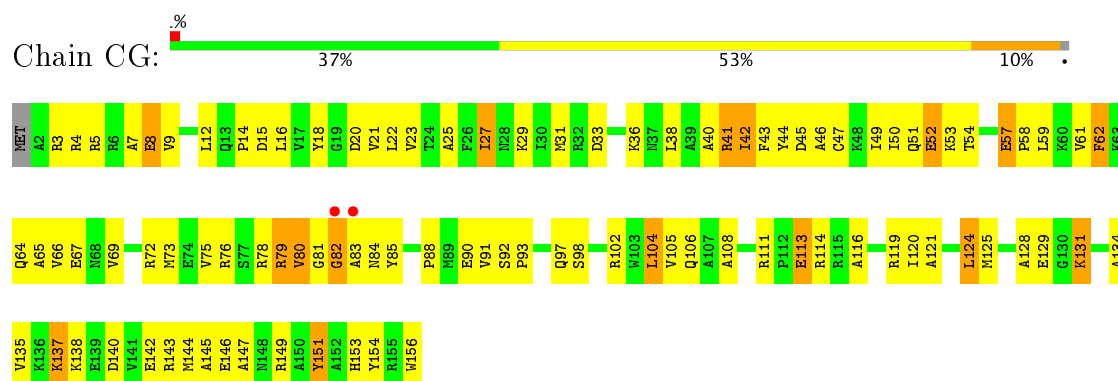
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



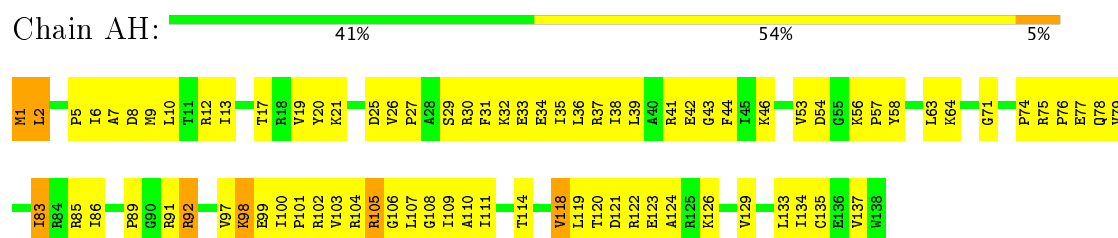
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



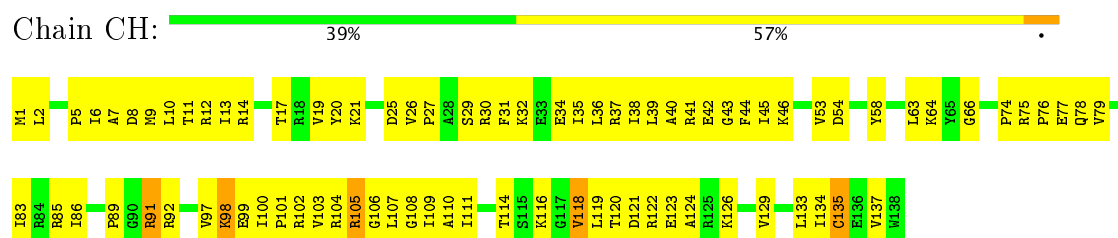
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



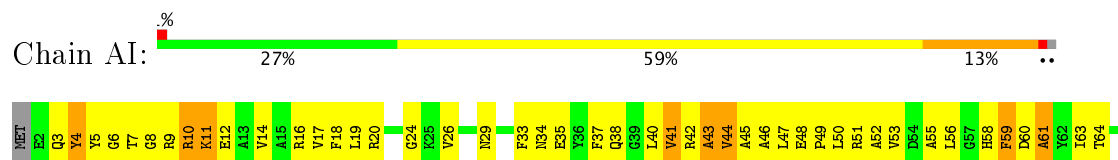
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



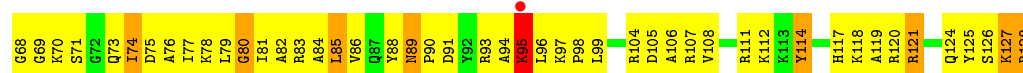
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



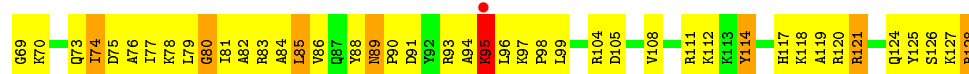
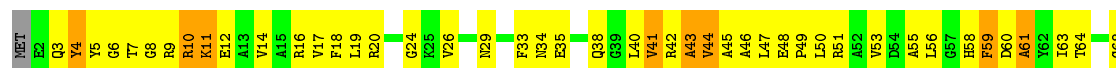
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



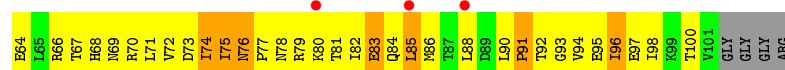
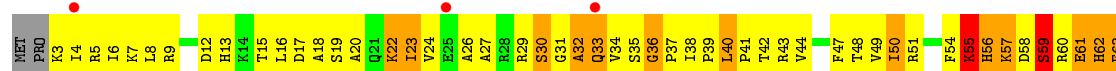
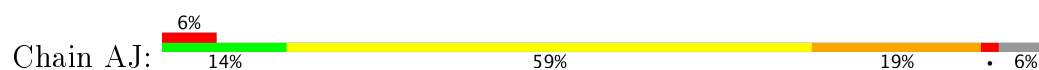




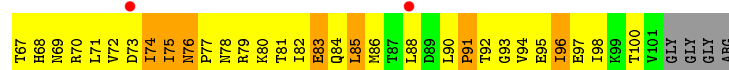
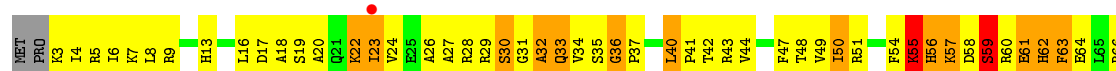
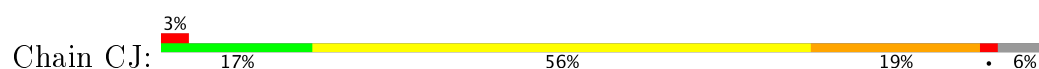
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

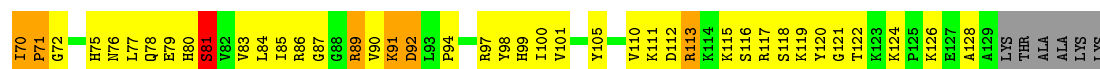
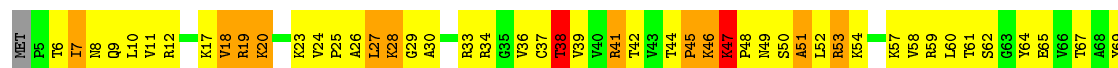


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

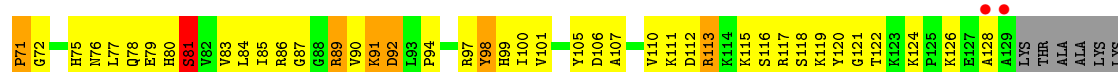
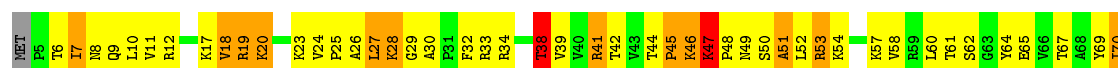




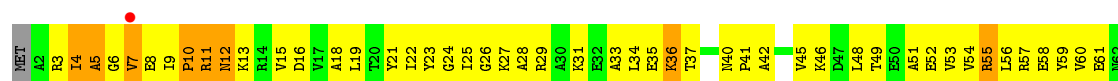
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



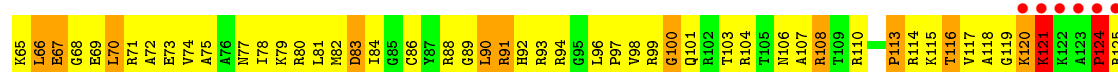
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 13: 30S RIBOSOMAL PROTEIN S13



- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN: 



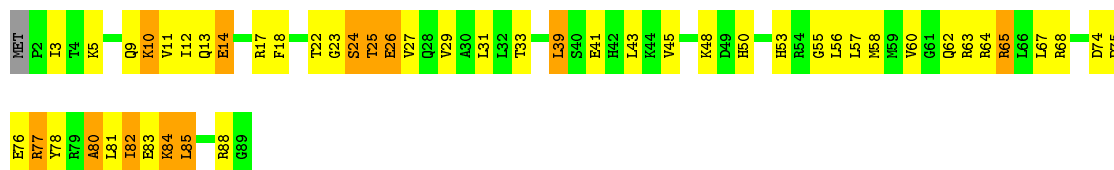
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN: 



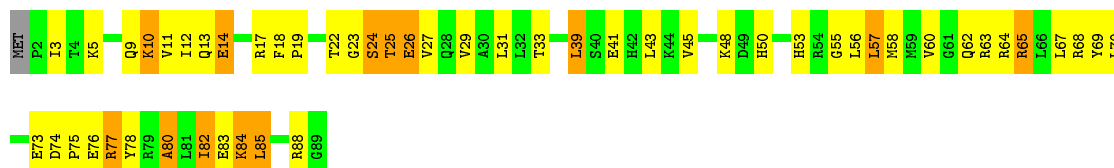
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO: 



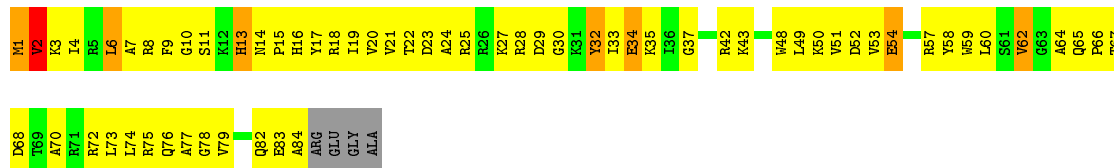
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO: 



- Molecule 16: 30S RIBOSOMAL PROTEIN S16

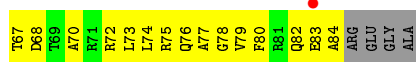
Chain AP: 



- Molecule 16: 30S RIBOSOMAL PROTEIN S16

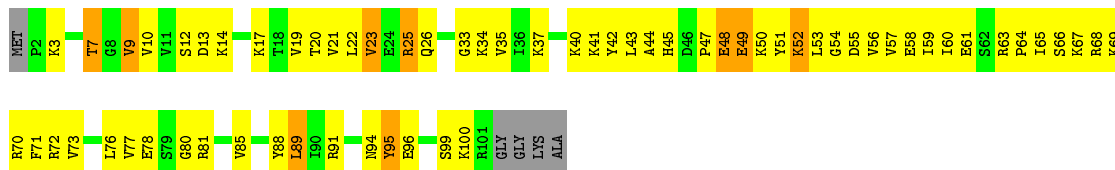
Chain CP: 





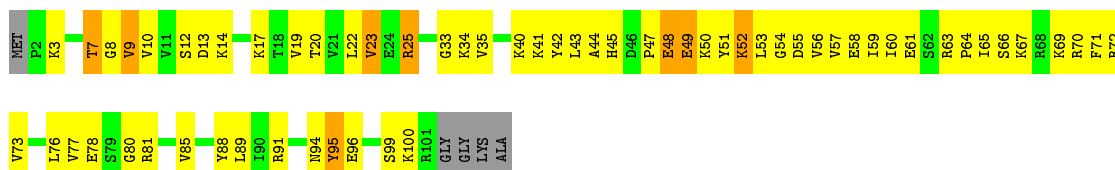
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ: 33% 53% 9% 5%



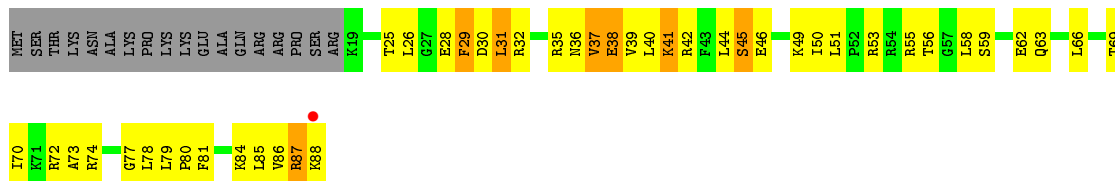
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ: 36% 51% 8% 5%



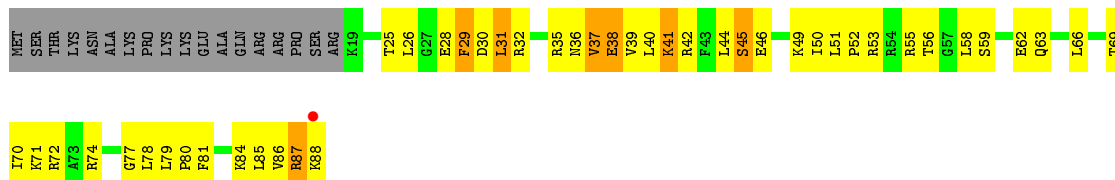
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR: 30% 42% 8% 20%



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

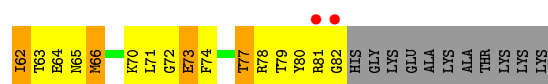
Chain CR: 28% 43% 8% 20%



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS: 2% 12% 45% 26% 15%

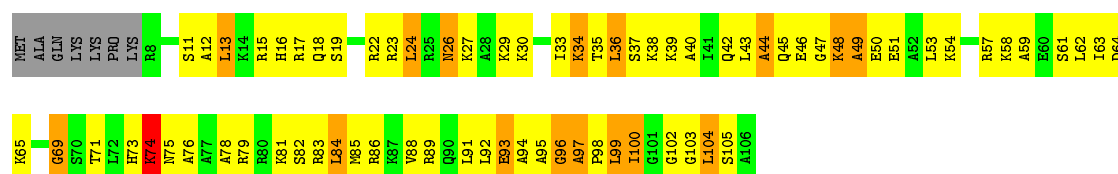




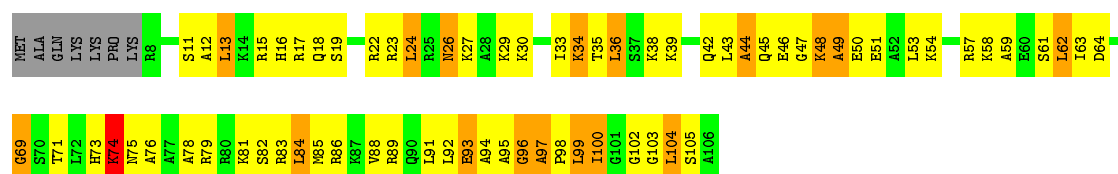
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



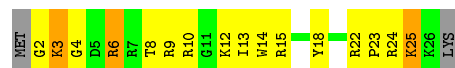
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

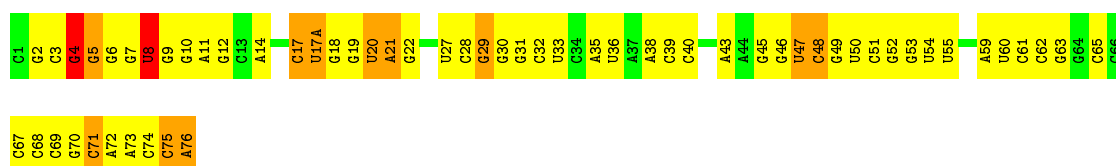


• Molecule 21: 30S RIBOSOMAL PROTEIN THX

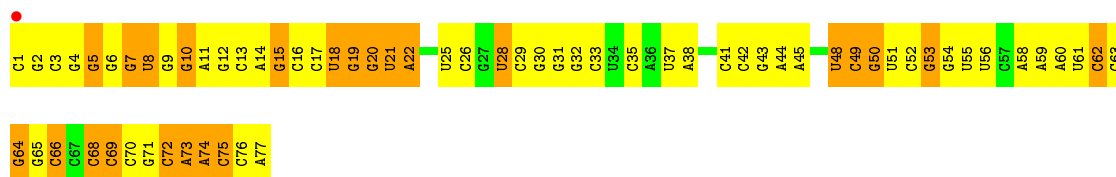
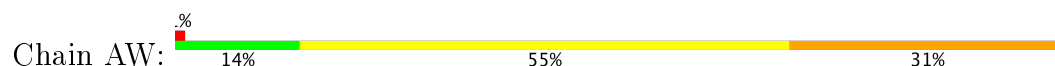


• Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)

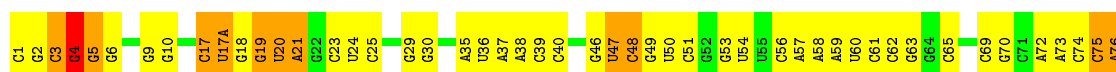




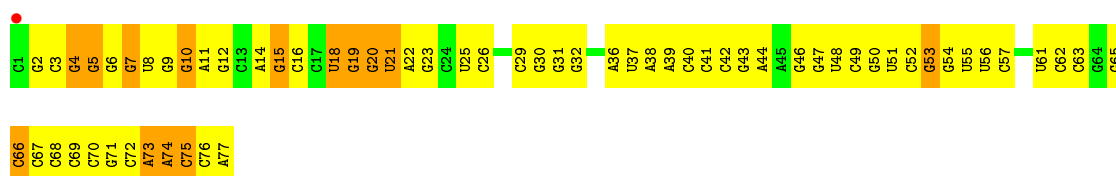
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



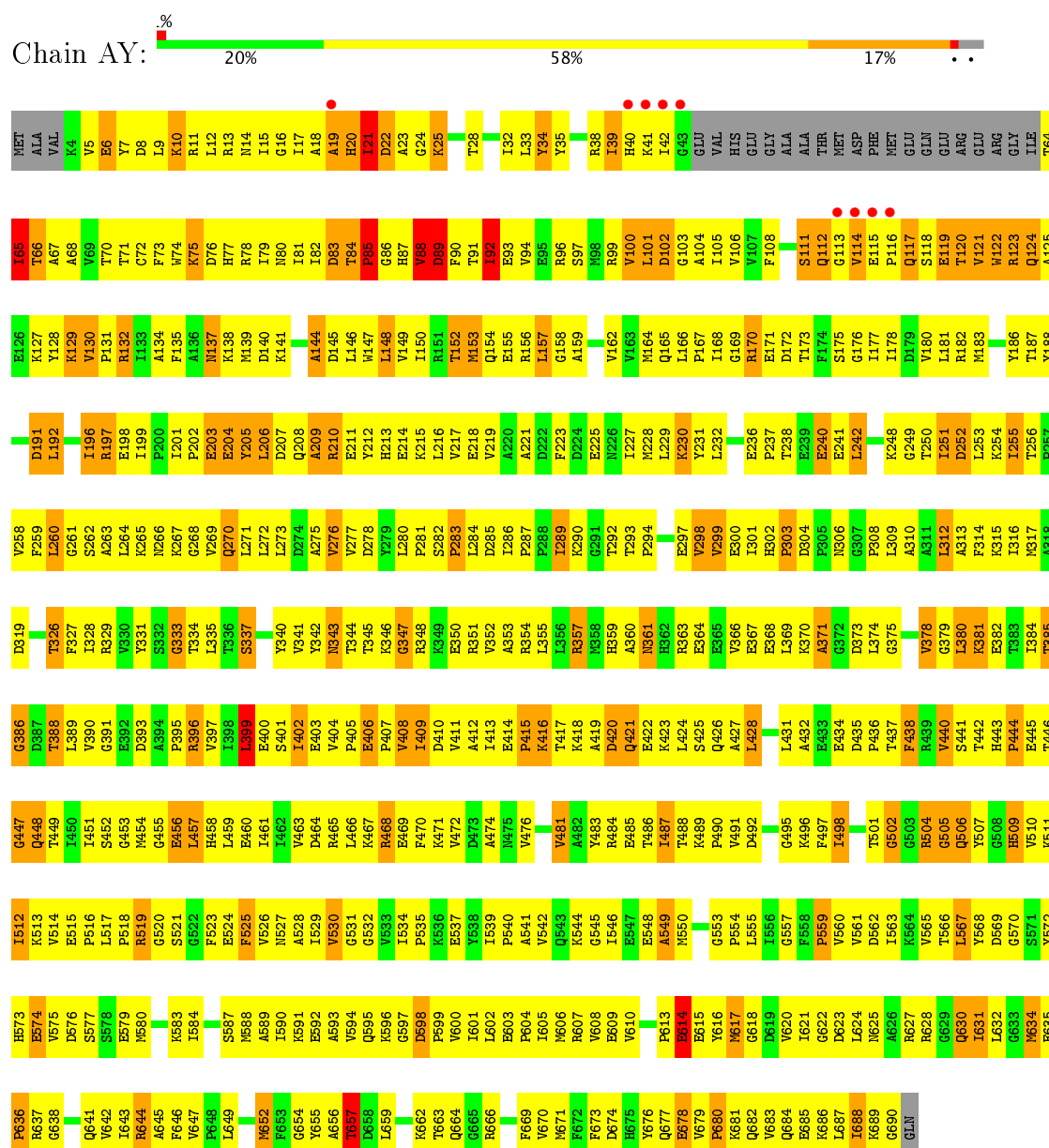
- Molecule 23: MRNA

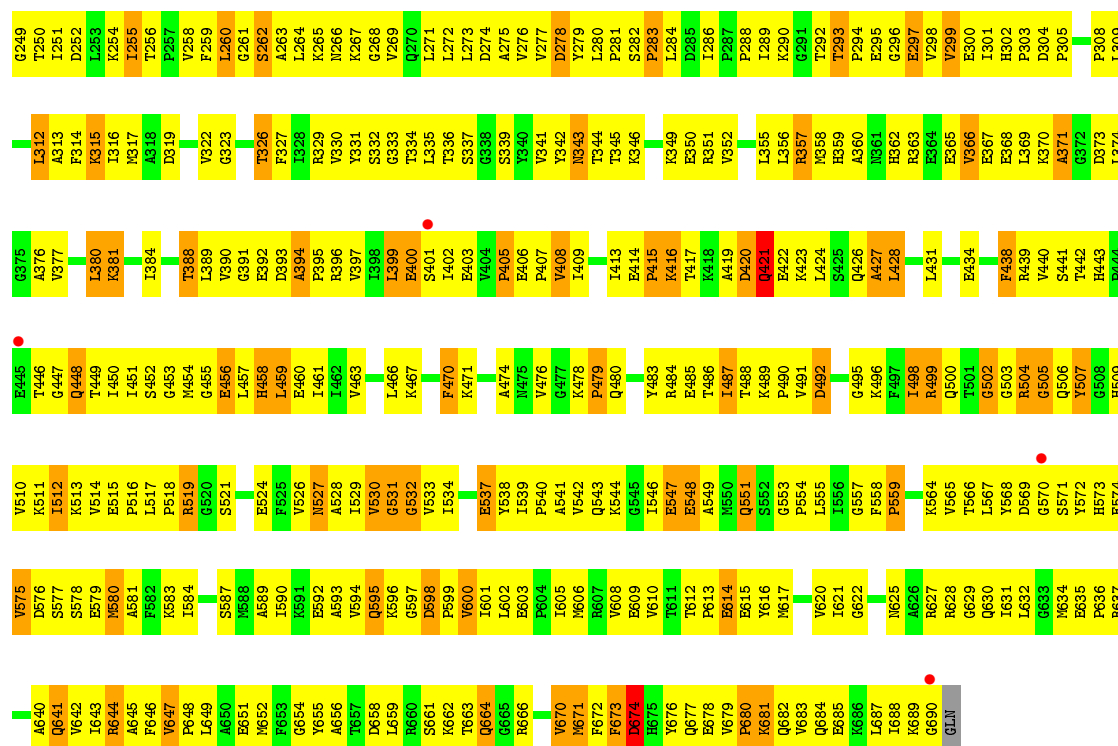


- Molecule 23: MRNA

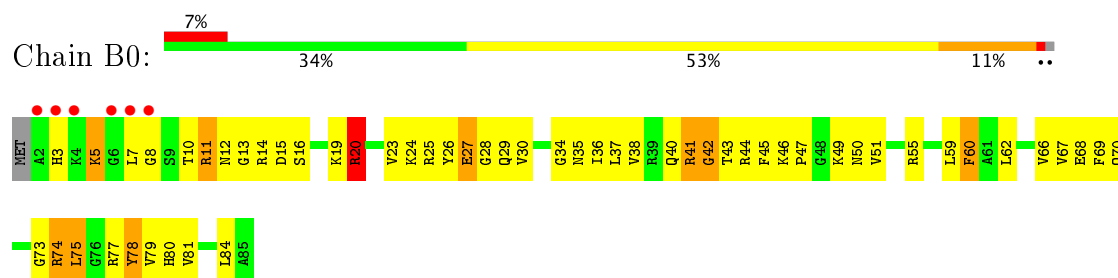


- Molecule 24: ELONGATION FACTOR G

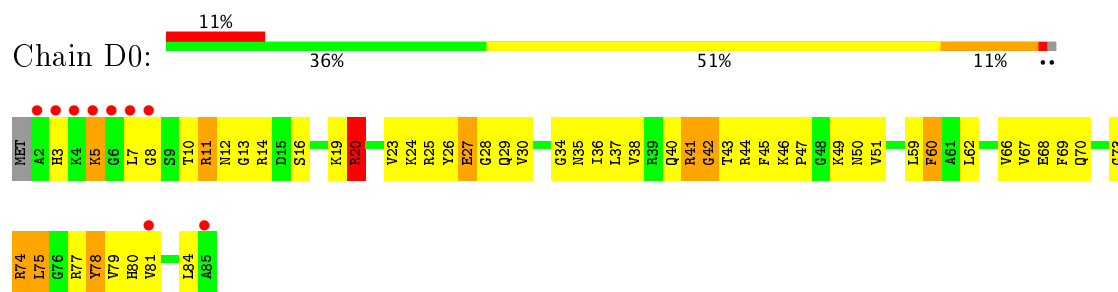




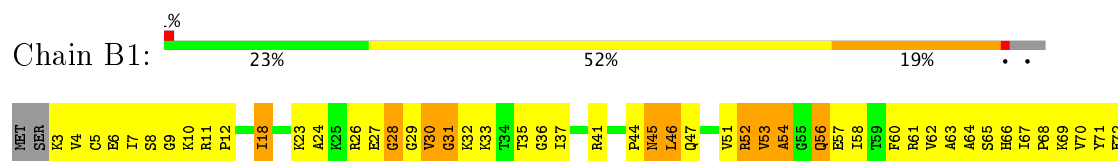
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



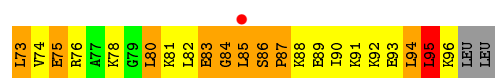
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



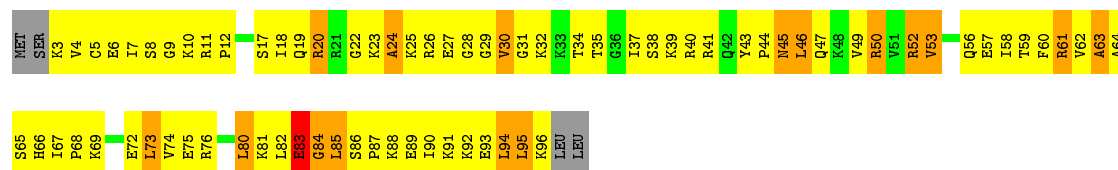
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



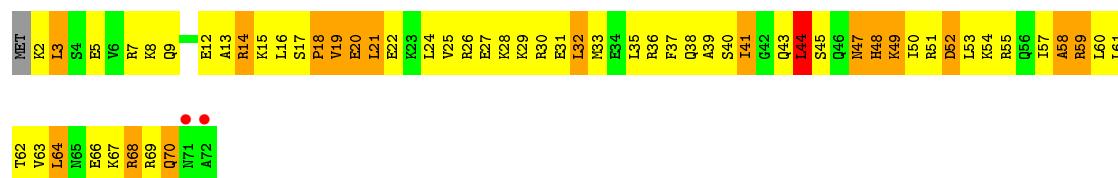




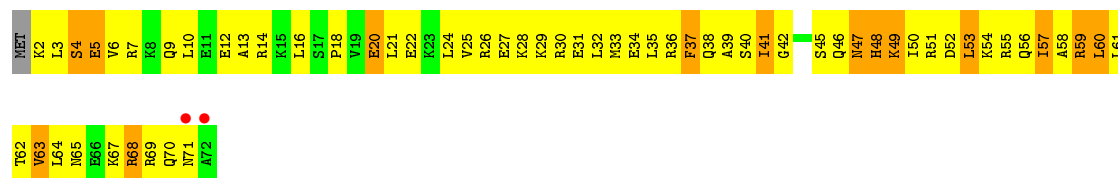
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



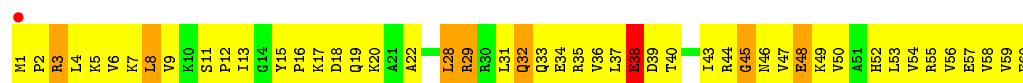
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



• Molecule 27: 50S RIBOSOMAL PROTEIN L29



• Molecule 28: 50S RIBOSOMAL PROTEIN L30

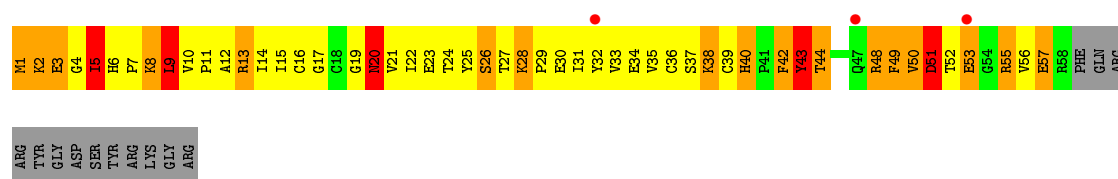


• Molecule 28: 50S RIBOSOMAL PROTEIN L30

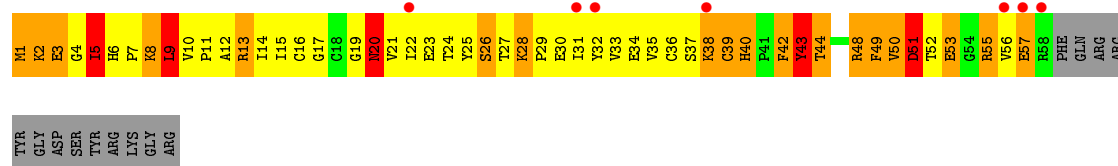


• Molecule 29: 50S RIBOSOMAL PROTEIN L31

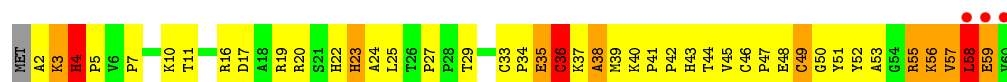




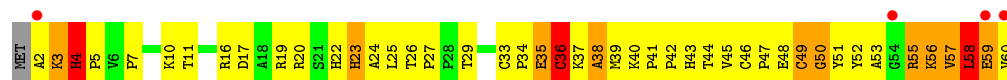
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



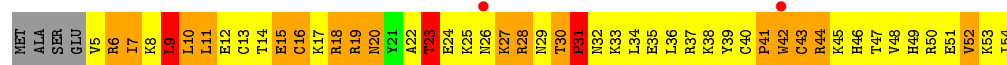
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



• Molecule 30: 50S RIBOSOMAL PROTEIN L32



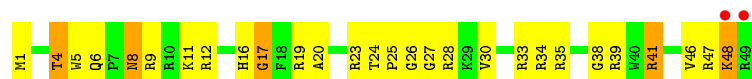
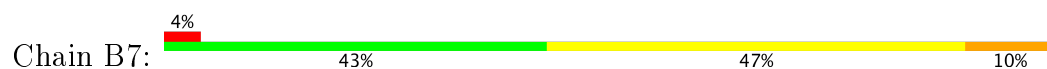
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



• Molecule 31: 50S RIBOSOMAL PROTEIN L33



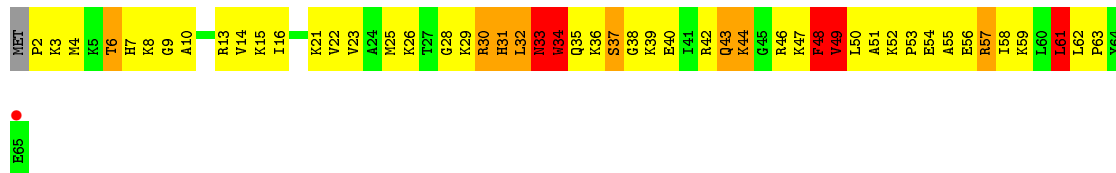
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



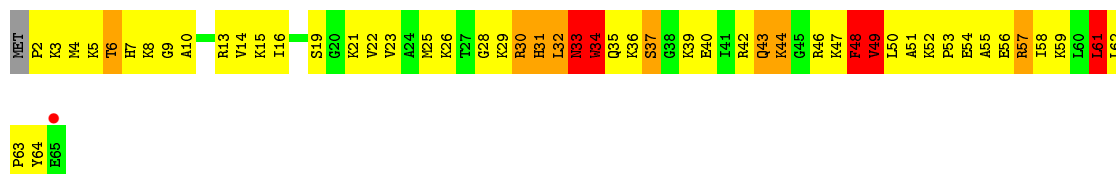
## • Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain D7:  45% 45% 10%

## • Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain B8:  2% 22% 57% 12% 8%

## • Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain D8:  2% 18% 60% 12% 8%

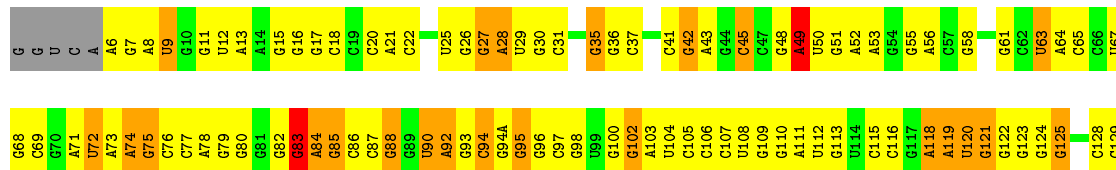
## • Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain B9:  30% 51% 16%

## • Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain D9:  3% 27% 54% 14% 5%

## • Molecule 35: 23S RIBOSOMAL RNA

Chain BA:  % 26% 56% 17%

G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	U1081	A1084	A1088	G1089	U1090	G1092	G1093	G1094	G1095	A1096	U1097	A1098	U1099	G1100	U1101	G1102	A1103	G1104	G1105	G1106	G1107	U1108	G1109	G1110	A1111	G1112	U1113	G1114	G1115	G1116	G1117	G1118	G1119	G1120	G1121	G1122	G1123	G1124	G1125	A1126	A1127	A1128	G1131																																																																																																																																																																																																																																																																																																																																																																																																																							
G942	U943	G944	A945	G946	G947	G948	G949	G950	G951	G952	A953	G954	G955	U958	A959	A960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	A973	G974	G975	G976	G977	G978	G979	A980	A981	G982	A983	A984	G985	G986	G987	G988	G989	G990	G991	G992	G993	A996	G997	G998	U999	A1000	A1001	G1002																																																																																																																																																																																																																																																																																																																																																																																																																						
G1005	G1006	G1007	G1008	G1009	A1010	G1011	G1012	G1013	G1014	G1015	G1016	U1019	A1020	G1021	G1022	U1023	G1024	G1025	A1026	A1027	A1028	A1029	A1030	U1033	G1034	U1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	A1045	A1046	G1047	A1048	G1049	A1050	G1051	G1052	G1053	A1054	A1057	G1058	G1059	U1060	G1061	G1062	G1063	G1064	A1067																																																																																																																																																																																																																																																																																																																																																																																																																								
C976	U977	A978	G979	G980	G981	G982	G983	G984	G985	G986	A987	G988	G989	A990	C993	C994	C995	C996	C997	C998	C999	A900	A901	C902	C903	C904	C905	C906	C907	C908	A909	A910	C911	C912	C913	C914	C915	C916	A917	A918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941																																																																																																																																																																																																																																																																																																											
U810	U811	A812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941																																																																																																																																																																																																																																							
C580	C581	C582	C583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	C600	C601	C602	C603	C604	C605	C606	C607	C608	C609	C610	C611	C612	C613	C614	C615	C616	C617	C618	C619	C620	C621	C622	C623	C624	C625	C626	C627	C628	C629	C630	C631	C632	C633	C634	C635	C636	C637	C638	C639	C640	C641	C642	C643	C644	C645	C646	C647	C648	C649	C650	C651	C652	C653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	
C516	C517	C518	C519	C520	C521	C522	C523	C524	C525	C526	C527	C528	C529	C530	C531	C532	C533	C534	C535	C536	C537	C538	C539	C540	C541	C542	C543	C544	C545	C546	C547	C548	C549	C550	C551	C552	C553	C554	C555	C556	C557	C558	C559	C560	C561	C562	C563	C564	C565	C566	C567	C568	C569	C570	C571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	C583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	C600	C601	C602	C603	C604	C605	C606	C607	C608	C609	C610	C611	C612	C613	C614	C615	C616	C617	C618	C619	C620	C621	C622	C623	C624	C625	C626	C627	C628	C629	C630	C631	C632	C633	C634	C635	C636	C637	C638	C639	C640	C641	C642	C643	C644	C645	C646	C647	C648	C649	C650	C651	C652	C653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978</



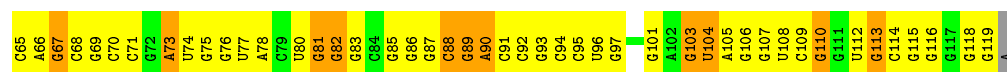




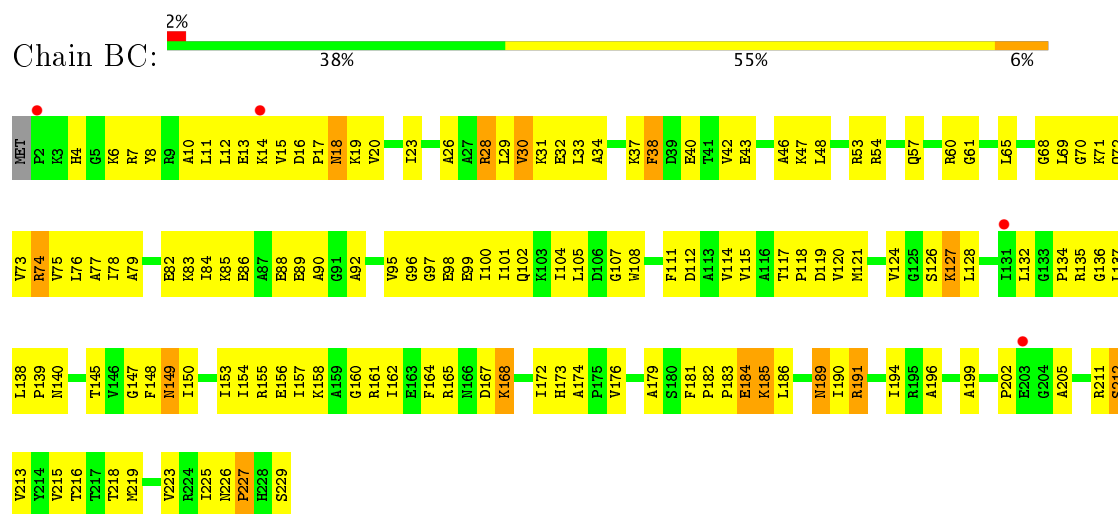




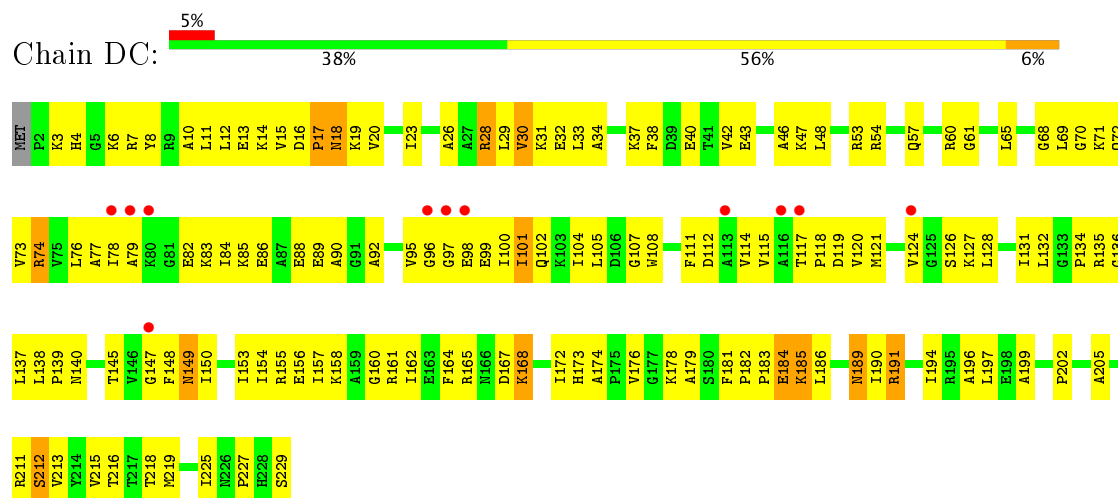




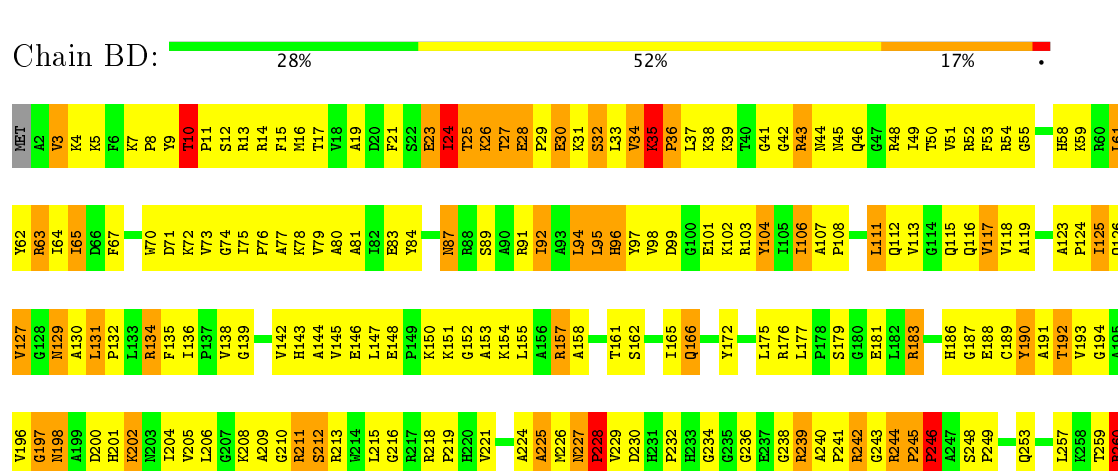
• Molecule 37: 50S RIBOSOMAL PROTEIN L1



• Molecule 37: 50S RIBOSOMAL PROTEIN L1



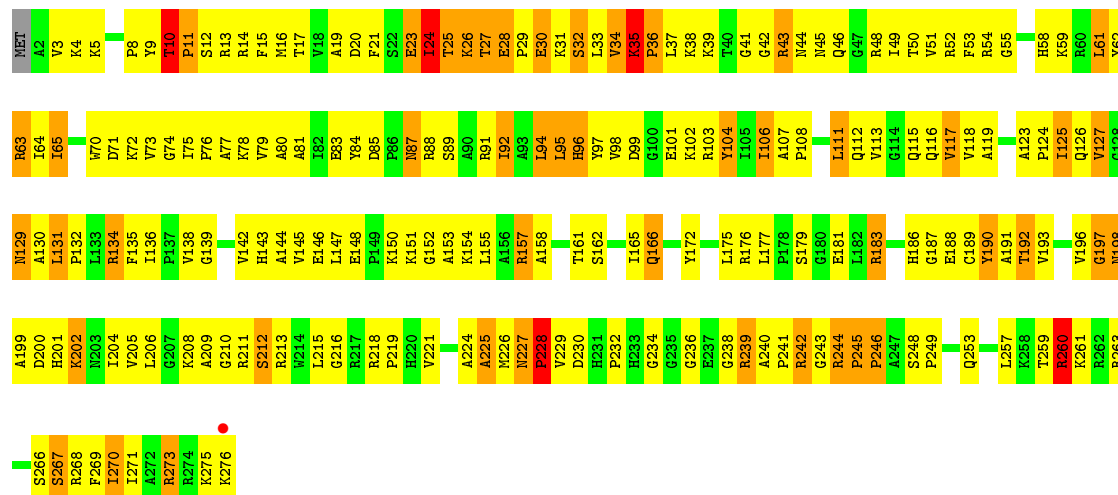
• Molecule 38: 50S RIBOSOMAL PROTEIN L2





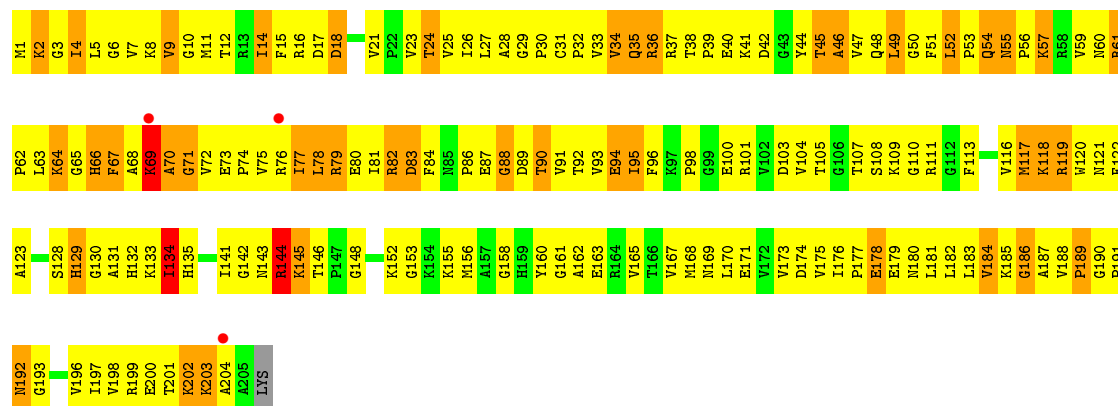
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain DD: 27% 54% 17%



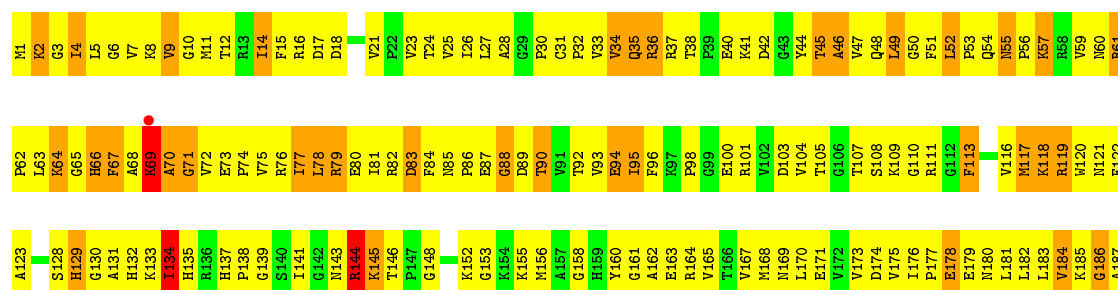
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain BE: 17% 60% 21%

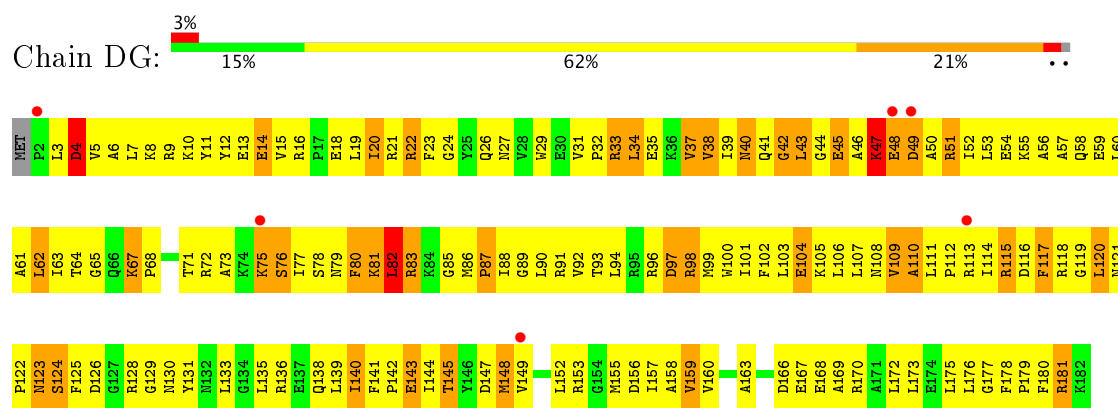


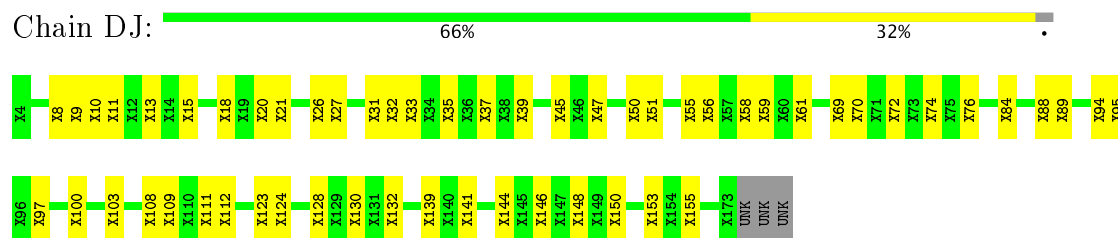
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain DE: 17% 62% 19%

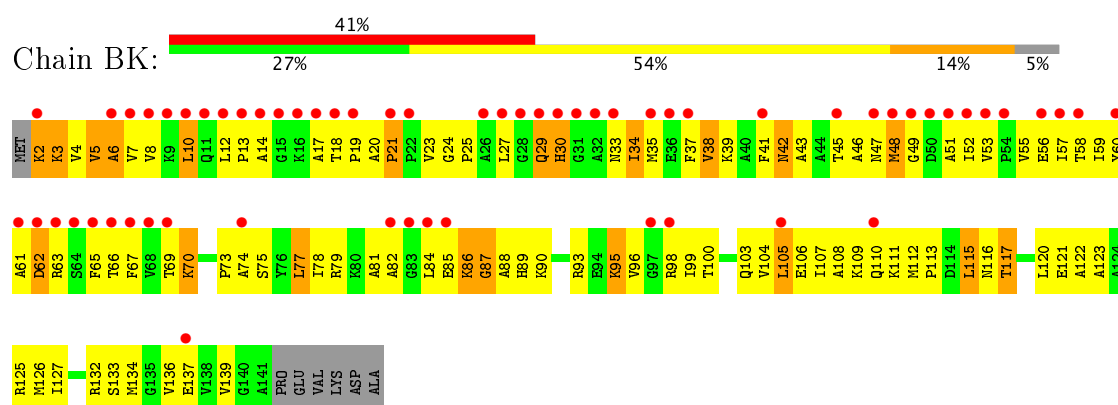




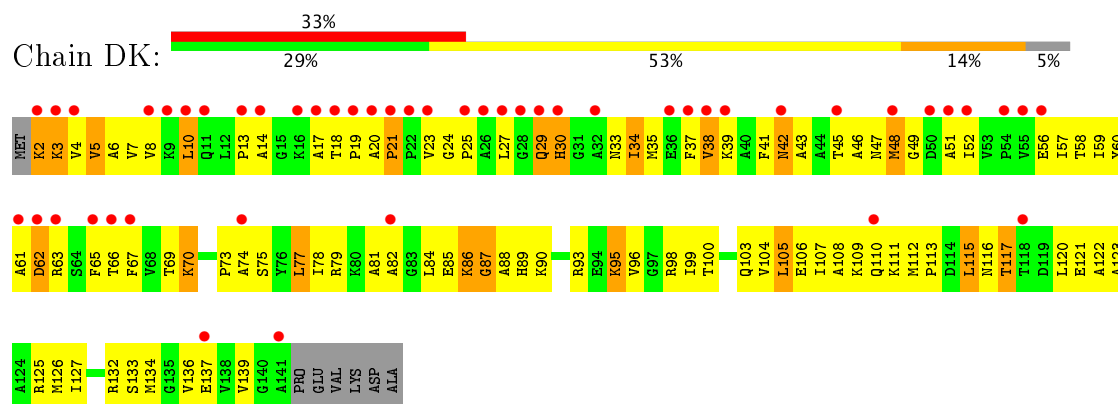




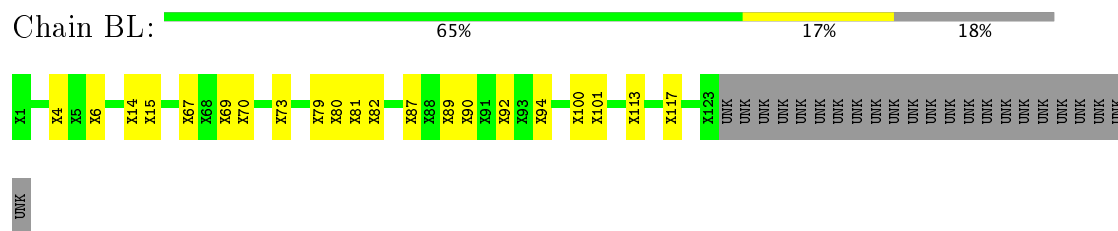
## ● Molecule 44: 50S RIBOSOMAL PROTEIN L11



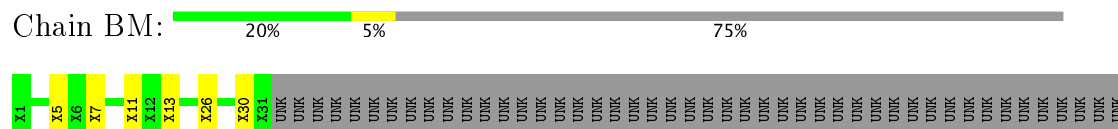
## ● Molecule 44: 50S RIBOSOMAL PROTEIN L11



## ● Molecule 45: 50S RIBOSOMAL PROTEIN L12



## ● Molecule 45: 50S RIBOSOMAL PROTEIN L12





[illegible][illegible]

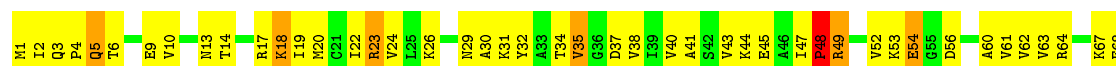
- Chain BN: 



- Chain DN: 



- Chain BO: 



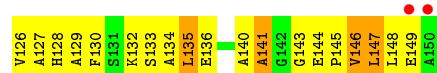
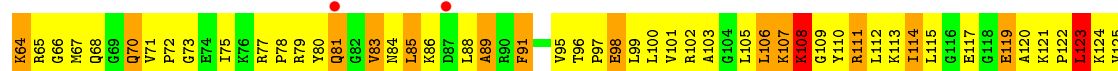
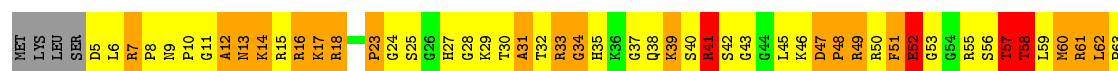
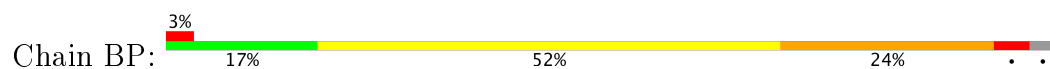
- Chain DO: 



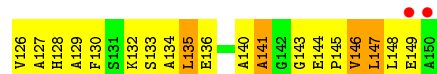
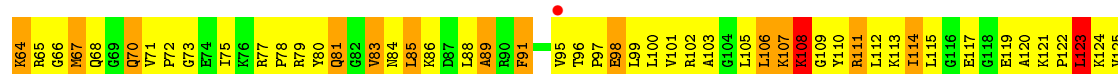
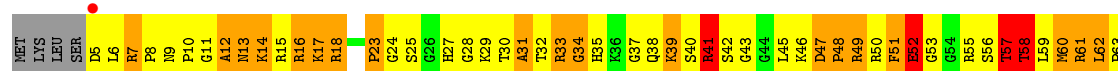
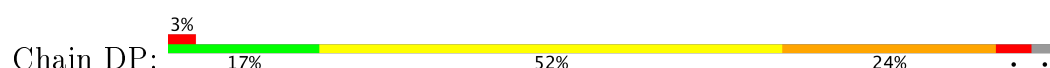




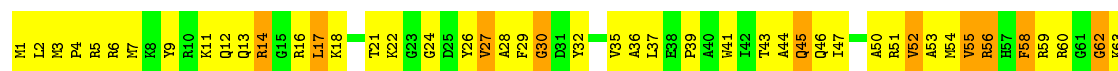
• Molecule 48: 50S RIBOSOMAL PROTEIN L15



• Molecule 48: 50S RIBOSOMAL PROTEIN L15

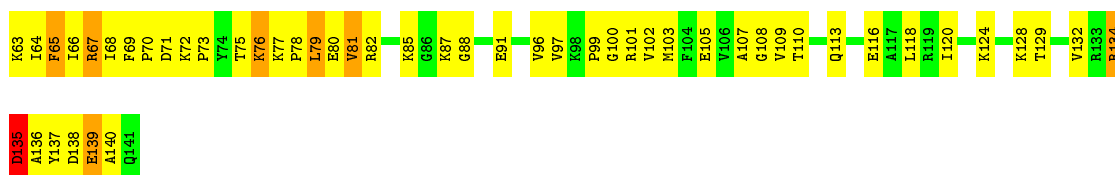


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

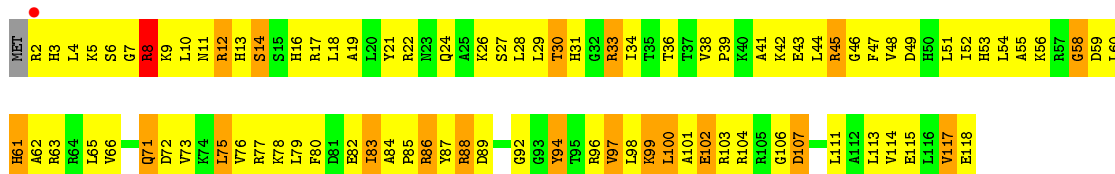


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

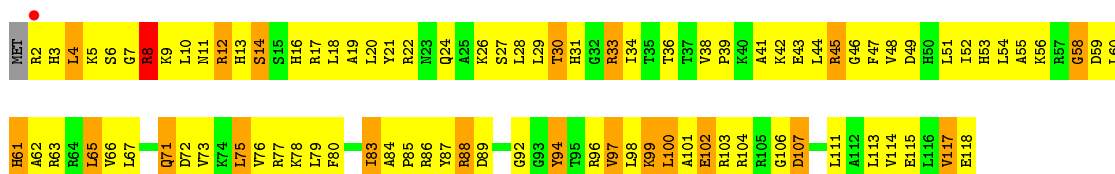




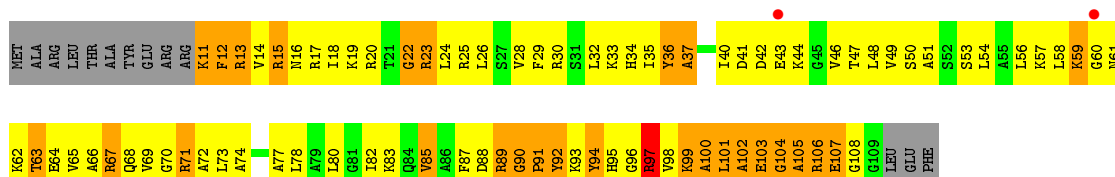
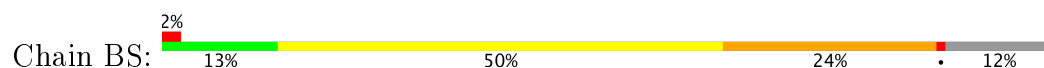
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



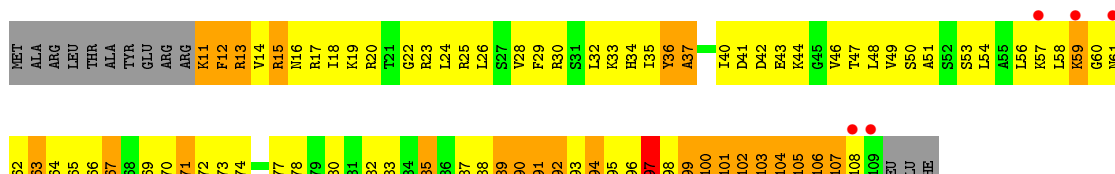
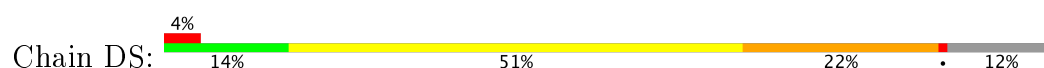
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



• Molecule 51: 50S RIBOSOMAL PROTEIN L18

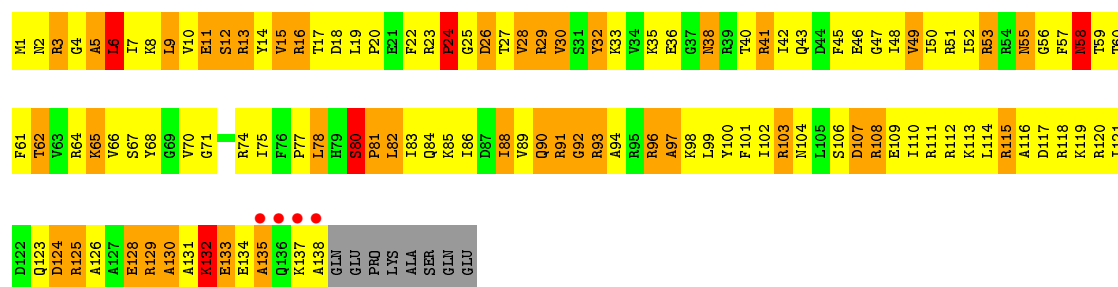


• Molecule 51: 50S RIBOSOMAL PROTEIN L18

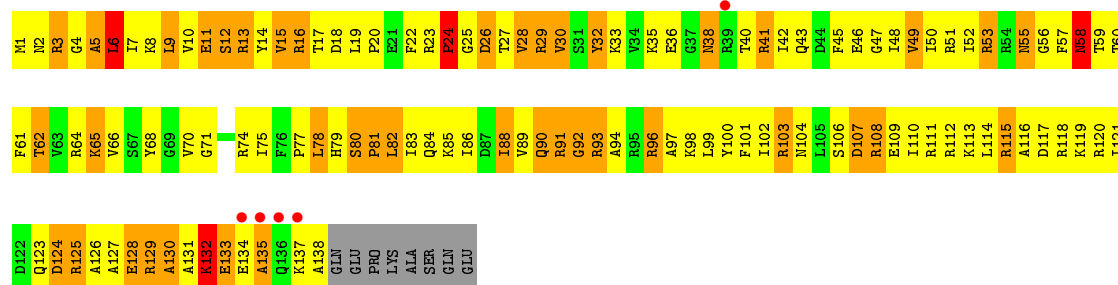
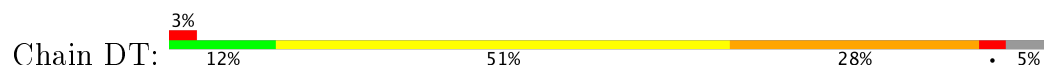


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

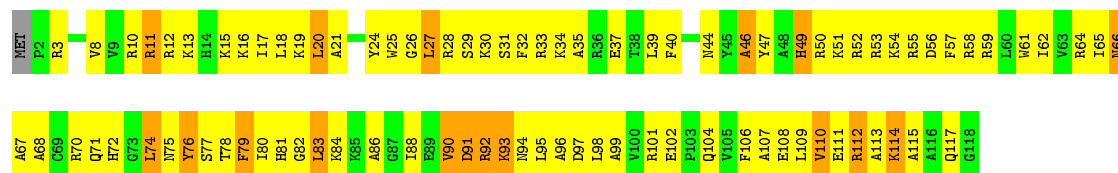




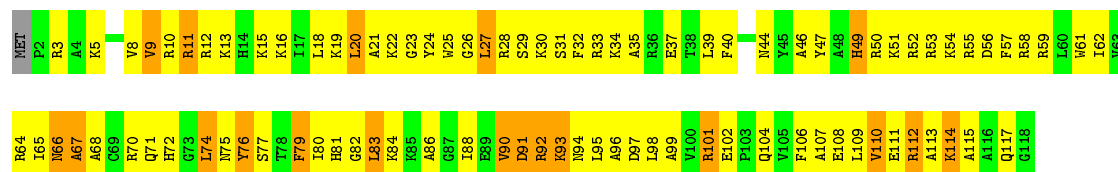
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



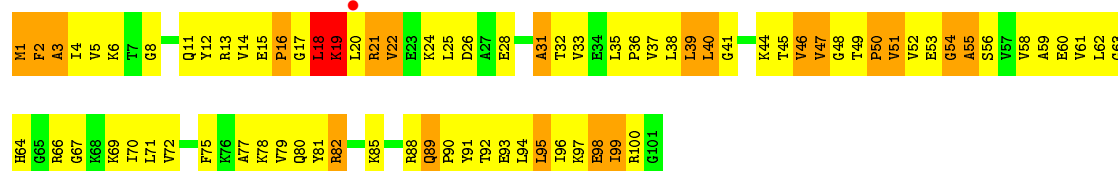
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



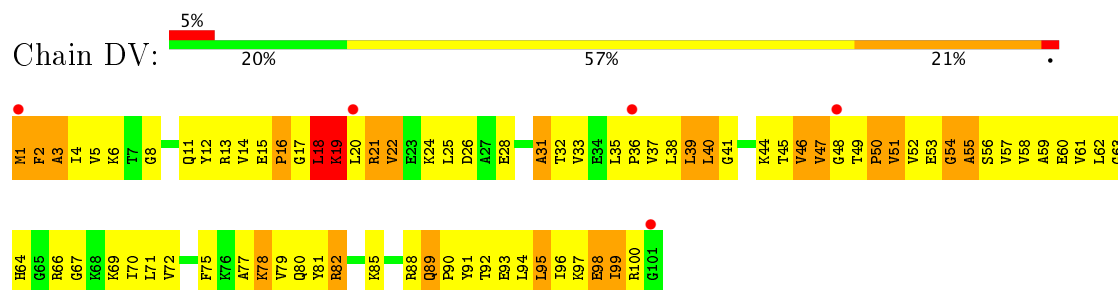
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



• Molecule 54: 50S RIBOSOMAL PROTEIN L21



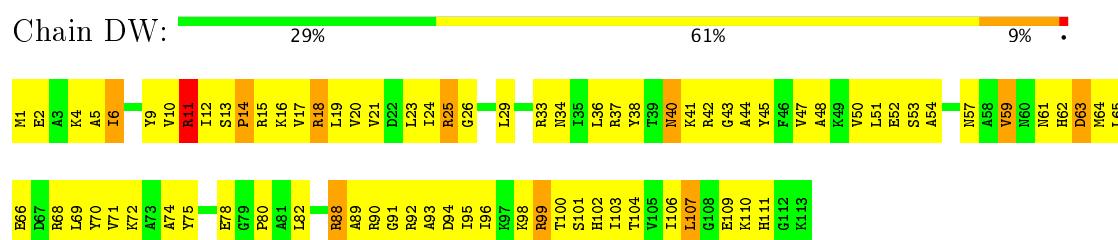
- Molecule 54: 50S RIBOSOMAL PROTEIN L21



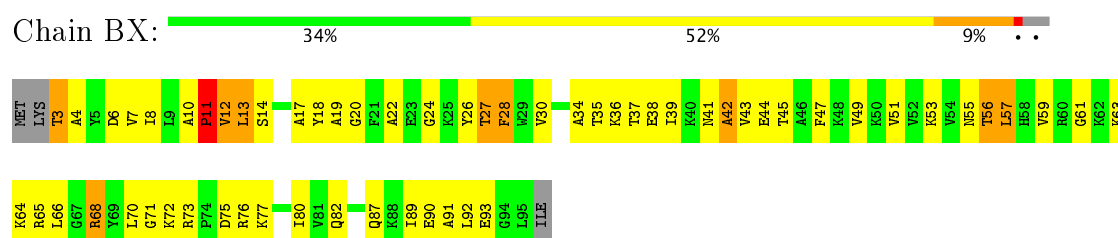
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



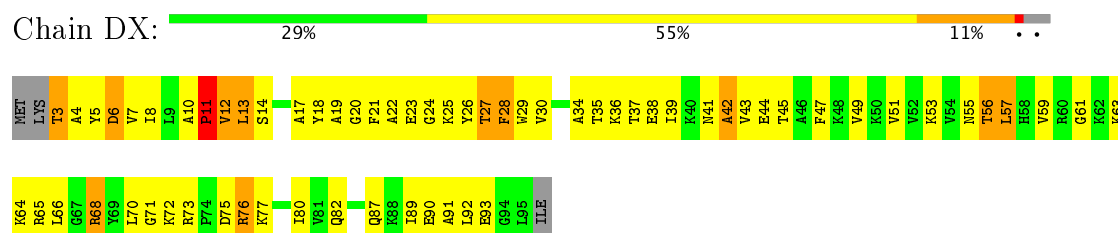
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



- Molecule 56: 50S RIBOSOMAL PROTEIN L23



- Molecule 56: 50S RIBOSOMAL PROTEIN L23



- Molecule 57: 50S RIBOSOMAL PROTEIN L24



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	291.84Å 270.36Å 402.36Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 49.57 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-3.60) 95.0 (49.57-3.40)	Depositor EDS
$R_{merge}$	0.37	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.227 , 0.260 0.227 , 0.227	Depositor DCC
$R_{free}$ test set	34394 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 34.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	311552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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: GDP, 5MU, ZN, MG, FUA

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	0.61	1/36190 (0.0%)	0.76	26/56486 (0.0%)
1	CA	0.60	2/36190 (0.0%)	0.76	20/56486 (0.0%)
2	AB	0.46	0/1936	0.70	0/2611
2	CB	0.44	0/1936	0.70	0/2611
3	AC	0.52	0/1637	0.69	0/2207
3	CC	0.46	0/1637	0.69	0/2207
4	AD	0.42	0/1733	0.66	0/2318
4	CD	0.41	0/1733	0.66	0/2318
5	AE	0.59	0/1163	0.72	0/1566
5	CE	0.55	0/1163	0.71	0/1566
6	AF	0.44	0/856	0.67	0/1154
6	CF	0.40	0/856	0.66	0/1154
7	AG	0.45	0/1276	0.65	0/1709
7	CG	0.45	0/1276	0.65	0/1709
8	AH	0.51	0/1136	0.74	0/1527
8	CH	0.46	0/1136	0.74	0/1527
9	AI	0.44	0/1027	0.68	0/1373
9	CI	0.41	0/1027	0.67	0/1373
10	AJ	0.47	0/808	0.72	0/1087
10	CJ	0.42	0/808	0.71	0/1087
11	AK	0.50	0/900	0.70	0/1213
11	CK	0.47	0/900	0.70	0/1213
12	AL	0.52	0/987	0.75	0/1322
12	CL	0.48	0/987	0.74	0/1322
13	AM	0.41	0/999	0.69	0/1338
13	CM	0.39	0/999	0.69	0/1338
14	AN	0.49	0/501	0.69	0/664
14	CN	0.47	0/501	0.69	0/664
15	AO	0.45	0/745	0.67	0/992
15	CO	0.43	0/745	0.66	0/992
16	AP	0.45	0/717	0.68	0/965
16	CP	0.43	0/717	0.68	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.51	0/837	0.69	0/1119
17	CQ	0.49	0/837	0.69	0/1119
18	AR	0.47	0/579	0.72	0/768
18	CR	0.45	0/579	0.73	0/768
19	AS	0.46	0/643	0.68	1/867 (0.1%)
19	CS	0.44	0/643	0.67	1/867 (0.1%)
20	AT	0.40	0/765	0.66	0/1007
20	CT	0.39	0/765	0.66	0/1007
21	AU	0.52	0/213	0.65	0/279
21	CU	0.50	0/213	0.65	0/279
22	AV	0.57	0/1810	0.73	0/2821
22	AW	0.41	0/1810	0.72	0/2821
22	CV	0.54	0/1810	0.70	0/2821
22	CW	0.38	0/1810	0.69	0/2821
23	AX	0.82	0/257	0.86	0/398
23	CX	0.79	0/257	0.84	1/398 (0.3%)
24	AY	0.40	0/5313	0.69	0/7195
24	CY	0.42	0/5313	0.69	1/7195 (0.0%)
25	B0	0.43	0/671	0.66	0/892
25	D0	0.42	0/671	0.67	0/892
26	B1	0.48	0/739	0.78	0/983
26	D1	0.45	0/739	0.69	0/983
27	B2	0.36	0/600	0.66	0/793
27	D2	0.37	0/600	0.62	0/793
28	B3	0.43	0/473	0.63	0/636
28	D3	0.43	0/473	0.64	0/636
29	B4	0.68	0/461	0.92	2/623 (0.3%)
29	D4	0.74	0/461	0.93	2/623 (0.3%)
30	B5	0.43	0/473	0.75	0/639
30	D5	0.44	0/473	0.74	0/639
31	B6	0.64	0/440	0.96	1/586 (0.2%)
31	D6	0.64	0/440	0.96	1/586 (0.2%)
32	B7	0.45	0/427	0.71	0/563
32	D7	0.45	0/427	0.71	0/563
33	B8	0.54	0/516	0.83	0/681
33	D8	0.54	0/516	0.83	0/681
34	B9	0.47	0/310	0.69	0/407
34	D9	0.46	0/310	0.70	0/407
35	BA	0.56	3/69972 (0.0%)	0.75	35/109237 (0.0%)
35	DA	0.55	4/69972 (0.0%)	0.75	36/109237 (0.0%)
36	BB	0.44	0/2853	0.72	1/4451 (0.0%)
36	DB	0.44	0/2853	0.72	0/4451
37	BC	0.35	0/1774	0.61	0/2391



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DC	0.34	0/1774	0.61	0/2391
38	BD	0.54	0/2195	0.83	0/2955
38	DD	0.53	0/2195	0.82	0/2955
39	BE	0.48	0/1597	0.74	0/2155
39	DE	0.46	0/1597	0.74	0/2155
40	BF	0.39	0/1659	0.66	0/2246
40	DF	0.38	0/1659	0.66	0/2246
41	BG	0.42	0/1498	0.78	1/2013 (0.0%)
41	DG	0.43	0/1498	0.74	0/2013
42	BH	0.36	0/1293	0.71	0/1746
42	DH	0.35	0/1293	0.69	0/1746
44	BK	0.35	0/1045	0.60	0/1418
44	DK	0.36	0/1045	0.60	0/1418
46	BN	0.40	0/1132	0.73	1/1527 (0.1%)
46	DN	0.39	0/1132	0.73	1/1527 (0.1%)
47	BO	0.49	0/943	0.72	0/1269
47	DO	0.47	0/943	0.72	0/1269
48	BP	0.44	0/1131	0.93	4/1504 (0.3%)
48	DP	0.44	0/1131	0.91	4/1504 (0.3%)
49	BQ	0.49	0/1143	0.69	0/1527
49	DQ	0.48	0/1143	0.70	0/1527
50	BR	0.39	0/974	0.68	0/1302
50	DR	0.38	0/974	0.68	1/1302 (0.1%)
51	BS	0.41	0/779	0.69	0/1038
51	DS	0.40	0/779	0.70	0/1038
52	BT	0.47	0/1156	0.79	2/1544 (0.1%)
52	DT	0.49	0/1156	0.79	1/1544 (0.1%)
53	BU	0.43	0/975	0.68	0/1297
53	DU	0.44	0/975	0.69	0/1297
54	BV	0.39	0/790	0.70	0/1057
54	DV	0.39	0/790	0.70	0/1057
55	BW	0.37	0/907	0.65	0/1216
55	DW	0.39	0/907	0.65	0/1216
56	BX	0.42	0/740	0.66	0/995
56	DX	0.42	0/740	0.66	0/995
57	BY	0.41	0/824	0.67	0/1100
57	DY	0.42	0/824	0.68	0/1100
58	BZ	0.48	0/1500	0.74	0/2037
58	DZ	0.46	0/1500	0.73	0/2037
All	All	0.53	10/333656 (0.0%)	0.74	143/497270 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	48
1	CA	0	43
22	AV	0	3
22	CV	0	1
23	AX	0	2
23	CX	0	1
35	BA	2	69
35	DA	2	58
36	BB	0	1
36	DB	0	1
37	BC	0	1
37	DC	0	1
44	BK	0	1
44	DK	0	1
46	DN	0	1
All	All	4	232

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	2506	U	N1-C2	7.05	1.44	1.38
35	DA	2506	U	N1-C2	6.48	1.44	1.38
35	BA	272(I)	U	C1'-N1	5.69	1.57	1.48
1	AA	1417	G	C6-O6	5.55	1.29	1.24
35	DA	272(I)	U	C1'-N1	5.49	1.56	1.48

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	1992	G	C2'-C3'-O3'	10.77	133.19	109.50
35	DA	1992	G	C2'-C3'-O3'	10.61	132.85	109.50
1	CA	575	G	C2'-C3'-O3'	9.68	130.80	109.50
1	AA	575	G	C2'-C3'-O3'	9.65	130.72	109.50
35	BA	945	A	N9-C1'-C2'	9.34	126.14	114.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	BA	1799	G	C3'
35	BA	1992	G	C3'

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Mol	Chain	Res	Type	Atom
35	DA	1799	G	C3'
35	DA	1992	G	C3'

5 of 232 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	108	G	Sidechain
1	AA	112	G	Sidechain
1	AA	30	U	Sidechain
1	AA	39	G	Sidechain
1	AA	5	U	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1236	0
1	CA	32329	0	16318	1267	0
2	AB	1901	0	1951	243	0
2	CB	1901	0	1951	241	2
3	AC	1613	0	1677	211	0
3	CC	1613	0	1677	216	0
4	AD	1703	0	1763	187	0
4	CD	1703	0	1763	191	0
5	AE	1147	0	1207	128	0
5	CE	1147	0	1207	134	0
6	AF	843	0	857	77	0
6	CF	843	0	857	79	0
7	AG	1257	0	1296	100	0
7	CG	1257	0	1296	95	0
8	AH	1116	0	1177	86	0
8	CH	1116	0	1177	88	0
9	AI	1010	0	1035	135	0
9	CI	1010	0	1035	132	0
10	AJ	795	0	840	180	0
10	CJ	795	0	840	176	0
11	AK	885	0	904	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CK	885	0	904	75	0
12	AL	971	0	1057	131	0
12	CL	971	0	1057	129	0
13	AM	988	0	1059	146	0
13	CM	988	0	1059	144	0
14	AN	492	0	530	68	0
14	CN	492	0	530	65	0
15	AO	734	0	771	66	0
15	CO	734	0	771	62	0
16	AP	701	0	720	78	0
16	CP	701	0	720	78	0
17	AQ	824	0	891	60	0
17	CQ	824	0	891	57	0
18	AR	574	0	644	71	0
18	CR	574	0	644	72	0
19	AS	630	0	652	119	0
19	CS	630	0	652	122	0
20	AT	763	0	861	96	0
20	CT	763	0	861	93	0
21	AU	209	0	221	19	0
21	CU	209	0	221	21	0
22	AV	1640	0	836	72	0
22	AW	1640	0	836	82	0
22	CV	1640	0	836	49	0
22	CW	1640	0	836	71	0
23	AX	230	0	119	26	0
23	CX	230	0	119	21	0
24	AY	5215	0	5287	798	0
24	CY	5215	0	5287	767	0
25	B0	662	0	688	86	0
25	D0	662	0	688	87	0
26	B1	732	0	808	131	0
26	D1	732	0	808	126	0
27	B2	598	0	653	106	0
27	D2	598	0	653	108	0
28	B3	468	0	523	60	0
28	D3	468	0	523	55	0
29	B4	451	0	448	99	0
29	D4	451	0	449	100	0
30	B5	459	0	480	108	0
30	D5	459	0	480	110	0
31	B6	433	0	461	176	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	D6	433	0	461	177	0
32	B7	419	0	467	38	0
32	D7	419	0	467	40	0
33	B8	508	0	576	107	0
33	D8	508	0	576	108	0
34	B9	307	0	335	39	0
34	D9	307	0	335	39	0
35	BA	62474	0	31497	2701	0
35	DA	62474	0	31497	2744	0
36	BB	2551	0	1295	127	0
36	DB	2551	0	1295	135	0
37	BC	1742	0	1798	169	0
37	DC	1742	0	1798	168	2
38	BD	2145	0	2234	302	0
38	DD	2145	0	2234	306	0
39	BE	1564	0	1629	280	0
39	DE	1564	0	1629	282	0
40	BF	1624	0	1677	261	0
40	DF	1624	0	1677	269	0
41	BG	1474	0	1534	288	0
41	DG	1474	0	1534	272	0
42	BH	1269	0	1337	231	0
42	DH	1269	0	1337	216	0
43	BJ	851	0	191	28	0
43	DJ	851	0	195	44	0
44	BK	1026	0	1066	151	0
44	DK	1026	0	1066	146	0
45	BL	506	0	111	14	0
45	BM	151	0	33	4	0
45	Bl	151	0	32	0	0
45	Bm	146	0	32	0	0
45	DL	506	0	115	17	0
45	DM	151	0	32	1	0
45	DI	151	0	32	0	0
45	Dm	146	0	31	0	0
46	BN	1105	0	1180	196	0
46	DN	1105	0	1180	196	0
47	BO	933	0	996	106	0
47	DO	933	0	996	106	0
48	BP	1114	0	1187	303	0
48	DP	1114	0	1187	304	0
49	BQ	1122	0	1179	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	DQ	1122	0	1179	150	0
50	BR	960	0	1021	163	0
50	DR	960	0	1021	160	0
51	BS	771	0	832	173	0
51	DS	771	0	832	161	0
52	BT	1142	0	1202	248	0
52	DT	1142	0	1202	244	0
53	BU	958	0	1015	171	0
53	DU	958	0	1015	174	0
54	BV	779	0	852	140	0
54	DV	779	0	852	145	0
55	BW	896	0	953	97	0
55	DW	896	0	953	91	0
56	BX	726	0	778	78	0
56	DX	726	0	778	85	0
57	BY	811	0	901	171	0
57	DY	811	0	901	174	0
58	BZ	1468	0	1492	238	0
58	DZ	1468	0	1492	275	0
59	AD	1	0	0	0	0
59	AN	1	0	0	1	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	0	0
60	AY	1	0	0	0	0
60	CY	1	0	0	0	0
61	AY	37	0	47	13	0
61	CY	37	0	47	22	0
62	AY	28	0	12	8	0
62	CY	28	0	12	8	0
All	All	311552	0	214129	22488	2

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 43.

The worst 5 of 22488 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)
42:DH:157:TYR:CE1	42:DH:171:LEU:HD22	1.61	1.35
42:BH:157:TYR:CE1	42:BH:171:LEU:HD22	1.62	1.32
42:DH:157:TYR:HE1	42:DH:171:LEU:CD2	1.50	1.24
42:BH:157:TYR:HE1	42:BH:171:LEU:CD2	1.50	1.24
40:DF:3:GLU:HA	40:DF:24:LEU:HG	1.24	1.20

All (2) 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	37:DC:28:ARG:NH2[2_646]	1.56	0.64
2:CB:65:GLY:O	37:DC:28:ARG:CZ[2_646]	1.87	0.33

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	139 (60%)	53 (23%)	41 (18%)	0	3
2	CB	233/256 (91%)	140 (60%)	51 (22%)	42 (18%)	0	3
3	AC	205/239 (86%)	133 (65%)	50 (24%)	22 (11%)	0	9
3	CC	205/239 (86%)	132 (64%)	52 (25%)	21 (10%)	1	10
4	AD	206/209 (99%)	134 (65%)	50 (24%)	22 (11%)	0	9
4	CD	206/209 (99%)	134 (65%)	51 (25%)	21 (10%)	1	10
5	AE	149/162 (92%)	119 (80%)	21 (14%)	9 (6%)	2	22
5	CE	149/162 (92%)	117 (78%)	24 (16%)	8 (5%)	2	24
6	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1	18
6	CF	99/101 (98%)	74 (75%)	18 (18%)	7 (7%)	1	18
7	AG	153/156 (98%)	109 (71%)	34 (22%)	10 (6%)	1	21
7	CG	153/156 (98%)	110 (72%)	32 (21%)	11 (7%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AH	136/138 (99%)	103 (76%)	30 (22%)	3 (2%)	8	47
8	CH	136/138 (99%)	105 (77%)	27 (20%)	4 (3%)	5	41
9	AI	121/128 (94%)	81 (67%)	26 (22%)	14 (12%)	0	7
9	CI	121/128 (94%)	82 (68%)	27 (22%)	12 (10%)	1	10
10	AJ	97/105 (92%)	60 (62%)	21 (22%)	16 (16%)	0	4
10	CJ	97/105 (92%)	61 (63%)	20 (21%)	16 (16%)	0	4
11	AK	117/129 (91%)	91 (78%)	20 (17%)	6 (5%)	2	26
11	CK	117/129 (91%)	91 (78%)	20 (17%)	6 (5%)	2	26
12	AL	123/132 (93%)	82 (67%)	23 (19%)	18 (15%)	0	5
12	CL	123/132 (93%)	82 (67%)	22 (18%)	19 (15%)	0	4
13	AM	123/126 (98%)	77 (63%)	25 (20%)	21 (17%)	0	3
13	CM	123/126 (98%)	77 (63%)	26 (21%)	20 (16%)	0	4
14	AN	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	19
14	CN	58/61 (95%)	46 (79%)	7 (12%)	5 (9%)	1	13
15	AO	86/89 (97%)	55 (64%)	23 (27%)	8 (9%)	1	11
15	CO	86/89 (97%)	53 (62%)	24 (28%)	9 (10%)	0	9
16	AP	82/88 (93%)	60 (73%)	15 (18%)	7 (8%)	1	13
16	CP	82/88 (93%)	60 (73%)	15 (18%)	7 (8%)	1	13
17	AQ	98/105 (93%)	78 (80%)	15 (15%)	5 (5%)	2	26
17	CQ	98/105 (93%)	78 (80%)	16 (16%)	4 (4%)	3	32
18	AR	68/88 (77%)	52 (76%)	11 (16%)	5 (7%)	1	16
18	CR	68/88 (77%)	51 (75%)	12 (18%)	5 (7%)	1	16
19	AS	77/93 (83%)	43 (56%)	14 (18%)	20 (26%)	0	1
19	CS	77/93 (83%)	43 (56%)	15 (20%)	19 (25%)	0	1
20	AT	97/106 (92%)	52 (54%)	30 (31%)	15 (16%)	0	4
20	CT	97/106 (92%)	53 (55%)	29 (30%)	15 (16%)	0	4
21	AU	23/27 (85%)	14 (61%)	6 (26%)	3 (13%)	0	6
21	CU	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	3
24	AY	663/691 (96%)	435 (66%)	137 (21%)	91 (14%)	0	5
24	CY	663/691 (96%)	449 (68%)	134 (20%)	80 (12%)	0	7
25	B0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	2	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	D0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	2	27
26	B1	92/98 (94%)	64 (70%)	15 (16%)	13 (14%)	0	5
26	D1	92/98 (94%)	67 (73%)	13 (14%)	12 (13%)	0	6
27	B2	69/72 (96%)	35 (51%)	18 (26%)	16 (23%)	0	1
27	D2	69/72 (96%)	29 (42%)	31 (45%)	9 (13%)	0	6
28	B3	58/60 (97%)	41 (71%)	12 (21%)	5 (9%)	1	13
28	D3	58/60 (97%)	41 (71%)	12 (21%)	5 (9%)	1	13
29	B4	56/71 (79%)	27 (48%)	14 (25%)	15 (27%)	0	0
29	D4	56/71 (79%)	28 (50%)	13 (23%)	15 (27%)	0	0
30	B5	57/60 (95%)	37 (65%)	9 (16%)	11 (19%)	0	2
30	D5	57/60 (95%)	38 (67%)	7 (12%)	12 (21%)	0	2
31	B6	48/54 (89%)	21 (44%)	12 (25%)	15 (31%)	0	0
31	D6	48/54 (89%)	22 (46%)	12 (25%)	14 (29%)	0	0
32	B7	47/49 (96%)	35 (74%)	11 (23%)	1 (2%)	8	48
32	D7	47/49 (96%)	35 (74%)	11 (23%)	1 (2%)	8	48
33	B8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	2
33	D8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	2
34	B9	35/37 (95%)	21 (60%)	9 (26%)	5 (14%)	0	5
34	D9	35/37 (95%)	21 (60%)	8 (23%)	6 (17%)	0	3
37	BC	226/229 (99%)	163 (72%)	51 (23%)	12 (5%)	2	25
37	DC	226/229 (99%)	163 (72%)	50 (22%)	13 (6%)	2	23
38	BD	273/276 (99%)	189 (69%)	50 (18%)	34 (12%)	0	7
38	DD	273/276 (99%)	188 (69%)	50 (18%)	35 (13%)	0	6
39	BE	203/206 (98%)	122 (60%)	45 (22%)	36 (18%)	0	3
39	DE	203/206 (98%)	124 (61%)	44 (22%)	35 (17%)	0	3
40	BF	206/210 (98%)	132 (64%)	44 (21%)	30 (15%)	0	5
40	DF	206/210 (98%)	133 (65%)	42 (20%)	31 (15%)	0	4
41	BG	177/182 (97%)	110 (62%)	43 (24%)	24 (14%)	0	5
41	DG	177/182 (97%)	115 (65%)	36 (20%)	26 (15%)	0	5
42	BH	165/180 (92%)	86 (52%)	40 (24%)	39 (24%)	0	1
42	DH	165/180 (92%)	86 (52%)	40 (24%)	39 (24%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BK	138/147 (94%)	92 (67%)	35 (25%)	11 (8%)	1	14
44	DK	138/147 (94%)	92 (67%)	35 (25%)	11 (8%)	1	14
46	BN	137/140 (98%)	88 (64%)	28 (20%)	21 (15%)	0	4
46	DN	137/140 (98%)	88 (64%)	28 (20%)	21 (15%)	0	4
47	BO	120/122 (98%)	91 (76%)	19 (16%)	10 (8%)	1	13
47	DO	120/122 (98%)	93 (78%)	17 (14%)	10 (8%)	1	13
48	BP	144/150 (96%)	72 (50%)	45 (31%)	27 (19%)	0	2
48	DP	144/150 (96%)	72 (50%)	44 (31%)	28 (19%)	0	2
49	BQ	139/141 (99%)	106 (76%)	26 (19%)	7 (5%)	2	26
49	DQ	139/141 (99%)	106 (76%)	26 (19%)	7 (5%)	2	26
50	BR	115/118 (98%)	81 (70%)	20 (17%)	14 (12%)	0	7
50	DR	115/118 (98%)	81 (70%)	20 (17%)	14 (12%)	0	7
51	BS	97/112 (87%)	41 (42%)	35 (36%)	21 (22%)	0	1
51	DS	97/112 (87%)	41 (42%)	35 (36%)	21 (22%)	0	1
52	BT	136/146 (93%)	76 (56%)	32 (24%)	28 (21%)	0	2
52	DT	136/146 (93%)	75 (55%)	32 (24%)	29 (21%)	0	2
53	BU	115/118 (98%)	66 (57%)	37 (32%)	12 (10%)	0	10
53	DU	115/118 (98%)	67 (58%)	35 (30%)	13 (11%)	0	8
54	BV	99/101 (98%)	69 (70%)	12 (12%)	18 (18%)	0	2
54	DV	99/101 (98%)	69 (70%)	12 (12%)	18 (18%)	0	2
55	BW	111/113 (98%)	80 (72%)	21 (19%)	10 (9%)	1	12
55	DW	111/113 (98%)	81 (73%)	21 (19%)	9 (8%)	1	14
56	BX	91/96 (95%)	56 (62%)	26 (29%)	9 (10%)	1	10
56	DX	91/96 (95%)	57 (63%)	25 (28%)	9 (10%)	1	10
57	BY	105/110 (96%)	42 (40%)	36 (34%)	27 (26%)	0	1
57	DY	105/110 (96%)	43 (41%)	36 (34%)	26 (25%)	0	1
58	BZ	183/206 (89%)	108 (59%)	42 (23%)	33 (18%)	0	3
58	DZ	183/206 (89%)	114 (62%)	37 (20%)	32 (18%)	0	3
All	All	13200/13966 (94%)	8607 (65%)	2874 (22%)	1719 (13%)	0	6

5 of 1719 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	12	GLU
2	AB	13	ALA
2	AB	15	VAL
2	AB	20	GLU
2	AB	95	GLN

### 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%)	179 (89%)	23 (11%)	7	35
2	CB	202/220 (92%)	179 (89%)	23 (11%)	7	35
3	AC	160/188 (85%)	142 (89%)	18 (11%)	7	35
3	CC	160/188 (85%)	142 (89%)	18 (11%)	7	35
4	AD	180/181 (99%)	160 (89%)	20 (11%)	7	37
4	CD	180/181 (99%)	160 (89%)	20 (11%)	7	37
5	AE	115/123 (94%)	100 (87%)	15 (13%)	5	29
5	CE	115/123 (94%)	100 (87%)	15 (13%)	5	29
6	AF	90/90 (100%)	83 (92%)	7 (8%)	15	51
6	CF	90/90 (100%)	83 (92%)	7 (8%)	15	51
7	AG	126/127 (99%)	117 (93%)	9 (7%)	17	55
7	CG	126/127 (99%)	117 (93%)	9 (7%)	17	55
8	AH	119/119 (100%)	110 (92%)	9 (8%)	15	52
8	CH	119/119 (100%)	112 (94%)	7 (6%)	23	62
9	AI	98/99 (99%)	90 (92%)	8 (8%)	13	49
9	CI	98/99 (99%)	90 (92%)	8 (8%)	13	49
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	5	31
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	5	31
11	AK	90/99 (91%)	84 (93%)	6 (7%)	19	58
11	CK	90/99 (91%)	84 (93%)	6 (7%)	19	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	104/109 (95%)	94 (90%)	10 (10%)	10	43
12	CL	104/109 (95%)	93 (89%)	11 (11%)	8	38
13	AM	99/101 (98%)	91 (92%)	8 (8%)	14	50
13	CM	99/101 (98%)	91 (92%)	8 (8%)	14	50
14	AN	49/50 (98%)	43 (88%)	6 (12%)	6	31
14	CN	49/50 (98%)	43 (88%)	6 (12%)	6	31
15	AO	79/80 (99%)	71 (90%)	8 (10%)	9	40
15	CO	79/80 (99%)	71 (90%)	8 (10%)	9	40
16	AP	72/74 (97%)	67 (93%)	5 (7%)	18	56
16	CP	72/74 (97%)	67 (93%)	5 (7%)	18	56
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	16	53
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	16	53
18	AR	61/77 (79%)	59 (97%)	2 (3%)	43	77
18	CR	61/77 (79%)	59 (97%)	2 (3%)	43	77
19	AS	69/80 (86%)	59 (86%)	10 (14%)	4	25
19	CS	69/80 (86%)	59 (86%)	10 (14%)	4	25
20	AT	76/82 (93%)	69 (91%)	7 (9%)	11	45
20	CT	76/82 (93%)	69 (91%)	7 (9%)	11	45
21	AU	19/22 (86%)	19 (100%)	0	100	100
21	CU	19/22 (86%)	19 (100%)	0	100	100
24	AY	563/582 (97%)	489 (87%)	74 (13%)	5	29
24	CY	563/582 (97%)	495 (88%)	68 (12%)	6	32
25	B0	66/67 (98%)	57 (86%)	9 (14%)	4	28
25	D0	66/67 (98%)	57 (86%)	9 (14%)	4	28
26	B1	78/83 (94%)	65 (83%)	13 (17%)	2	17
26	D1	78/83 (94%)	70 (90%)	8 (10%)	8	40
27	B2	66/67 (98%)	59 (89%)	7 (11%)	8	38
27	D2	66/67 (98%)	58 (88%)	8 (12%)	6	32
28	B3	51/52 (98%)	47 (92%)	4 (8%)	15	51
28	D3	51/52 (98%)	47 (92%)	4 (8%)	15	51
29	B4	51/63 (81%)	38 (74%)	13 (26%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	D4	51/63 (81%)	37 (72%)	14 (28%)	0	4
30	B5	51/52 (98%)	45 (88%)	6 (12%)	6	33
30	D5	51/52 (98%)	45 (88%)	6 (12%)	6	33
31	B6	49/52 (94%)	39 (80%)	10 (20%)	1	10
31	D6	49/52 (94%)	38 (78%)	11 (22%)	1	7
32	B7	41/42 (98%)	36 (88%)	5 (12%)	6	31
32	D7	41/42 (98%)	36 (88%)	5 (12%)	6	31
33	B8	53/55 (96%)	44 (83%)	9 (17%)	2	17
33	D8	53/55 (96%)	43 (81%)	10 (19%)	2	11
34	B9	34/34 (100%)	30 (88%)	4 (12%)	6	33
34	D9	34/34 (100%)	29 (85%)	5 (15%)	3	24
37	BC	180/181 (99%)	170 (94%)	10 (6%)	25	63
37	DC	180/181 (99%)	169 (94%)	11 (6%)	22	61
38	BD	217/218 (100%)	177 (82%)	40 (18%)	2	12
38	DD	217/218 (100%)	178 (82%)	39 (18%)	2	13
39	BE	165/166 (99%)	139 (84%)	26 (16%)	3	21
39	DE	165/166 (99%)	140 (85%)	25 (15%)	3	22
40	BF	165/166 (99%)	153 (93%)	12 (7%)	16	54
40	DF	165/166 (99%)	153 (93%)	12 (7%)	16	54
41	BG	155/156 (99%)	131 (84%)	24 (16%)	3	21
41	DG	155/156 (99%)	126 (81%)	29 (19%)	2	12
42	BH	136/148 (92%)	126 (93%)	10 (7%)	16	53
42	DH	136/148 (92%)	126 (93%)	10 (7%)	16	53
44	BK	104/111 (94%)	89 (86%)	15 (14%)	4	25
44	DK	104/111 (94%)	90 (86%)	14 (14%)	4	28
46	BN	117/119 (98%)	103 (88%)	14 (12%)	6	32
46	DN	117/119 (98%)	102 (87%)	15 (13%)	5	29
47	BO	100/100 (100%)	92 (92%)	8 (8%)	14	50
47	DO	100/100 (100%)	92 (92%)	8 (8%)	14	50
48	BP	112/116 (97%)	91 (81%)	21 (19%)	2	12
48	DP	112/116 (97%)	91 (81%)	21 (19%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BQ	111/111 (100%)	95 (86%)	16 (14%)	4	25
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	5	30
50	BR	100/101 (99%)	89 (89%)	11 (11%)	7	37
50	DR	100/101 (99%)	88 (88%)	12 (12%)	6	32
51	BS	77/88 (88%)	68 (88%)	9 (12%)	6	34
51	DS	77/88 (88%)	68 (88%)	9 (12%)	6	34
52	BT	120/127 (94%)	97 (81%)	23 (19%)	1	11
52	DT	120/127 (94%)	97 (81%)	23 (19%)	1	11
53	BU	92/94 (98%)	83 (90%)	9 (10%)	9	42
53	DU	92/94 (98%)	83 (90%)	9 (10%)	9	42
54	BV	82/82 (100%)	71 (87%)	11 (13%)	4	28
54	DV	82/82 (100%)	71 (87%)	11 (13%)	4	28
55	BW	91/92 (99%)	84 (92%)	7 (8%)	15	52
55	DW	91/92 (99%)	84 (92%)	7 (8%)	15	52
56	BX	74/78 (95%)	64 (86%)	10 (14%)	4	28
56	DX	74/78 (95%)	64 (86%)	10 (14%)	4	28
57	BY	87/91 (96%)	75 (86%)	12 (14%)	4	27
57	DY	87/91 (96%)	75 (86%)	12 (14%)	4	27
58	BZ	162/179 (90%)	134 (83%)	28 (17%)	2	15
58	DZ	162/179 (90%)	144 (89%)	18 (11%)	7	37
All	All	11080/11566 (96%)	9776 (88%)	1304 (12%)	6	33

5 of 1304 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	BU	108	GLU
5	CE	75	THR
51	DS	11	LYS
55	BW	98	LYS
2	CB	24	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 348 such sidechains are listed below:

Mol	Chain	Res	Type
53	BU	94	ASN
6	CF	27	GLN
50	DR	23	ASN
56	BX	41	ASN
2	CB	204	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	270 (17%)	43 (2%)
1	CA	1503/1522 (98%)	266 (17%)	43 (2%)
22	AV	76/77 (98%)	15 (19%)	0
22	AW	76/77 (98%)	25 (32%)	1 (1%)
22	CV	76/77 (98%)	14 (18%)	0
22	CW	76/77 (98%)	19 (25%)	1 (1%)
23	AX	11/25 (44%)	4 (36%)	1 (9%)
23	CX	11/25 (44%)	4 (36%)	1 (9%)
35	BA	2900/2915 (99%)	597 (20%)	71 (2%)
35	DA	2900/2915 (99%)	594 (20%)	71 (2%)
36	BB	118/122 (96%)	25 (21%)	0
36	DB	118/122 (96%)	25 (21%)	0
All	All	9368/9476 (98%)	1858 (19%)	232 (2%)

5 of 1858 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	33	A
1	AA	39	G

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2611	U
1	CA	428	G
35	DA	2344	U
35	BA	2762	G
1	CA	60	A

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

4 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
22	5MU	AV	54	22	14,21,23	1.21	2 (14%)	15,30,35	4.07	2 (13%)
22	5MU	AW	55	22	14,21,23	1.19	2 (14%)	15,30,35	4.13	2 (13%)
22	5MU	CV	54	22	14,21,23	1.14	2 (14%)	15,30,35	4.10	2 (13%)
22	5MU	CW	55	22	14,21,23	1.19	2 (14%)	15,30,35	4.09	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	AV	54	22	-	0/3/25/26	0/2/2/2
22	5MU	AW	55	22	-	0/3/25/26	0/2/2/2
22	5MU	CV	54	22	-	0/3/25/26	0/2/2/2
22	5MU	CW	55	22	-	0/3/25/26	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CW	55	5MU	C6-N1	2.06	1.38	1.35
22	CV	54	5MU	C6-N1	2.08	1.38	1.35
22	AW	55	5MU	C6-N1	2.09	1.38	1.35
22	AV	54	5MU	C6-N1	2.11	1.38	1.35
22	CV	54	5MU	C4-N3	3.12	1.38	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AW	55	5MU	C5-C4-N3	-3.32	115.19	123.12
22	CV	54	5MU	C5-C4-N3	-3.32	115.20	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CW	55	5MU	C5-C4-N3	-3.30	115.23	123.12
22	AV	54	5MU	C5-C4-N3	-3.18	115.52	123.12
22	AV	54	5MU	C4-N3-C2	15.32	127.29	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AV	54	5MU	2	0
22	AW	55	5MU	1	0
22	CV	54	5MU	1	0
22	CW	55	5MU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
61	FUA	AY	702	-	37,40,40	1.71	6 (16%)	45,64,64	1.72	7 (15%)
62	GDP	AY	703	60	25,30,30	1.28	3 (12%)	26,47,47	2.03	6 (23%)
61	FUA	CY	702	-	37,40,40	1.72	6 (16%)	45,64,64	1.57	9 (20%)
62	GDP	CY	703	60	25,30,30	1.32	3 (12%)	26,47,47	2.25	8 (30%)

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	FUA	AY	702	-	-	0/10/92/92	0/4/4/4
62	GDP	AY	703	60	-	0/12/32/32	0/3/3/3
61	FUA	CY	702	-	-	0/10/92/92	0/4/4/4
62	GDP	CY	703	60	-	0/12/32/32	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CY	702	FUA	C23-C22	-6.57	1.39	1.51
61	AY	702	FUA	C23-C22	-6.39	1.39	1.51
61	AY	702	FUA	C23-C24	-4.14	1.39	1.53
61	CY	702	FUA	C23-C24	-4.14	1.39	1.53
61	CY	702	FUA	C24-C25	-3.25	1.39	1.50

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	CY	703	GDP	N3-C2-N1	-5.00	120.16	127.46
62	AY	703	GDP	N3-C2-N1	-4.99	120.17	127.46
61	AY	702	FUA	C13-C12-C11	-4.41	105.84	111.97
61	CY	702	FUA	C16-O2-C31	-4.15	110.67	117.10
62	CY	703	GDP	C4'-O4'-C1'	-3.90	105.62	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	AY	702	FUA	13	0
62	AY	703	GDP	8	0
61	CY	702	FUA	22	0
62	CY	703	GDP	8	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	AI	2
9	CI	2
45	BL	1
41	DG	1
41	BG	1
45	DL	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DL	30:UNK	C	52:UNK	N	38.40
1	BL	30:UNK	C	52:UNK	N	36.36
1	BG	112:PRO	C	113:ARG	N	3.27
1	DG	112:PRO	C	113:ARG	N	3.05
1	CI	53:VAL	C	54:ASP	N	2.98

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1504/1522 (98%)	-0.27	22 (1%) 74 61	23, 62, 148, 220	0
1	CA	1504/1522 (98%)	-0.52	15 (0%) 82 70	26, 65, 148, 220	0
2	AB	235/256 (91%)	-0.31	3 (1%) 77 64	40, 81, 147, 159	0
2	CB	235/256 (91%)	-0.33	1 (0%) 92 87	43, 82, 147, 158	0
3	AC	207/239 (86%)	-0.41	0 100 100	31, 72, 113, 118	0
3	CC	207/239 (86%)	-0.38	0 100 100	33, 75, 115, 121	0
4	AD	208/209 (99%)	-0.39	0 100 100	47, 79, 115, 124	0
4	CD	208/209 (99%)	-0.43	0 100 100	48, 80, 116, 125	0
5	AE	151/162 (93%)	-0.49	1 (0%) 87 78	25, 50, 90, 112	0
5	CE	151/162 (93%)	-0.46	1 (0%) 87 78	27, 52, 91, 112	0
6	AF	101/101 (100%)	-0.44	0 100 100	55, 85, 110, 118	0
6	CF	101/101 (100%)	-0.29	0 100 100	60, 87, 111, 118	0
7	AG	155/156 (99%)	-0.39	1 (0%) 89 81	51, 79, 109, 136	0
7	CG	155/156 (99%)	-0.39	2 (1%) 77 64	55, 81, 111, 136	0
8	AH	138/138 (100%)	-0.41	0 100 100	32, 54, 75, 82	0
8	CH	138/138 (100%)	-0.49	0 100 100	35, 56, 76, 83	0
9	AI	127/128 (99%)	-0.23	1 (0%) 86 75	50, 83, 114, 120	0
9	CI	127/128 (99%)	-0.37	1 (0%) 86 75	53, 86, 114, 120	0
10	AJ	99/105 (94%)	0.08	6 (6%) 22 16	47, 100, 155, 159	0
10	CJ	99/105 (94%)	0.17	3 (3%) 51 37	50, 102, 156, 159	0
11	AK	119/129 (92%)	-0.34	2 (1%) 70 57	42, 59, 100, 123	0
11	CK	119/129 (92%)	-0.28	1 (0%) 86 75	44, 60, 102, 124	0
12	AL	125/132 (94%)	-0.49	0 100 100	38, 57, 87, 127	0
12	CL	125/132 (94%)	-0.44	2 (1%) 72 59	39, 58, 88, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	125/126 (99%)	-0.15	6 (4%)	31 22	68, 111, 139, 171	0
13	CM	125/126 (99%)	-0.16	8 (6%)	20 14	70, 112, 139, 172	0
14	AN	60/61 (98%)	-0.41	1 (1%)	70 57	39, 59, 92, 97	0
14	CN	60/61 (98%)	-0.42	0	100 100	44, 61, 93, 98	0
15	AO	88/89 (98%)	-0.57	0	100 100	35, 61, 91, 100	0
15	CO	88/89 (98%)	-0.55	0	100 100	38, 61, 94, 100	0
16	AP	84/88 (95%)	-0.45	0	100 100	54, 73, 96, 131	0
16	CP	84/88 (95%)	-0.43	1 (1%)	79 66	57, 74, 98, 132	0
17	AQ	100/105 (95%)	-0.56	0	100 100	43, 64, 89, 98	0
17	CQ	100/105 (95%)	-0.50	0	100 100	46, 66, 90, 97	0
18	AR	70/88 (79%)	-0.42	1 (1%)	75 62	42, 69, 94, 108	0
18	CR	70/88 (79%)	-0.51	1 (1%)	75 62	45, 70, 95, 109	0
19	AS	79/93 (84%)	-0.02	2 (2%)	58 43	77, 106, 144, 149	0
19	CS	79/93 (84%)	0.15	4 (5%)	29 20	78, 107, 144, 150	0
20	AT	99/106 (93%)	-0.37	0	100 100	63, 84, 126, 129	0
20	CT	99/106 (93%)	-0.37	0	100 100	64, 85, 127, 129	0
21	AU	25/27 (92%)	-0.24	0	100 100	63, 82, 118, 122	0
21	CU	25/27 (92%)	0.12	0	100 100	66, 86, 120, 123	0
22	AV	76/77 (98%)	-0.49	0	100 100	32, 67, 110, 127	0
22	AW	76/77 (98%)	-0.43	1 (1%)	77 64	71, 168, 192, 201	0
22	CV	76/77 (98%)	-0.62	0	100 100	47, 84, 121, 151	0
22	CW	76/77 (98%)	-0.37	1 (1%)	77 64	78, 176, 200, 210	0
23	AX	11/25 (44%)	0.08	0	100 100	28, 94, 149, 166	0
23	CX	11/25 (44%)	0.00	0	100 100	45, 106, 156, 168	0
24	AY	667/691 (96%)	-0.18	9 (1%)	77 64	61, 99, 140, 150	0
24	CY	667/691 (96%)	0.07	23 (3%)	46 33	73, 108, 148, 161	0
25	B0	84/85 (98%)	0.04	6 (7%)	17 12	67, 82, 140, 163	0
25	D0	84/85 (98%)	0.37	9 (10%)	7 6	69, 84, 141, 163	0
26	B1	94/98 (95%)	-0.46	1 (1%)	80 67	41, 70, 118, 128	0
26	D1	94/98 (95%)	-0.34	0	100 100	53, 80, 123, 131	0
27	B2	71/72 (98%)	-0.30	2 (2%)	53 40	77, 116, 150, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	D2	71/72 (98%)	-0.15	2 (2%) 53 40	95, 119, 146, 163	0
28	B3	60/60 (100%)	-0.09	1 (1%) 70 57	63, 88, 114, 135	0
28	D3	60/60 (100%)	-0.02	2 (3%) 47 35	64, 89, 114, 134	0
29	B4	58/71 (81%)	0.07	3 (5%) 28 20	76, 135, 220, 222	0
29	D4	58/71 (81%)	0.27	7 (12%) 5 5	77, 137, 220, 222	0
30	B5	59/60 (98%)	-0.08	3 (5%) 29 20	52, 80, 153, 172	0
30	D5	59/60 (98%)	-0.03	4 (6%) 18 13	52, 80, 153, 172	0
31	B6	50/54 (92%)	-0.00	2 (4%) 39 28	56, 89, 107, 117	0
31	D6	50/54 (92%)	-0.26	1 (2%) 65 51	56, 90, 108, 117	0
32	B7	49/49 (100%)	-0.34	2 (4%) 38 27	47, 64, 119, 132	0
32	D7	49/49 (100%)	-0.39	0 100 100	47, 64, 120, 132	0
33	B8	64/65 (98%)	-0.37	1 (1%) 72 59	63, 75, 105, 125	0
33	D8	64/65 (98%)	-0.26	1 (1%) 72 59	65, 76, 105, 126	0
34	B9	37/37 (100%)	-0.43	0 100 100	60, 71, 85, 89	0
34	D9	37/37 (100%)	-0.30	1 (2%) 55 41	60, 73, 87, 91	0
35	BA	2901/2915 (99%)	-0.40	27 (0%) 84 72	30, 76, 162, 221	0
35	DA	2901/2915 (99%)	-0.53	32 (1%) 80 67	29, 77, 162, 221	0
36	BB	119/122 (97%)	-0.54	0 100 100	65, 106, 138, 183	0
36	DB	119/122 (97%)	-0.72	0 100 100	66, 108, 138, 183	0
37	BC	228/229 (99%)	-0.13	4 (1%) 69 55	42, 97, 147, 160	0
37	DC	228/229 (99%)	0.09	11 (4%) 31 22	43, 98, 148, 162	0
38	BD	275/276 (99%)	-0.52	0 100 100	31, 52, 82, 101	0
38	DD	275/276 (99%)	-0.51	1 (0%) 92 87	32, 52, 82, 101	0
39	BE	205/206 (99%)	-0.33	3 (1%) 74 61	44, 77, 128, 135	0
39	DE	205/206 (99%)	-0.29	3 (1%) 74 61	44, 77, 128, 134	0
40	BF	208/210 (99%)	0.01	10 (4%) 31 22	53, 110, 166, 177	0
40	DF	208/210 (99%)	-0.01	12 (5%) 24 17	53, 111, 166, 176	0
41	BG	181/182 (99%)	-0.27	4 (2%) 62 48	63, 95, 131, 143	0
41	DG	181/182 (99%)	-0.03	6 (3%) 47 35	86, 110, 137, 151	0
42	BH	167/180 (92%)	0.06	6 (3%) 43 32	81, 117, 143, 159	0
42	DH	167/180 (92%)	0.04	4 (2%) 59 45	81, 118, 143, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BJ	0/173	-	-	-	-
43	DJ	0/173	-	-	-	-
44	BK	140/147 (95%)	1.96	61 (43%) 0 0	162, 180, 186, 188	0
44	DK	140/147 (95%)	1.68	49 (35%) 0 1	162, 180, 186, 187	0
45	BL	0/125	-	-	-	-
45	BM	0/125	-	-	-	-
45	Bl	0/125	-	-	-	-
45	Bm	0/125	-	-	-	-
45	DL	0/125	-	-	-	-
45	DM	0/125	-	-	-	-
45	Dl	0/125	-	-	-	-
45	Dm	0/125	-	-	-	-
46	BN	139/140 (99%)	-0.30	2 (1%) 75 62	60, 91, 132, 137	0
46	DN	139/140 (99%)	-0.25	1 (0%) 87 78	61, 91, 132, 137	0
47	BO	122/122 (100%)	-0.46	0 100 100	35, 60, 73, 86	0
47	DO	122/122 (100%)	-0.44	0 100 100	36, 61, 73, 88	0
48	BP	146/150 (97%)	0.02	4 (2%) 55 41	46, 111, 137, 157	0
48	DP	146/150 (97%)	0.10	4 (2%) 55 41	50, 113, 137, 157	0
49	BQ	141/141 (100%)	-0.38	0 100 100	45, 65, 88, 119	0
49	DQ	141/141 (100%)	-0.41	0 100 100	45, 66, 89, 120	0
50	BR	117/118 (99%)	-0.37	1 (0%) 84 72	49, 81, 101, 128	0
50	DR	117/118 (99%)	-0.28	1 (0%) 84 72	53, 82, 101, 128	0
51	BS	99/112 (88%)	-0.19	2 (2%) 65 51	82, 116, 140, 144	0
51	DS	99/112 (88%)	0.28	5 (5%) 29 20	83, 117, 141, 145	0
52	BT	138/146 (94%)	-0.13	4 (2%) 52 38	55, 83, 149, 176	0
52	DT	138/146 (94%)	-0.18	5 (3%) 43 32	57, 84, 149, 177	0
53	BU	117/118 (99%)	-0.37	0 100 100	62, 80, 114, 135	0
53	DU	117/118 (99%)	-0.36	0 100 100	62, 81, 115, 134	0
54	BV	101/101 (100%)	-0.03	1 (0%) 82 70	59, 116, 133, 141	0
54	DV	101/101 (100%)	0.17	5 (4%) 30 21	61, 116, 134, 140	0
55	BW	113/113 (100%)	-0.28	0 100 100	61, 79, 119, 158	0
55	DW	113/113 (100%)	-0.16	0 100 100	63, 80, 120, 159	0
56	BX	93/96 (96%)	-0.18	0 100 100	76, 91, 110, 114	0
56	DX	93/96 (96%)	-0.22	0 100 100	76, 92, 111, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
57	BY	107/110 (97%)	0.08	2 (1%) 67 53	78, 127, 149, 155	0
57	DY	107/110 (97%)	0.41	4 (3%) 42 31	78, 127, 149, 155	0
58	BZ	185/206 (89%)	-0.23	1 (0%) 90 84	47, 90, 135, 143	0
58	DZ	185/206 (89%)	-0.09	1 (0%) 90 84	68, 99, 138, 146	0
All	All	22794/24788 (91%)	-0.29	444 (1%) 67 53	23, 82, 155, 222	0

The worst 5 of 444 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BA	654(K)	C	14.8
1	CA	1036	G	13.4
52	BT	138	ALA	13.1
35	DA	654(D)	G	13.0
35	BA	654(F)	C	11.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
22	5MU	CV	54	20/22	0.97	0.11	-	89,92,95,96	0
22	5MU	AV	54	20/22	0.95	0.13	-	82,84,86,86	0
22	5MU	AW	55	20/22	0.83	0.14	-	161,165,168,168	0
22	5MU	CW	55	20/22	0.81	0.13	-	178,179,186,186	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.



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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
61	FUA	AY	702	37/37	0.90	0.43	1.99	98,102,110,111	0
59	ZN	AD	301	1/1	1.00	0.28	1.61	32,32,32,32	0
59	ZN	CD	301	1/1	0.99	0.28	1.04	49,49,49,49	0
61	FUA	CY	702	37/37	0.90	0.35	0.41	102,104,107,109	0
59	ZN	B9	101	1/1	0.99	0.15	0.02	62,62,62,62	0
59	ZN	AN	101	1/1	1.00	0.16	-0.23	35,35,35,35	0
59	ZN	D9	101	1/1	1.00	0.12	-0.51	86,86,86,86	0
62	GDP	AY	703	28/28	0.96	0.17	-0.57	78,82,83,84	0
59	ZN	CN	101	1/1	1.00	0.16	-0.86	66,66,66,66	0
59	ZN	D4	101	1/1	0.89	0.07	-1.04	164,164,164,164	0
59	ZN	B4	101	1/1	0.91	0.12	-1.48	122,122,122,122	0
62	GDP	CY	703	28/28	0.95	0.15	-1.65	81,87,94,95	0
60	MG	AY	701	1/1	0.98	0.22	-	30,30,30,30	0
60	MG	CY	701	1/1	0.99	0.12	-	39,39,39,39	0

## 6.5 Other polymers

There are no such residues in this entry.