



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:46 PM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

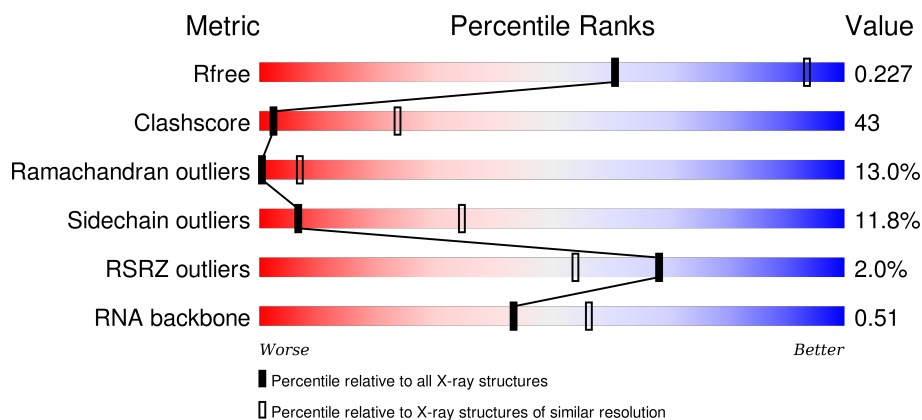
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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.



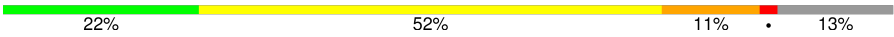
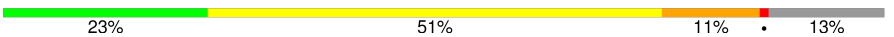



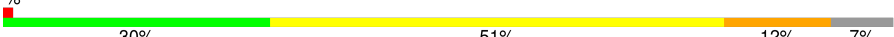
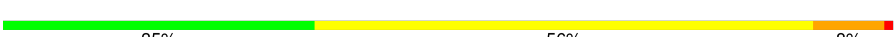
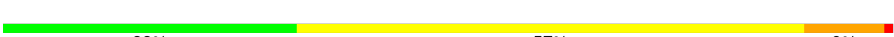
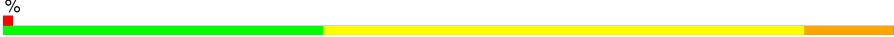

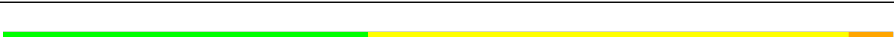
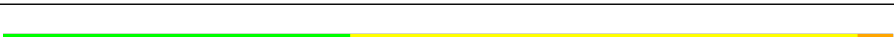

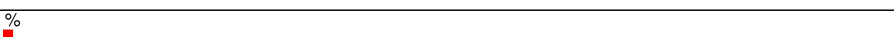
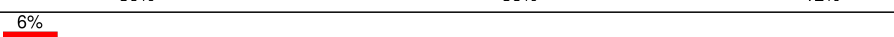
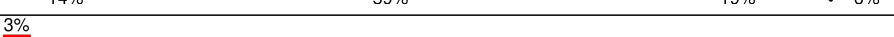



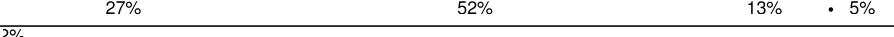
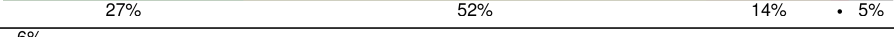
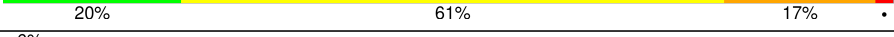
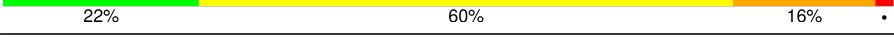


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)
RNA backbone	2183	1058 (4.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>2%</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>


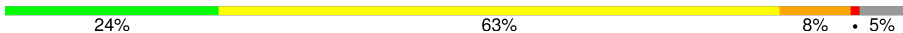
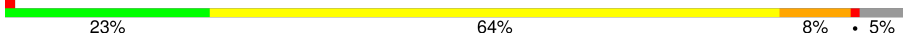


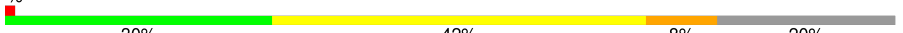
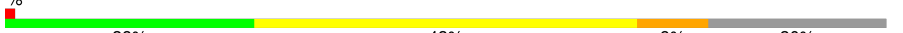




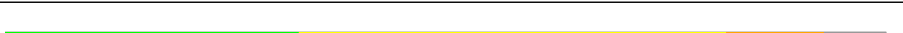





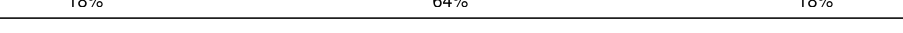


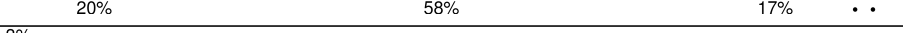
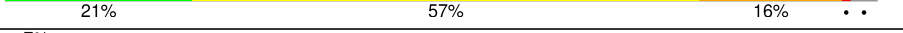


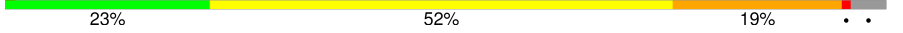
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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126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



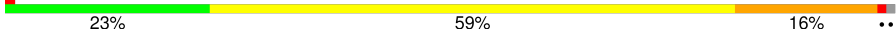
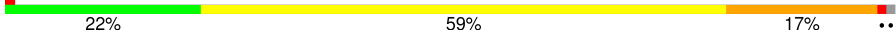
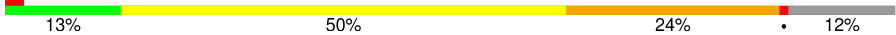
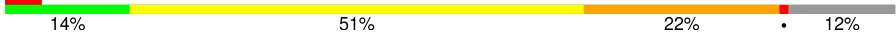
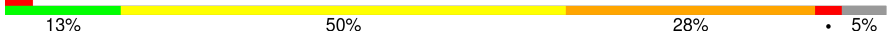
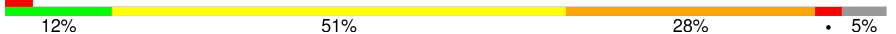
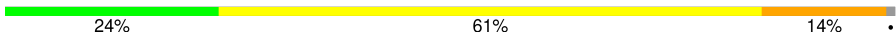
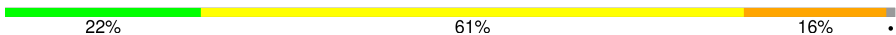
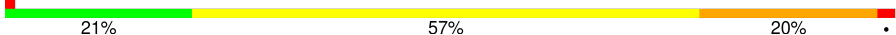
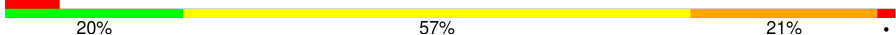
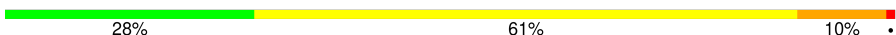







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Mol	Chain	Length	Quality of chain
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BJ	173	
43	DJ	173	
44	BK	147	
44	DK	147	
45	BL	125	
45	BM	125	
45	Bl	125	
45	Bm	125	
45	DL	125	
45	DM	125	
45	Dl	125	
45	Dm	125	
46	BN	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 RRNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	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			

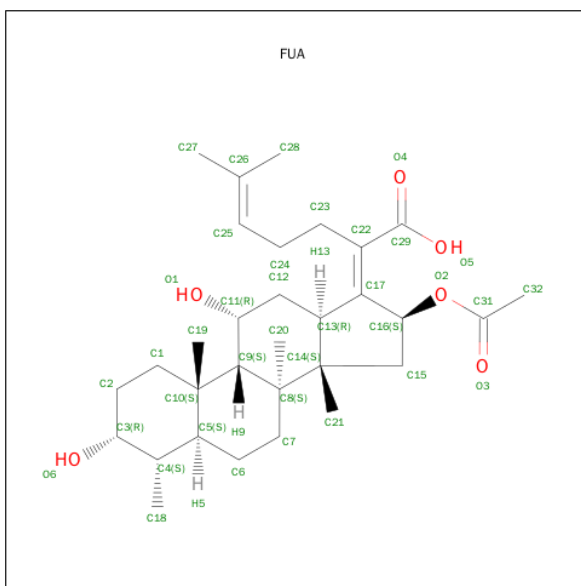
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

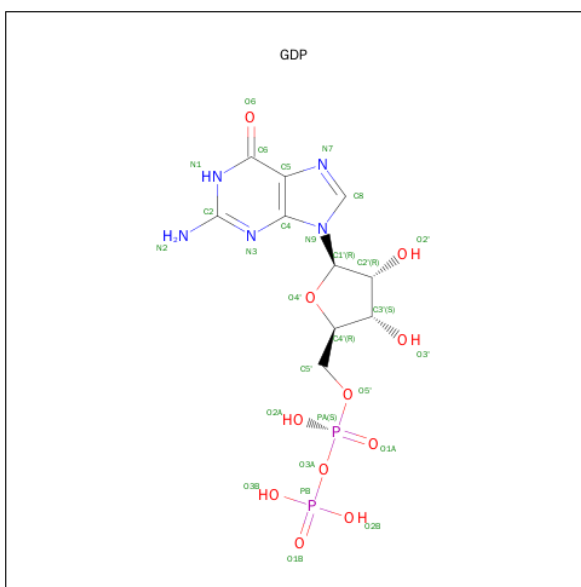
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AY	1	Total	Mg	0	0
			1	1		
60	CY	1	Total	Mg	0	0
			1	1		

- 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 37 31 6	0	0
61	CY	1	Total C O 37 31 6	0	0

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

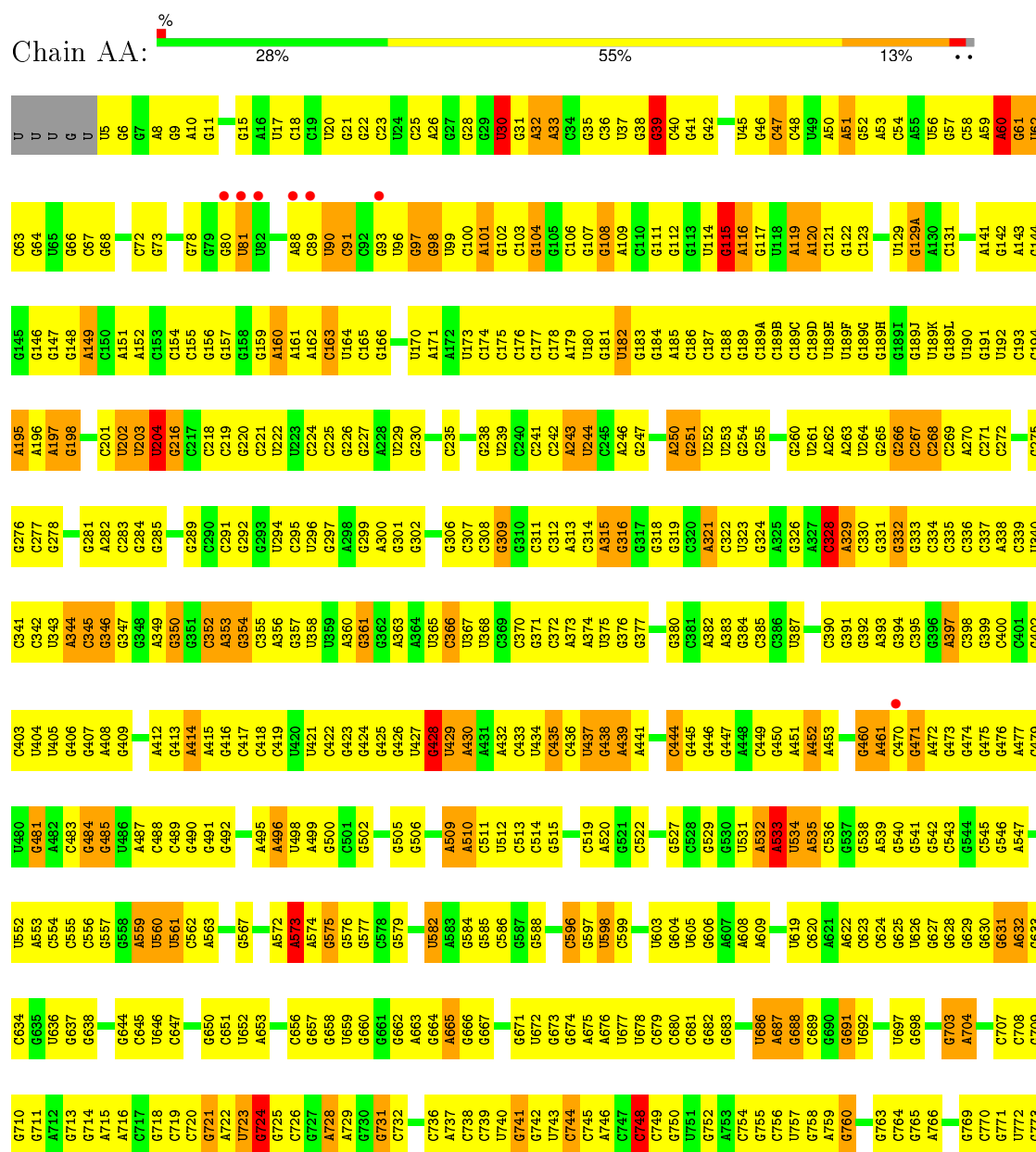


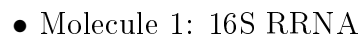
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
62	AY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
62	CY	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

3 Residue-property plots

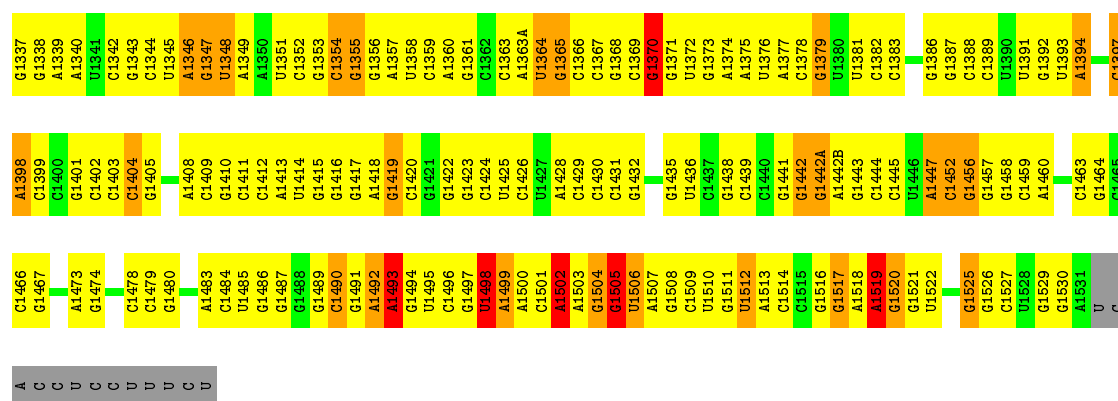
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S rRNA

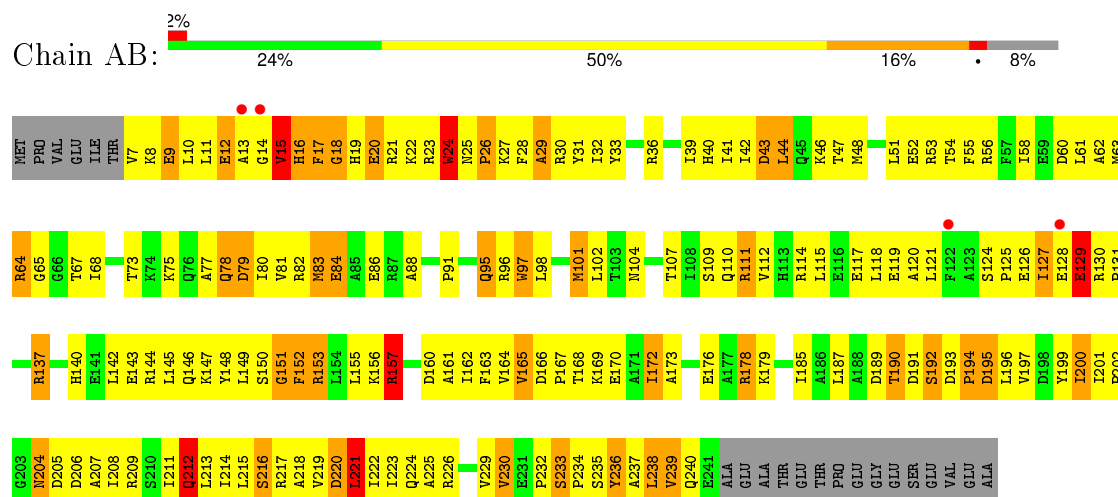




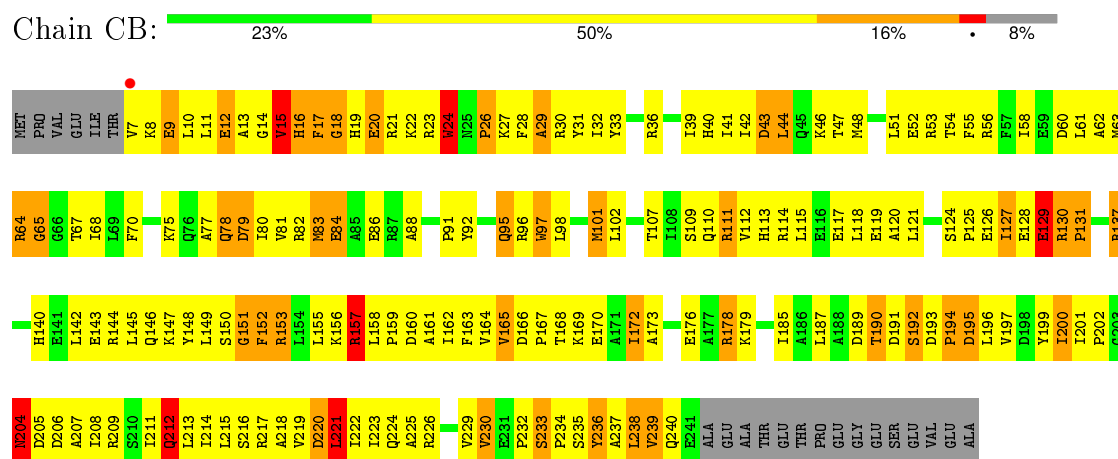
G1277	U1211	G1143	G1001A	G939	G854	G778	A712	G638	C556	U486	A408	A344	G278	A195
U1278	U1212	G1144	G1002	G940	G858	G779	G713	G641	G557	A487	G409	C345	G281	A196
A1279	A1213	C1145	G1003	G941	A780	A781	G714	U641	G558	C488	A412	G346	A282	A197
A1280	C1214	A1146	A1004	G942	A859	A782	A715	U646	U560	C489	A413	G347	C283	G198
U1281	G1215	C1147	A1005	G943	A860	A783	G716	U647	U561	G490	A414	A348	G284	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	U1150	U1150	C1008	G946	A865	G785	G719	G651	A573	A495	C417	C352	G289	U204
A1285	A1151	A1151	G1009	G947	C866	A787	G720	C651	A574	U496	C418	A353	C290	G216
A1286	C1152	A1080	G1010	C948	C867	A787	A722	A653	A575	U498	C419	G354	C291	C217
A1287	G1081	G1081	A1014	G949	C868	G791	U723	G656	G575	A499	U420	C355	G292	C218
A1288	G1082	U1083	A1015	U950	C869	A792	G724	G657	G576	G500	U421	A356	G293	C219
G1290	U1083	U1083	A1016	U951	G874	U793	G725	G658	G577	G501	C422	G357	U294	G220
G1291	A1157	U1089	A1017	G953	G878	U794	G726	G659	C579	G502	G423	U358	C295	G221
U1292	C1158	U1090	C1018	G954	C879	C796	G727	U659	G579	U359	G424	U359	U296	U222
G1293	U1159	U1090	C1019	U955	C879	C796	A728	G660	G579	U359	G425	A360	C297	U223
G1294	G1160	U1095	U1020	U956	C882	C797	A729	G661	U582	G505	G428	G362	A298	U229
G1295	C1161	U1095	U1021	U957	C883	A802	G730	G662	A583	G506	U429	G363	G299	U230
C1296	C1162	C1162	U1025	A958	C884	G803	G731	A663	G584	A509	U430	A364	A300	G230
C1297	C1163	C1163	U1026	A959	C885	G803	C732	A664	G585	A510	A431	A365	G301	C235
C1298	C1164	C1164	C1027	U960	C886	A807	A733	A665	G586	C511	A432	C366	G302	C235
A1299	C1165	C1165	C1028	U961	C887	C808	A736	G666	G587	C512	C433	U367	G306	G238
G1300	C1166	C1166	C1029	G962	C888	C808	A737	G667	C586	C513	C434	U368	C307	U239
U1301	A1168	A1168	G1030	G963	C889	C817	A738	U672	U588	C514	C435	C369	C308	G240
U1302	A1169	A1169	G1030A	A964	C890	C818	G739	G673	U589	C515	C436	C370	G309	C241
C1303	A1170	A1170	C1030B	A965	C891	C819	C740	G674	C599	C516	C437	C371	G310	C242
G1304	G1171	G1171	G1030C	G966	C892	U820	U740	A675	A607	C517	C438	C372	C311	A243
G1305	C1172	C1172	A1030D	C967	C893	G821	G741	A676	A608	G520	C439	C373	C312	U244
A1306	G1173	G1173	G1031	A968	C894	A815	G742	A677	A609	G521	A441	A374	C313	C245
U1307	G1174	C1113	G1032	A969	C895	A816	U743	U677	U603	C522	U441	A375	C314	A246
U1308	G1175	C1114	G1033	C970	C896	C817	C744	U678	G604	A523	C444	U375	A315	G247
G1309	G1176	C1115	G1034	G971	C897	G818	A747	C679	G605	C524	G445	G376	G316	A250
G1310	A1179	C1116	A1035	C972	A900	A819	C748	C680	G606	C525	G446	G377	G317	G251
G1311	G1180	C1117	G1036	G973	A901	U820	C749	C681	A607	C526	G447	C380	G318	U252
U1312	G1181	C1118	C1037	A974	A902	G821	G750	G682	A608	C527	C448	C381	G319	U253
C1313	G1182	C1119	C1038	A975	A903	C822	G751	G683	A609	C528	C449	C382	C320	G254
C1314	G1183	G1120	C1039	C976	A904	G823	G752	G684	U610	C529	C450	A383	C322	G255
U1315	U1121	U1121	G1047	A977	C910	C824	C753	U686	G617	C530	C451	G384	U323	U256
G1316	A1122	A1122	C1048	C978	A913	C825	G754	A687	C618	C531	C452	C385	G324	G257
C1317	A1123	A1123	U1049	C979	A914	C826	G755	A688	U619	C532	C453	C386	A325	G260
A1318	G1124	G1124	U1049	C980	A915	C827	G756	C689	U619	C533	C454	C387	A326	U261
A1319	U1125	U1125	G1050	U981	A916	C828	G757	C690	C620	C534	C455	C388	C327	G262
C1320	U1126	U1126	G1051	U982	U921	G829	A759	G691	A621	C535	C456	C389	A328	G263
C1321	G1127	G1127	G1052	A983	G922	G830	G760	U692	A622	C536	C457	C390	A329	A264
C1322	C1128	C1128	A1054	A984	A923	U831	G761	G693	C623	C537	C458	C391	A330	G265
G1323	C1129	C1129	A1055	A985	C924	C832	G762	A694	C624	C538	C459	C392	A331	G266
A1324	G1130	G1130	U1056	G987	G925	U833	G763	A695	G625	C539	C460	C393	A332	G267
C1325	U1131	U1131	G1057	U988	G926	C834	G764	A696	U626	C540	C461	C394	A333	C268
C1326	C1132	C1132	G1058	U989	G927	U835	G765	U697	G627	C541	C462	C395	A334	C269
G1327	G1133	G1133	C1059	U991	G928	U836	A766	G698	G628	C542	C463	C396	A335	A270
C1328	U1134	U1134	C1060	U992	C930	C837	A767	G699	C629	C543	C464	C397	A336	C271
A1329	G1135	G1135	U1061	A994	C931	U839	A768	C703	G630	C544	C465	C398	A337	C272
U1330	U1136	U1136	U1062	C995	C932	U840	G769	A704	G631	C545	C466	C399	A338	G275
G1331	C1137	C1137	C1063	A996	G933	U841	C770	G705	G632	C546	C467	C401	A339	G276
A1332	G1138	G1138	G1064	U997	G934	C848	U772	C707	A632	C547	C468	C402	A340	G277
A1333	U1065	U1065	U1065	G998	A935	C849	G773	C708	G633	C548	C469	C403	A341	G278
G1334	C1066	C1066	A1067	C999	C936	G851	G774	G709	G634	C549	C470	C404	A342	G279
C1335	A1068	A1068	G1068	U1000	A937	G852	G775	G710	G635	C550	C471	C405	A343	G280
G1336	G1068	G1068	G1068	A1001	A938	G853	A777	G711	G637	C551	C472	C406	A344	G281



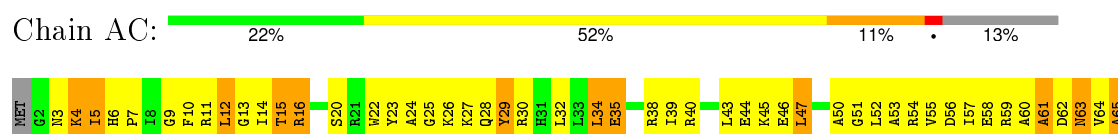
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

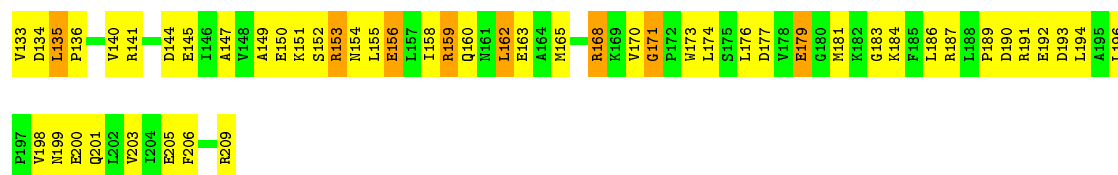


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

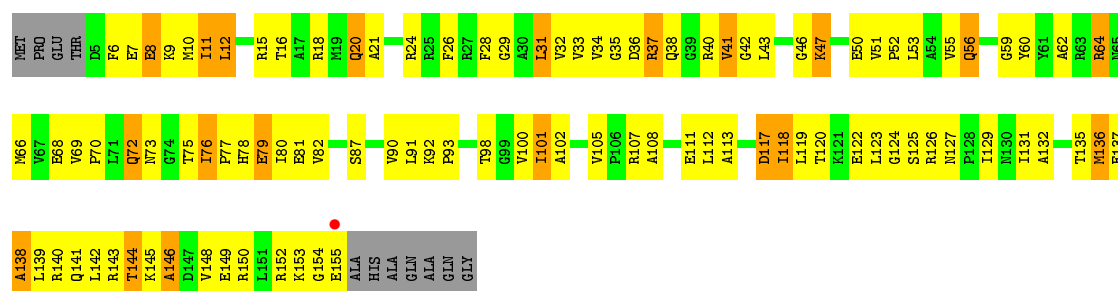


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

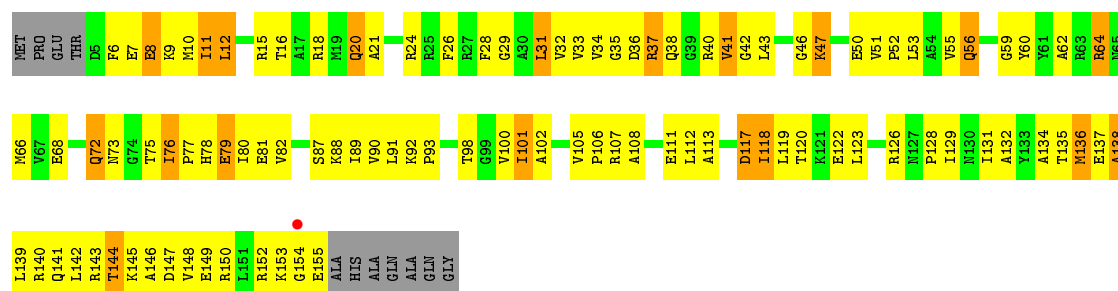




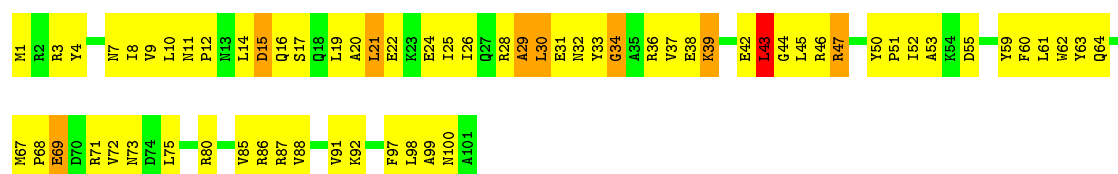
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



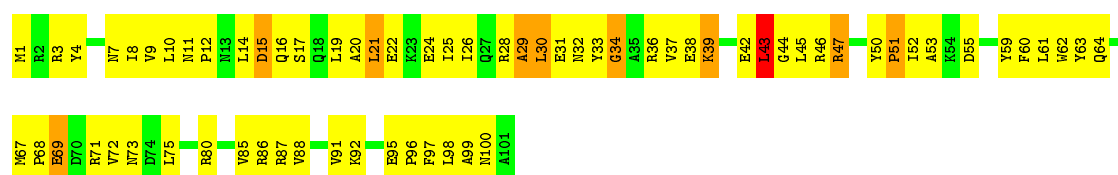
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



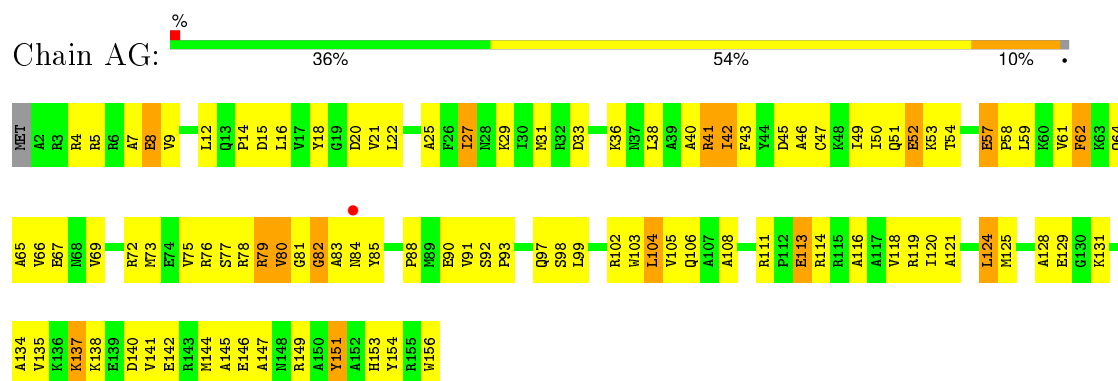
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



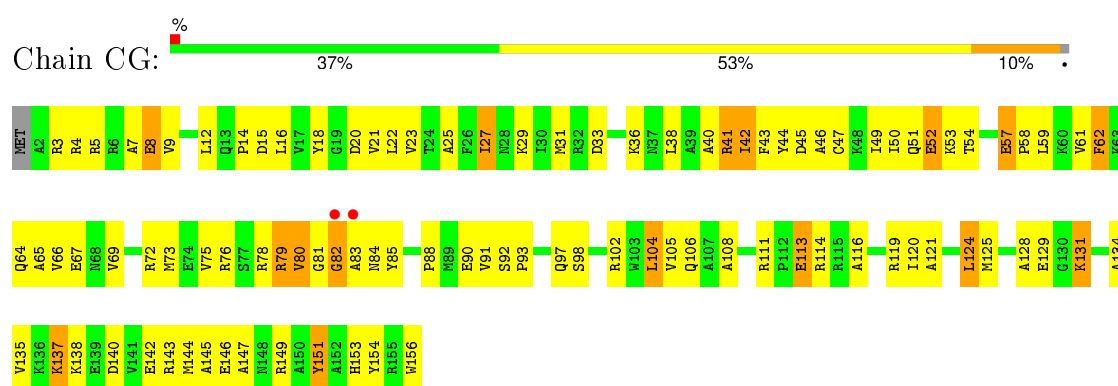
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



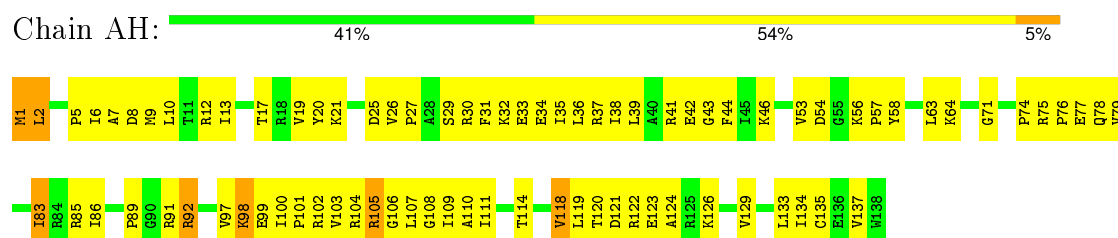
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



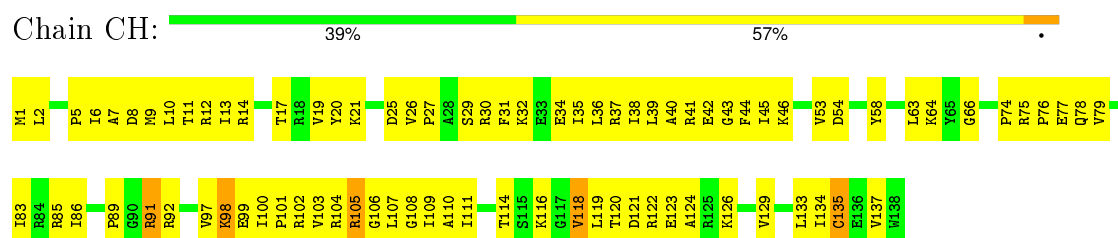
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



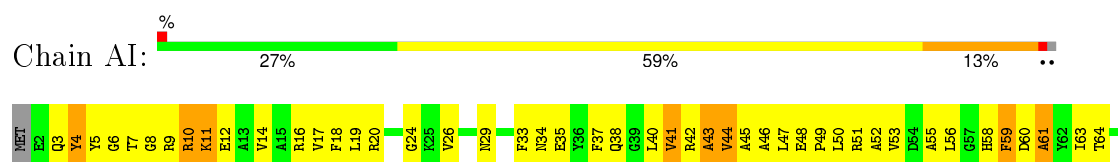
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

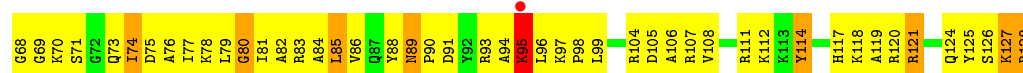


- Molecule 8: 30S RIBOSOMAL PROTEIN S8

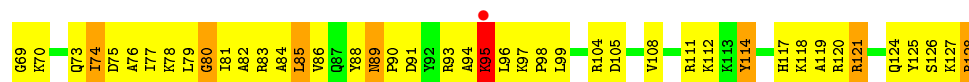
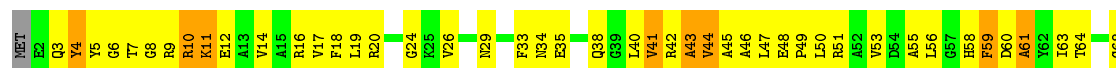


- Molecule 9: 30S RIBOSOMAL PROTEIN S9

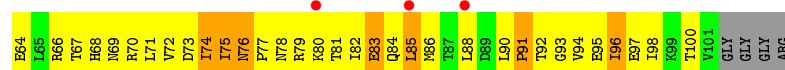
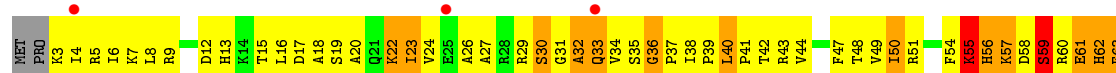
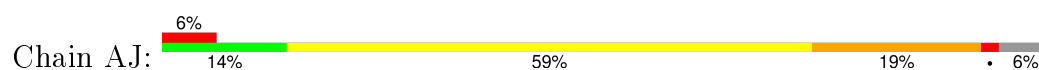




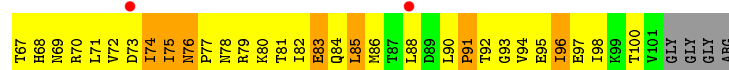
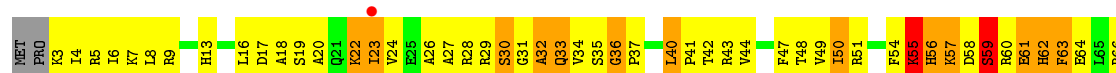
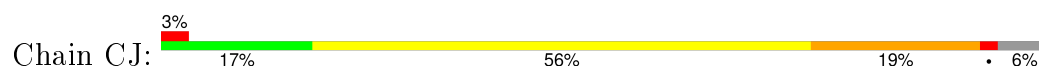
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11



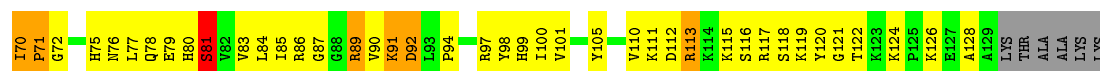
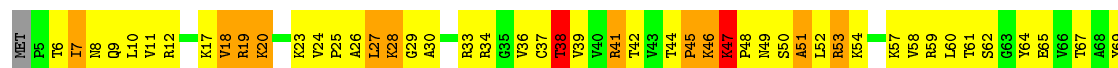
• Molecule 11: 30S RIBOSOMAL PROTEIN S11





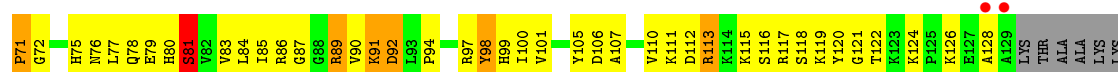
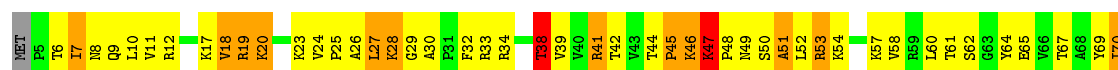
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL: 27% 52% 13% 5%



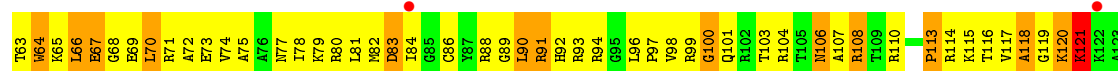
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL: 2% 27% 52% 14% 5%



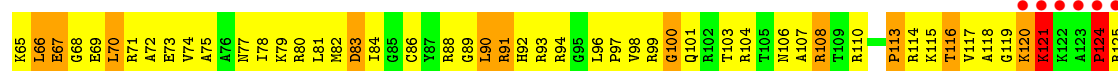
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM: 6% 20% 61% 17% ..



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM: 6% 22% 60% 16% ..



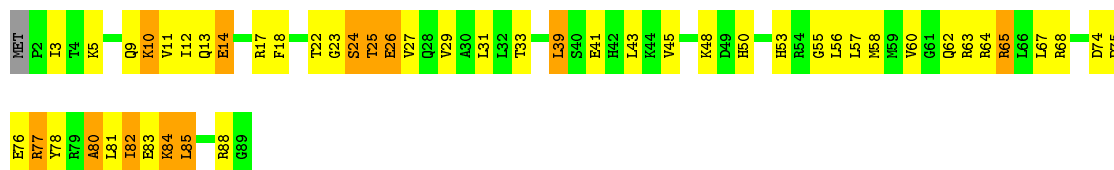
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:  2% 39% 48% 7% 5%

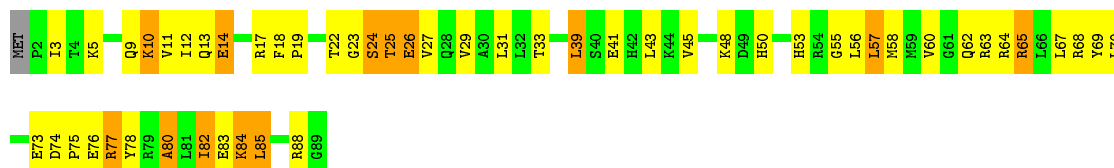
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN:  33% 54% 7% 5%

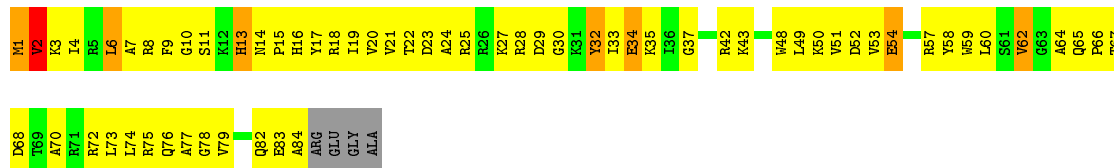
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:  44% 42% 13%

• Molecule 15: 30S RIBOSOMAL PROTEIN S15

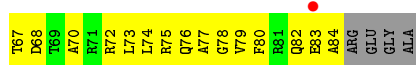
Chain CO:  40% 44% 15%

• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:  24% 63% 8% 5%

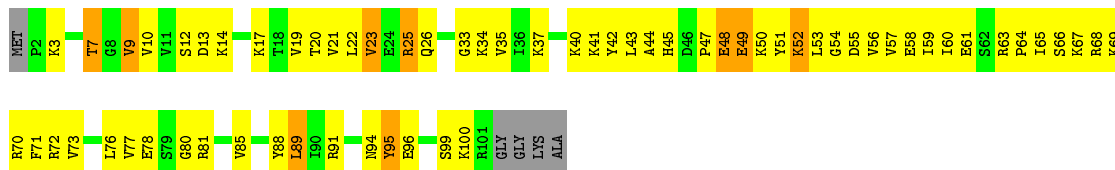
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:  23% 64% 8% 5%



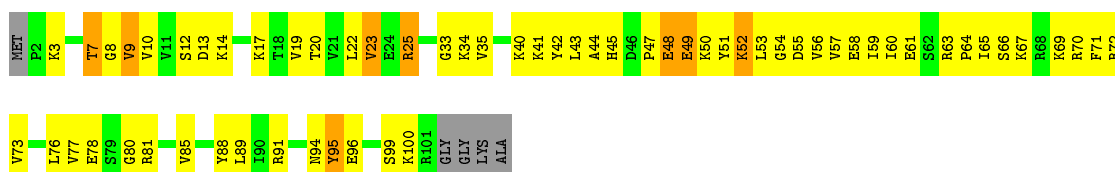
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ: 33% 53% 9% 5%



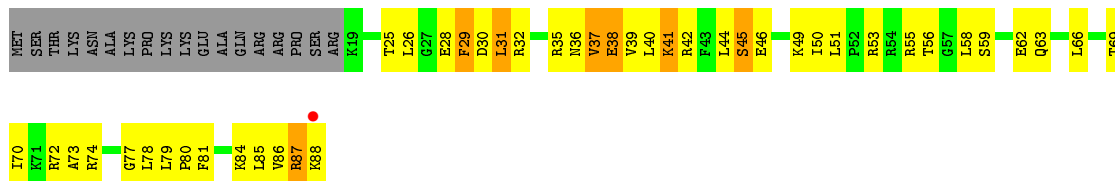
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ: 36% 51% 8% 5%



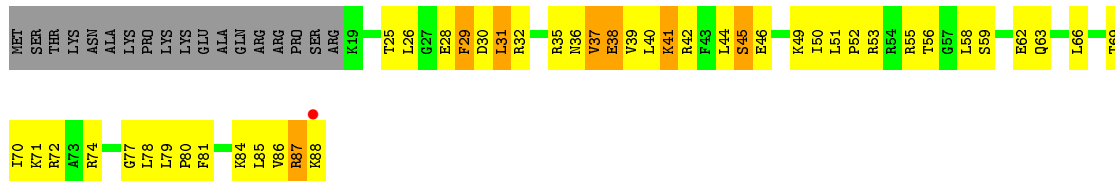
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR: 30% 42% 8% 20%



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

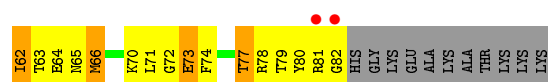
Chain CR: 28% 43% 8% 20%



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

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

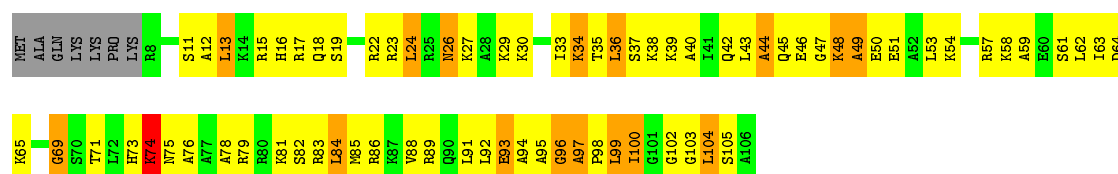


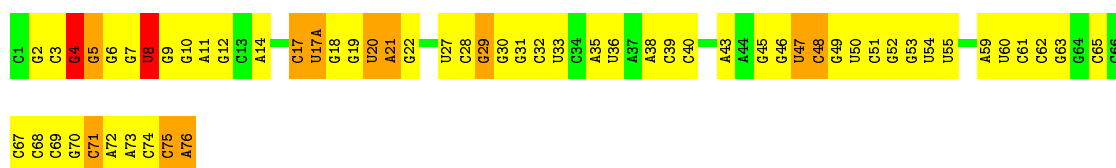


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

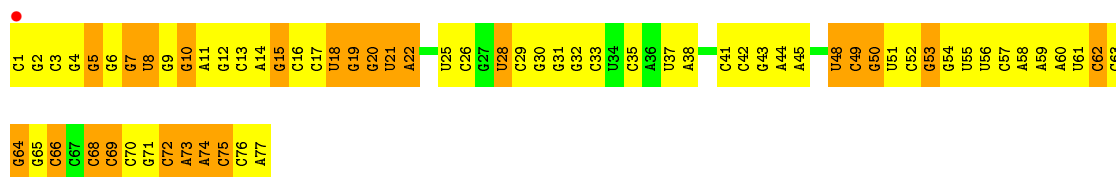
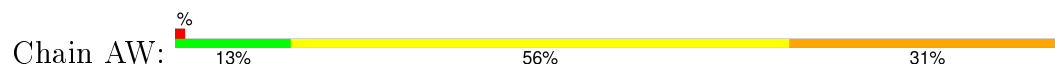


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

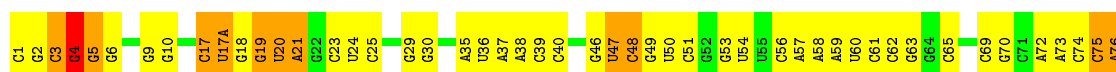




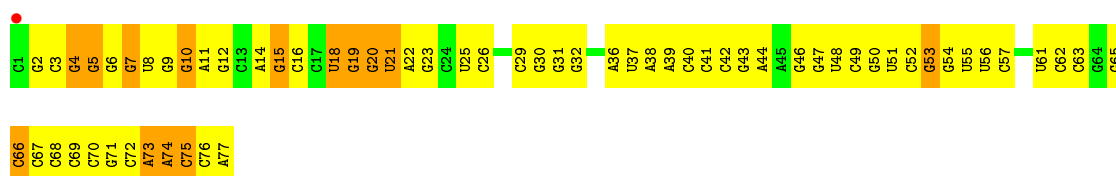
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)



- 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)



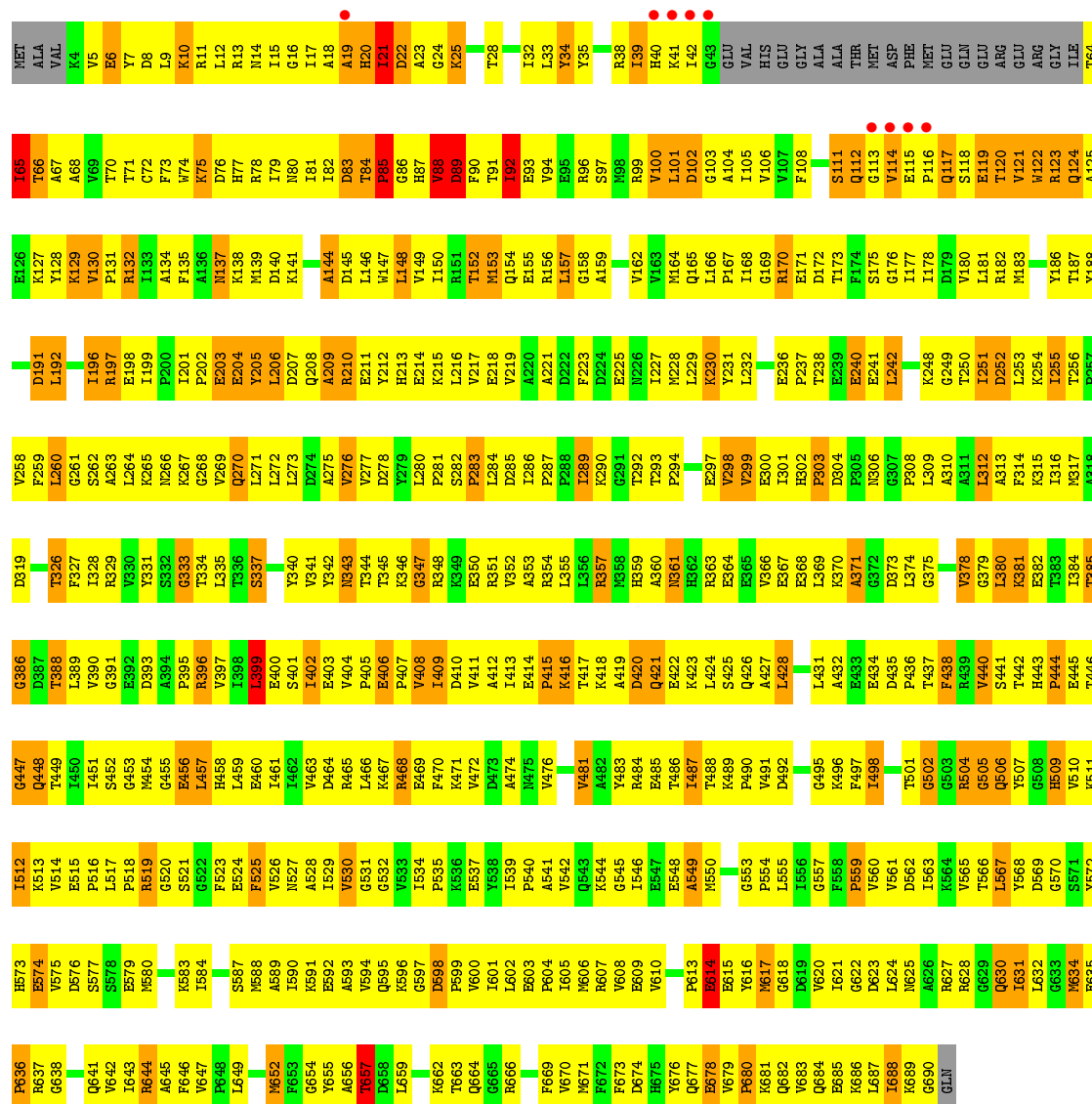
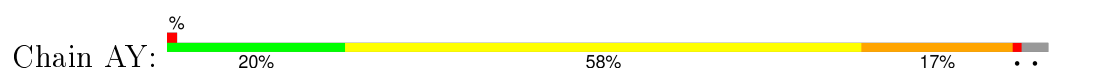
- Molecule 23: MRNA



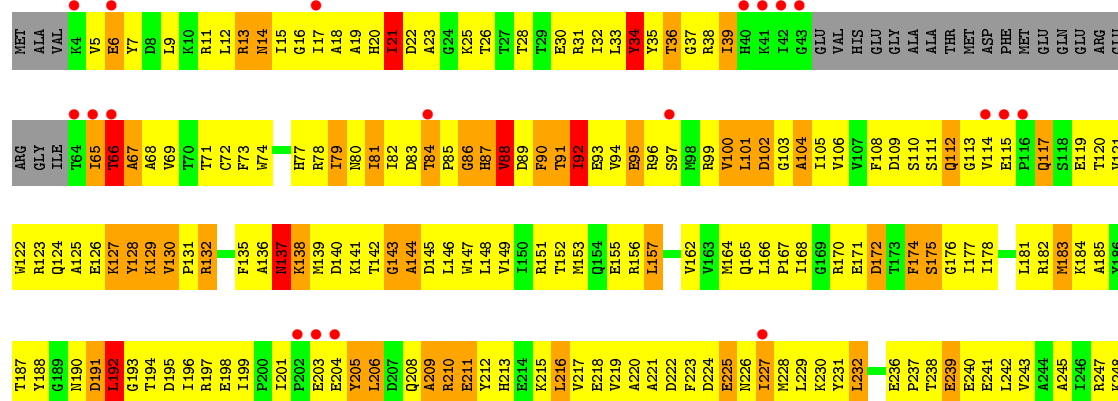
- Molecule 23: MRNA

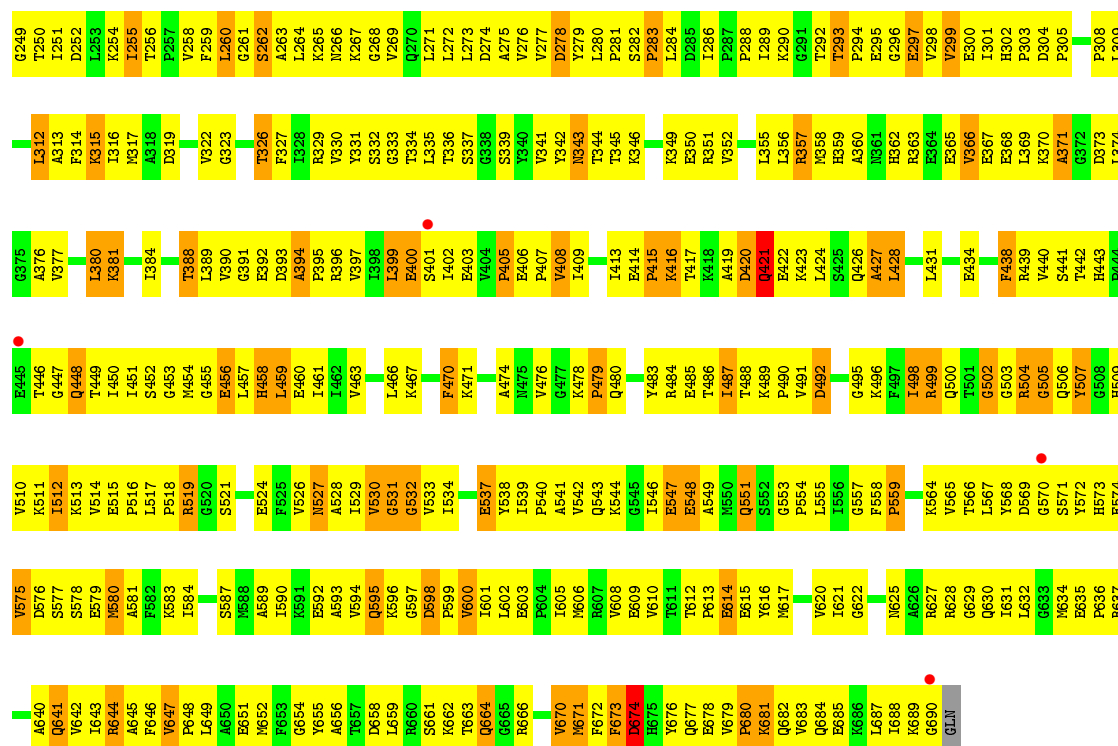


- Molecule 24: ELONGATION FACTOR G

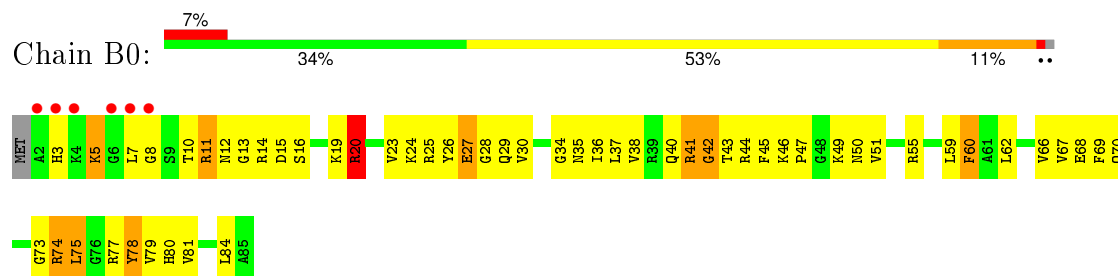


● Molecule 24: ELONGATION FACTOR G

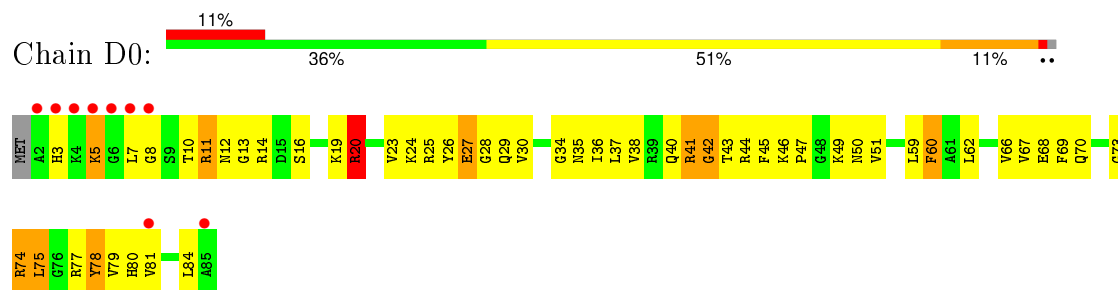




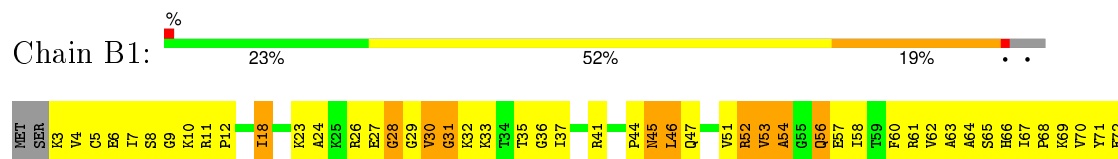
• Molecule 25: 50S RIBOSOMAL PROTEIN L27

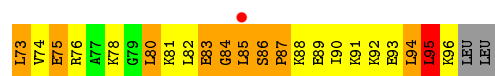


• Molecule 25: 50S RIBOSOMAL PROTEIN L27

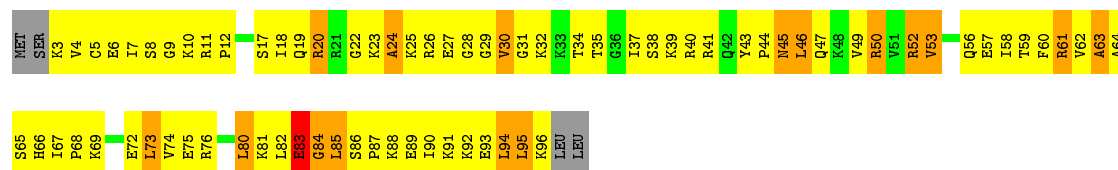


• Molecule 26: 50S RIBOSOMAL PROTEIN L28

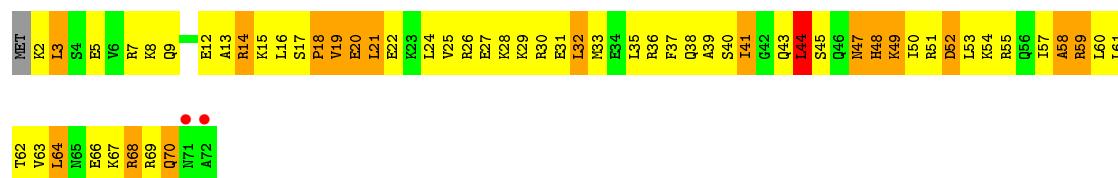




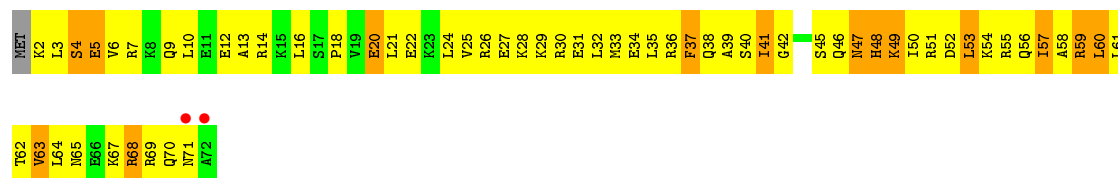
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



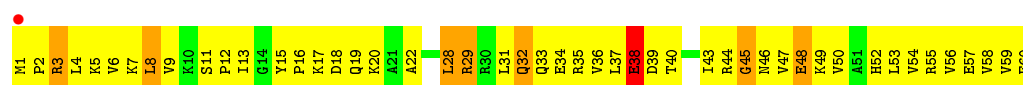
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



• Molecule 27: 50S RIBOSOMAL PROTEIN L29



• Molecule 28: 50S RIBOSOMAL PROTEIN L30

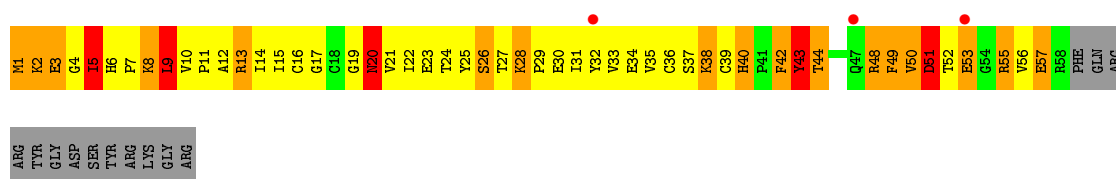


• Molecule 28: 50S RIBOSOMAL PROTEIN L30

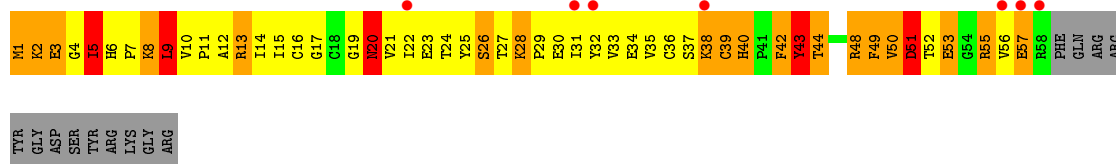


• Molecule 29: 50S RIBOSOMAL PROTEIN L31

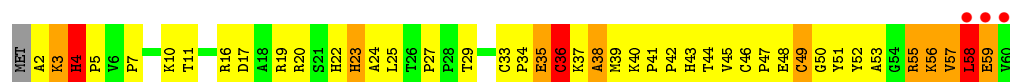




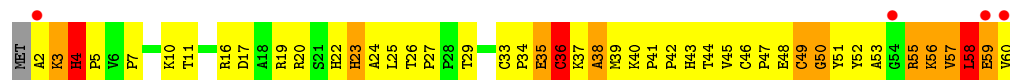
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



• Molecule 30: 50S RIBOSOMAL PROTEIN L32



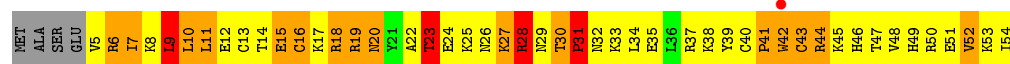
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



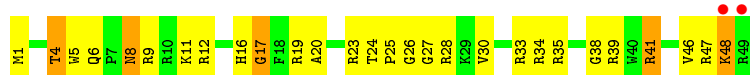
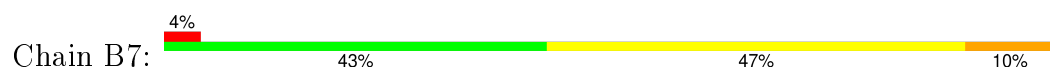
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



• Molecule 31: 50S RIBOSOMAL PROTEIN L33



• Molecule 32: 50S RIBOSOMAL PROTEIN L34



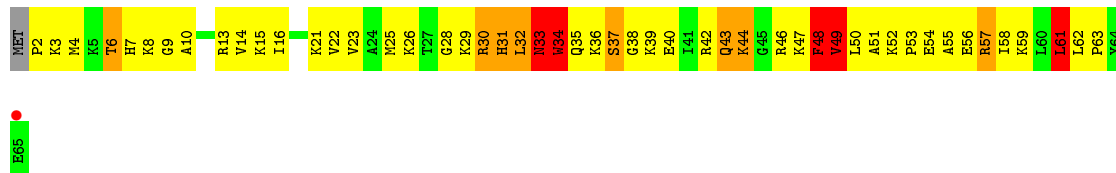
- Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain D7: 



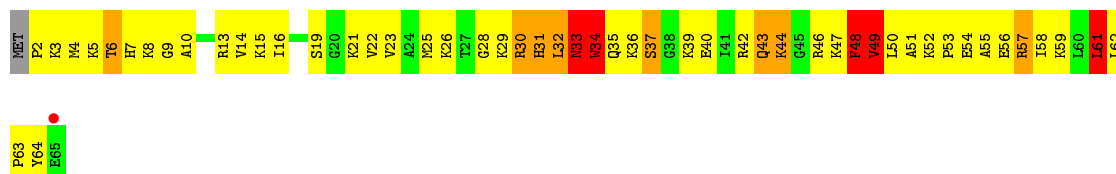
- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain B8: 



- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain D8: 



- Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain B9: 



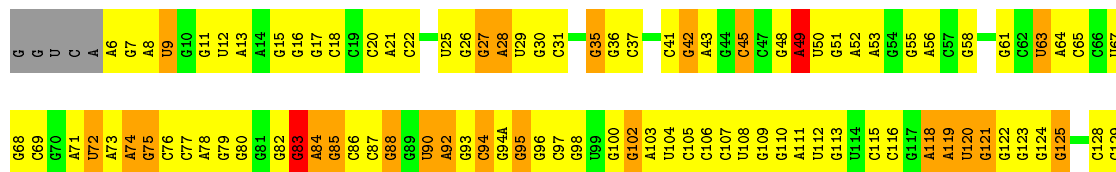
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain D9: 



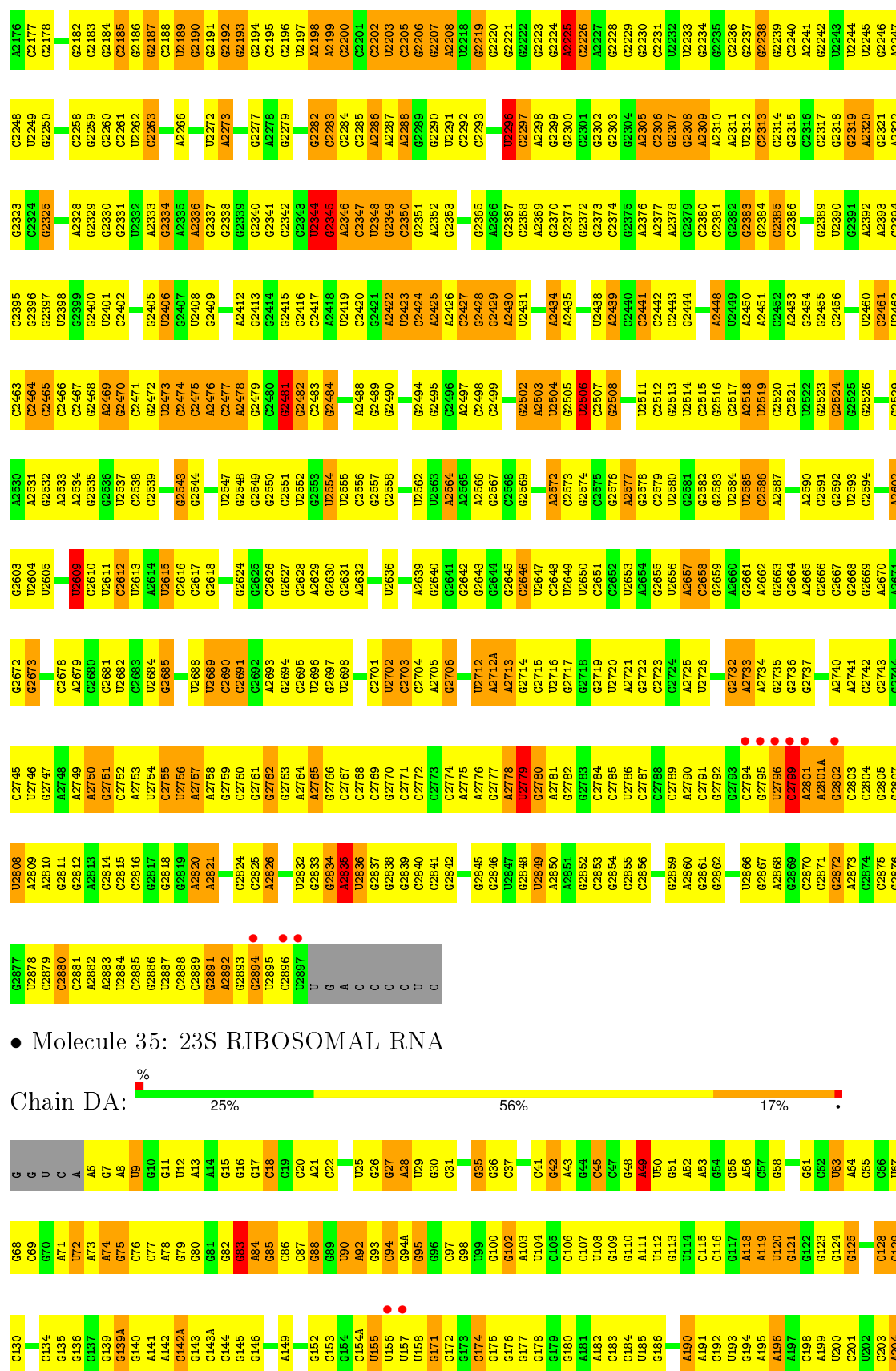
- Molecule 35: 23S RIBOSOMAL RNA

Chain BA: 



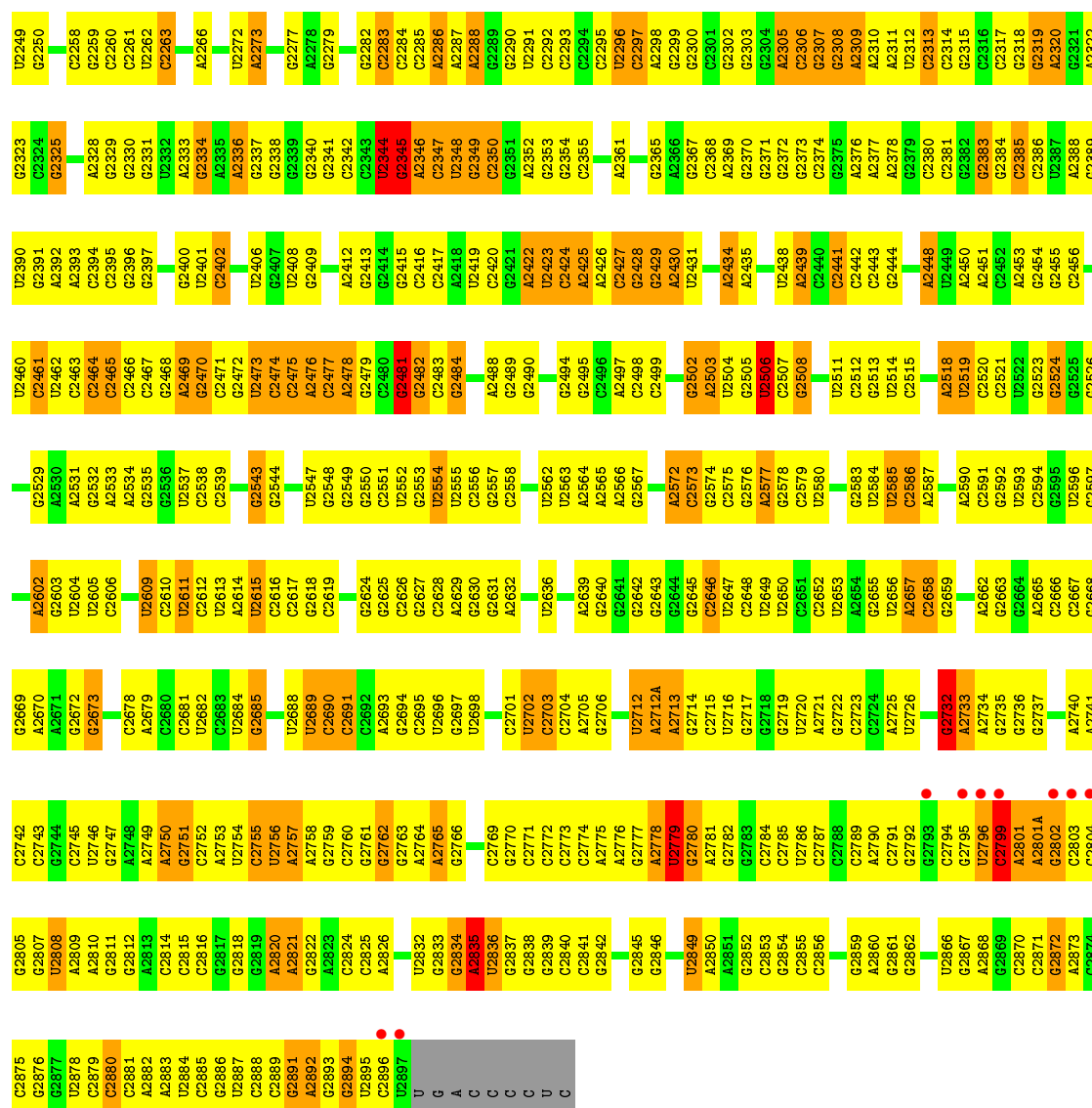
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G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711																																																																																																																																																																																																																																																																																				
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G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711																																																																						
C302	C303	C304	C305	C306	C307	C308	C309	C310	C311	C312	C313	C314	C315	C316	C317	C318	C319	C320	C321	C322	C323	C324	C325	C326	C327	C328	C329	C330	C331	C332	C333	C334	C335	C336	C337	C338	C339	C340	C341	C342	C343	C344	C345	C346	C347	C348	C349	C350	C351	C352	C353	C354	C355	C356	C357	C358	C359	C360	C361	C362	C363	C364	C365	C366	C367	C368	C369	C370	C371	C372	C373	C374	C375	C376	C377	C378	C379	C380	C381	C382	C383	C384	C385	C386	C387	C388	C389	C390	C391	C392	C393	C394	C395	C396	C397	C398	C399	C400	C401	C402	C403	C404	C405	C406	C407	C408	C409	C410	C411	C412	C413	C414	C415	C416	C417	C418	C419	C420	C421	C422	C423	C424	C425	C426	C427	C428	C429	C430	C431	C432	C433	C434	C435	C436	C437	C438	C439	C440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451	C452	C453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	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
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U2113	C2043	G1973	G1907	G1828	U1766	G1601	A1535	G1465	A1395	U1326	G1256	G1192	G1131
A2114	G2046	C1974	C1908	A1829	C1767	U1602	C1536	G1466	U1396	C1327	C1257	G1193	A1132
G2116		C1983	G1909	G1830	U1768	A1603	G1538	C1467	U1397	U1329	G1258		U1133
A2117	C2050	G1984	G1910	G1831	G1769		G1539	A1472	G1398	U1329	G1259	C1196	G1136
U2118	A2051	G1985	U1911	G1832	G1770	A1608	U1540	G1473	G1399	C1330	G1260	G1197	
G2119	C2052	G1986	U1912	U1833	G1771	A1609	G1541	C1474	G1401	A1331	C1261	U1198	G1137
G2120	G2053	C1987	C1914	U1834	G1772	U1610	A1542	G1475	C1402	G1332	U1263		G1138
G2121	A2054	C1988	U1917	G1835	A1773	G1611	C1543	C1476	C1403	G1334	G1264	A1203	G1139
G2122	C2055	G1989	A1918	G1836	G1681		A1544	A1477	C1404	U1335	A1265	U1205	U1141
G2123	G2056	G1990	G1919	G1837	G1682	A1614	A1545	G1478	U1405	U1336	G1266	G1206	U1142
A2126	A2057	G1992	U1920	U1838	C1684	G1615	C1546	G1482	U1407	G1337	U1267		A1142
G2127	A2058	U1993	G1921	U1839	U1778	A1616		G1484	C1408	G1338	A1268	G1209	A1142A
G2128	A2059		G1922	G1842	U1779	A1618	C1551	G1485	C1409	U1341	A1269	A1210	A1143
C2129	A2060	C1996		C1843	A1780		A1552	G1486	C1410	U1342	G1270	U1211	G1144
A2130	A2062	G1997	G1925	G1844	U1781		A1553	A1486	C1411	G1343	G1271	G1212	C1145
G2131		G1998	U1926	G1845	U1782	G1623	A1554	G1487		G1343	A1272	A1213	C1146
G2132	C2065	G1999	C1925	G1846	C1783	G1624	G1555	G1488	U1415	G1344	U1273	G1215	G1147
U2133		C2000	U1926	A1847	C1694	C1625	C1556	U1489	U1416	C1345	A1274	G1216	A1148
G2134	C2066	A2001	G1929	U1848			C1557	A1490	C1417	G1346	A1275	G1217	G1149
A2135	G2067	G2002	G1930	G1849	G1697	U1629	A1558	G1491	U1420	G1347	G1276	G1218	C1150
G2136	U2068	C2003	U1931	G1850	A1787	G1630	G1559	G1492	C1493	G1348	U1277	G1219	G1151
C2136	G2069	G2004	A1932	U1851	G1699		G1560	C1493	U1420	A1349	G1278		C1152
G2137	U2070		G1933	C1852	A1700	A1632	G1561	A1494	G1421		G1279	G1220	G1153
C2138	G2071	C2007	C1934	A1853	G1713	G1633	G1562	A1495		A1353		A1221	G1154
G2139	G2072	C2008	G1935	A1854	G1714	A1641	G1563	A1496	A1427	A1354	G1285	C1221A	A1155
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G2141	U2074	C2010	U1937	C1856	C1710	G1635	C1565	U1497	G1429	G1356	A1287	G1223	G1157
C2142	U2075	U2011	A1938	G1857	G1711	G1636	A1566	C1498	C1430	U1357	C1288	G1224	C1158
G2143	G2076	G2012	G1938	G1858	C1712	G1638	A1567	C1499	U1431	G1358	U1289	G1225	U1159
	A2077	A2013	C1941	A1859	U1713	U1639	G1568	G1500	C1432	A1359	C1290	A1226	G1160
G2146	C2078	G2014	C1942	G1859	G1714	C1640	A1569	U1503	U1433	A1360	C1291	G1227	G1161
G2147	U2079	A2015	U1943	C1860	G1717	A1641	A1570	C1504	U1434	G1361	C1292	G1228	G1162
G2148	G2080	U2016	G1944	G1861	G1718		A1571	C1505	G1435	A1434	G1229	G1230	G1163
G2149	C2081	U2017	U1945	A1802	G1719	C1644	A1572	C1506	G1436	C1363	C1230	G1231	G1164
U2150	U2082	G2018	U1946	G1865	G1720	G1645	G1573		C1437	G1364	G1231	G1232	U1165
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G2152	U2086	A2020	G1948	A1876	G1722	G1647	C1575	A1509A	A1439	A1366	U1300	G1233	U1167
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G2155	U2089	G2023	U1951		A1741	G1650	U1578	C1511	G1442		G1236	A1237	G1170
C2156	G2090	G2024	A1952	U1808	G1742	G1651	A1579	U1512		G1374	C1305	G1237	G1171
G2157	U2091	C2025	A1953	G1882	C1743			C1513	A1445	C1375	C1306	G1238	G1173
A2158	U2092	G2026	G1954	A1883	G1744	A1654	C1582	U1514	C1445A	C1376	A1307	G1239	A1174
G2159	G2093	G2027	U1955	A1885		A1655	A1583	G1515	C1446	G1377	A1308	U1240	U1175
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C2161	C2097	G2029	C1957	G1887	G1748	C1657	A1586	G1517	G1448	A1379	G1310	A1242	A1177
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C2164	G2100	G2032	A1960	G1890	C1751	C1660	C1589	G1524	C1451	G1382	C1314	G1245	C1181
		A2033	G1891	U1817	G1752	G1661	U1590	G1525	A1452	C1383	C1315	A1246	A1182
U2167	C2103	U2034	U1963	U1818	G1753	C1662	G1591	G1526	U1453	G1384	U1316	A1247	G1183
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A2171	C2107		A1901	G1823		G1666	A1596	G1529	A1460	G1388		G1252	G1187
		C2038	A1902	G1824	A1762	G1667	A1597	C1530	G1461	G1389	A1322	G1253	U1188
G2172		C2039	C1902	G1825	G1763	A1668	C1598	G1531	C1462	U1390	G1323	A1254	A1189
A2173	G2110	U2041	A1970	G1826	G1764	A1669	C1599		C1463	U1391	G1324	A1255	G1190
C2174	G2111		G1971		G1826			U1534					G1191
G2175	G2112	A2042	A1972	C1827	C1765	C1670	C1600						



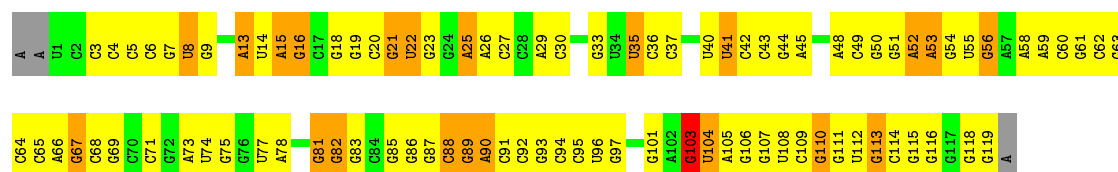


C2177	C2178	A2114	C2040	C1967	G1822	A1759	G1667	A1597	C1530	C1462	U1391	U1326	C1261	U1198
G2115	U2041	G2116	U2041	G1968	G1823	G1762	A1668	C1598	C1531	C1463	U1391	C1327	A1262	U1198
A2117	C2042	G2118	A2042	A1969	G1824	G1763	A1669	C1599	U1334	C1464	A1395	C1328	U1263	G1203
U2113	C2043	A2119	G1903	A1970	G1825	G1764	C1670	C1600	A1536	G1465	U1396	U1329	G1264	A1204
G2120	G2046	U2118	G1904	A1972	C1827	G1765	U1671	U1602	A1536	G1466	C1398	C1330	U1265	U1205
G2121	C2050	G2122	C1905	G1973	G1828	U1766	G1674	A1603	G1537	A1467	C1399	G1332	U1267	G1209
U2121	A2051	U2122	G1907	C1974	A1829	C1767	C1675	A1603	G1538	U1472	G1400	G1333	A1268	A1210
G2123	C2052	G2123	C1908	C1983	C1830	U1768	A1676	C1607	G1539	G1473	G1401	G1334	A1269	U1211
U2189	G2053	G1984	C1909	G1983	G1831	U1769	A1677	A1608	U1540	C1474	C1402	U1335	G1270	G1211
G2184	A2054	G1985	G1910	G1983	G1832	G1770	G1678	A1609	G1541	G1475	C1403	U1336	C1271	G1212
A2126	C2055	A1986	U1911	U1834	G1833	G1771	U1679	A1610	A1542	C1476	U1404	G1337	A1272	A1213
G2127	G2056	G1987	U1912	U1835	U1834	G1772	G1680	C1611	C1543	A1477	U1405	U1341	U1273	A1214
C2128	A2057	G1989	A1913	G1836	G1881	A1773	G1681	A1614	A1544	G1478	U1406	U1342	A1274	G1215
U2129	C2058	U1993	C1913	C1837	G1682	C1774	G1682	C1615	A1545	U1482	C1407	G1343	A1275	G1216
G2130	A2059	G1992	G1914	C1837	G1683	U1775	C1684	A1616	C1546	G1484	C1408	G1344	A1276	G1217
U2131	G2061	C1994	U1917	G1838	G1776	G1776	U1688	C1617	U1551	G1485	C1409	G1345	A1277	G1218
G2132	A2062	C1994	A1918	G1839	U1777	U1778	A1688	A1618	G1552	A1486	C1411	G1346	A1278	G1219
A2133	C2063	C1994	A1919	G1840	U1778	U1779	A1689	U1689	G1553	U1487	A1412	G1347	G1279	A1220
A2134	A2064	U1995	A1920	U1841	U1779	U1780	A1689	U1689	A1554	G1488	A1412	G1348	G1285	A1221
A2135	C2065	C1996	G1921	U1842	U1780	U1781	A1689	U1689	A1554	G1488	C1407	G1349	G1286	C1221A
C2136	C2066	G1997	G1921	C1843	C1781	U1781	U1692	G1624	G1555	U1489	U1415	A1349	A1287	C1222
C2137	G2067	G1998	G1922	C1844	C1782	U1782	U1693	C1625	G1556	U1490	G1416	A1350	A1287	G1223
U2138	G2068	C2000	C1925	G1845	A1783	C1694	C1694	U1628	C1557	G1491	G1417	G1351	U1288	G1224
C2139	G2069	A2001	U1926	G1846	A1784	U1697	U1697	U1629	A1558	G1492	U1420	U1352	C1289	G1225
C2140	G2070	G2004	U1926	A1847	A1785	A1698	A1698	G1630	G1559	G1493	G1421	A1353	C1290	A1226
G2141	U2071	U2071	G1929	G1848	A1786	A1698	A1698	U1630	G1560	A1494	G1421	A1354	C1291	G1227
C2142	U2072	G2004	G1930	G1849	A1787	A1699	A1699	G1630	G1561	A1495	U1427	A1355	U1292	G1228
C2143	U2073	C2008	U1931	G1850	C1788	A1700	A1700	G1632	U1562	A1496	A1427	U1356	C1293	G1229
C2146	U2074	C2008	U1932	G1851	A1789	C1790	U1708	G1633	G1564	U1497	G1428	G1358	U1294	C1230
C2147	U2075	C2009	G1933	C1852	C1790	A1791	U1709	G1634	C1565	C1498	G1429	G1359	C1297	G1231
G2148	C2076	G2010	C1934	A1853	C1791	U1791	U1710	G1635	G1566	C1499	C1430	A1359	C1298	G1232
U2078	U2077	U2011	G1935	A1854	U1792	U1793	C1711	C1636	G1567	G1500	C1431	A1360	C1299	C1233
U2079	G2080	A2013	G1936	G1855	U1794	U1795	C1712	A1637	C1568	C1501	C1432	A1361	U1299	U1234
C2081	C2081	A2014	A1937	G1856	U1796	U1796	U1713	U1638	G1569	C1502	C1433	C1362	U1300	G1235
A2082	C2082	A2015	A1938	G1857	U1796	U1796	U1714	U1639	A1570	C1503	A1434	G1363	A1301	G1236
U2086	U2086	U2016	A1938	G1858	U1796	U1796	G1714	C1640	A1571	C1504	G1435	G1364	A1302	A1237
G2087	G2087	U2017	C1941	A1859	C1793	C1800	G1717	A1641	A1571	C1505	G1436	A1365	G1303	G1238
G2088	G2088	C2018	C1942	G1862	C1801	C1801	G1718	C1644	A1572	C1506	C1437	A1366	G1304	G1239
U2089	U2089	A2019	U1943	G1863	G1802	G1802	G1719	G1645	G1573	U1509	U1438	A1367	C1305	U1240
G2090	G2090	C2021	U1944	U1864	A1803	A1803	U1720	G1646	C1574	C1509A	A1439	G1368	C1306	A1241
U2091	U2091	U2022	U1945	G1865	C1804	C1804	G1721	C1647	G1575	A1509A	G1440	G1369	A1307	A1242
C2097	U2097	G2023	U1946	C1866	U1805	U1805	A1722	G1648	C1577	A1509B	G1441	U1374	A1308	G1243
U2097	C2097	C2023	C1947	A1876	C1806	C1806	U1739	C1648	C1577	C1510	G1442	U1375	G1309	G1244
U2098	U2098	C2026	G1948	A1877	G1807	G1807	G1740	G1649	U1578	C1511	U1445	C1376	G1310	G1245
G2100	G2100	G2027	G1950	G1878	U1808	U1808	G1742	G1650	A1579	C1512	A1445	C1377	U1312	A1246
C2103	C2103	U2028	U1951	C1882	A1810	A1810	C1743	A1654	C1582	C1513	C1445A	G1377	U1312	A1247
G2104	G2104	A2030	U1952	G1883	A1811	A1811	G1744	A1655	A1583	U1514	C1446	A1378	U1313	G1248
C2105	C2105	C2032	U1955	A1884	G1812	G1812	G1747A	C1656	C1584	U1515	G1447	A1379	C1314	U1249
G2106	C2106	A2033	U1956	A1885	A1813	A1813	U1748	C1657	A1586	G1516	G1448	G1380	C1315	G1250
C2107	C2107	U2034	U1957	C1886	G1814	G1814	G1749	C1658	A1587	C1517	U1450A	G1381	U1316	C1251
A2171	A2171	C2035	C1957	G1888	A1815	A1815	U1750	U1659	C1588	U1523	C1451	G1382	A1317	G1252
U2172	U2172	C2035	A1960	G1889	G1816	G1816	C1751	G1661	C1589	G1524	A1452	A1383	C1318	A1253
C2036	C2036	C2036	U1963	A1890	G1817	G1817	C1752	C1662	U1590	G1525	U1453	C1384	G1319	A1254
G2110	G2110	G2037	U1964	G1891	U1818	U1818	G1753	C1663	G1591	G1526	G1455	C1385	G1385	U1255
C2111	C2111	U2038	G1964	G1891	U1819	U1819	G1755	C1664	G1594	G1527	G1459	C1387	A1322	G1257
G2112	G2112	C2038	U1964	G1891	U1820	U1820	A1755	A1665	G1595	A1528	G1460	G1388	U1323	G1258
U2113	U2113	C2039	U1964	G1892	A1821	A1821	U1755	A1666	A1596	A1528A	G1461	U1390	G1324	G1260



• Molecule 36: 5S RIBOSOMAL RNA

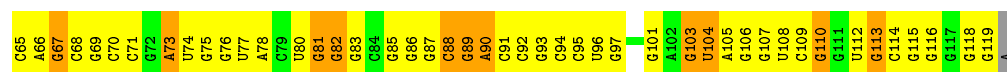
Chain BB: 22% 57% 17% ..



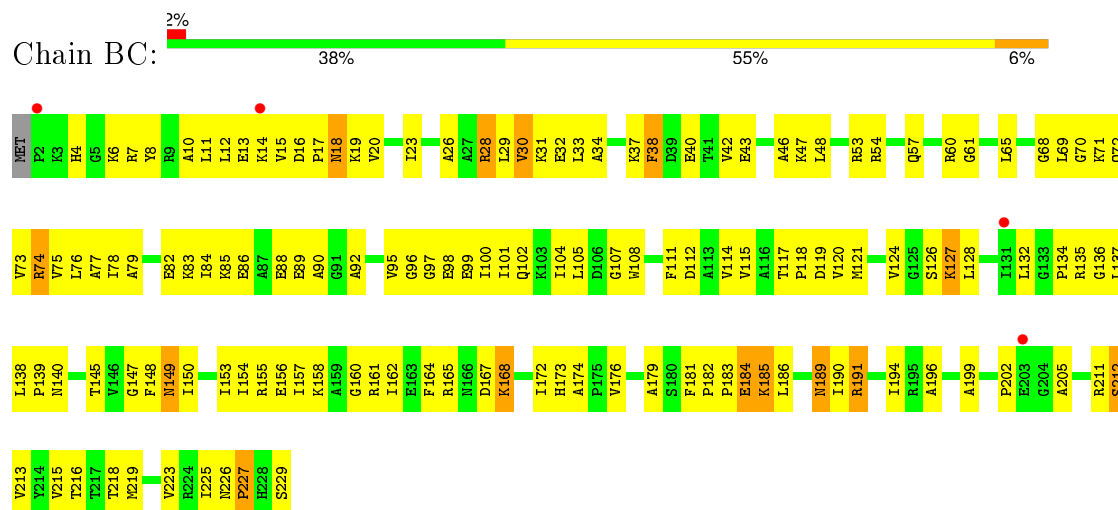
• Molecule 36: 5S RIBOSOMAL RNA

Chain DB: 20% 57% 20% .

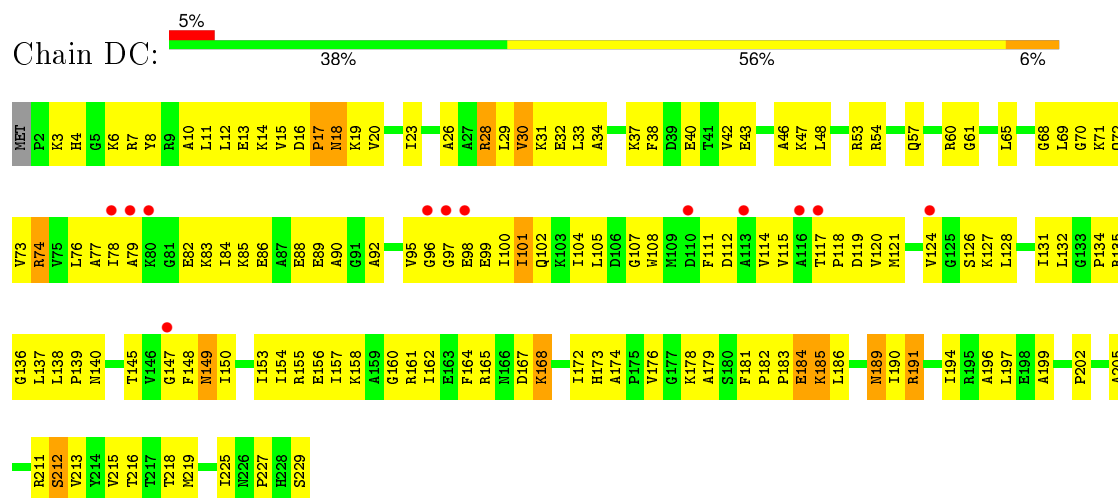




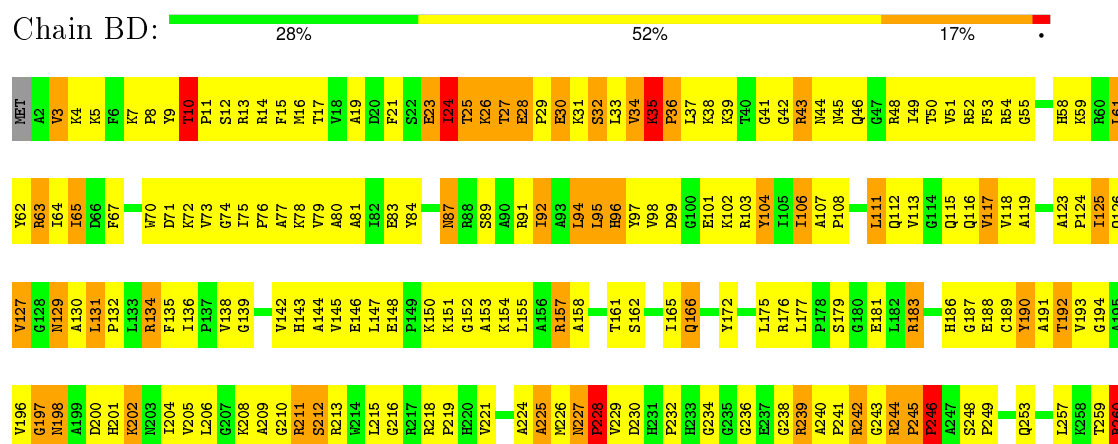
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

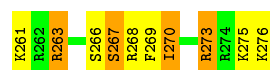


• Molecule 37: 50S RIBOSOMAL PROTEIN L1



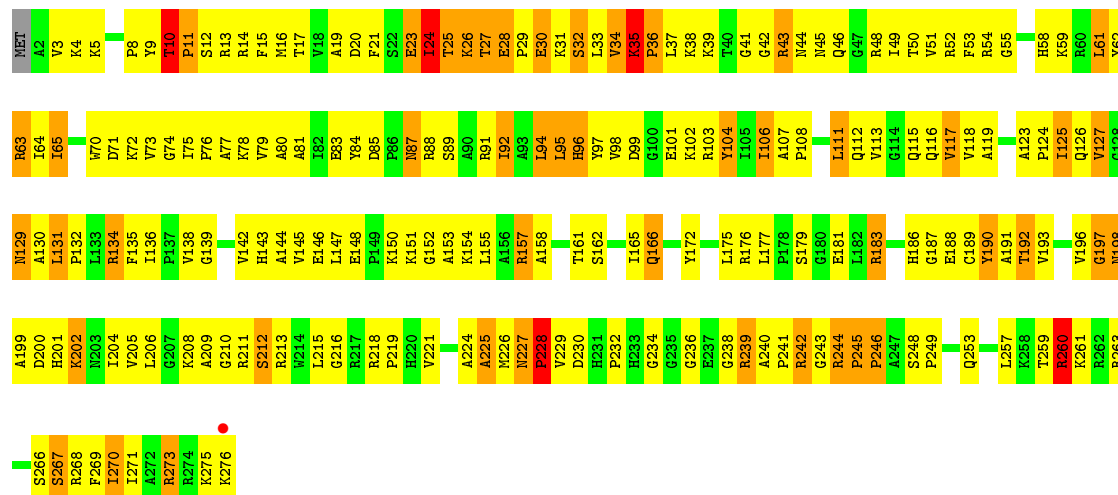
• Molecule 38: 50S RIBOSOMAL PROTEIN L2





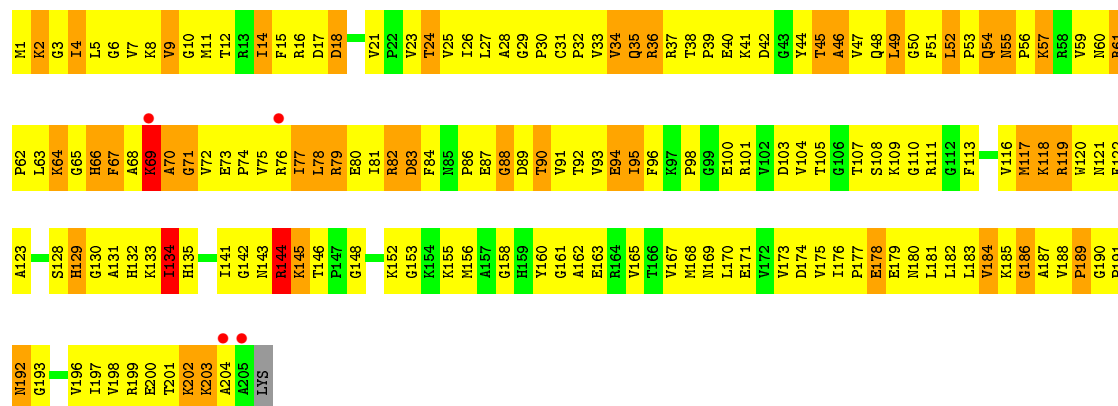
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain DD: 27% 54% 17%



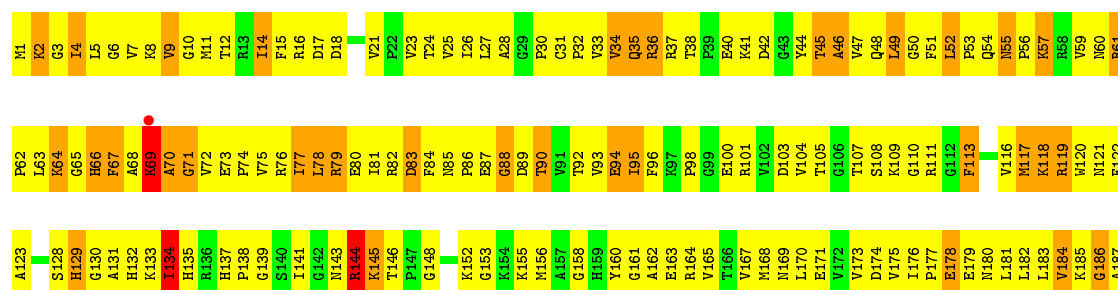
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

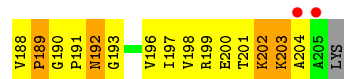
Chain BE: 2% 17% 60% 21%



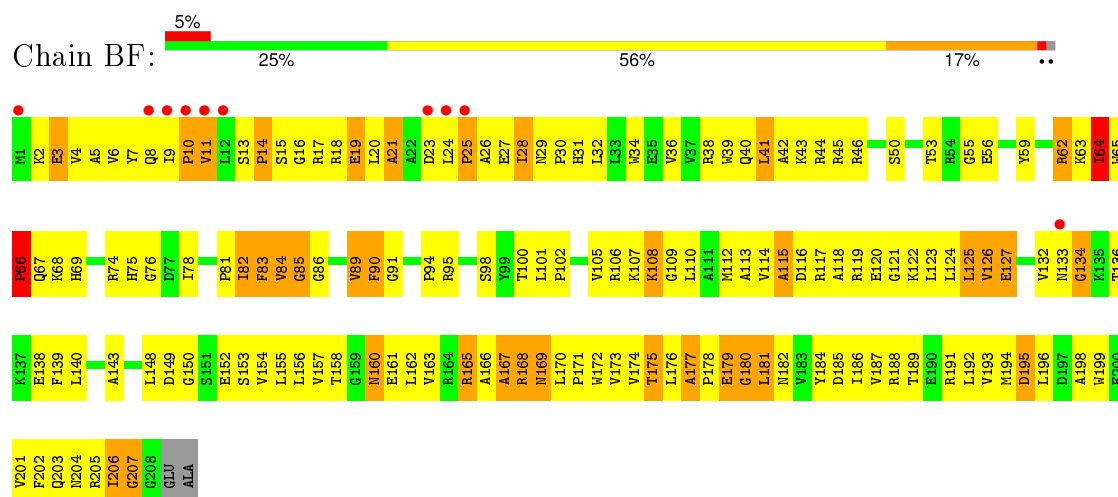
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain DE: 17% 62% 19%

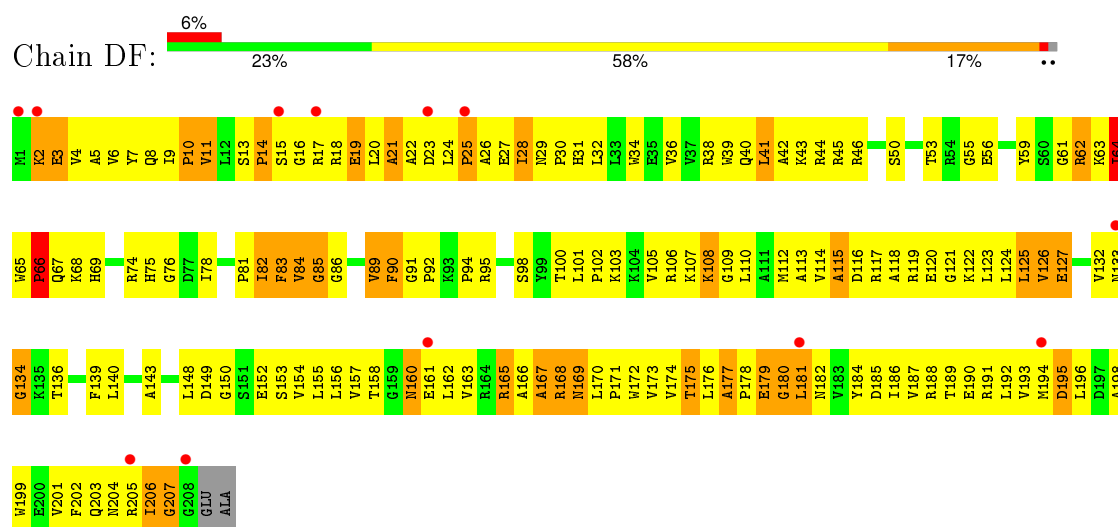




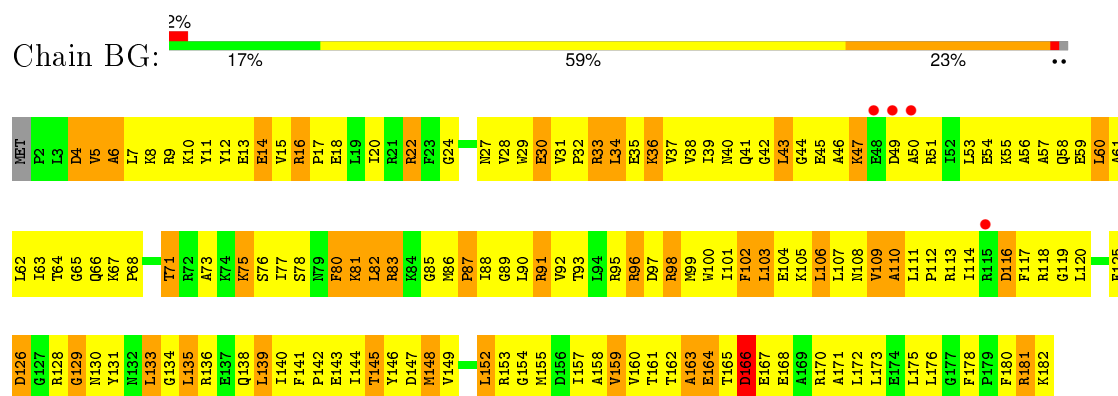
• Molecule 40: 50S RIBOSOMAL PROTEIN L4



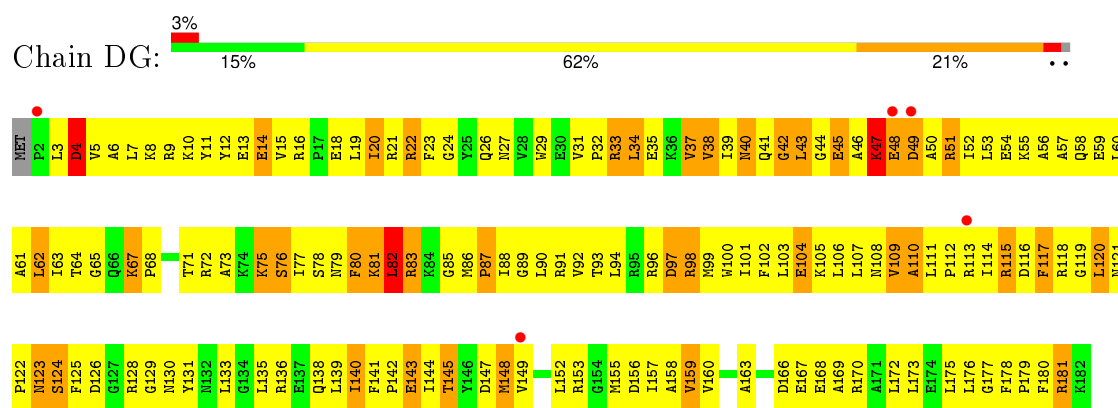
• Molecule 40: 50S RIBOSOMAL PROTEIN L4



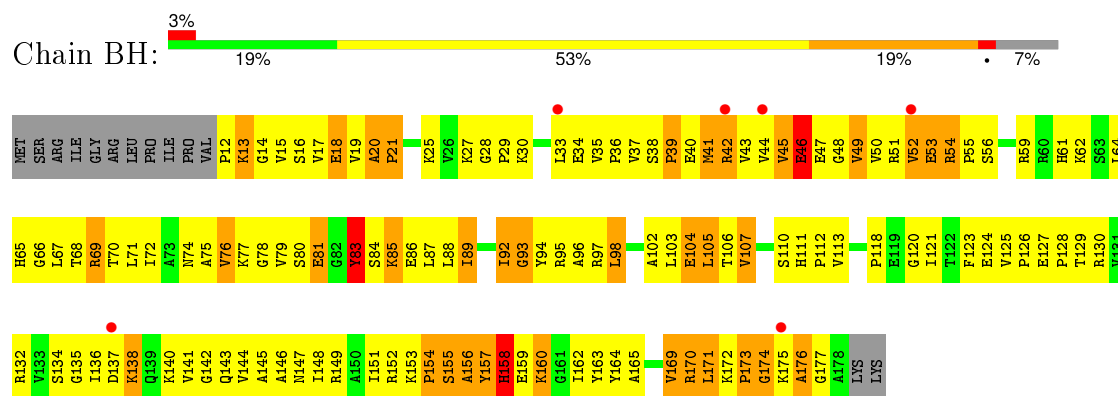
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



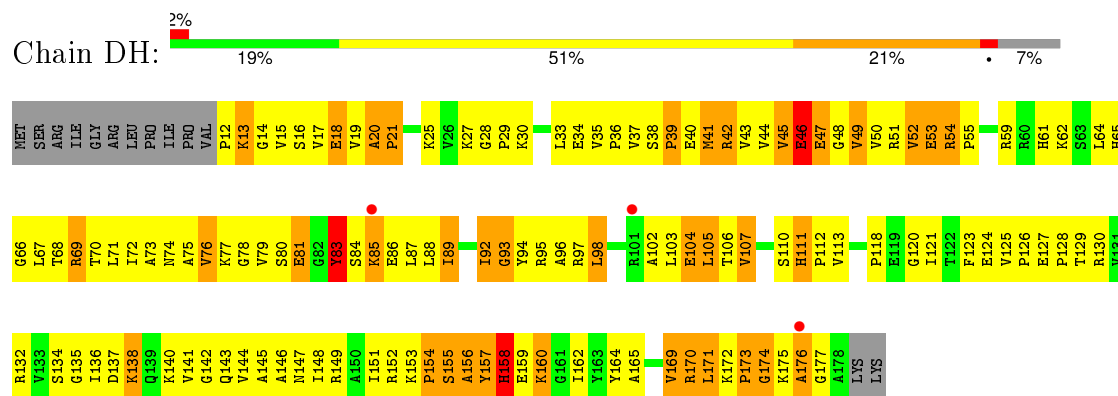
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



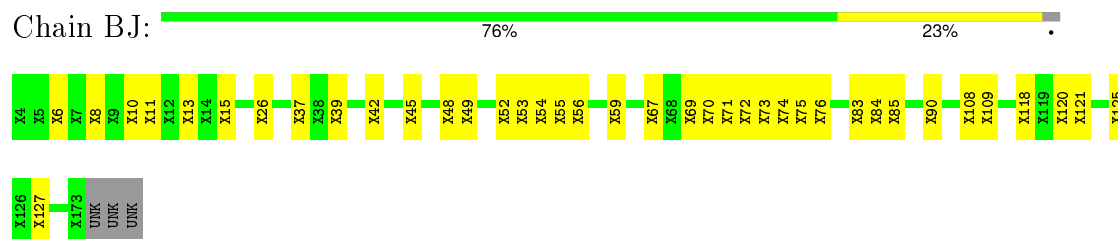
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



• Molecule 42: 50S RIBOSOMAL PROTEIN L6



• Molecule 43: 50S RIBOSOMAL PROTEIN L10



[illegible]

H130	Q131	A132	Q133	R134	P135	E136	K137	L138	E139	VAL
------	------	------	------	------	------	------	------	------	------	-----

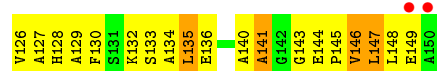
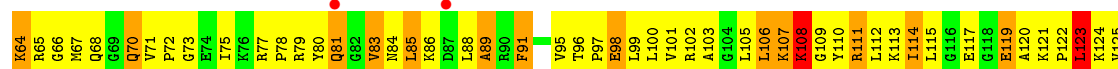
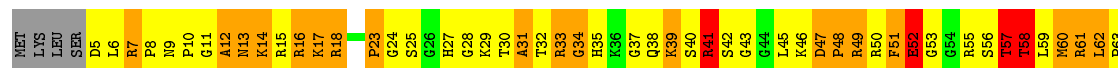
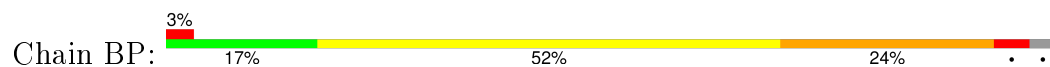
P129	H130	Q131	A132	Q133	R134	P135	E136	K137	L138	E139	VAL
------	------	------	------	------	------	------	------	------	------	------	-----

I69	A76	D80	N81	A83	A84	V85	I86	N88	N89	Q90	L91	E92	R97	V98	F99	G100	A103	R104	E105	L106	R107	E108	K109	G110	F111	M112	K113	I114	V115	S116	L117	A118	P119	E120	V121	I122
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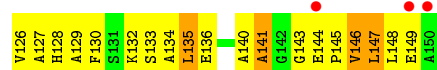
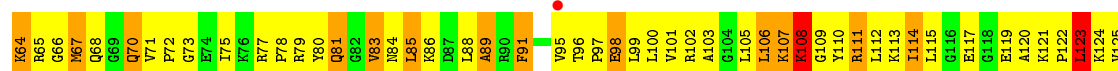
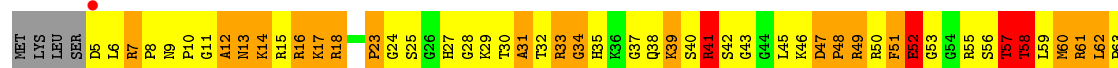
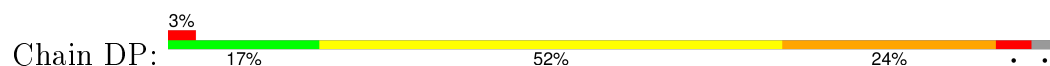
M1	I2	Q3	P4	Q5	T6	E9	V10	M13	T14	G15	A16	R17	K18	I19	M20	C21	I22	R23	K24	V24	L25	K26	N29	A30	Y31	K32	A33	T34	V35	G36	D37	V38	I39	V40	A41	V43	K44	E45	A46	I47	P48	R49	V52	K53	E54	G55	D56	A60	V61	V62	V63	R64	T67
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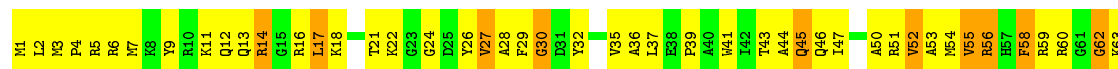
• Molecule 48: 50S RIBOSOMAL PROTEIN L15



• Molecule 48: 50S RIBOSOMAL PROTEIN L15

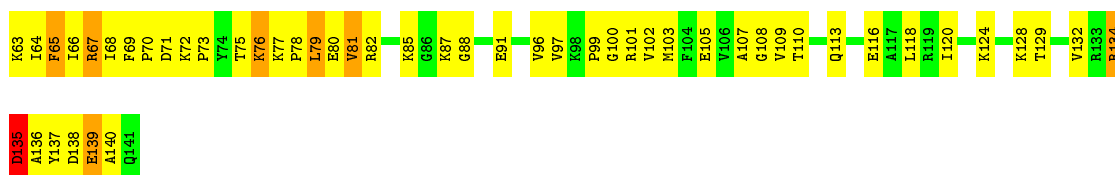


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

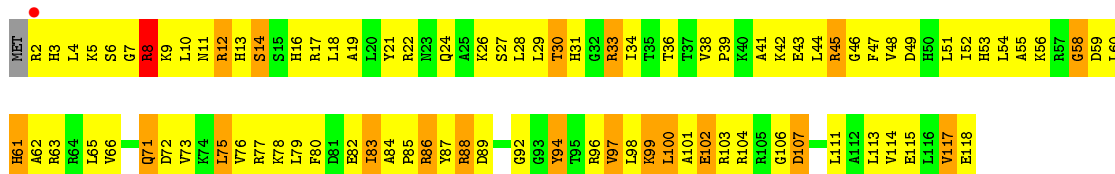


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

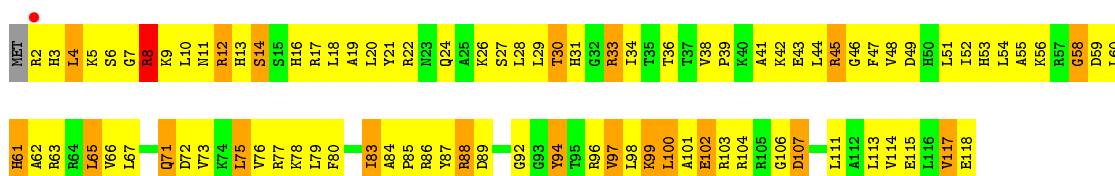




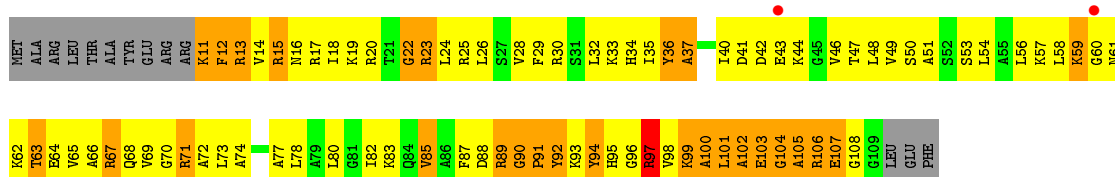
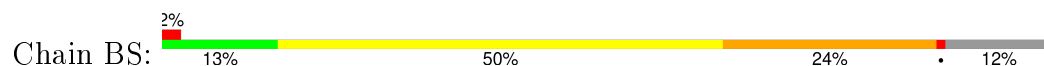
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



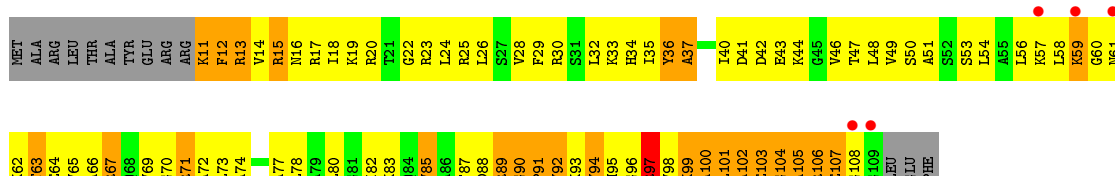
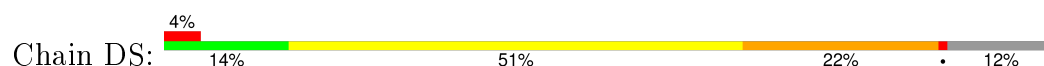
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



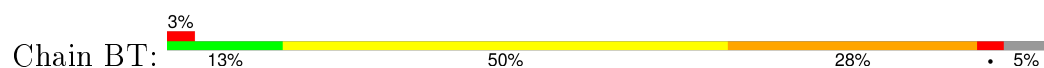
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

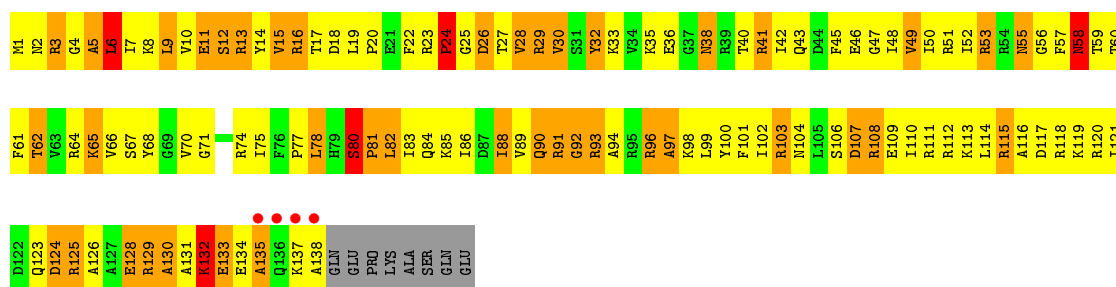


• Molecule 51: 50S RIBOSOMAL PROTEIN L18

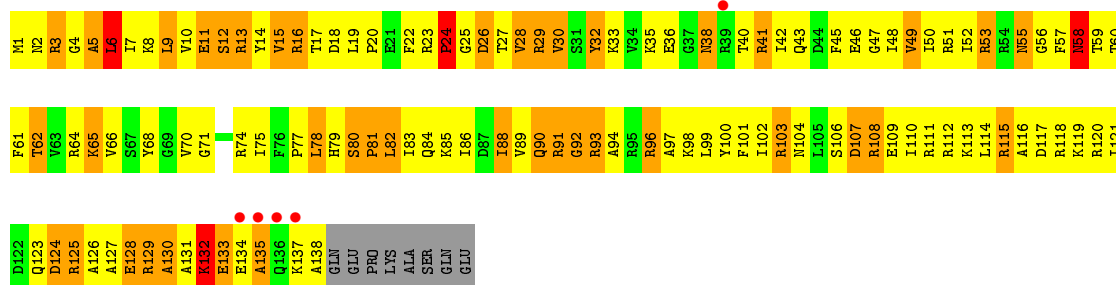
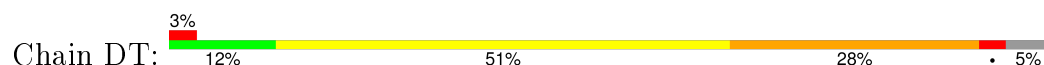


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

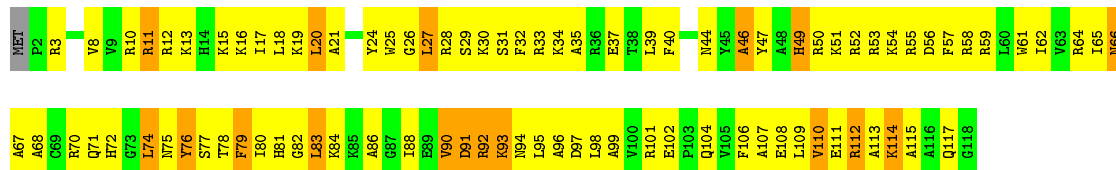




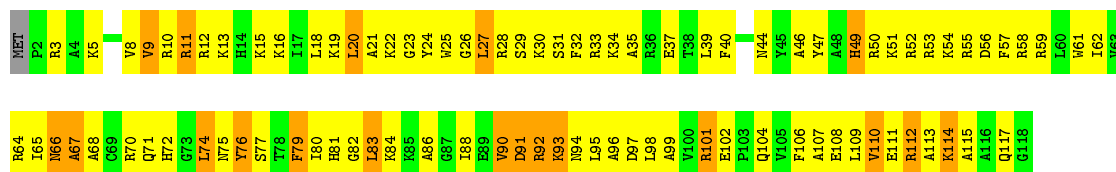
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



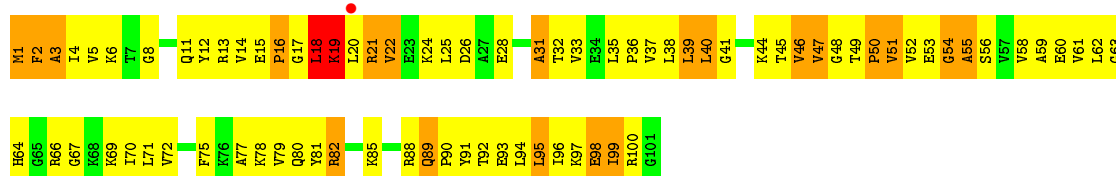
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



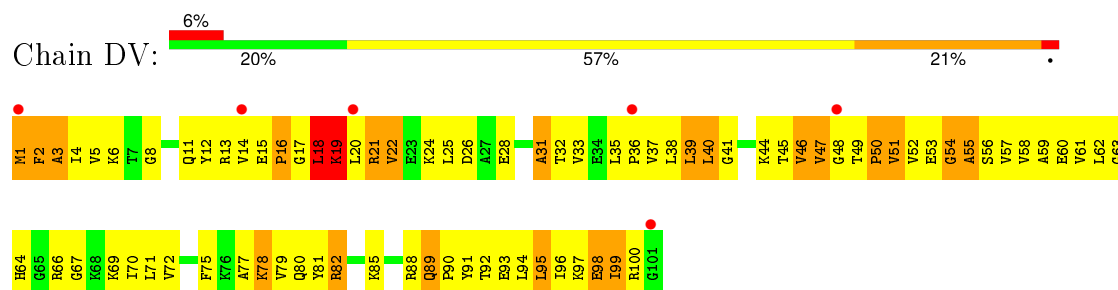
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



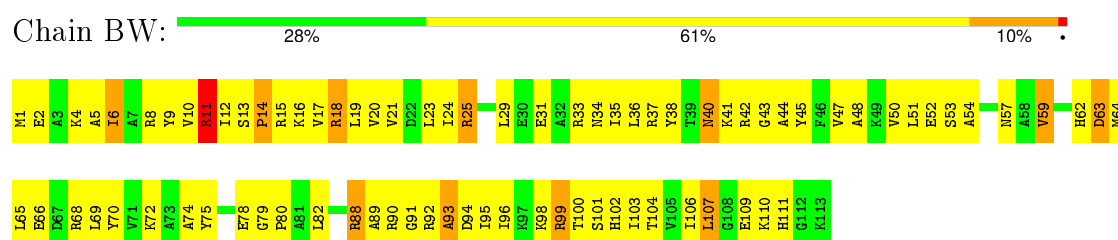
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



- Molecule 54: 50S RIBOSOMAL PROTEIN L21



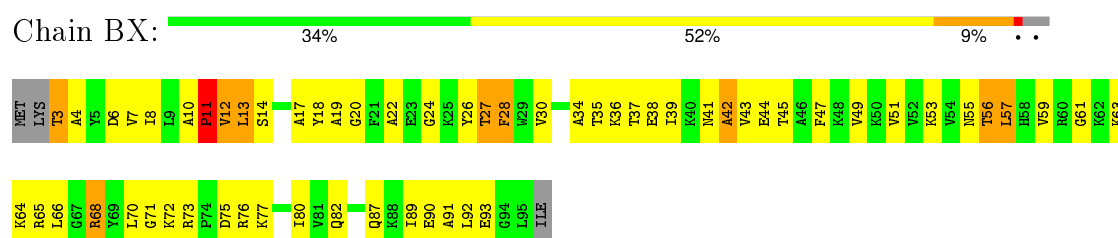
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



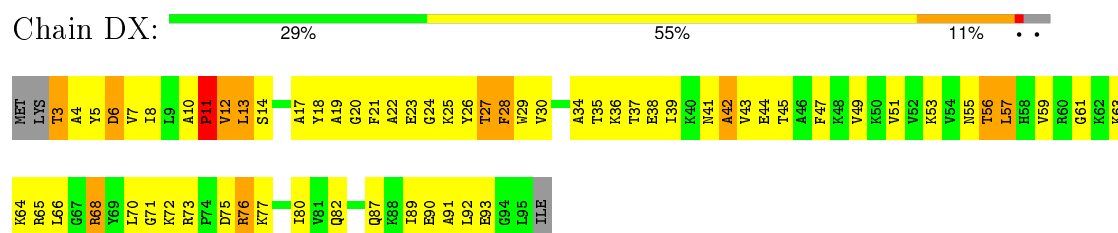
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



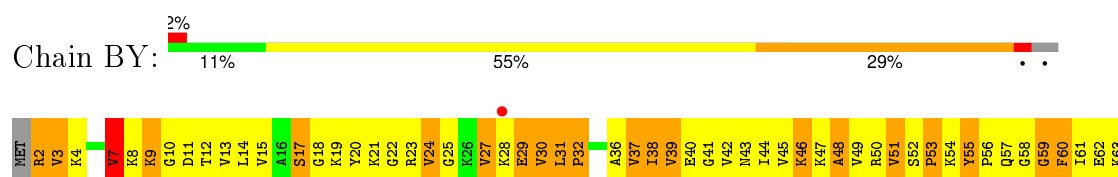
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



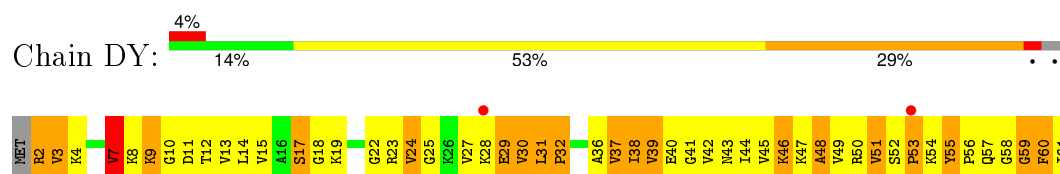
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



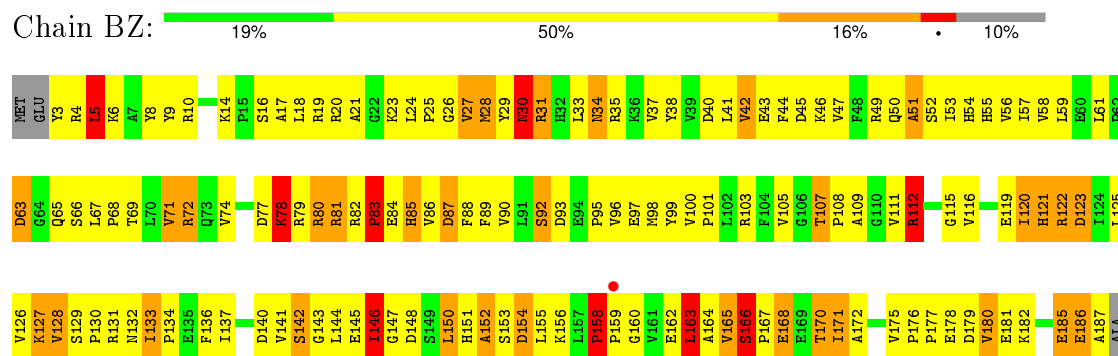
- Molecule 57: 50S RIBOSOMAL PROTEIN L24



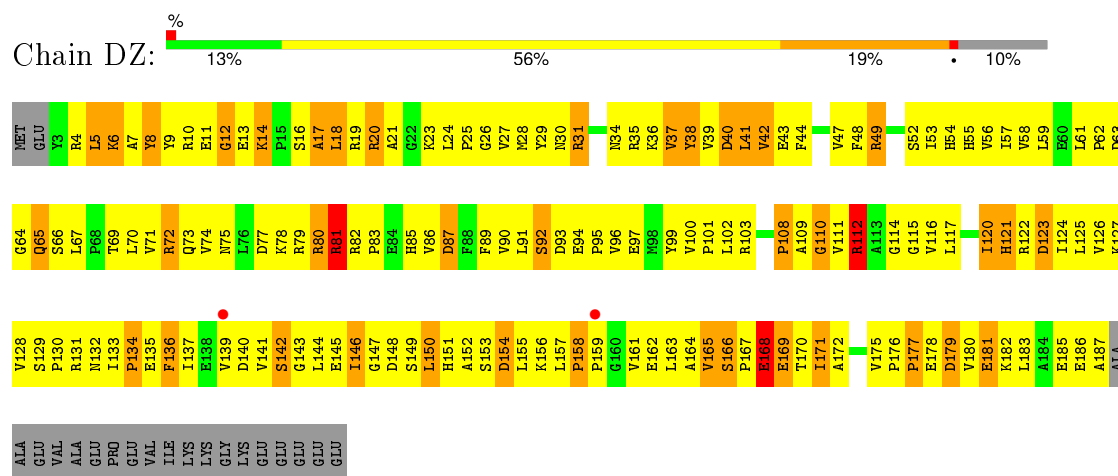
• Molecule 57: 50S RIBOSOMAL PROTEIN L24



• Molecule 58: 50S RIBOSOMAL PROTEIN L25



• Molecule 58: 50S RIBOSOMAL PROTEIN L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	78.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 34.7	EDS
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 810659 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	311552	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1237	0
1	CA	32329	0	16318	1268	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	83	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	2706	0
35	DA	62474	0	31497	2749	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	Dl	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	22501	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 22501 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	10
3	CC	205/239 (86%)	132 (64%)	52 (25%)	21 (10%)	1	11
4	AD	206/209 (99%)	134 (65%)	50 (24%)	22 (11%)	0	10
4	CD	206/209 (99%)	134 (65%)	51 (25%)	21 (10%)	1	11
5	AE	149/162 (92%)	119 (80%)	21 (14%)	9 (6%)	2	24
5	CE	149/162 (92%)	117 (78%)	24 (16%)	8 (5%)	2	27
6	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1	19
6	CF	99/101 (98%)	74 (75%)	18 (18%)	7 (7%)	1	19
7	AG	153/156 (98%)	109 (71%)	34 (22%)	10 (6%)	1	22
7	CG	153/156 (98%)	110 (72%)	32 (21%)	11 (7%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
8	AH	136/138 (99%)	103 (76%)	30 (22%)	3 (2%)	8	51	
8	CH	136/138 (99%)	105 (77%)	27 (20%)	4 (3%)	6	44	
9	AI	121/128 (94%)	81 (67%)	26 (22%)	14 (12%)	0	9	
9	CI	121/128 (94%)	82 (68%)	27 (22%)	12 (10%)	1	12	
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	28	
11	CK	117/129 (91%)	91 (78%)	20 (17%)	6 (5%)	2	28	
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	20	
14	CN	58/61 (95%)	46 (79%)	7 (12%)	5 (9%)	1	14	
15	AO	86/89 (97%)	55 (64%)	23 (27%)	8 (9%)	1	13	
15	CO	86/89 (97%)	53 (62%)	24 (28%)	9 (10%)	1	10	
16	AP	82/88 (93%)	60 (73%)	15 (18%)	7 (8%)	1	14	
16	CP	82/88 (93%)	60 (73%)	15 (18%)	7 (8%)	1	14	
17	AQ	98/105 (93%)	78 (80%)	15 (15%)	5 (5%)	2	28	
17	CQ	98/105 (93%)	78 (80%)	16 (16%)	4 (4%)	3	34	
18	AR	68/88 (77%)	52 (76%)	11 (16%)	5 (7%)	1	18	
18	CR	68/88 (77%)	51 (75%)	12 (18%)	5 (7%)	1	18	
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	7	
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	6	
24	CY	663/691 (96%)	449 (68%)	134 (20%)	80 (12%)	0	8	
25	B0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	3	29	

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	D0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	3	29
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	7
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	7
28	B3	58/60 (97%)	41 (71%)	12 (21%)	5 (9%)	1	14
28	D3	58/60 (97%)	41 (71%)	12 (21%)	5 (9%)	1	14
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%)	9	52
32	D7	47/49 (96%)	35 (74%)	11 (23%)	1 (2%)	9	52
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	27
37	DC	226/229 (99%)	163 (72%)	50 (22%)	13 (6%)	2	25
38	BD	273/276 (99%)	189 (69%)	50 (18%)	34 (12%)	0	8
38	DD	273/276 (99%)	188 (69%)	50 (18%)	35 (13%)	0	7
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	5
41	BG	177/182 (97%)	110 (62%)	43 (24%)	24 (14%)	0	6
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	16
44	DK	138/147 (94%)	92 (67%)	35 (25%)	11 (8%)	1	16
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	15
47	DO	120/122 (98%)	93 (78%)	17 (14%)	10 (8%)	1	15
48	BP	144/150 (96%)	72 (50%)	45 (31%)	27 (19%)	0	3
48	DP	144/150 (96%)	72 (50%)	44 (31%)	28 (19%)	0	2
49	BQ	139/141 (99%)	106 (76%)	26 (19%)	7 (5%)	3	29
49	DQ	139/141 (99%)	106 (76%)	26 (19%)	7 (5%)	3	29
50	BR	115/118 (98%)	81 (70%)	20 (17%)	14 (12%)	0	8
50	DR	115/118 (98%)	81 (70%)	20 (17%)	14 (12%)	0	8
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%)	1	11
53	DU	115/118 (98%)	67 (58%)	35 (30%)	13 (11%)	0	9
54	BV	99/101 (98%)	69 (70%)	12 (12%)	18 (18%)	0	3
54	DV	99/101 (98%)	69 (70%)	12 (12%)	18 (18%)	0	3
55	BW	111/113 (98%)	80 (72%)	21 (19%)	10 (9%)	1	13
55	DW	111/113 (98%)	81 (73%)	21 (19%)	9 (8%)	1	15
56	BX	91/96 (95%)	56 (62%)	26 (29%)	9 (10%)	1	12
56	DX	91/96 (95%)	57 (63%)	25 (28%)	9 (10%)	1	12
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	7

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	36
2	CB	202/220 (92%)	179 (89%)	23 (11%)	7	36
3	AC	160/188 (85%)	142 (89%)	18 (11%)	7	37
3	CC	160/188 (85%)	142 (89%)	18 (11%)	7	37
4	AD	180/181 (99%)	160 (89%)	20 (11%)	8	38
4	CD	180/181 (99%)	160 (89%)	20 (11%)	8	38
5	AE	115/123 (94%)	100 (87%)	15 (13%)	5	30
5	CE	115/123 (94%)	100 (87%)	15 (13%)	5	30
6	AF	90/90 (100%)	83 (92%)	7 (8%)	16	55
6	CF	90/90 (100%)	83 (92%)	7 (8%)	16	55
7	AG	126/127 (99%)	117 (93%)	9 (7%)	18	59
7	CG	126/127 (99%)	117 (93%)	9 (7%)	18	59
8	AH	119/119 (100%)	110 (92%)	9 (8%)	16	56
8	CH	119/119 (100%)	112 (94%)	7 (6%)	24	66
9	AI	98/99 (99%)	90 (92%)	8 (8%)	14	53
9	CI	98/99 (99%)	90 (92%)	8 (8%)	14	53
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	6	32
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	6	32
11	AK	90/99 (91%)	84 (93%)	6 (7%)	20	62
11	CK	90/99 (91%)	84 (93%)	6 (7%)	20	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	104/109 (95%)	94 (90%)	10 (10%)	10	45
12	CL	104/109 (95%)	93 (89%)	11 (11%)	8	40
13	AM	99/101 (98%)	91 (92%)	8 (8%)	15	54
13	CM	99/101 (98%)	91 (92%)	8 (8%)	15	54
14	AN	49/50 (98%)	43 (88%)	6 (12%)	6	32
14	CN	49/50 (98%)	43 (88%)	6 (12%)	6	32
15	AO	79/80 (99%)	71 (90%)	8 (10%)	9	43
15	CO	79/80 (99%)	71 (90%)	8 (10%)	9	43
16	AP	72/74 (97%)	67 (93%)	5 (7%)	19	60
16	CP	72/74 (97%)	67 (93%)	5 (7%)	19	60
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	17	57
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	17	57
18	AR	61/77 (79%)	59 (97%)	2 (3%)	45	80
18	CR	61/77 (79%)	59 (97%)	2 (3%)	45	80
19	AS	69/80 (86%)	59 (86%)	10 (14%)	4	26
19	CS	69/80 (86%)	59 (86%)	10 (14%)	4	26
20	AT	76/82 (93%)	69 (91%)	7 (9%)	11	48
20	CT	76/82 (93%)	69 (91%)	7 (9%)	11	48
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	30
24	CY	563/582 (97%)	495 (88%)	68 (12%)	6	33
25	B0	66/67 (98%)	57 (86%)	9 (14%)	5	29
25	D0	66/67 (98%)	57 (86%)	9 (14%)	5	29
26	B1	78/83 (94%)	65 (83%)	13 (17%)	3	19
26	D1	78/83 (94%)	70 (90%)	8 (10%)	9	42
27	B2	66/67 (98%)	59 (89%)	7 (11%)	8	40
27	D2	66/67 (98%)	58 (88%)	8 (12%)	6	33
28	B3	51/52 (98%)	47 (92%)	4 (8%)	16	55
28	D3	51/52 (98%)	47 (92%)	4 (8%)	16	55
29	B4	51/63 (81%)	38 (74%)	13 (26%)	1	6

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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	34
30	D5	51/52 (98%)	45 (88%)	6 (12%)	6	34
31	B6	49/52 (94%)	39 (80%)	10 (20%)	1	11
31	D6	49/52 (94%)	38 (78%)	11 (22%)	1	8
32	B7	41/42 (98%)	36 (88%)	5 (12%)	6	32
32	D7	41/42 (98%)	36 (88%)	5 (12%)	6	32
33	B8	53/55 (96%)	44 (83%)	9 (17%)	2	18
33	D8	53/55 (96%)	43 (81%)	10 (19%)	2	13
34	B9	34/34 (100%)	30 (88%)	4 (12%)	6	34
34	D9	34/34 (100%)	29 (85%)	5 (15%)	4	25
37	BC	180/181 (99%)	170 (94%)	10 (6%)	26	68
37	DC	180/181 (99%)	169 (94%)	11 (6%)	23	65
38	BD	217/218 (100%)	177 (82%)	40 (18%)	2	14
38	DD	217/218 (100%)	178 (82%)	39 (18%)	2	15
39	BE	165/166 (99%)	139 (84%)	26 (16%)	3	22
39	DE	165/166 (99%)	140 (85%)	25 (15%)	3	24
40	BF	165/166 (99%)	153 (93%)	12 (7%)	17	58
40	DF	165/166 (99%)	153 (93%)	12 (7%)	17	58
41	BG	155/156 (99%)	131 (84%)	24 (16%)	3	23
41	DG	155/156 (99%)	126 (81%)	29 (19%)	2	13
42	BH	136/148 (92%)	126 (93%)	10 (7%)	17	57
42	DH	136/148 (92%)	126 (93%)	10 (7%)	17	57
44	BK	104/111 (94%)	89 (86%)	15 (14%)	4	26
44	DK	104/111 (94%)	90 (86%)	14 (14%)	5	29
46	BN	117/119 (98%)	103 (88%)	14 (12%)	6	33
46	DN	117/119 (98%)	102 (87%)	15 (13%)	5	31
47	BO	100/100 (100%)	92 (92%)	8 (8%)	15	54
47	DO	100/100 (100%)	92 (92%)	8 (8%)	15	54
48	BP	112/116 (97%)	91 (81%)	21 (19%)	2	13
48	DP	112/116 (97%)	91 (81%)	21 (19%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BQ	111/111 (100%)	95 (86%)	16 (14%)	4	26
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	5	31
50	BR	100/101 (99%)	89 (89%)	11 (11%)	8	39
50	DR	100/101 (99%)	88 (88%)	12 (12%)	6	33
51	BS	77/88 (88%)	68 (88%)	9 (12%)	7	35
51	DS	77/88 (88%)	68 (88%)	9 (12%)	7	35
52	BT	120/127 (94%)	97 (81%)	23 (19%)	2	12
52	DT	120/127 (94%)	97 (81%)	23 (19%)	2	12
53	BU	92/94 (98%)	83 (90%)	9 (10%)	10	44
53	DU	92/94 (98%)	83 (90%)	9 (10%)	10	44
54	BV	82/82 (100%)	71 (87%)	11 (13%)	5	29
54	DV	82/82 (100%)	71 (87%)	11 (13%)	5	29
55	BW	91/92 (99%)	84 (92%)	7 (8%)	16	56
55	DW	91/92 (99%)	84 (92%)	7 (8%)	16	56
56	BX	74/78 (95%)	64 (86%)	10 (14%)	5	29
56	DX	74/78 (95%)	64 (86%)	10 (14%)	5	29
57	BY	87/91 (96%)	75 (86%)	12 (14%)	4	28
57	DY	87/91 (96%)	75 (86%)	12 (14%)	4	28
58	BZ	162/179 (90%)	134 (83%)	28 (17%)	2	17
58	DZ	162/179 (90%)	144 (89%)	18 (11%)	8	38
All	All	11080/11566 (96%)	9776 (88%)	1304 (12%)	6	34

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	11,21,23	1.33	2 (18%)	15,30,35	3.54	2 (13%)
22	5MU	AW	55	22	11,21,23	1.31	2 (18%)	15,30,35	3.59	2 (13%)
22	5MU	CV	54	22	11,21,23	1.26	1 (9%)	15,30,35	3.57	2 (13%)
22	5MU	CW	55	22	11,21,23	1.31	1 (9%)	15,30,35	3.56	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 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AW	55	5MU	C6-N1	2.00	1.38	1.35
22	AV	54	5MU	C6-N1	2.02	1.38	1.35
22	CV	54	5MU	C4-N3	3.01	1.38	1.33
22	AV	54	5MU	C4-N3	3.09	1.38	1.33
22	CW	55	5MU	C4-N3	3.13	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	-3.09	115.19	123.12
22	CV	54	5MU	C5-C4-N3	-3.09	115.20	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CW	55	5MU	C5-C4-N3	-3.07	115.23	123.12
22	AV	54	5MU	C5-C4-N3	-2.96	115.52	123.12
22	AV	54	5MU	C4-N3-C2	13.28	127.29	114.14

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	1.70	6 (16%)	45,64,64	1.66	7 (15%)
62	GDP	AY	703	60	23,30,30	1.36	3 (13%)	30,47,47	1.81	7 (23%)
61	FUA	CY	702	-	37,40,40	1.72	6 (16%)	45,64,64	1.53	7 (15%)
62	GDP	CY	703	60	23,30,30	1.41	3 (13%)	30,47,47	2.13	10 (33%)

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	-6.14	1.39	1.51
61	AY	702	FUA	C23-C22	-5.97	1.39	1.51
61	AY	702	FUA	C23-C24	-4.18	1.39	1.53
61	CY	702	FUA	C23-C24	-4.17	1.39	1.53
61	CY	702	FUA	C24-C25	-3.98	1.39	1.50

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	CY	703	GDP	N3-C2-N1	-4.78	120.16	127.44
62	AY	703	GDP	N3-C2-N1	-4.77	120.17	127.44
61	AY	702	FUA	C13-C12-C11	-4.51	105.84	111.95
62	CY	703	GDP	PA-O3A-PB	-4.34	118.11	132.67
62	CY	703	GDP	C2'-C1'-N9	-4.25	107.79	114.29

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	-0.22	22 (1%) 76 64	23, 62, 148, 220	0
1	CA	1504/1522 (98%)	-0.46	15 (0%) 84 73	26, 65, 148, 220	0
2	AB	235/256 (91%)	-0.28	4 (1%) 73 59	40, 81, 147, 159	0
2	CB	235/256 (91%)	-0.30	1 (0%) 93 88	43, 82, 147, 158	0
3	AC	207/239 (86%)	-0.38	0 100 100	31, 72, 113, 118	0
3	CC	207/239 (86%)	-0.35	0 100 100	33, 75, 115, 121	0
4	AD	208/209 (99%)	-0.36	0 100 100	47, 79, 115, 124	0
4	CD	208/209 (99%)	-0.40	0 100 100	48, 80, 116, 125	0
5	AE	151/162 (93%)	-0.46	1 (0%) 89 81	25, 50, 90, 112	0
5	CE	151/162 (93%)	-0.43	1 (0%) 89 81	27, 52, 91, 112	0
6	AF	101/101 (100%)	-0.41	0 100 100	55, 85, 110, 118	0
6	CF	101/101 (100%)	-0.26	0 100 100	60, 87, 111, 118	0
7	AG	155/156 (99%)	-0.35	1 (0%) 90 83	51, 79, 109, 136	0
7	CG	155/156 (99%)	-0.36	2 (1%) 79 66	55, 81, 111, 136	0
8	AH	138/138 (100%)	-0.38	0 100 100	32, 54, 75, 82	0
8	CH	138/138 (100%)	-0.46	0 100 100	35, 56, 76, 83	0
9	AI	127/128 (99%)	-0.20	1 (0%) 87 78	50, 83, 114, 120	0
9	CI	127/128 (99%)	-0.34	1 (0%) 87 78	53, 86, 114, 120	0
10	AJ	99/105 (94%)	0.10	6 (6%) 25 16	47, 100, 155, 159	0
10	CJ	99/105 (94%)	0.20	3 (3%) 54 38	50, 102, 156, 159	0
11	AK	119/129 (92%)	-0.31	2 (1%) 73 59	42, 59, 100, 123	0
11	CK	119/129 (92%)	-0.25	1 (0%) 87 78	44, 60, 102, 124	0
12	AL	125/132 (94%)	-0.46	0 100 100	38, 57, 87, 127	0
12	CL	125/132 (94%)	-0.40	2 (1%) 74 61	39, 58, 88, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	-0.12	7 (5%) 28 19	68, 111, 139, 171	0
13	CM	125/126 (99%)	-0.14	8 (6%) 23 15	70, 112, 139, 172	0
14	AN	60/61 (98%)	-0.38	1 (1%) 73 59	39, 59, 92, 97	0
14	CN	60/61 (98%)	-0.39	0 100 100	44, 61, 93, 98	0
15	AO	88/89 (98%)	-0.54	0 100 100	35, 61, 91, 100	0
15	CO	88/89 (98%)	-0.52	0 100 100	38, 61, 94, 100	0
16	AP	84/88 (95%)	-0.42	0 100 100	54, 73, 96, 131	0
16	CP	84/88 (95%)	-0.39	1 (1%) 81 69	57, 74, 98, 132	0
17	AQ	100/105 (95%)	-0.53	0 100 100	43, 64, 89, 98	0
17	CQ	100/105 (95%)	-0.47	0 100 100	46, 66, 90, 97	0
18	AR	70/88 (79%)	-0.39	1 (1%) 78 65	42, 69, 94, 108	0
18	CR	70/88 (79%)	-0.48	1 (1%) 78 65	45, 70, 95, 109	0
19	AS	79/93 (84%)	0.00	2 (2%) 61 46	77, 106, 144, 149	0
19	CS	79/93 (84%)	0.18	4 (5%) 32 22	78, 107, 144, 150	0
20	AT	99/106 (93%)	-0.35	0 100 100	63, 84, 126, 129	0
20	CT	99/106 (93%)	-0.34	0 100 100	64, 85, 127, 129	0
21	AU	25/27 (92%)	-0.21	0 100 100	63, 82, 118, 122	0
21	CU	25/27 (92%)	0.14	0 100 100	66, 86, 120, 123	0
22	AV	76/77 (98%)	-0.43	0 100 100	32, 67, 110, 127	0
22	AW	76/77 (98%)	-0.38	1 (1%) 79 66	71, 168, 192, 201	0
22	CV	76/77 (98%)	-0.56	0 100 100	47, 84, 121, 151	0
22	CW	76/77 (98%)	-0.32	1 (1%) 79 66	78, 176, 200, 210	0
23	AX	11/25 (44%)	0.12	0 100 100	28, 94, 149, 166	0
23	CX	11/25 (44%)	0.05	0 100 100	45, 106, 156, 168	0
24	AY	667/691 (96%)	-0.15	9 (1%) 79 66	61, 99, 140, 150	0
24	CY	667/691 (96%)	0.10	23 (3%) 49 35	73, 108, 148, 161	0
25	B0	84/85 (98%)	0.07	6 (7%) 19 12	67, 82, 140, 163	0
25	D0	84/85 (98%)	0.39	9 (10%) 8 6	69, 84, 141, 163	0
26	B1	94/98 (95%)	-0.43	1 (1%) 82 70	41, 70, 118, 128	0
26	D1	94/98 (95%)	-0.32	0 100 100	53, 80, 123, 131	0
27	B2	71/72 (98%)	-0.28	2 (2%) 56 42	77, 116, 150, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	-0.12	2 (2%) 56 42	95, 119, 146, 163	0
28	B3	60/60 (100%)	-0.06	1 (1%) 73 59	63, 88, 114, 135	0
28	D3	60/60 (100%)	0.00	2 (3%) 50 36	64, 89, 114, 134	0
29	B4	58/71 (81%)	0.10	3 (5%) 31 22	76, 135, 220, 222	0
29	D4	58/71 (81%)	0.30	7 (12%) 6 5	77, 137, 220, 222	0
30	B5	59/60 (98%)	-0.05	3 (5%) 32 22	52, 80, 153, 172	0
30	D5	59/60 (98%)	0.00	4 (6%) 20 13	52, 80, 153, 172	0
31	B6	50/54 (92%)	0.03	2 (4%) 42 29	56, 89, 107, 117	0
31	D6	50/54 (92%)	-0.23	1 (2%) 68 54	56, 90, 108, 117	0
32	B7	49/49 (100%)	-0.31	2 (4%) 41 29	47, 64, 119, 132	0
32	D7	49/49 (100%)	-0.36	0 100 100	47, 64, 120, 132	0
33	B8	64/65 (98%)	-0.34	1 (1%) 74 61	63, 75, 105, 125	0
33	D8	64/65 (98%)	-0.23	1 (1%) 74 61	65, 76, 105, 126	0
34	B9	37/37 (100%)	-0.40	0 100 100	60, 71, 85, 89	0
34	D9	37/37 (100%)	-0.27	1 (2%) 58 43	60, 73, 87, 91	0
35	BA	2901/2915 (99%)	-0.34	27 (0%) 85 75	30, 76, 162, 221	0
35	DA	2901/2915 (99%)	-0.47	32 (1%) 82 70	29, 77, 162, 221	0
36	BB	119/122 (97%)	-0.48	0 100 100	65, 106, 138, 183	0
36	DB	119/122 (97%)	-0.65	0 100 100	66, 108, 138, 183	0
37	BC	228/229 (99%)	-0.10	4 (1%) 71 58	42, 97, 147, 160	0
37	DC	228/229 (99%)	0.11	12 (5%) 30 21	43, 98, 148, 162	0
38	BD	275/276 (99%)	-0.49	0 100 100	31, 52, 82, 101	0
38	DD	275/276 (99%)	-0.48	1 (0%) 93 88	32, 52, 82, 101	0
39	BE	205/206 (99%)	-0.30	4 (1%) 68 54	44, 77, 128, 135	0
39	DE	205/206 (99%)	-0.26	3 (1%) 76 64	44, 77, 128, 134	0
40	BF	208/210 (99%)	0.03	10 (4%) 34 24	53, 110, 166, 177	0
40	DF	208/210 (99%)	0.01	12 (5%) 26 18	53, 111, 166, 176	0
41	BG	181/182 (99%)	-0.24	4 (2%) 65 50	63, 95, 131, 143	0
41	DG	181/182 (99%)	-0.01	5 (2%) 56 42	86, 110, 137, 151	0
42	BH	167/180 (92%)	0.08	6 (3%) 46 33	81, 117, 143, 159	0
42	DH	167/180 (92%)	0.07	3 (1%) 71 58	81, 118, 143, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BJ	0/173	-	-	-	-
43	DJ	0/173	-	-	-	-
44	BK	140/147 (95%)	1.97	61 (43%) 0 0	162, 180, 186, 188	0
44	DK	140/147 (95%)	1.69	49 (35%) 0 0	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%)	-0.27	2 (1%) 78 65	60, 91, 132, 137	0
46	DN	139/140 (99%)	-0.23	1 (0%) 89 81	61, 91, 132, 137	0
47	BO	122/122 (100%)	-0.43	0 100 100	35, 60, 73, 86	0
47	DO	122/122 (100%)	-0.41	0 100 100	36, 61, 73, 88	0
48	BP	146/150 (97%)	0.05	4 (2%) 58 43	46, 111, 137, 157	0
48	DP	146/150 (97%)	0.12	5 (3%) 49 35	50, 113, 137, 157	0
49	BQ	141/141 (100%)	-0.35	0 100 100	45, 65, 88, 119	0
49	DQ	141/141 (100%)	-0.38	0 100 100	45, 66, 89, 120	0
50	BR	117/118 (99%)	-0.34	1 (0%) 85 75	49, 81, 101, 128	0
50	DR	117/118 (99%)	-0.26	1 (0%) 85 75	53, 82, 101, 128	0
51	BS	99/112 (88%)	-0.17	2 (2%) 68 54	82, 116, 140, 144	0
51	DS	99/112 (88%)	0.30	5 (5%) 32 22	83, 117, 141, 145	0
52	BT	138/146 (94%)	-0.10	4 (2%) 55 40	55, 83, 149, 176	0
52	DT	138/146 (94%)	-0.15	5 (3%) 46 33	57, 84, 149, 177	0
53	BU	117/118 (99%)	-0.34	0 100 100	62, 80, 114, 135	0
53	DU	117/118 (99%)	-0.33	0 100 100	62, 81, 115, 134	0
54	BV	101/101 (100%)	-0.00	1 (0%) 84 73	59, 116, 133, 141	0
54	DV	101/101 (100%)	0.20	6 (5%) 26 17	61, 116, 134, 140	0
55	BW	113/113 (100%)	-0.25	0 100 100	61, 79, 119, 158	0
55	DW	113/113 (100%)	-0.13	0 100 100	63, 80, 120, 159	0
56	BX	93/96 (96%)	-0.15	0 100 100	76, 91, 110, 114	0
56	DX	93/96 (96%)	-0.20	0 100 100	76, 92, 111, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
57	BY	107/110 (97%)	0.10	2 (1%) 70 56	78, 127, 149, 155	0
57	DY	107/110 (97%)	0.43	4 (3%) 45 32	78, 127, 149, 155	0
58	BZ	185/206 (89%)	-0.20	1 (0%) 91 86	47, 90, 135, 143	0
58	DZ	185/206 (89%)	-0.07	2 (1%) 82 70	68, 99, 138, 146	0
All	All	22794/24788 (91%)	-0.25	449 (1%) 68 54	23, 82, 155, 222	0

The worst 5 of 449 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BA	654(K)	C	14.3
52	BT	138	ALA	13.1
1	CA	1036	G	13.0
35	DA	654(D)	G	12.6
35	BA	654(F)	C	11.0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
61	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	0.01	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	0.90	0.07	-1.04	164,164,164,164	0
59	ZN	B4	101	1/1	0.91	0.12	-1.47	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.