



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 2, 2024 – 10:04 am GMT

PDB ID : 4V8N
Title : The crystal structure of agmatidine tRNA-Ile2 bound to the 70S ribosome in the A and P site.
Authors : Voorhees, R.M.; Mandal, D.; Neubauer, C.; Koehrer, C.; RajBhandary, U.L.; Ramakrishnan, V.
Deposited on : 2013-02-13
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

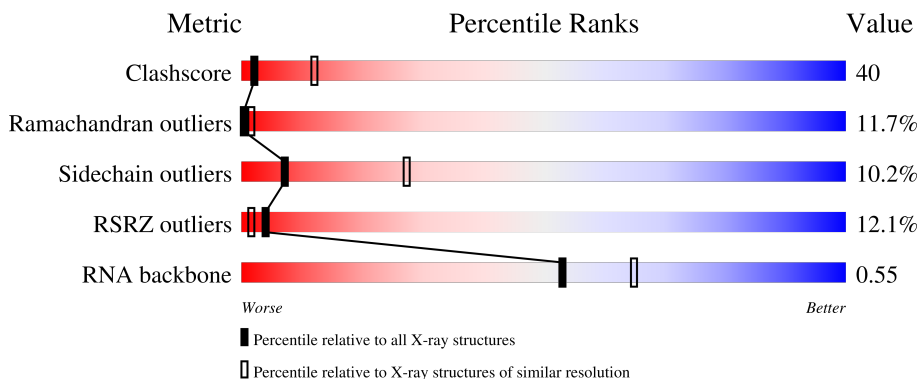
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	
1	CA	1522	
2	AB	256	
2	CB	256	
3	AC	239	

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Mol	Chain	Length	Quality of chain
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	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	

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Mol	Chain	Length	Quality of chain
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	78	
22	AY	78	
22	CV	78	
22	CY	78	
23	AW	78	
23	CW	78	
24	AX	24	
24	CX	24	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	
27	B2	72	

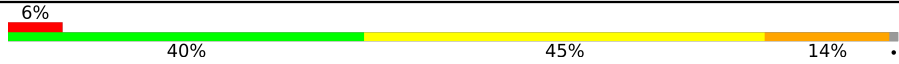
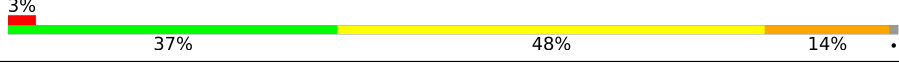
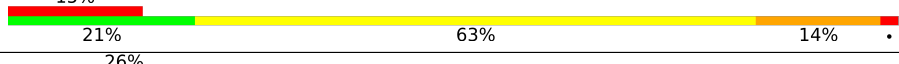
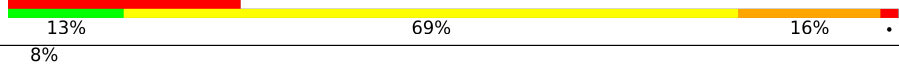
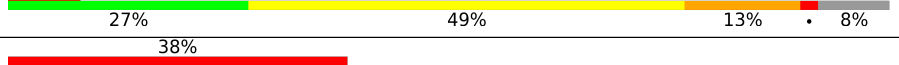
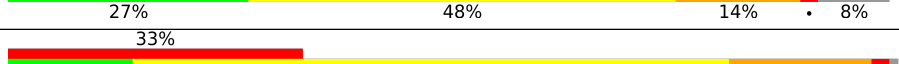
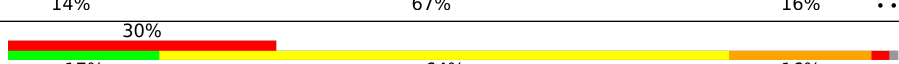
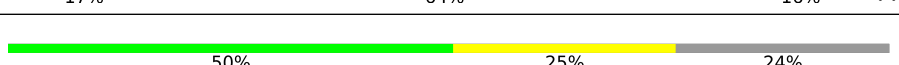
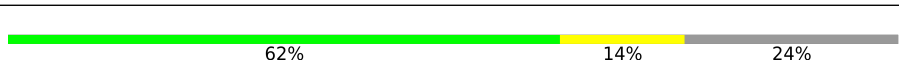

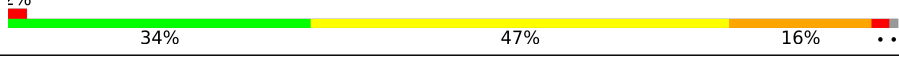
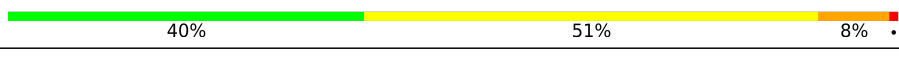
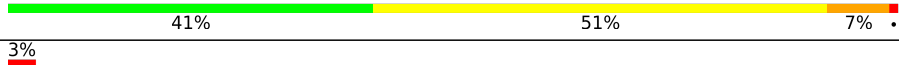
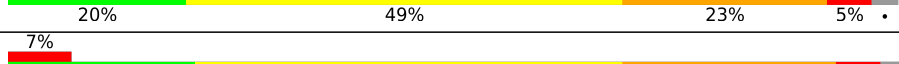
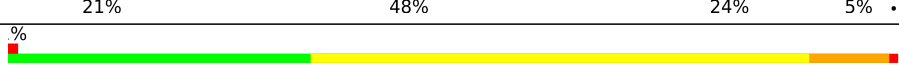
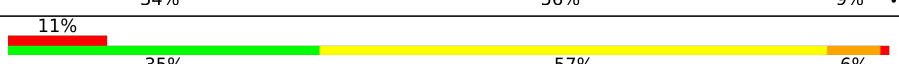
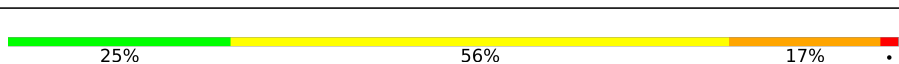
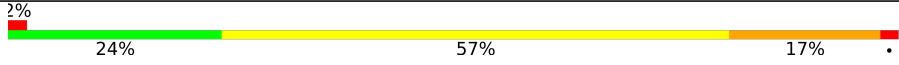
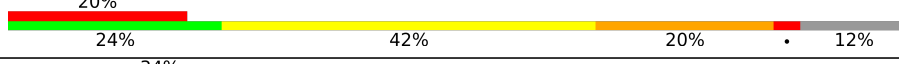
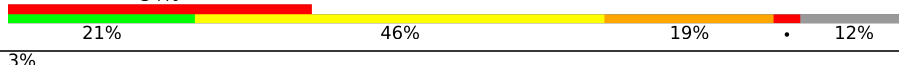





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Mol	Chain	Length	Quality of chain
27	D2	72	6% 35% 50% 11% ..
28	B3	60	3% 38% 53% 7% .
28	D3	60	25% 38% 53% 8%
29	B4	71	17% 21% 32% 24% . 18%
29	D4	71	20% 24% 31% 24% . 18%
30	B5	60	40% 35% 17% . 7%
30	D5	60	2% 42% 33% 17% . 7%
31	B6	54	72% 11% 52% 28% . 7%
31	D6	54	76% 11% 52% 28% . 7%
32	B7	49	2% 53% 41% . .
32	D7	49	2% 51% 45% . .
33	B8	65	3% 23% 57% 14% 5% .
33	D8	65	11% 26% 54% 14% 5% .
34	B9	37	95% 35% 62% .
34	D9	37	97% 32% 65% .
35	BA	2915	4% 40% 46% 11% ..
35	DA	2915	5% 38% 48% 11% ..
36	BB	122	% 36% 52% 10% .
36	DB	122	7% 37% 51% 10% .
37	BC	229	37% 17% 33% . 48%
37	DC	229	35% 17% 33% . 48%
38	BD	276	% 30% 51% 16% ..
38	DD	276	% 29% 54% 15% ..
39	BE	206	3% 29% 50% 18% .
39	DE	206	3% 28% 52% 16% .

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Mol	Chain	Length	Quality of chain
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BI	148	
43	DI	148	
44	BJ	173	
44	DJ	173	
45	BN	140	
45	DN	140	
46	BO	122	
46	DO	122	
47	BP	150	
47	DP	150	
48	BQ	141	
48	DQ	141	
49	BR	118	
49	DR	118	
50	BS	112	
50	DS	112	
51	BT	146	
51	DT	146	
52	BU	118	

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Mol	Chain	Length	Quality of chain
52	DU	118	
53	BV	101	
53	DV	101	
54	BW	113	
54	DW	113	
55	BX	96	
55	DX	96	
56	BY	110	
56	DY	110	
57	BZ	206	
57	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
22	AG9	AV	36	X	-	-	-
22	AG9	AY	36	X	-	X	-
22	AG9	CV	36	X	-	X	-
22	AG9	CY	36	X	-	-	X
58	ZN	AD	1000	-	-	X	-
58	ZN	AN	1000	-	-	X	-
58	ZN	CD	1000	-	-	X	-
58	ZN	CN	1000	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 298096 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
			Total	C	N	O	P			
1	AA	1504	Total 32329	C 14390	N 5992	O 10444	P 1503	0	0	0
1	CA	1504	Total 32329	C 14390	N 5992	O 10444	P 1503	0	0	0

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
10	CJ	99	795	499	157	138	1	0	0	1

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

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	1	MET	-	expression tag	UNP Q5SHN3
AL	2	VAL	-	expression tag	UNP Q5SHN3
AL	3	ALA	-	expression tag	UNP Q5SHN3
AL	4	LEU	-	expression tag	UNP Q5SHN3
CL	1	MET	-	expression tag	UNP Q5SHN3
CL	2	VAL	-	expression tag	UNP Q5SHN3
CL	3	ALA	-	expression tag	UNP Q5SHN3
CL	4	LEU	-	expression tag	UNP Q5SHN3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AM	119	938	579	194	163	2	0	0	1
13	CM	119	938	579	194	163	2	0	0	1

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	78	Total	C	N	O	P	0	0	0
			1667	746	299	545	77			
22	AY	78	Total	C	N	O	P	0	0	0
			1667	746	299	545	77			
22	CV	78	Total	C	N	O	P	0	0	0
			1667	746	299	545	77			
22	CY	78	Total	C	N	O	P	0	0	0
			1667	746	299	545	77			

- Molecule 23 is a RNA chain called A-SITE TRNA ILE2 AGMATIDINE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	78	Total	C	N	O	P	0	0	0
			1659	741	295	546	77			
23	CW	78	Total	C	N	O	P	0	0	0
			1659	741	295	546	77			

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	12	Total	C	N	O	P	0	0	0
			257	118	54	74	11			
24	CX	12	Total	C	N	O	P	0	0	0
			257	118	54	74	11			

- 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
			734	460	148	125	1			
26	D1	94	Total	C	N	O	S	0	0	1
			734	460	148	125	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	ARG	LYS	conflict	UNP P60494
D1	81	ARG	LYS	conflict	UNP P60494

- 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	56	Total	C	N	O	S	0	0	1
			428	267	87	69	5			
30	D5	56	Total	C	N	O	S	0	0	1
			428	267	87	69	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			
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	48	Total	C	N	O	S	0	0	1
			410	251	103	54	2			
32	D7	48	Total	C	N	O	S	0	0	1
			410	251	103	54	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	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			
35	DA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			

- 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	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			
37	DC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
38	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			
42	DH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
43	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BJ	131	Total	C	N	O	0	0	1
			651	390	131	130			
44	DJ	131	Total	C	N	O	0	0	1
			651	390	131	130			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BN	139	Total 1105	C 712	N 207	O 182	S 4	0	0	1
45	DN	139	Total 1105	C 712	N 207	O 182	S 4	0	0	1

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	BQ	141	Total 1113	C 710	N 211	O 185	S 7	0	0	1
48	DQ	141	Total 1113	C 710	N 211	O 185	S 7	0	0	1

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BT	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	1			
51	DT	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	1			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	BY	101	776	500	149	123	4	0	0	1
56	DY	101	776	500	149	123	4	0	0	1

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

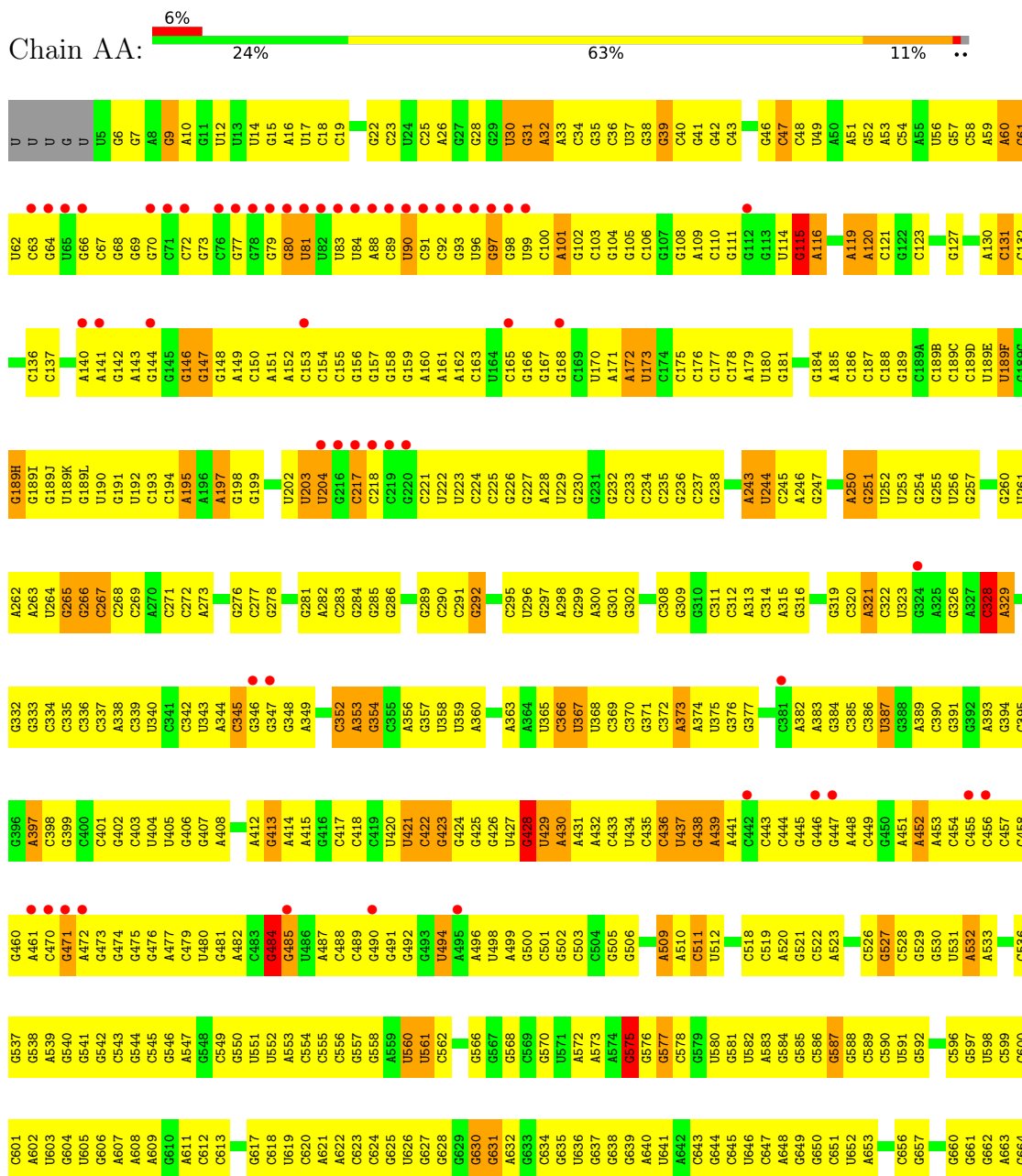
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

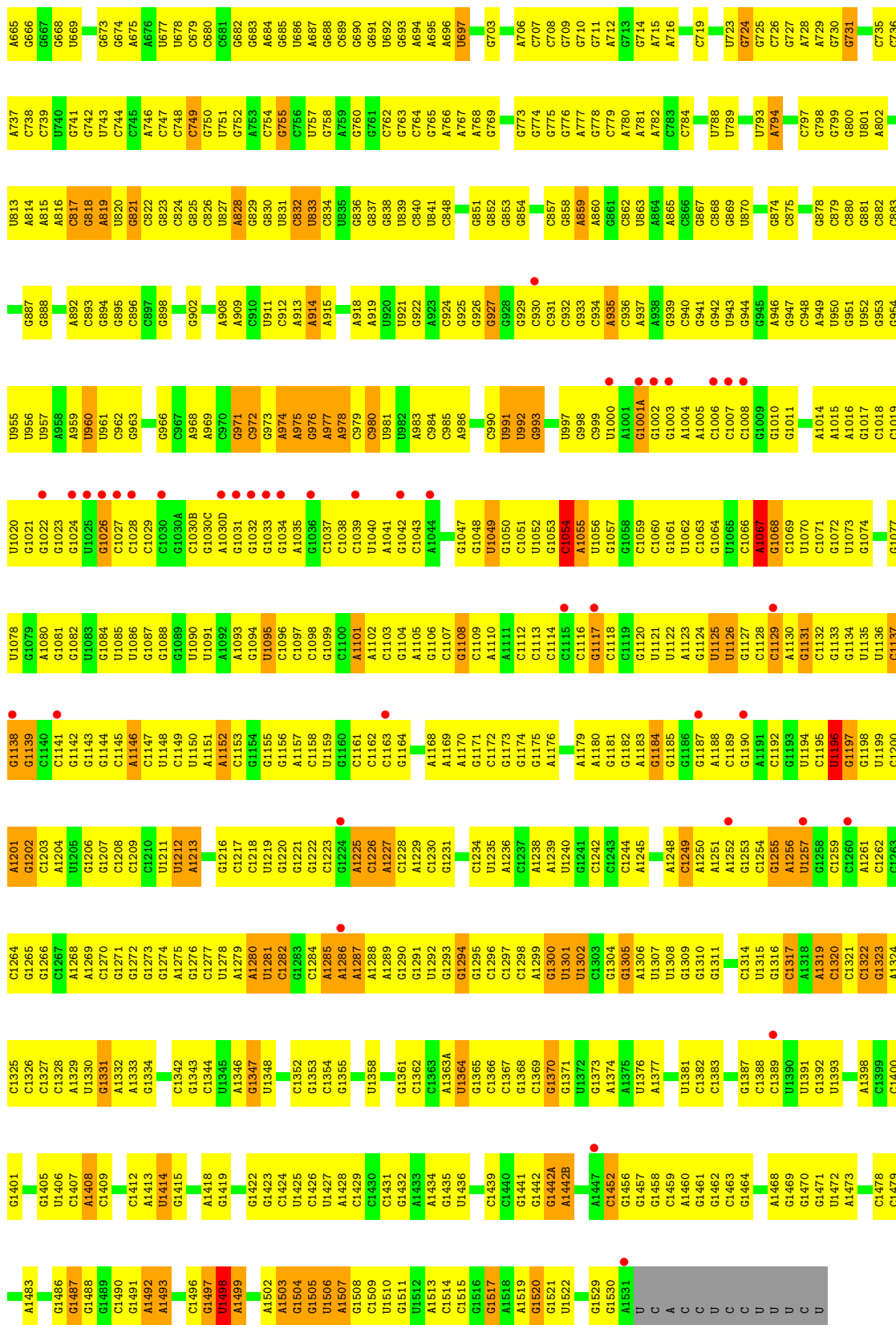
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AD	1	Total 1	Zn 1	0	0
58	AN	1	Total 1	Zn 1	0	0
58	CD	1	Total 1	Zn 1	0	0
58	CN	1	Total 1	Zn 1	0	0

3 Residue-property plots

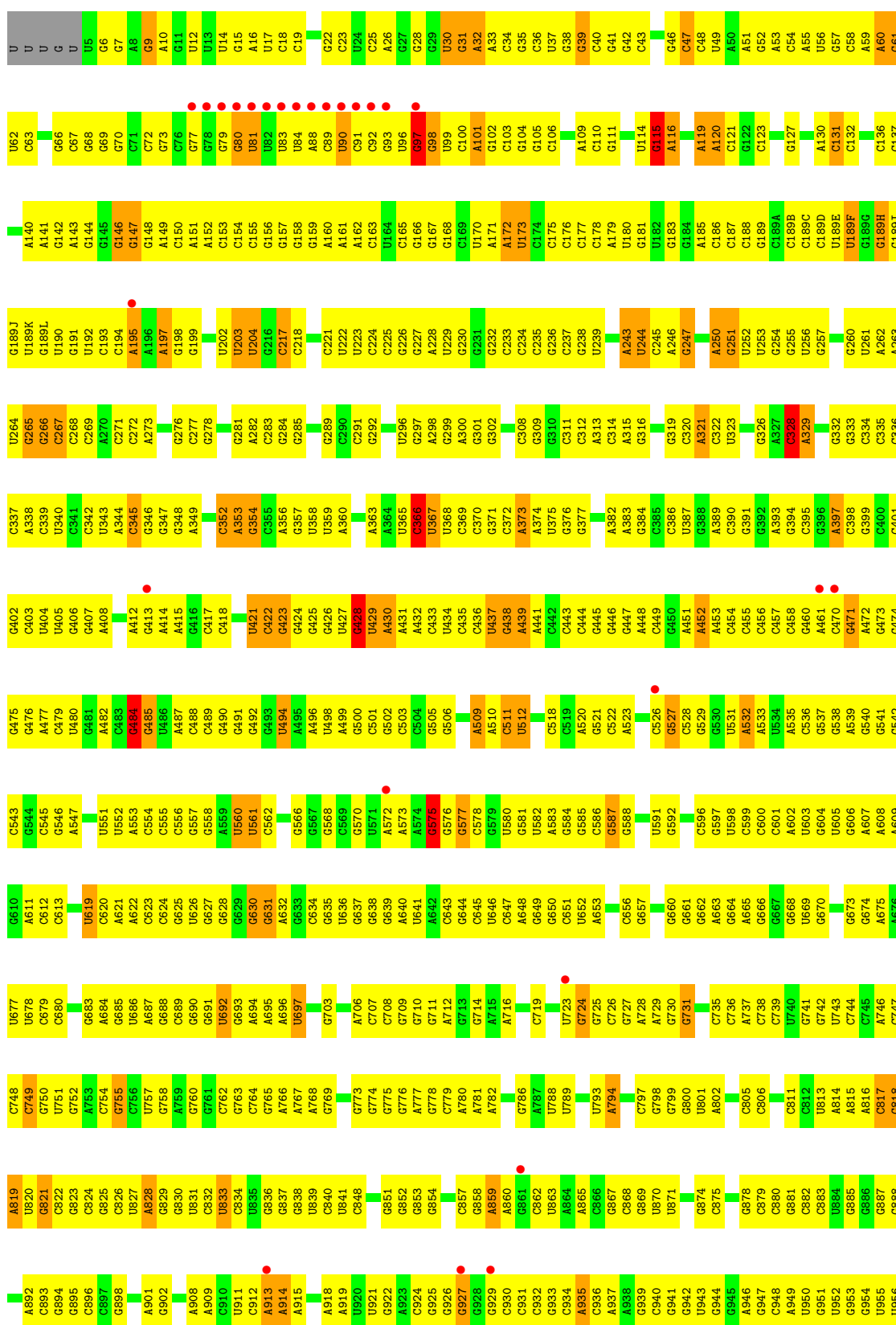
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

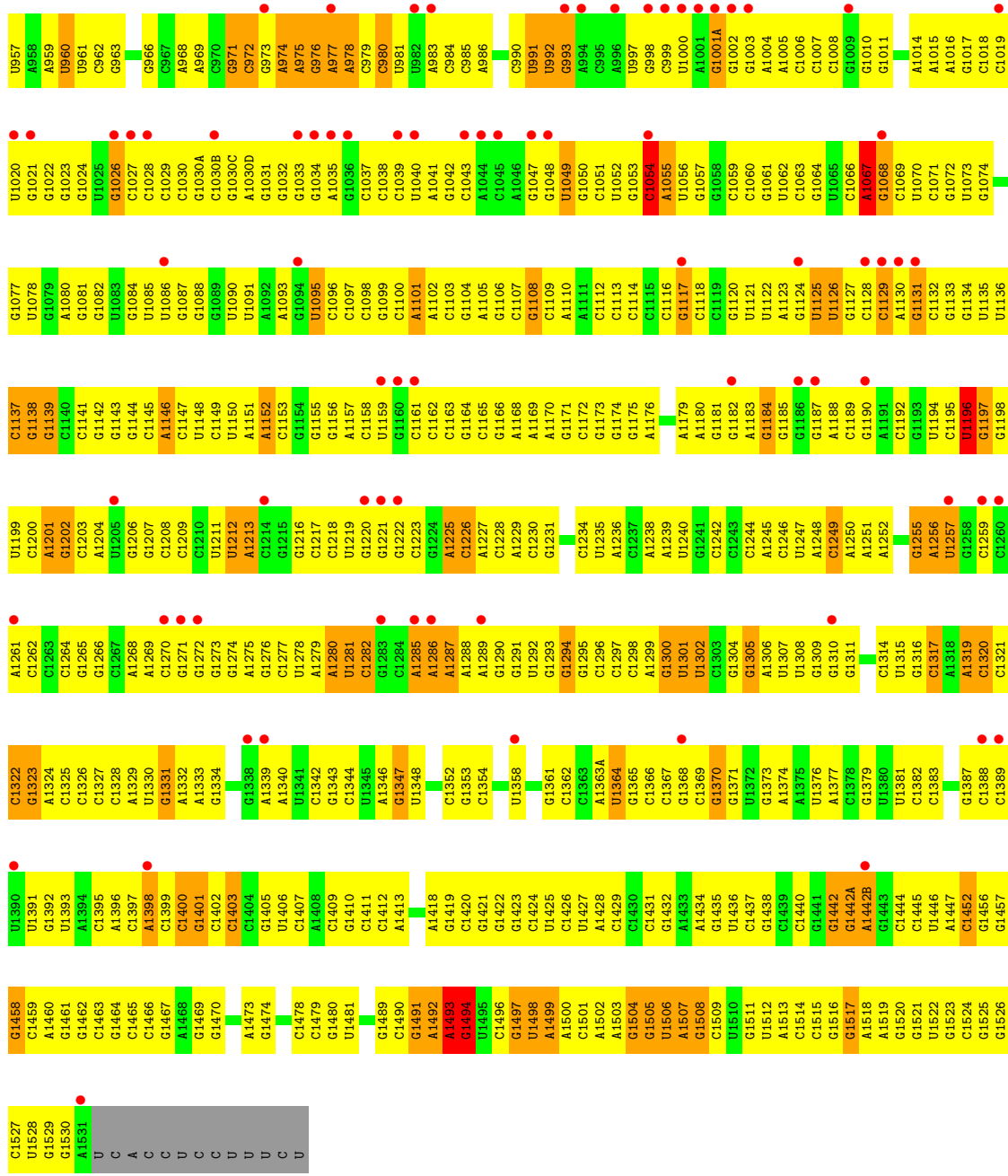
- Molecule 1: 16S RRNA



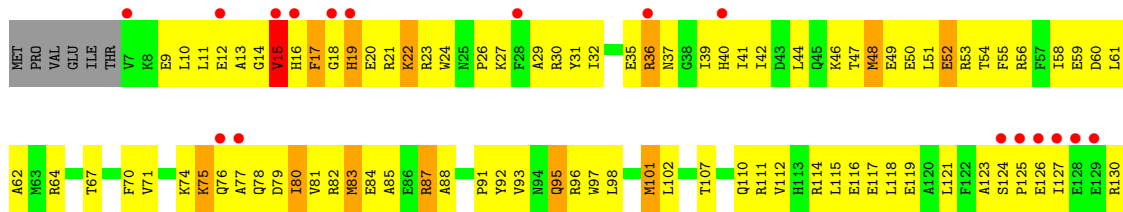


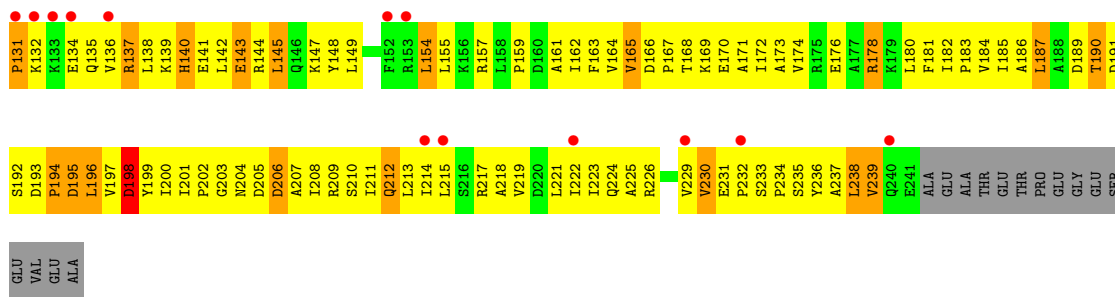
• Molecule 1: 16S rRNA



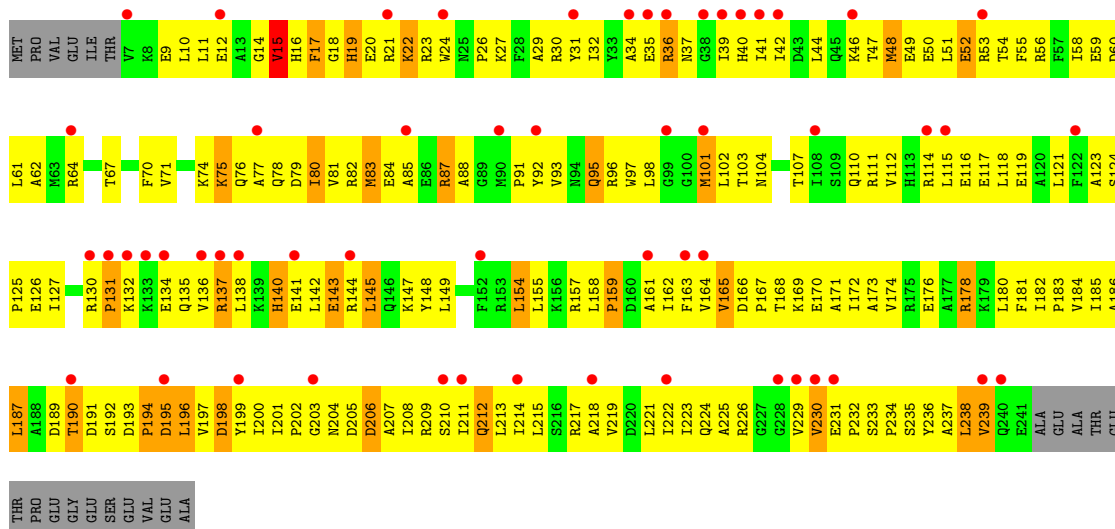


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

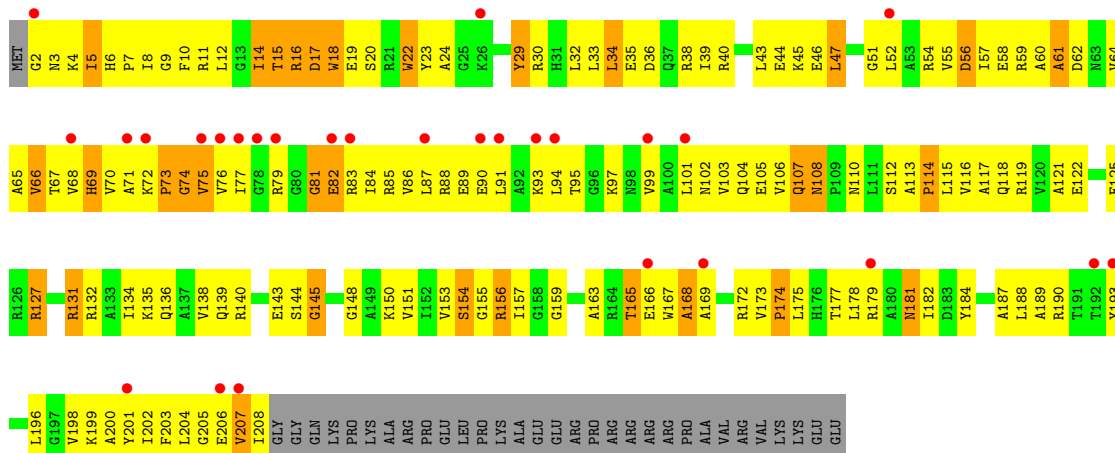




• Molecule 2: 30S RIBOSOMAL PROTEIN S2

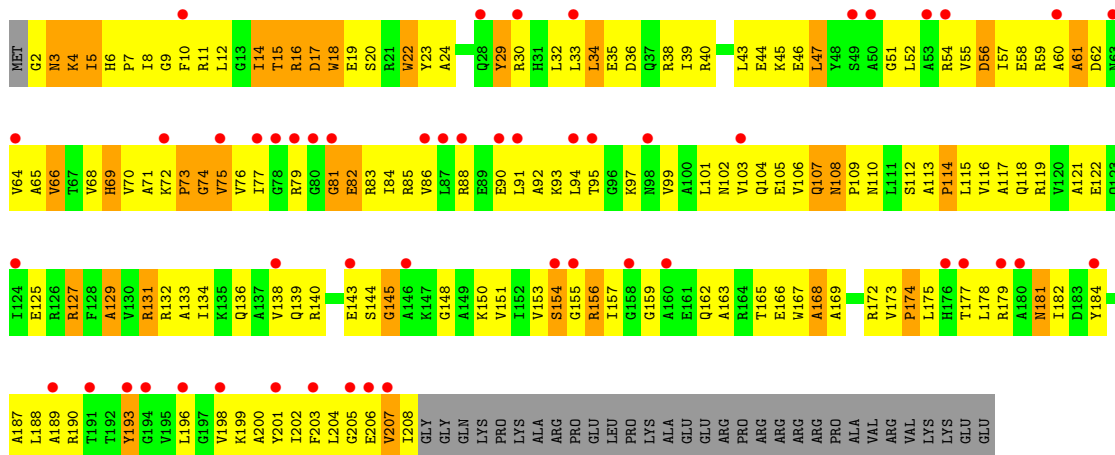


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

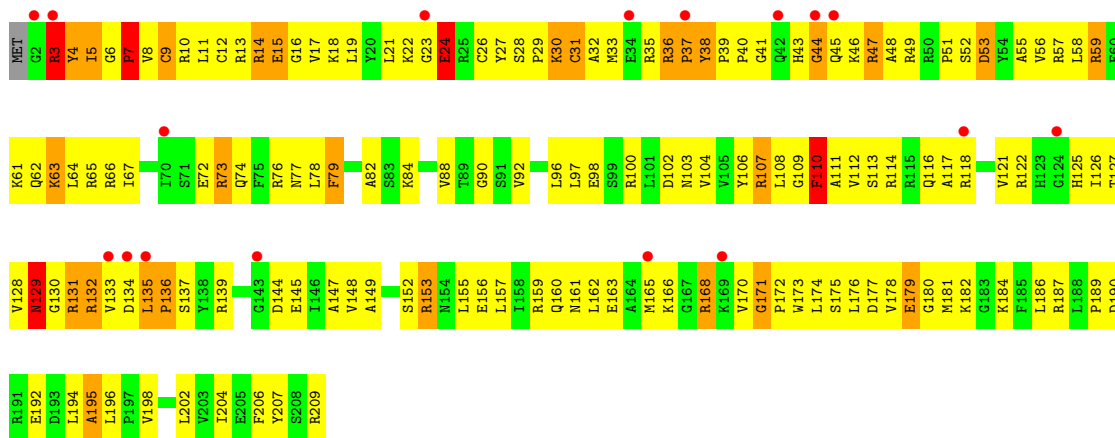


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

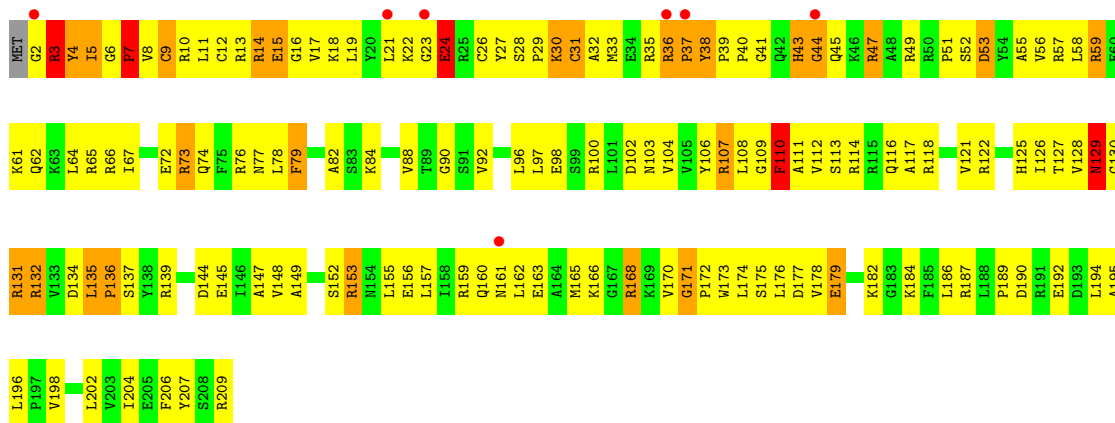




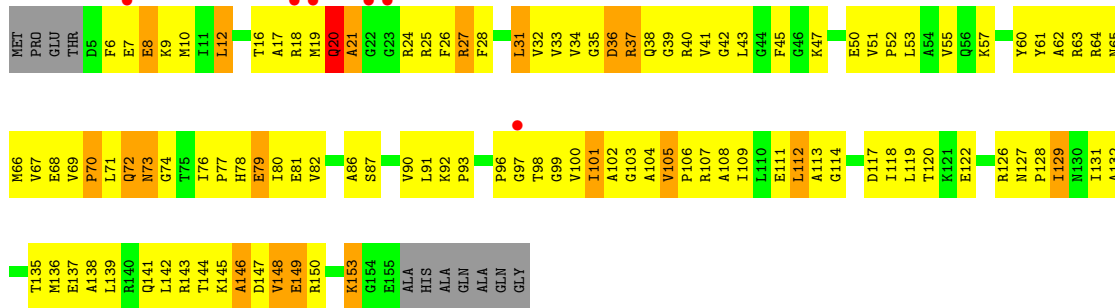
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



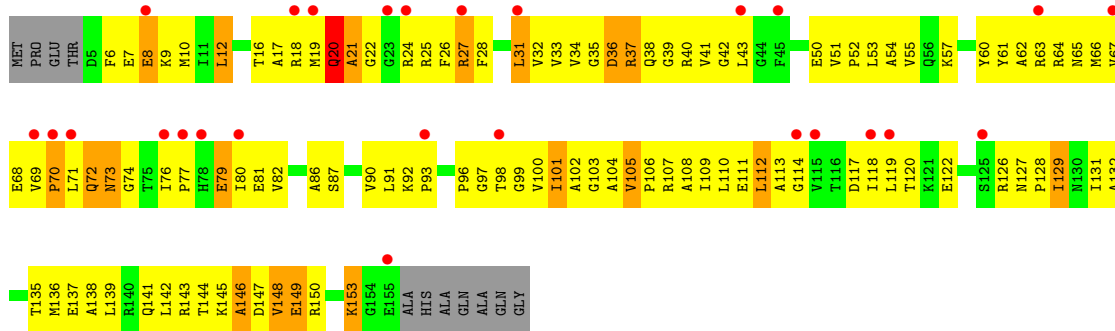
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



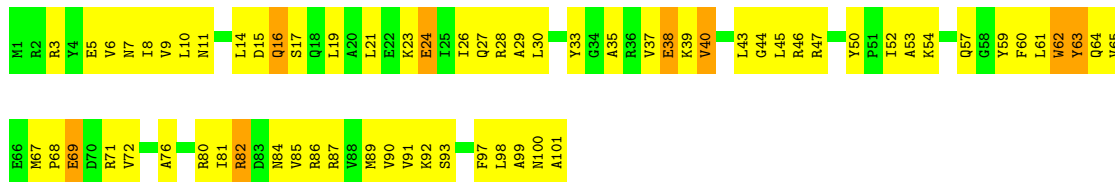
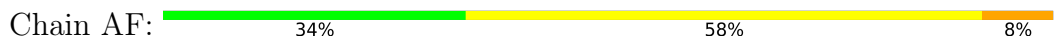
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



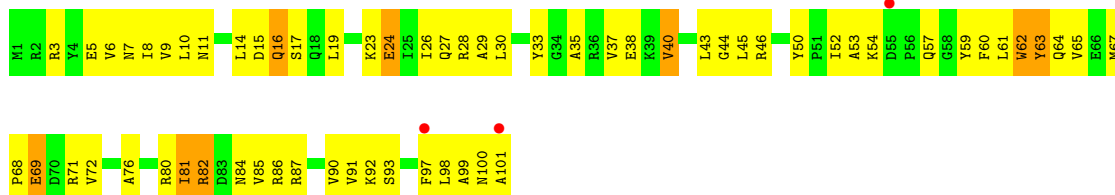
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

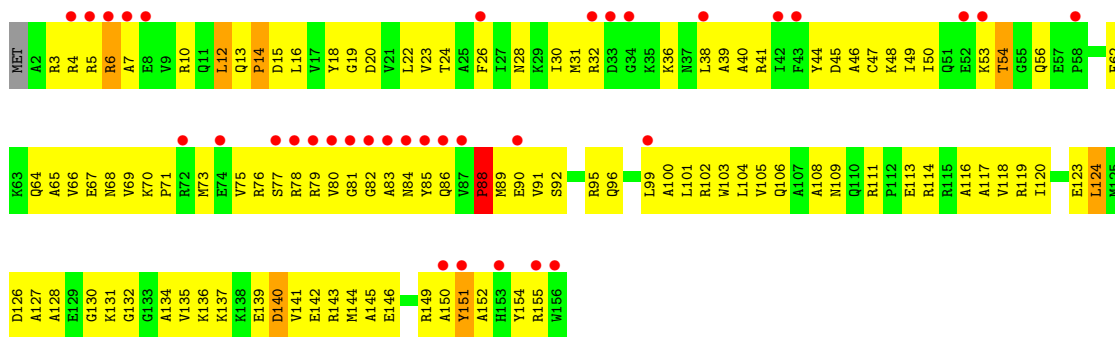


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

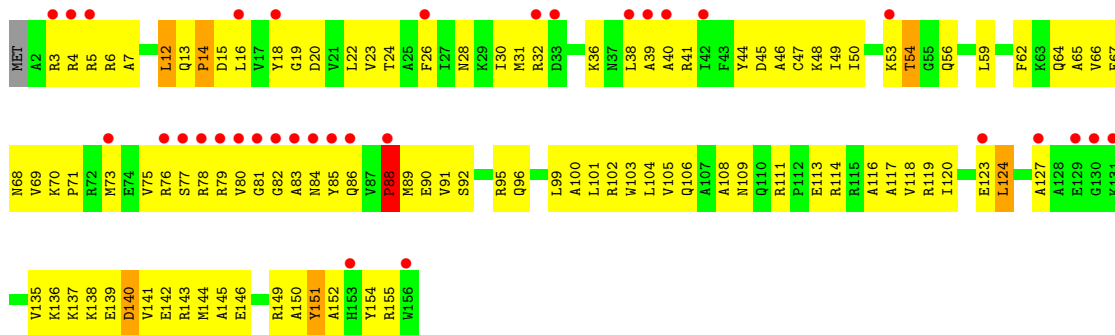


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

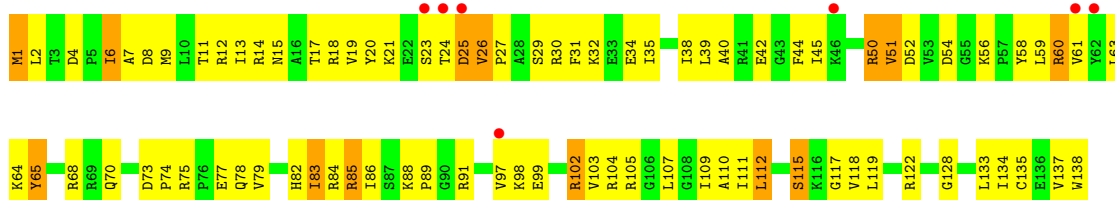




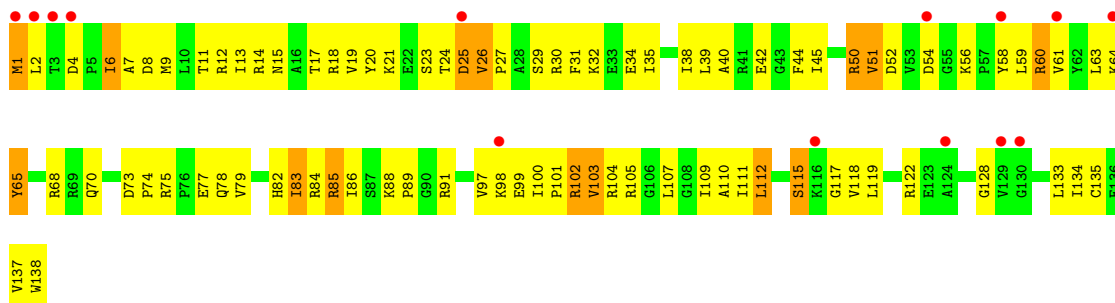
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



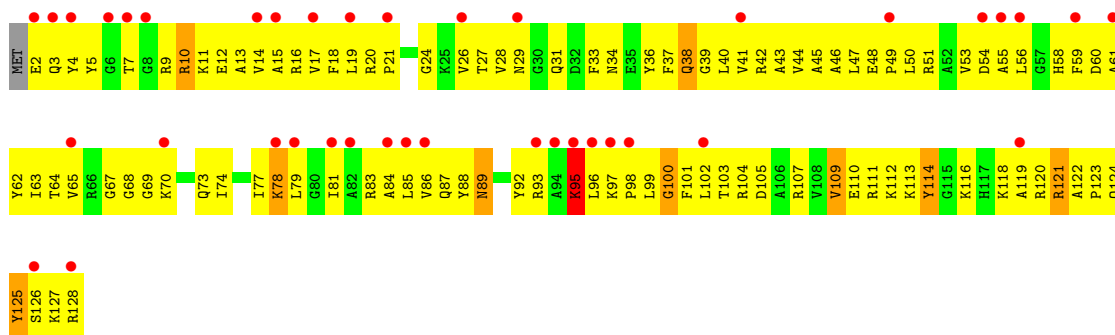
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



- Molecule 8: 30S RIBOSOMAL PROTEIN S8



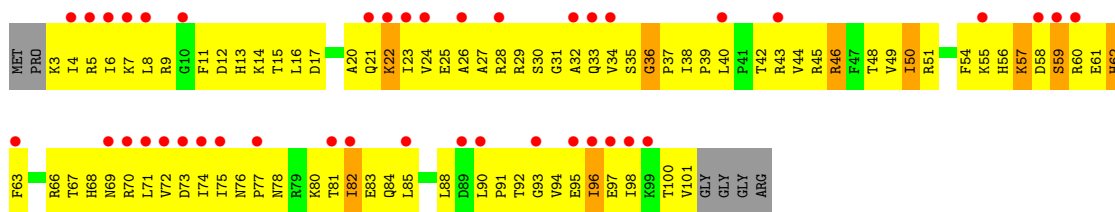
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



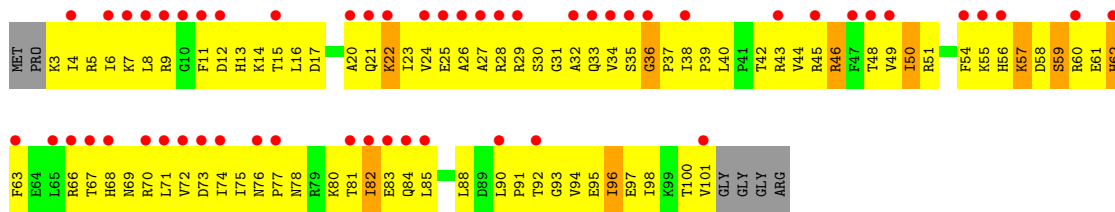
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



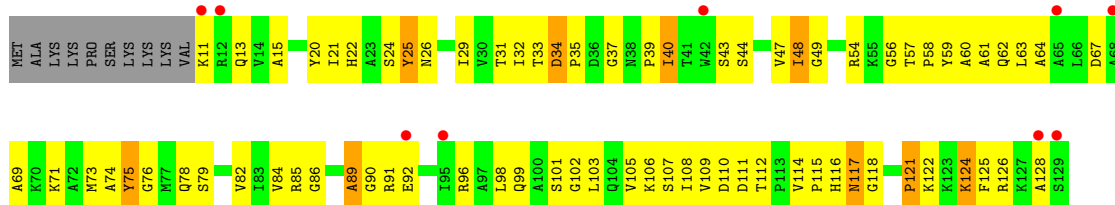
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



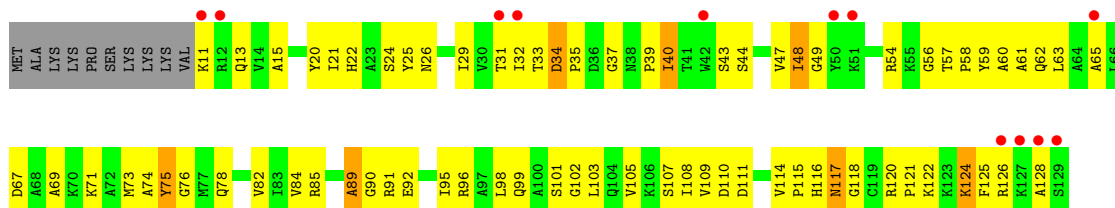
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



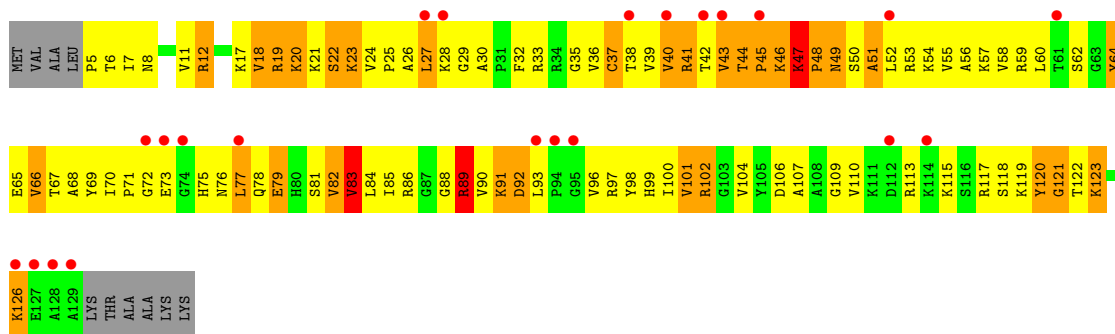
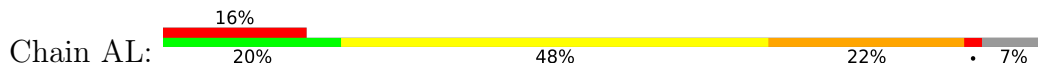
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



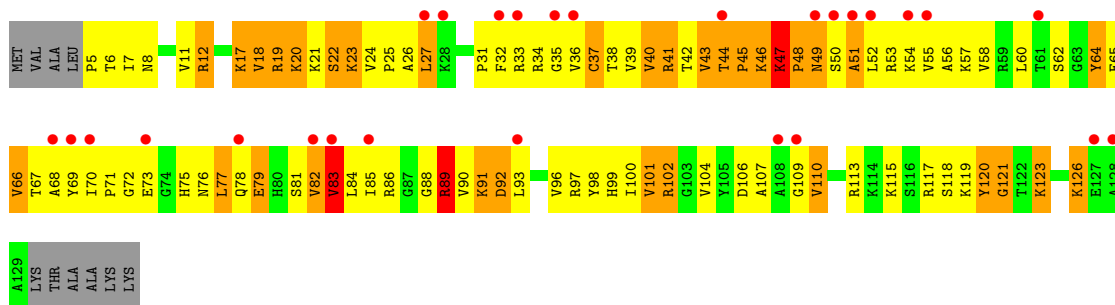
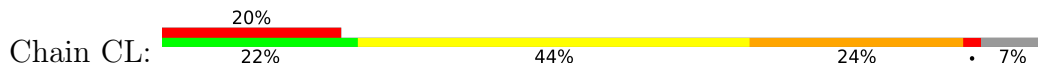
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



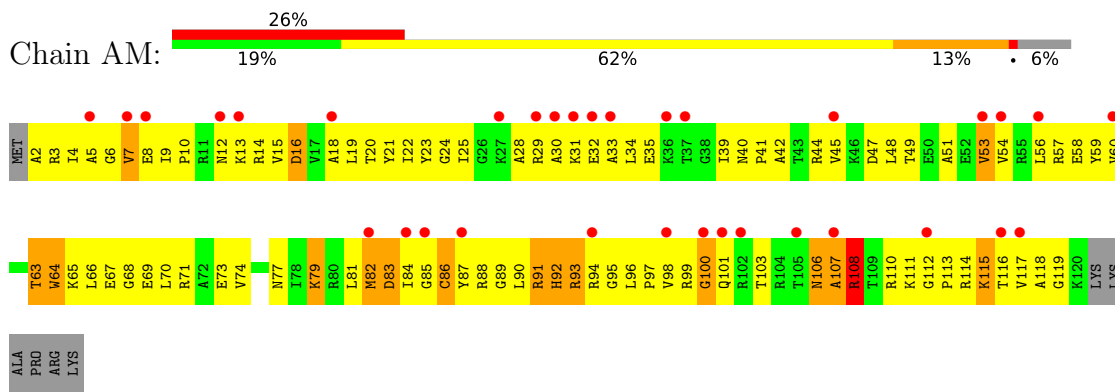
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



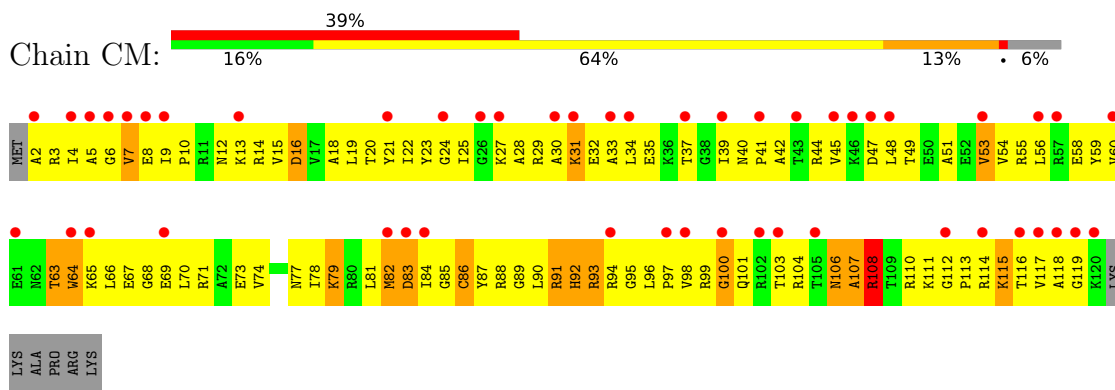
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



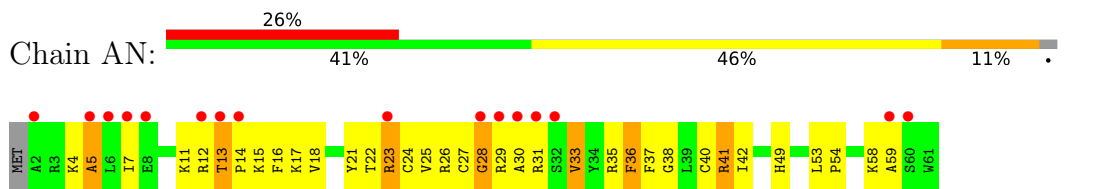
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



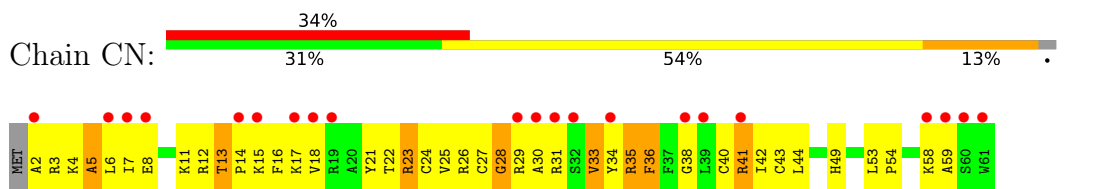
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



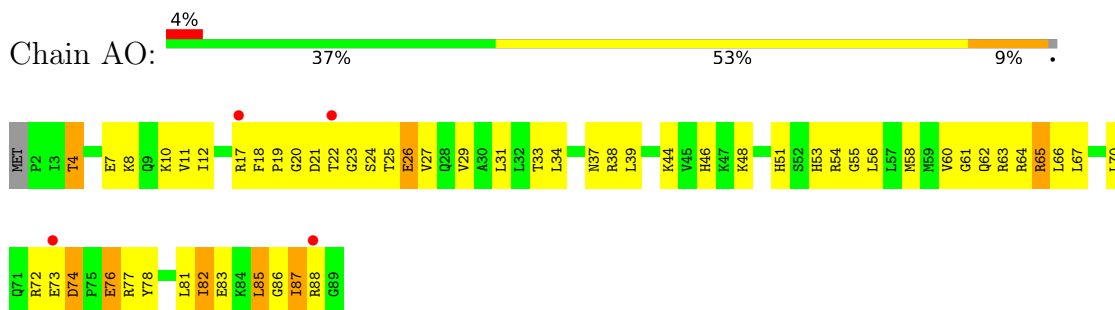
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



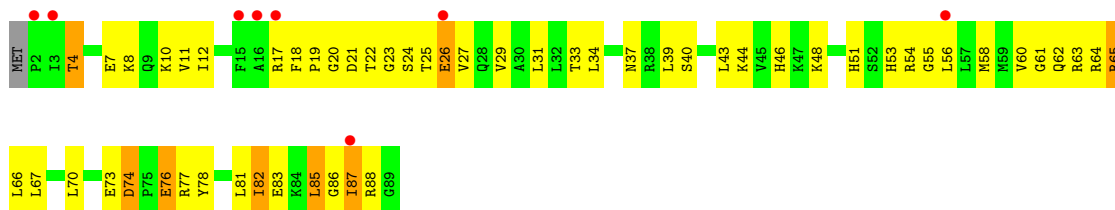
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



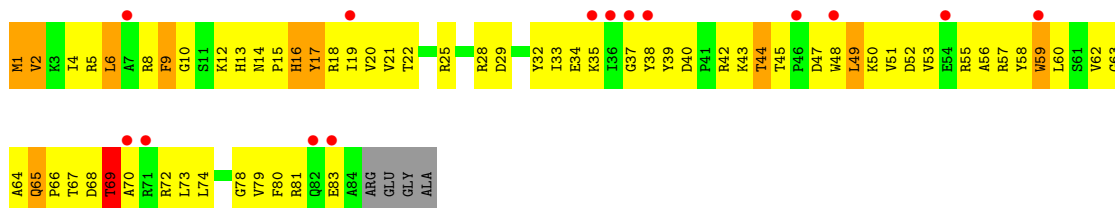
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 15: 30S RIBOSOMAL PROTEIN S15



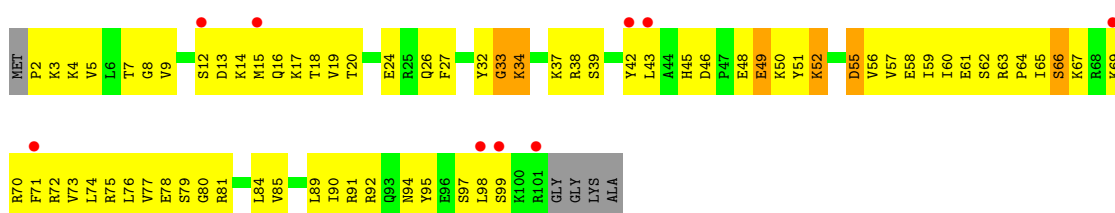
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



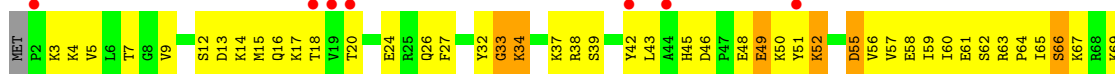
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

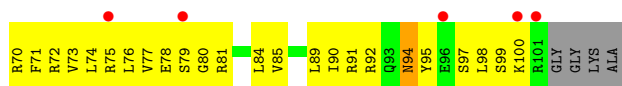


- Molecule 17: 30S RIBOSOMAL PROTEIN S17

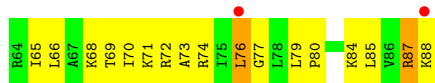
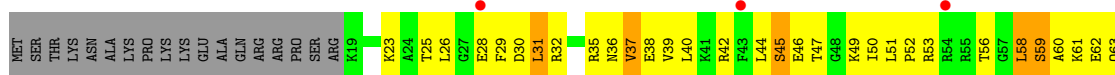


- Molecule 17: 30S RIBOSOMAL PROTEIN S17

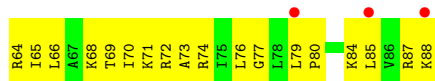
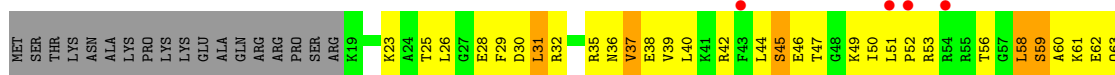




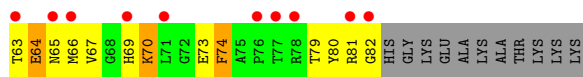
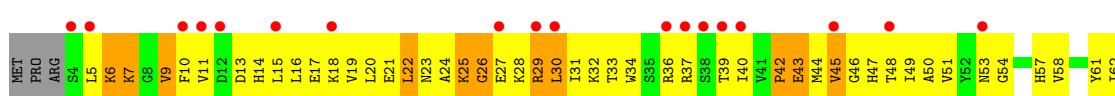
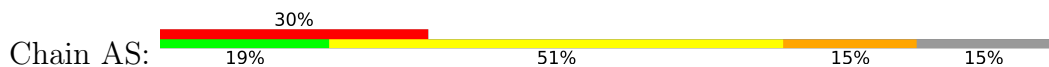
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



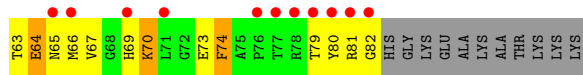
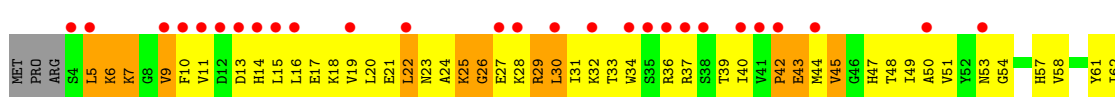
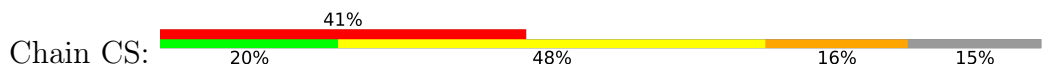
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

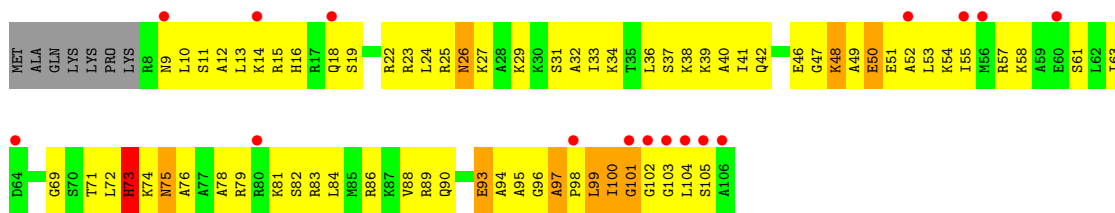


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

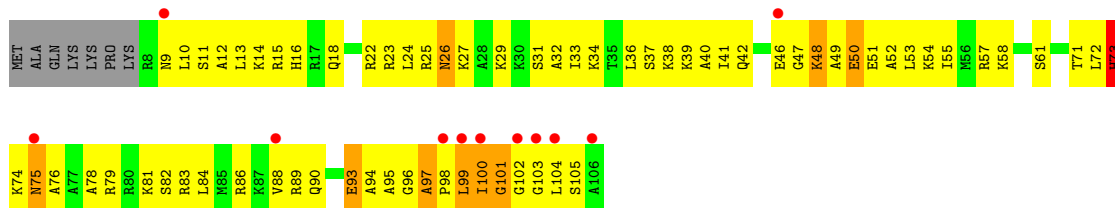


• Molecule 20: 30S RIBOSOMAL PROTEIN S20





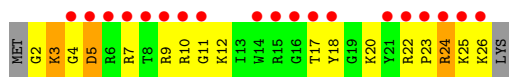
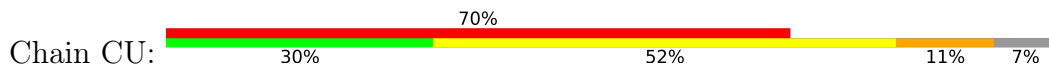
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



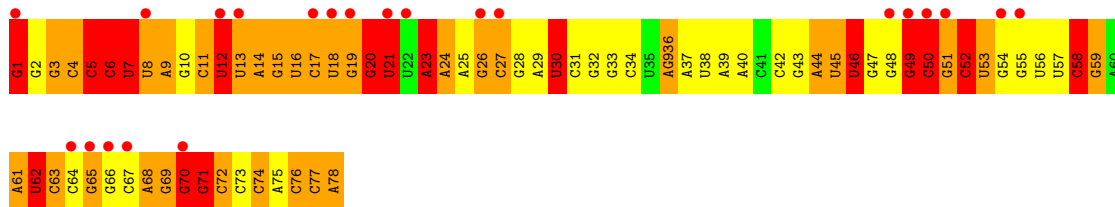
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 22: E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE

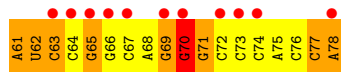
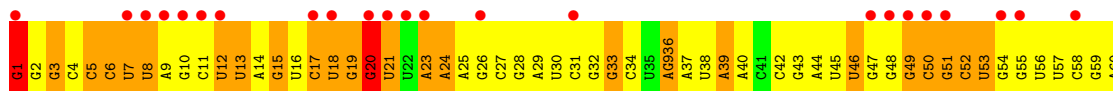


• Molecule 22: E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE





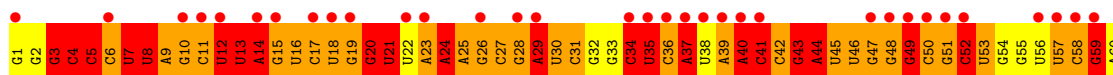
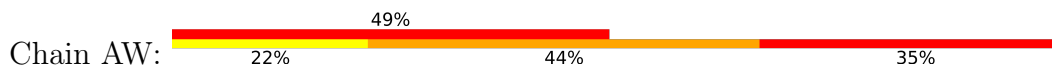
- Molecule 22: E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE



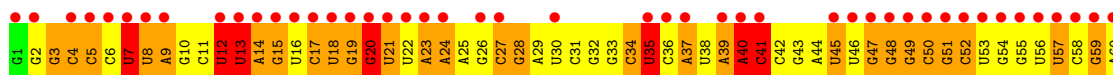
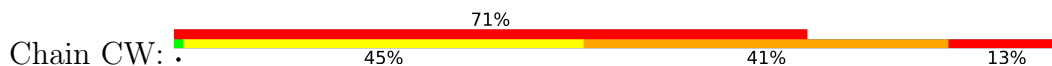
- Molecule 22: E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE



- Molecule 23: A-SITE TRNA ILE2 AGMATIDINE

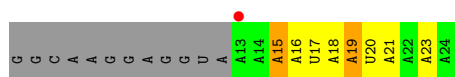


- Molecule 23: A-SITE TRNA ILE2 AGMATIDINE

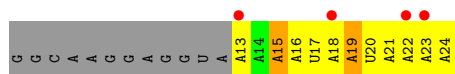


- Molecule 24: MRNA

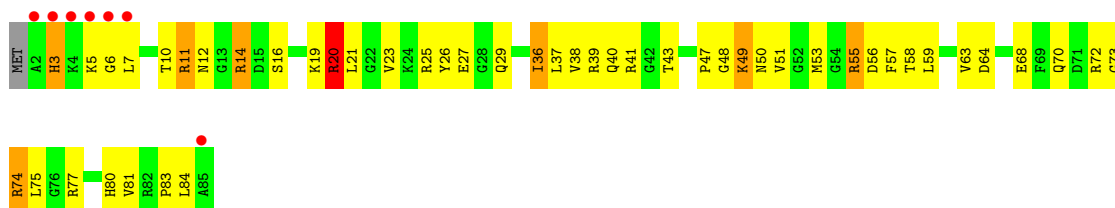




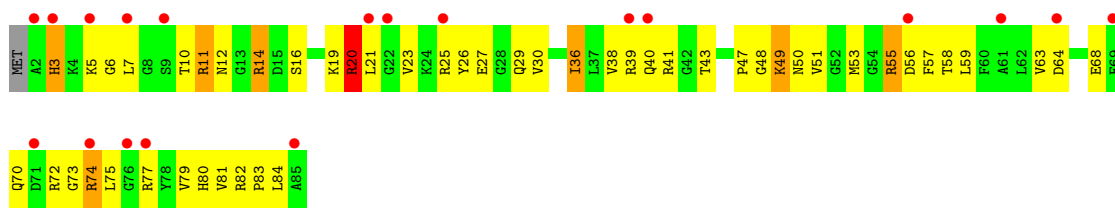
● Molecule 24: MRNA



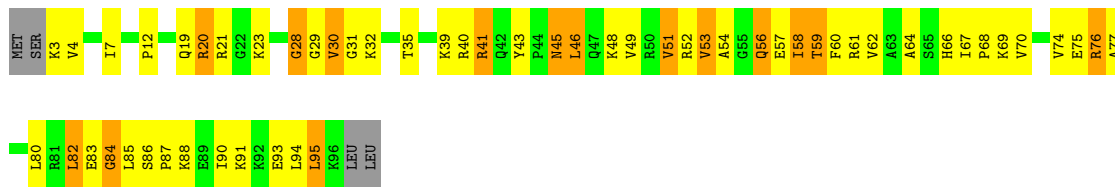
● Molecule 25: 50S RIBOSOMAL PROTEIN L27



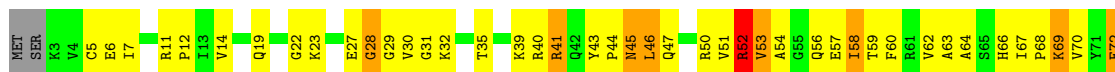
● Molecule 25: 50S RIBOSOMAL PROTEIN L27

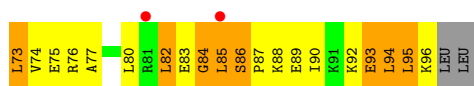


● Molecule 26: 50S RIBOSOMAL PROTEIN L28

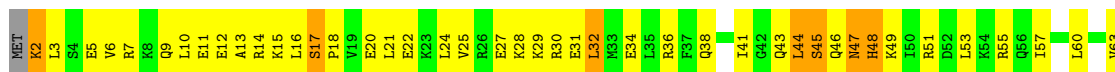


● Molecule 26: 50S RIBOSOMAL PROTEIN L28





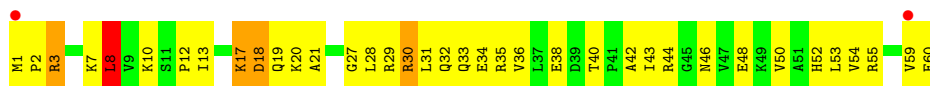
● Molecule 27: 50S RIBOSOMAL PROTEIN L29



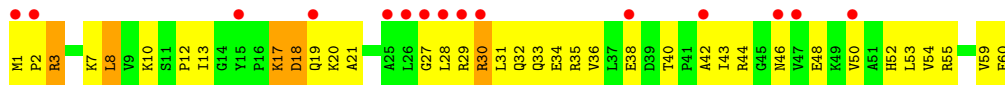
● Molecule 27: 50S RIBOSOMAL PROTEIN L29



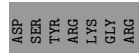
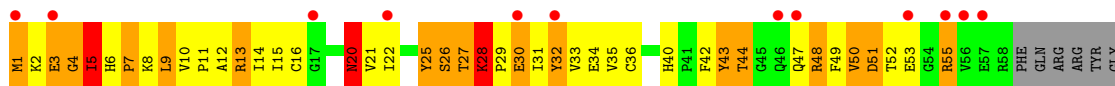
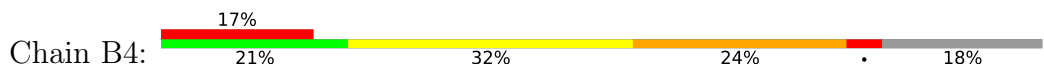
● Molecule 28: 50S RIBOSOMAL PROTEIN L30



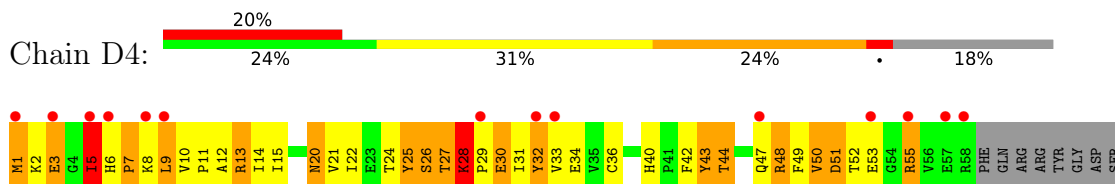
● Molecule 28: 50S RIBOSOMAL PROTEIN L30



● Molecule 29: 50S RIBOSOMAL PROTEIN L31

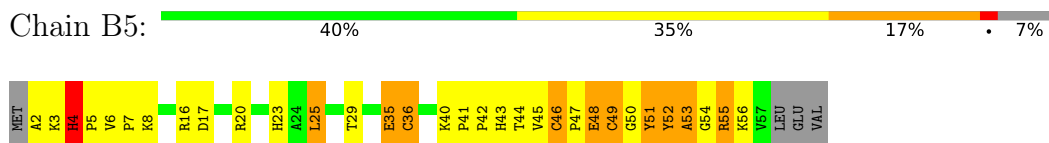


● Molecule 29: 50S RIBOSOMAL PROTEIN L31

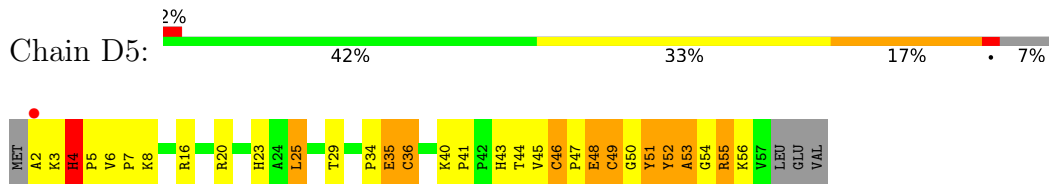


TYR
ARG
LYS
GLY
ARG

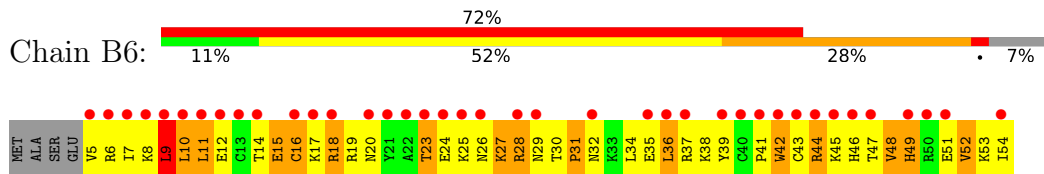
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



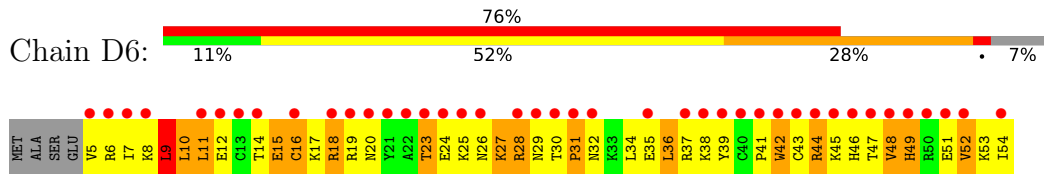
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



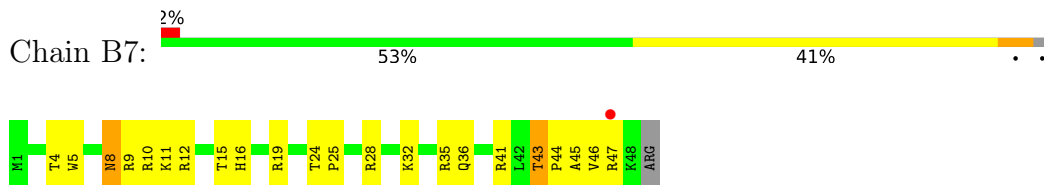
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



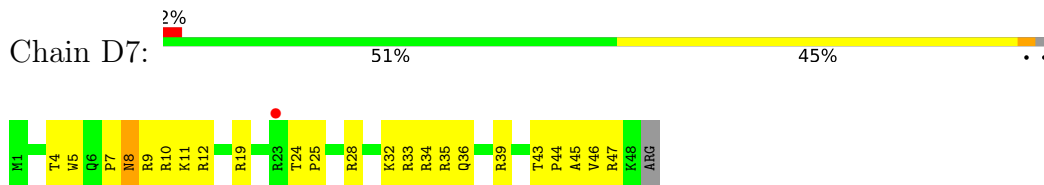
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



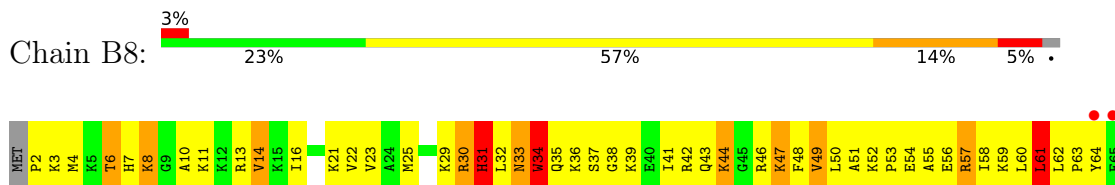
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



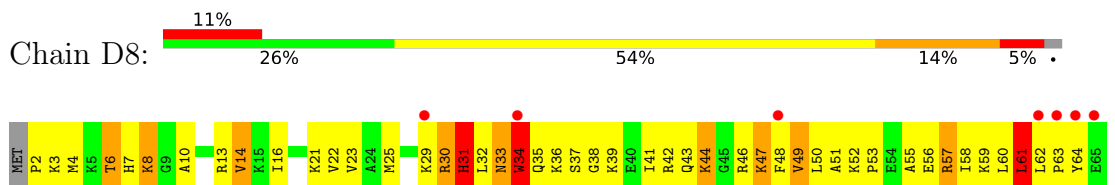
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



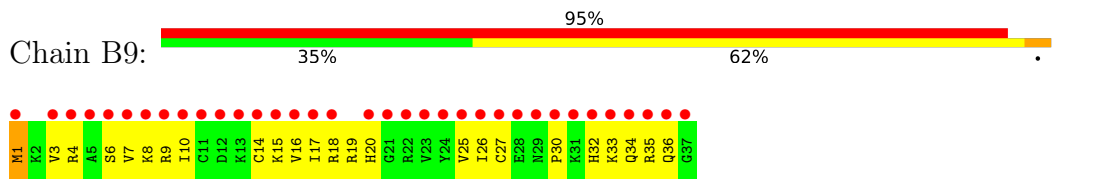
• Molecule 33: 50S RIBOSOMAL PROTEIN L35



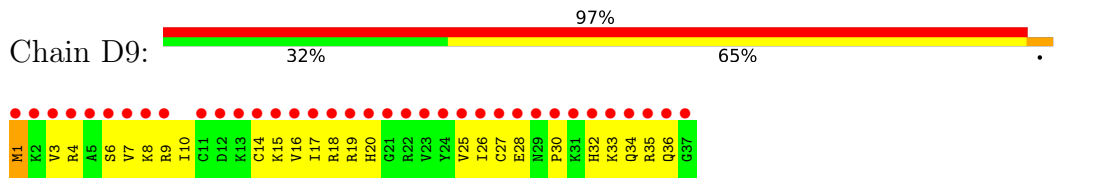
• Molecule 33: 50S RIBOSOMAL PROTEIN L35



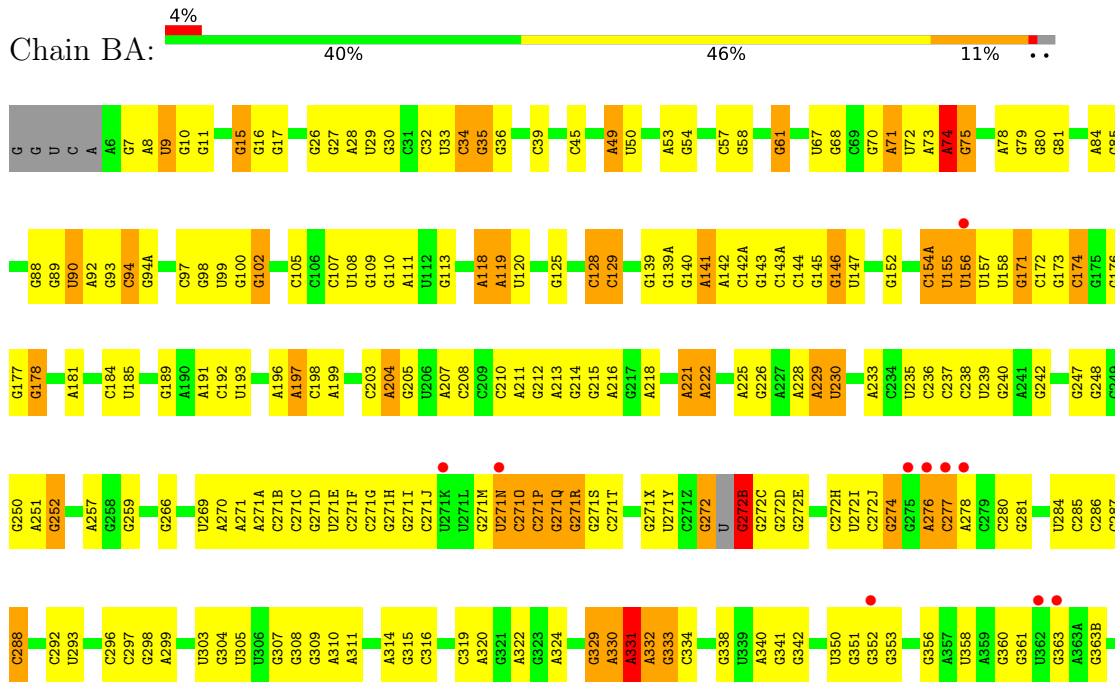
• Molecule 34: 50S RIBOSOMAL PROTEIN L36

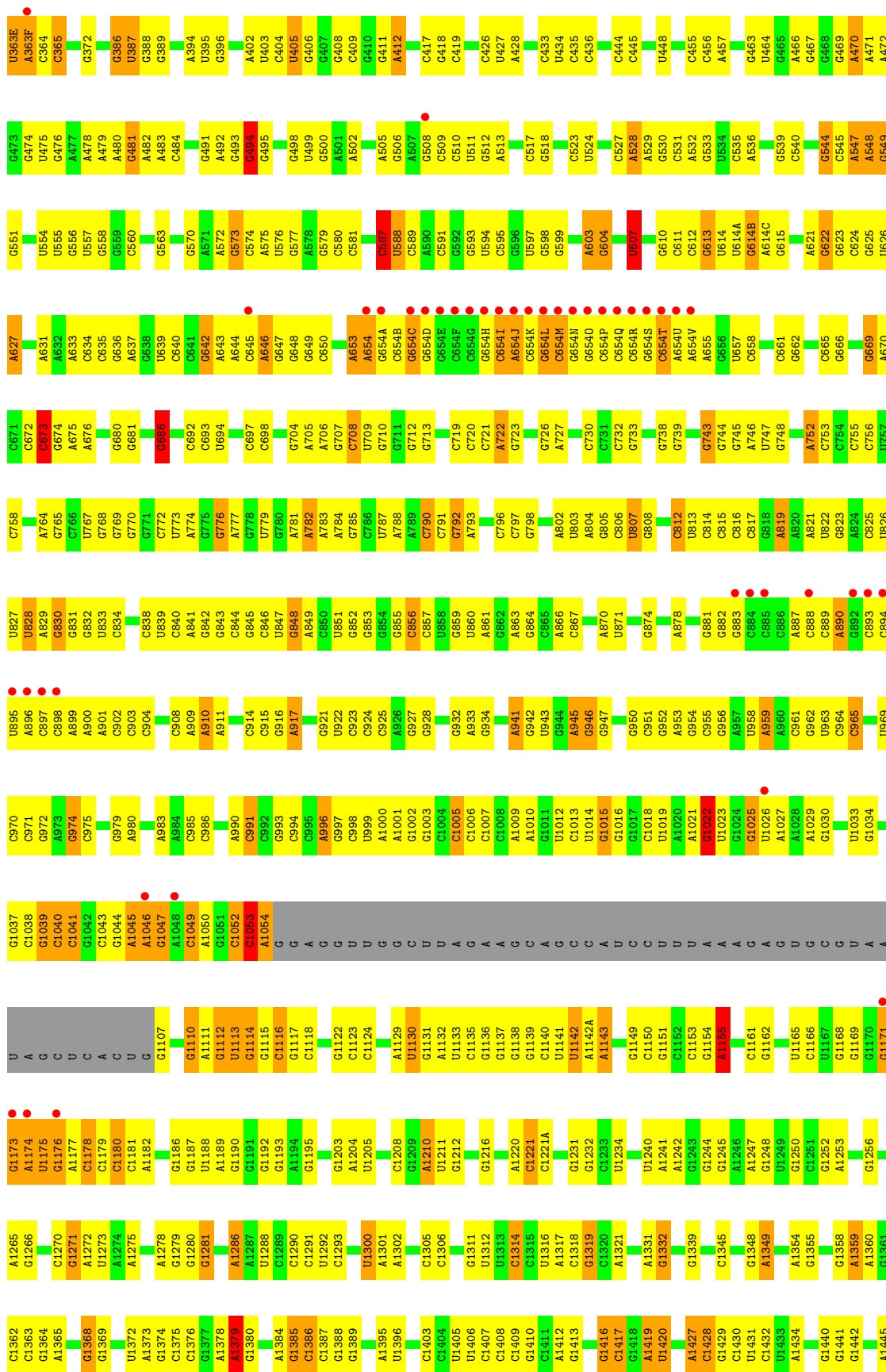


• Molecule 34: 50S RIBOSOMAL PROTEIN L36

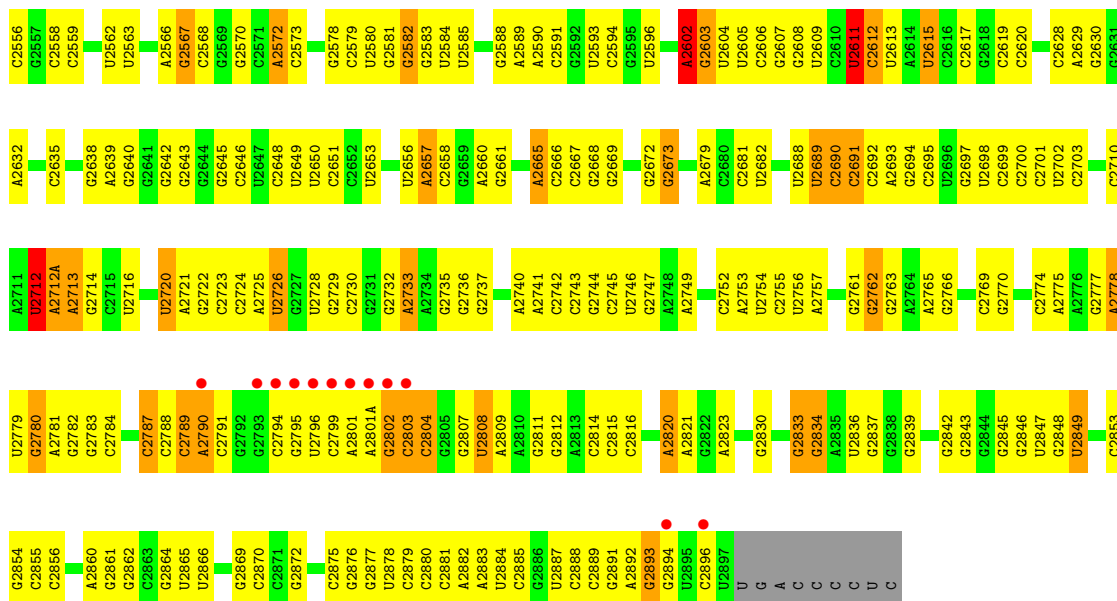


• Molecule 35: 23S RIBOSOMAL RNA

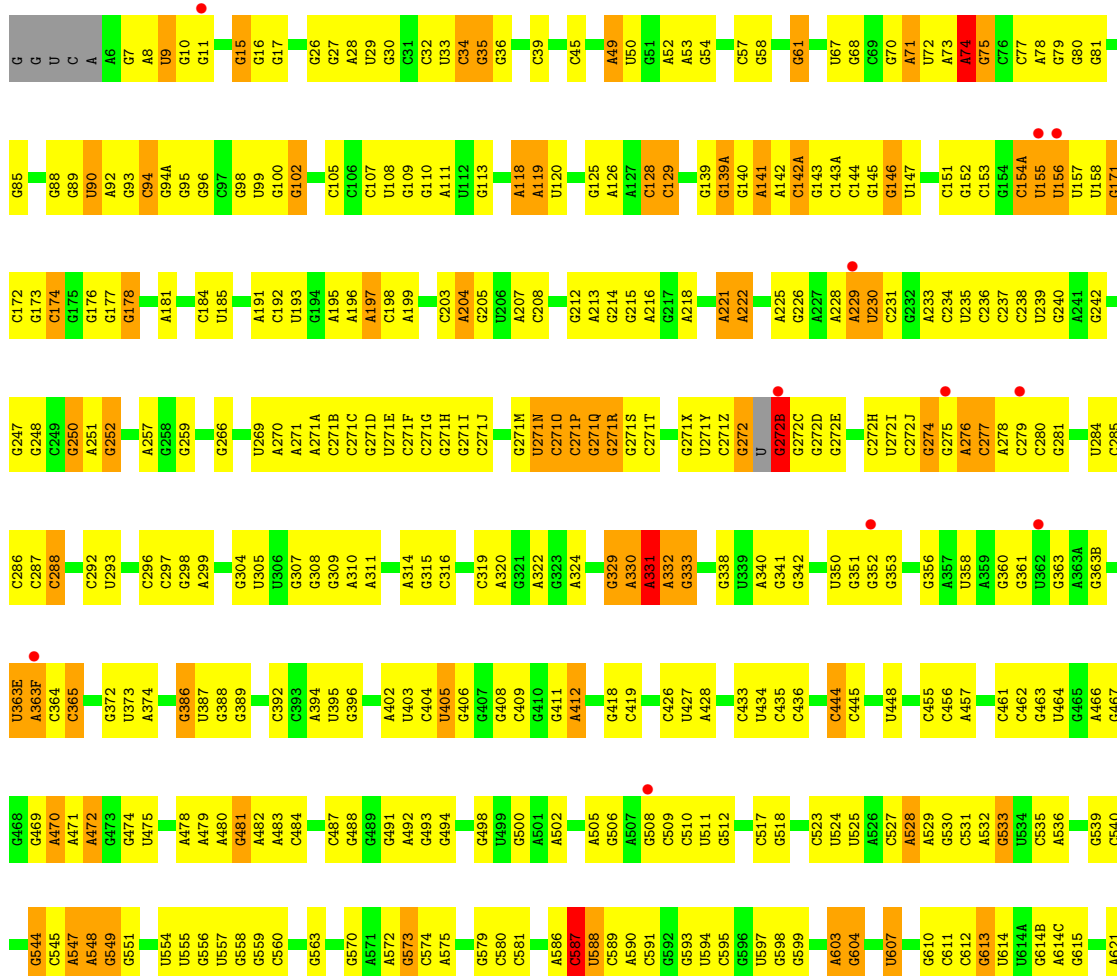




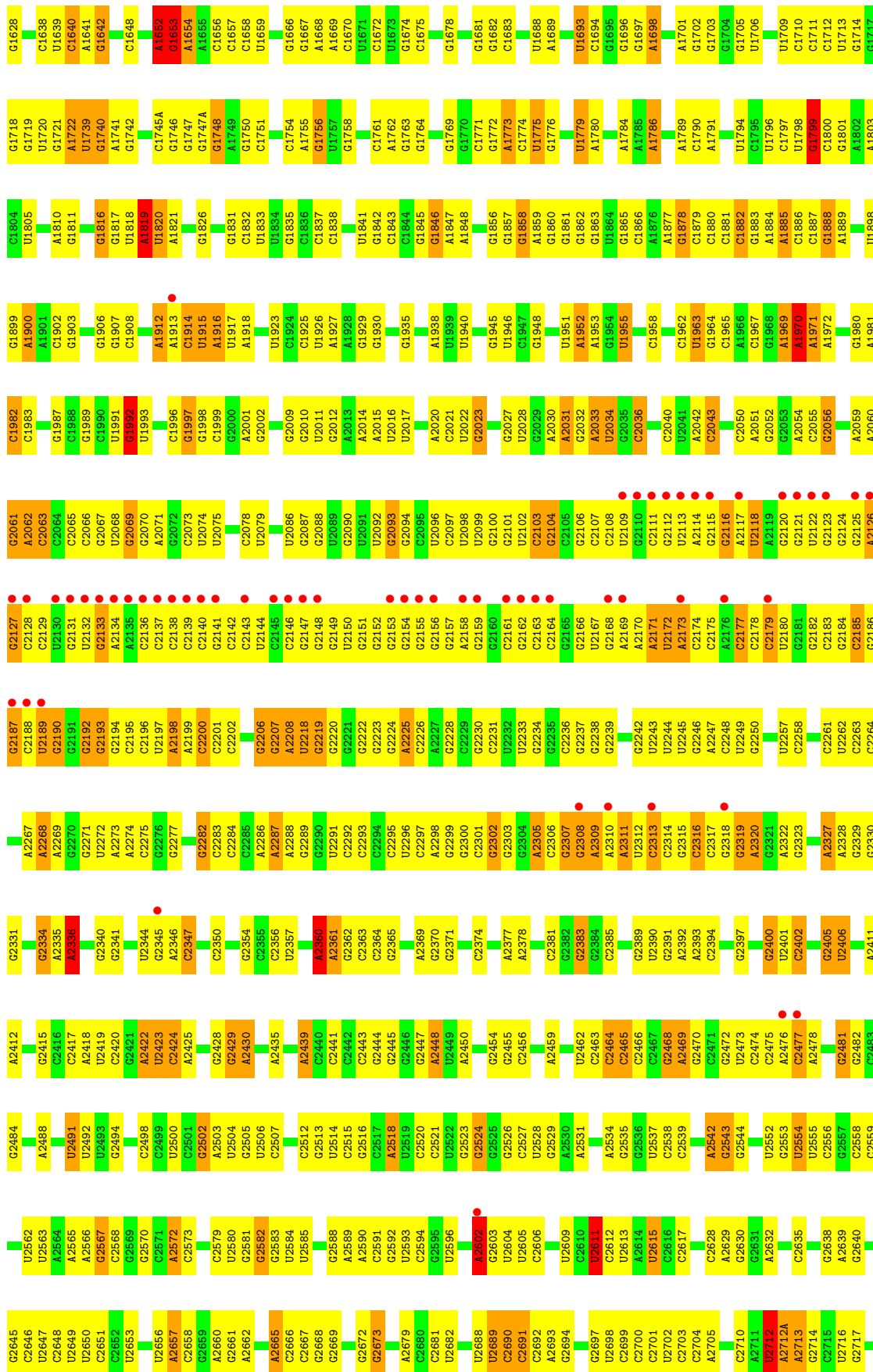
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G2791	G2792	G2793	G2794	G2795	G2796	A2459	G2378	C2312	U2104	G2168	G1932	A1844	G1770	C1651	C1642	G1575	C1513
G2797	G2798	G2799	G2800	G2801	G2802	A2460	G2379	C2313	G2105	G2169	G1933	A1845	G1771	C1652	C1643	G1576	C1514
G2803	G2804	G2805	G2806	G2807	G2808	A2461	G2380	C2314	U2105	G2170	G1934	A1846	G1772	C1653	C1644	G1577	C1515
G2809	G2810	G2811	G2812	G2813	G2814	A2462	G2381	C2315	G2106	G2171	G1935	A1847	G1773	C1654	C1645	G1578	C1516
G2815	G2816	G2817	G2818	G2819	G2820	A2463	G2382	C2316	U2106	G2172	G1936	A1848	G1774	C1655	C1646	G1579	C1517
G2821	G2822	G2823	G2824	G2825	G2826	A2464	G2383	C2317	G2107	G2173	G1937	A1849	G1775	C1656	C1647	G1580	C1518
G2827	G2828	G2829	G2830	G2831	G2832	A2465	G2384	C2318	U2107	G2174	G1938	A1850	G1776	C1657	C1648	G1581	C1519
G2833	G2834	G2835	G2836	G2837	G2838	A2466	G2385	C2319	G2108	G2175	G1939	A1851	G1777	C1658	C1649	G1582	C1520
G2839	G2840	G2841	G2842	G2843	G2844	A2467	G2386	C2320	U2108	G2176	G1940	A1852	G1778	C1659	C1650	G1583	C1521
G2845	G2846	G2847	G2848	G2849	G2850	A2468	G2387	C2321	G2109	G2177	G1941	A1853	G1779	C1660	C1651	G1584	C1522
G2851	G2852	G2853	G2854	G2855	G2856	A2469	G2388	C2322	U2109	G2178	G1942	A1854	G1780	C1661	C1652	G1585	C1523
G2857	G2858	G2859	G2860	G2861	G2862	A2470	G2389	C2323	G2110	G2179	G1943	A1855	G1781	C1662	C1653	G1586	C1524
G2863	G2864	G2865	G2866	G2867	G2868	A2471	G2390	C2324	U2110	G2180	G1944	A1856	G1782	C1663	C1654	G1587	C1525
G2869	G2																

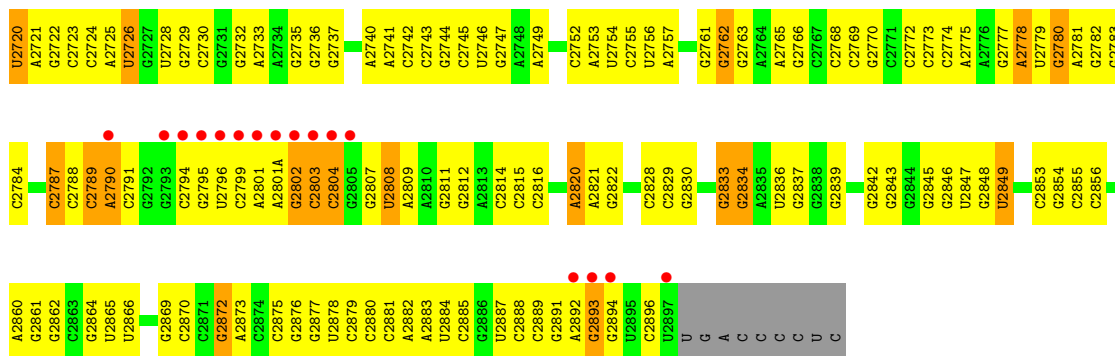


● Molecule 35: 23S RIBOSOMAL RNA

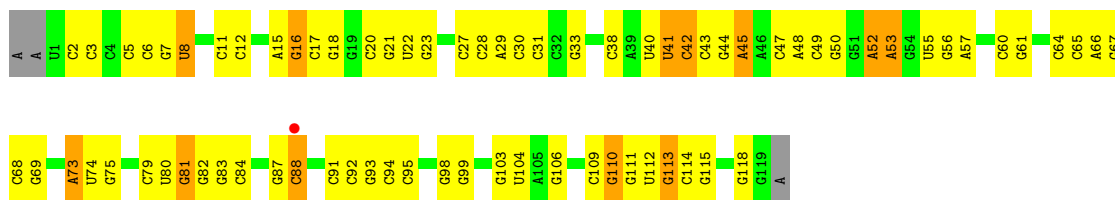


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G1541	C1474	U1397	U1313	U1234	C1150	U1019	G952	U822	C753	G666	G623
A1543	G1475	C1398	C1314	G1235	G1151	A1021	A953	G823	C754	G669	C624
A1544	G1478	G1399	C1315	U1240	C1153	G1022	C955	A824	C755	U825	G625
A1545	G1400	G1401	A1317	A1241	G1154	U1023	G956	C825	C756	A826	A627
C1546	C1318	C1402	C1318	A1242	A1155	G1024	G957	U827	U757	C671	U826
C1547	G1319	C1403	C1319	G1243	A1156	G1025	U958	U828	C758	C672	A627
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C1549	A1321	U1406	A1321	G1245	G1162	A1027	A960	G830	A764	G674	A632
A1554	A1331	C1407	A1331	A1247	U1165	A1028	G961	G831	G765	A675	A633
A1558	G1332	C1408	G1332	U1248	C1166	A1029	G962	G832	G768	A676	A634
G1559	A1336	C1409	A1336	G1249	U1167	G1030	G963	G833	G769	G680	G635
C1564	G1337	G1410	G1337	G1250	U1168	U1033	U964	A835	G770	G681	A637
C1565	G1338	G1411	G1338	C1251	G1169	G1034	A965	G836	G771	A685	G639
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A1570	G1344	G1416	G1344	G1256	G1173	G1039	A973	C839	U773	U688	G642
A1571	C1345	C1417	C1345	G1259	U1174	C1040	A974	A841	G774	C692	A644
A1572	G1348	A1418	G1348	G1260	U1175	G1041	G974	G842	G775	C693	C645
C1501	A1349	A1419	A1349	A1262	A1177	G1042	C975	G843	A777	U694	A646
C1502	A1354	U1420	A1354	G1265	C1178	G1044	G979	G844	U778	G704	G647
U1503	G1355	A1427	G1355	A1266	C1179	A1045	A980	G845	U779	A705	G649
C1504	G1358	C1428	A1358	A1265	C1180	U1046	A983	G846	A782	A706	C850
C1505	A1359	G1429	A1359	G1266	A1181	G1047	A984	U847	C782	A707	A653
C1506	U1360	C1430	U1360	G1270	A1182	U1048	A985	G848	A784	C708	A654
A1507	G1362	U1431	G1362	C1271	G1186	C1049	C985	G852	G785	U709	G654A
A1508	G1363	C1432	G1363	A1272	U1187	A1050	C986	G853	C786	G710	G654B
C1509	A1365	U1433	A1365	A1273	G1188	G1051	A990	G854	U787	G711	G654C
A1509A	G1368	A1434	G1368	G1280	U1189	C1052	C991	G855	A788	G712	G654D
C1584	G1369	U1438	G1369	U1282	A1191	A1054	C992	G856	C790	G713	G654E
A1586	U1372	A1439	U1372	G1283	G1192	G	G993	C857	C791	G717	C654F
A1587	A1373	G1440	A1373	A1284	G1193	G	C994	G858	G792	A718	C654G
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C1589	C1375	G1442	C1375	A1286	U1195	G	A996	U860	C796	C720	C654I
U1602	C1376	A1445	U1376	U1287	G1203	G	C997	A861	C797	C721	C654J
A1603	A1377	G1448	A1377	G1288	G1204	U	C998	G862	A798	A722	C654K
C1607	G1378	A1449	G1378	A1288	U1205	U	C999	A863	G798	G723	C654L
A1608	A1379	G1450	A1379	U1289	U1206	G	A1000	G864	C802	G726	C654M
A1609	G1380	U1453	G1380	U1290	C1208	C	A1001	A866	U802	G727	G654N
A1610	A1384	G1459	A1384	C1291	G1209	U	A1002	G867	U803	A727	G654O
A1614	G1385	A1460	G1385	U1292	A1210	U	C1003	G868	A804	C730	C654P
C1617	C1386	G1461	C1386	C1293	U1211	A	C1004	A870	C906	C736	C654Q
A1618	U1388	A1464	U1388	U1293	G1212	G	C1005	U871	U807	C737	C654R
	G1389	C1467	G1389	G1336	G1215	A	C1006	G874	G808	C738	C654T
	A1395	A1300	A1395	G1137	G1216	G	C1007	U877	C812	G739	A654U
		A1301	A1396	G1138	G1217	A	A1009	U878	U813	G739	A655
		A1302	A1397	G1139	G1218	C	A1010	A879	C813	G743	G656
		C1305	G1388	G1141	A1220	G	A945	G879	C815	G744	U657
		C1306	G1389	U1142	C1221A	C	A946	G880	C816	G745	C658
		G1311	A1395	U1143	U1143	A	G947	G881	C817	A746	C661
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					C	C	G950	G884	A820	G748	

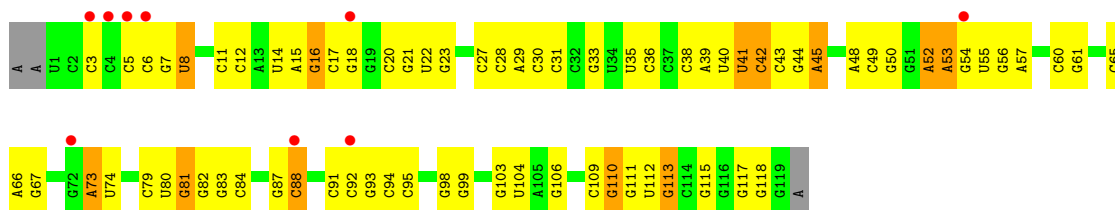




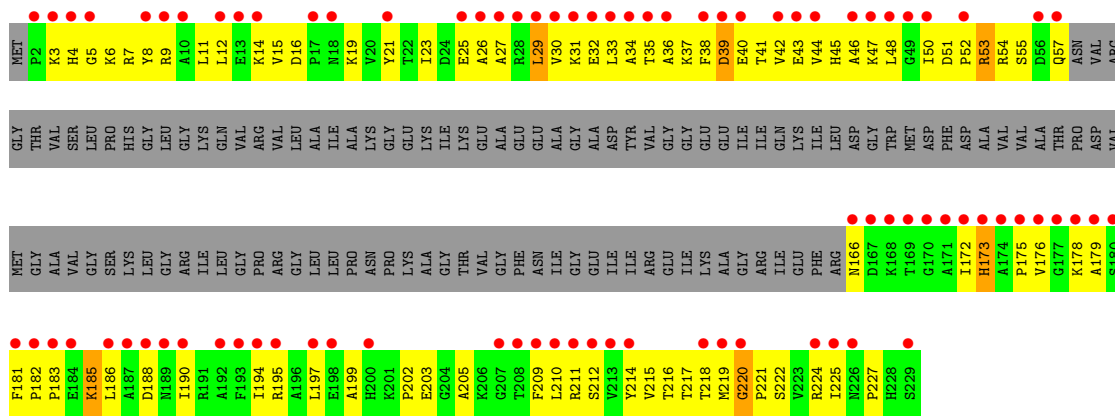
● Molecule 36: 5S RIBOSOMAL RNA



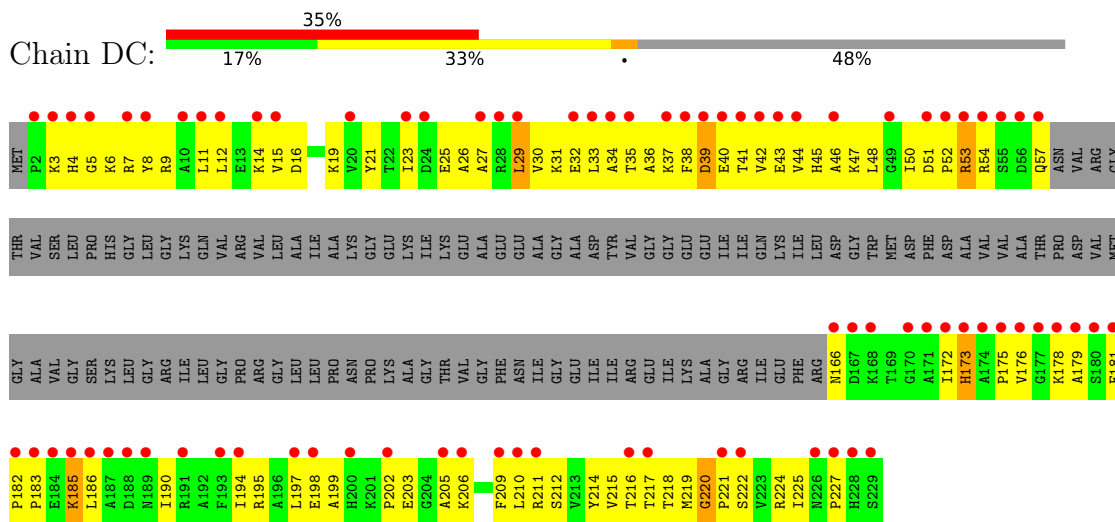
● Molecule 36: 5S RIBOSOMAL RNA



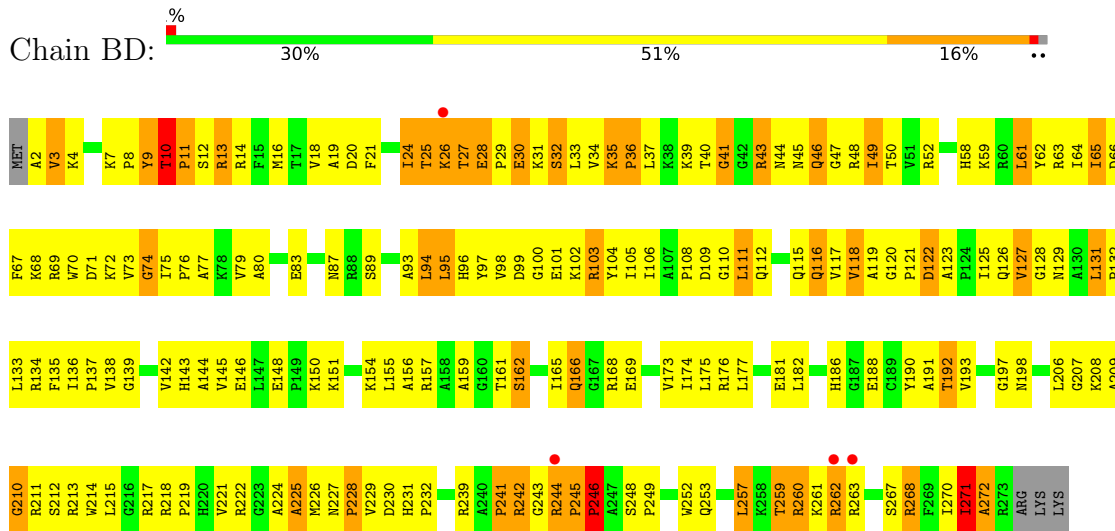
● Molecule 37: 50S RIBOSOMAL PROTEIN L1



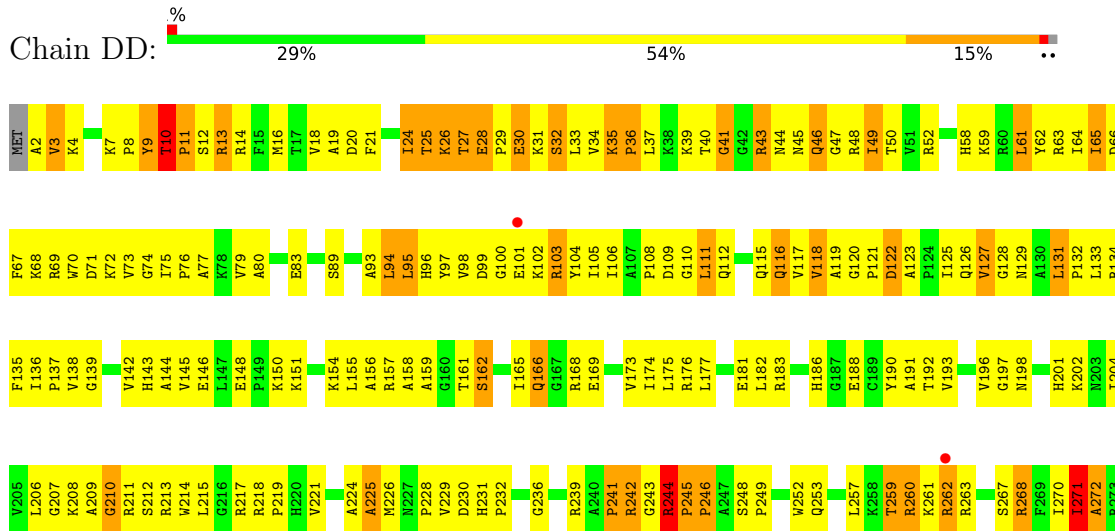
● Molecule 37: 50S RIBOSOMAL PROTEIN L1



• Molecule 38: 50S RIBOSOMAL PROTEIN L2

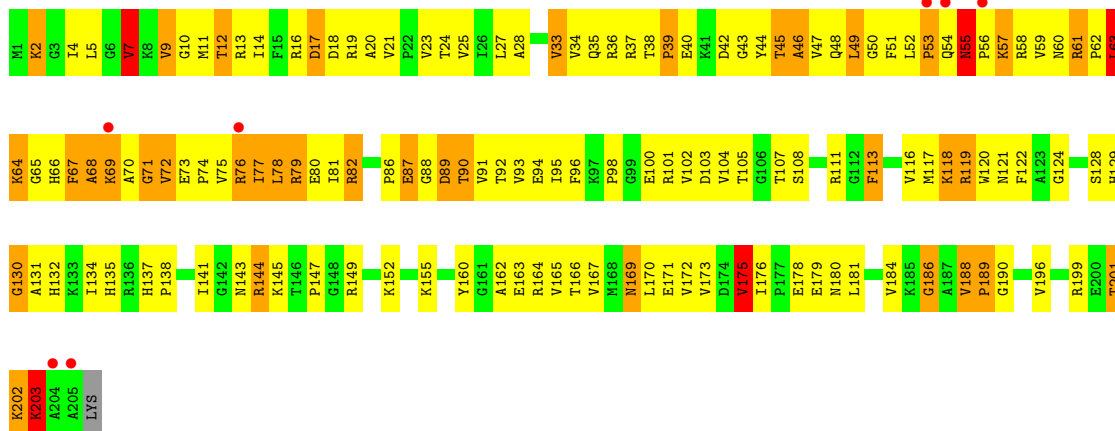


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

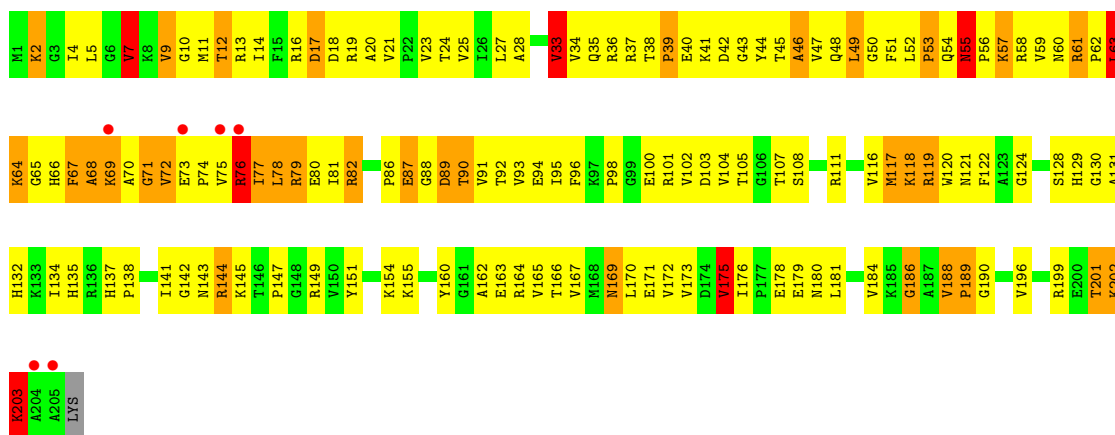
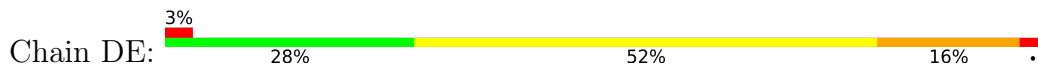


ARG
LYS
LYS

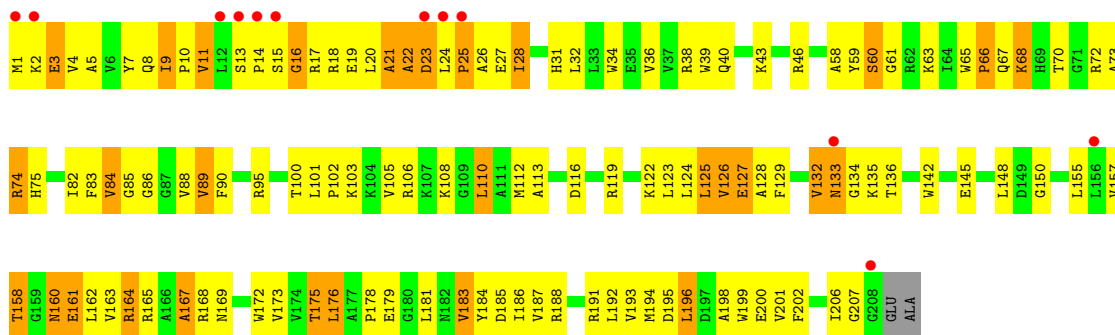
• Molecule 39: 50S RIBOSOMAL PROTEIN L3



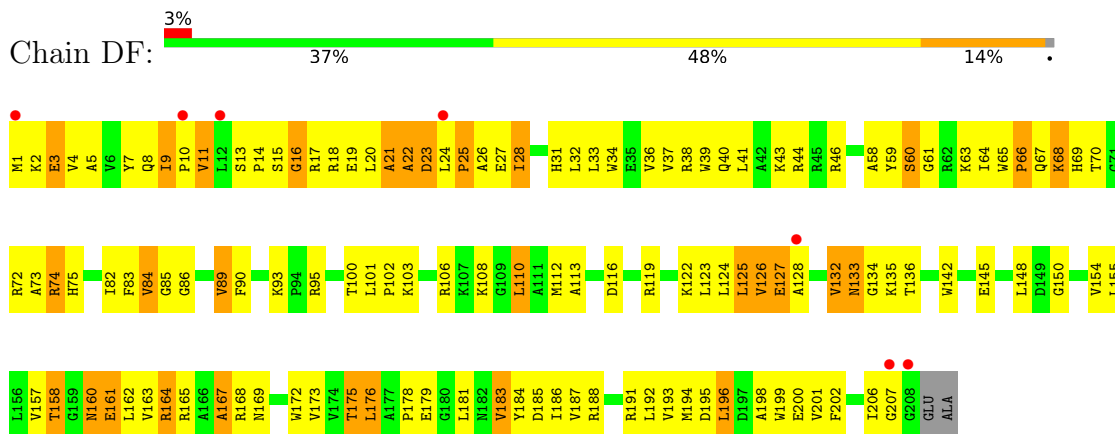
• Molecule 39: 50S RIBOSOMAL PROTEIN L3



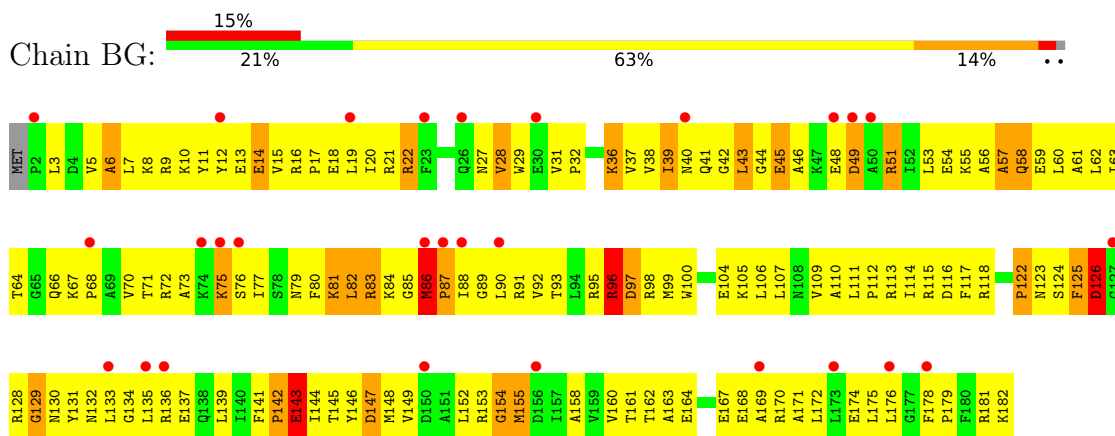
• Molecule 40: 50S RIBOSOMAL PROTEIN L4



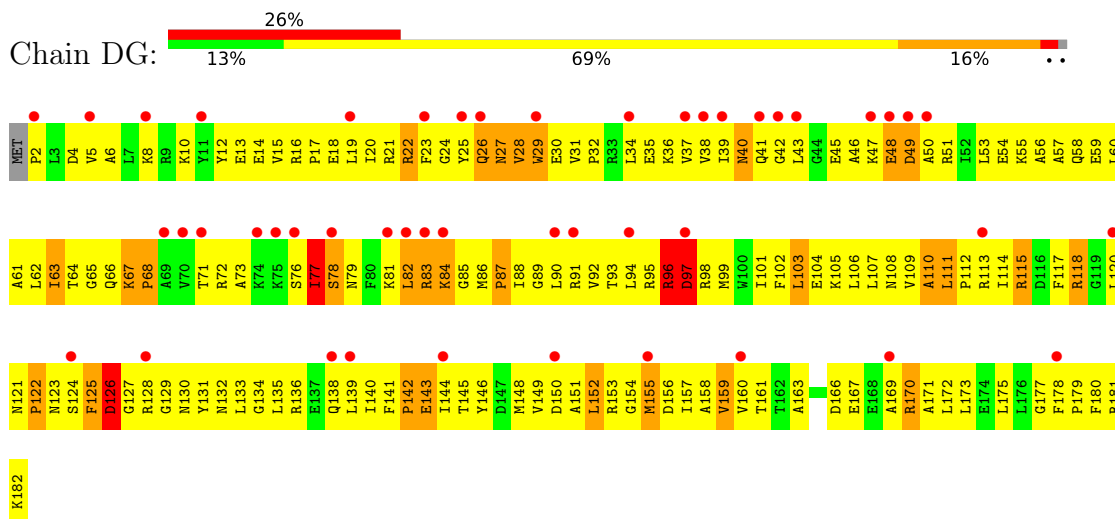
- Molecule 40: 50S RIBOSOMAL PROTEIN L4



- Molecule 41: 50S RIBOSOMAL PROTEIN L5

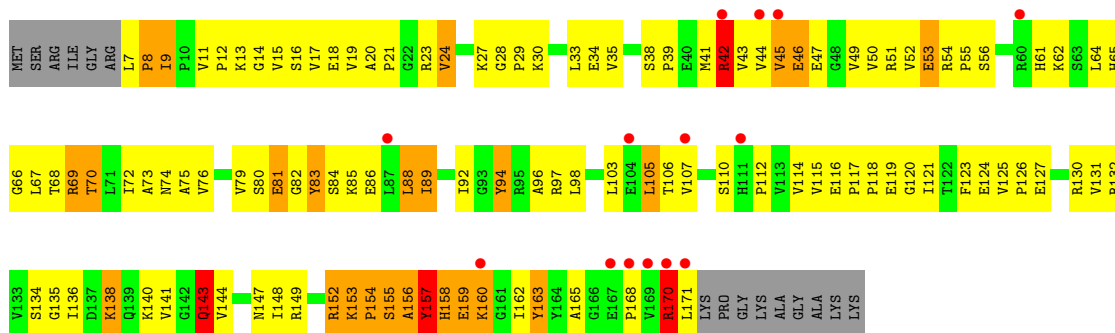


- Molecule 41: 50S RIBOSOMAL PROTEIN L5

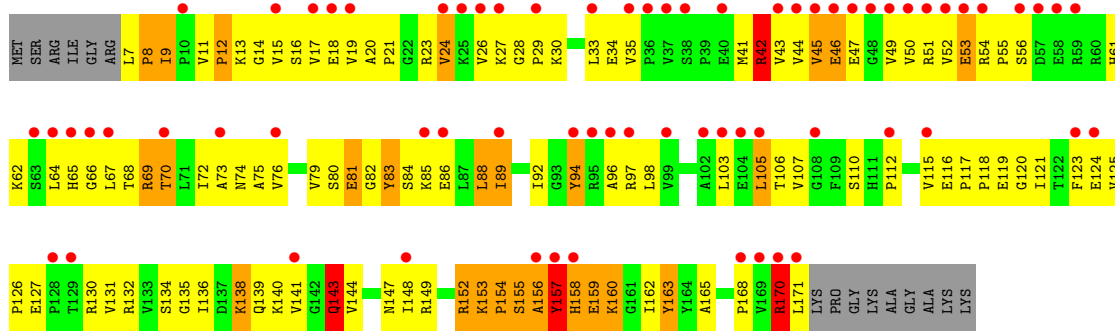


- Molecule 42: 50S RIBOSOMAL PROTEIN L6

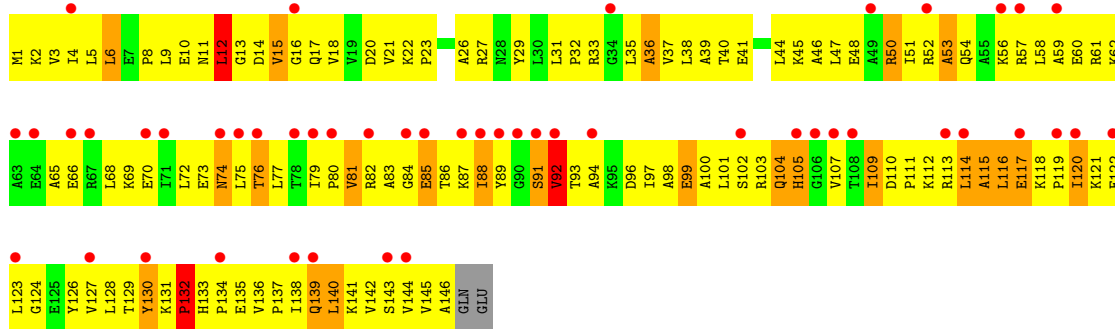




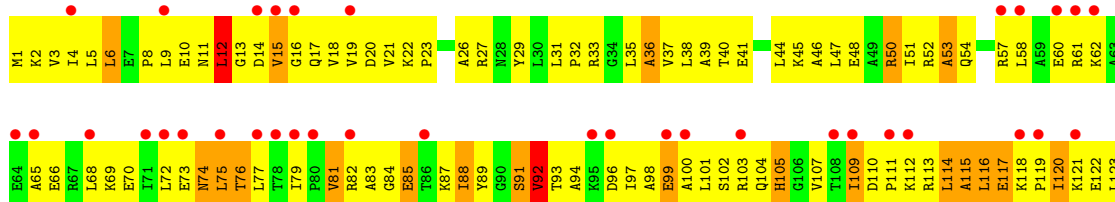
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

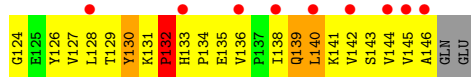


• Molecule 43: 50S RIBOSOMAL PROTEIN L9



• Molecule 43: 50S RIBOSOMAL PROTEIN L9

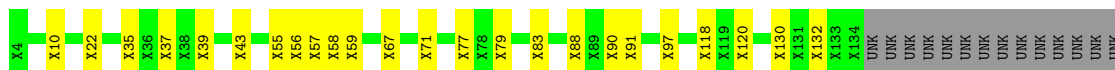




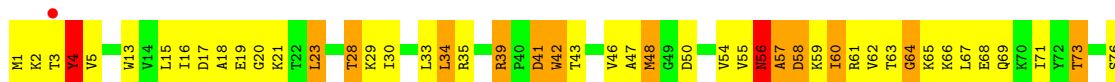
- Molecule 44: 50S RIBOSOMAL PROTEIN L10



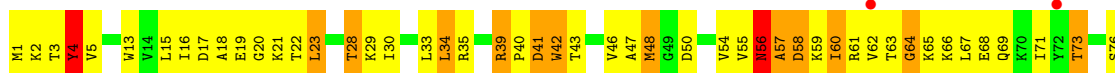
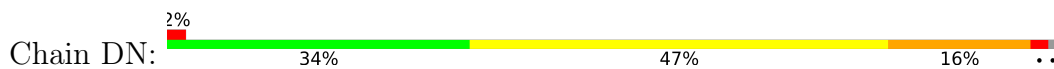
- Molecule 44: 50S RIBOSOMAL PROTEIN L10



- Molecule 45: 50S RIBOSOMAL PROTEIN L13

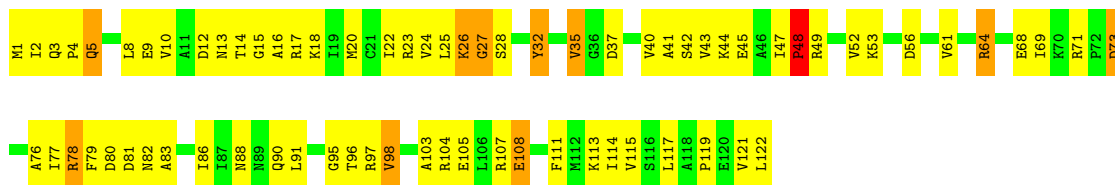


- Molecule 45: 50S RIBOSOMAL PROTEIN L13

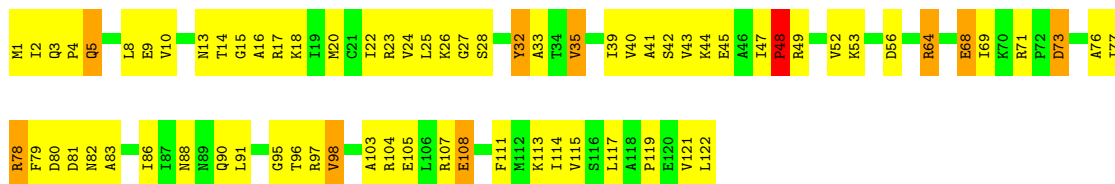


- Molecule 46: 50S RIBOSOMAL PROTEIN L14

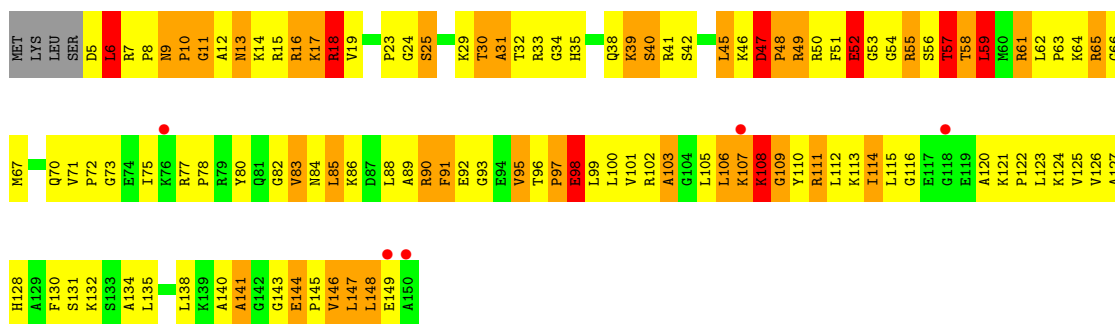
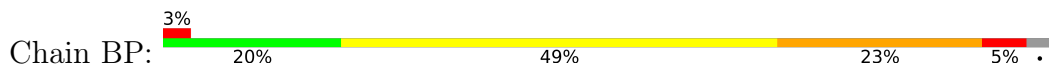




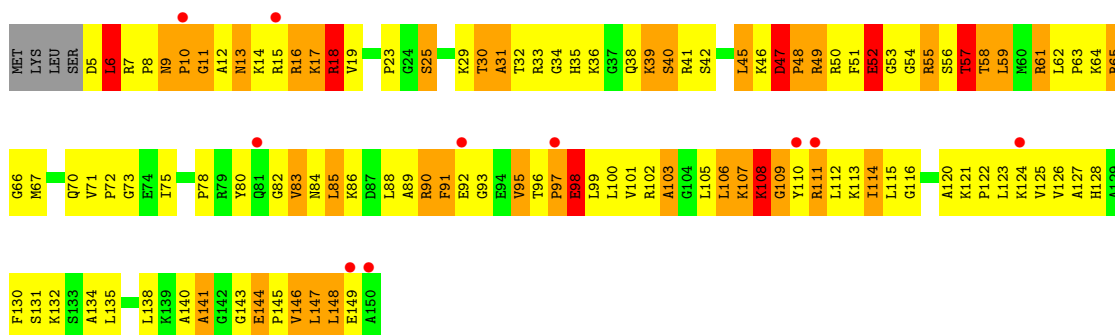
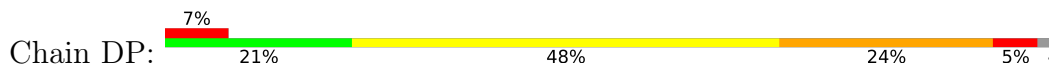
• Molecule 46: 50S RIBOSOMAL PROTEIN L14



• Molecule 47: 50S RIBOSOMAL PROTEIN L15

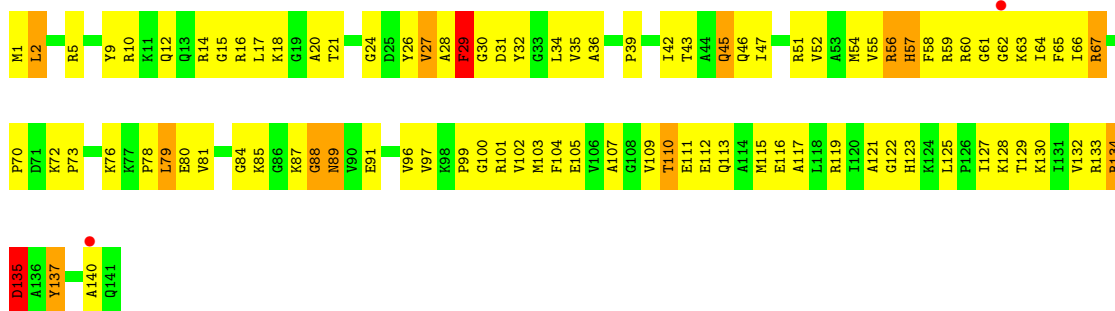


• Molecule 47: 50S RIBOSOMAL PROTEIN L15

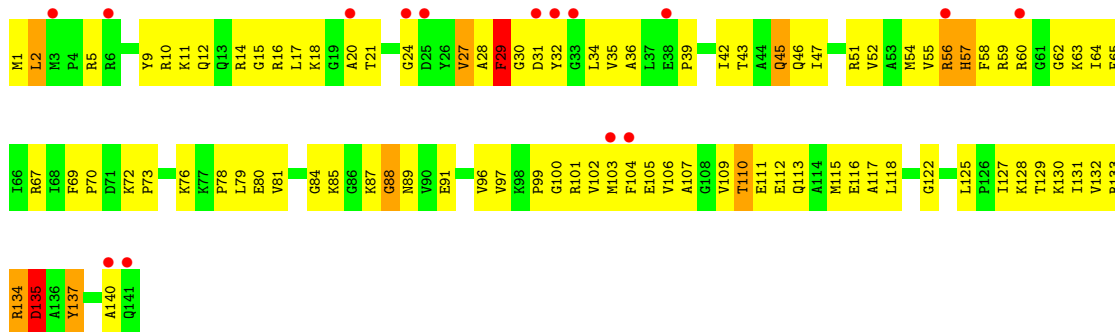


• Molecule 48: 50S RIBOSOMAL PROTEIN L16

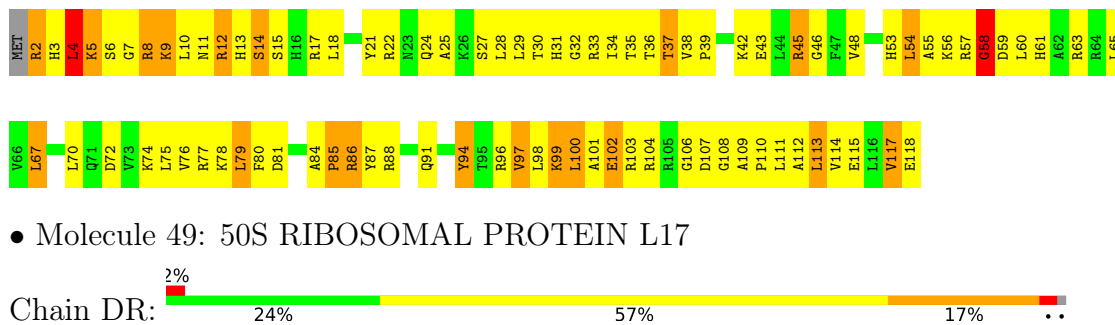




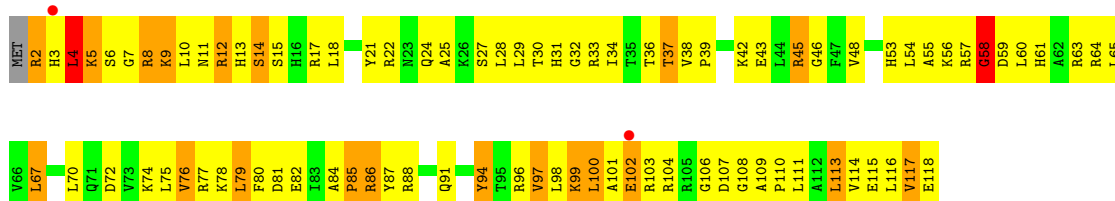
- Molecule 48: 50S RIBOSOMAL PROTEIN L16



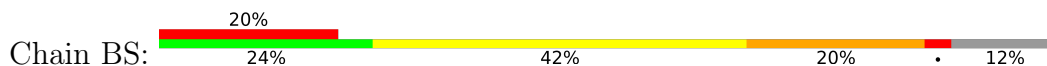
- Molecule 49: 50S RIBOSOMAL PROTEIN L17

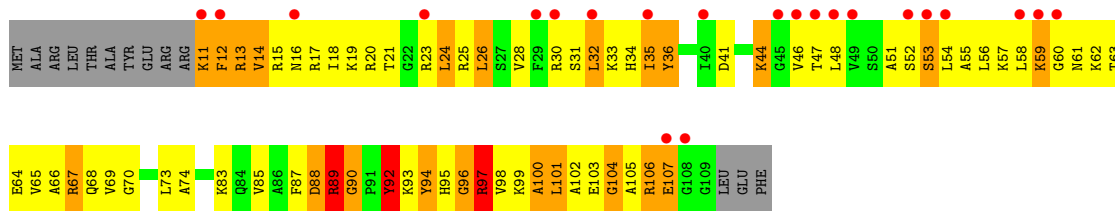


- Molecule 49: 50S RIBOSOMAL PROTEIN L17

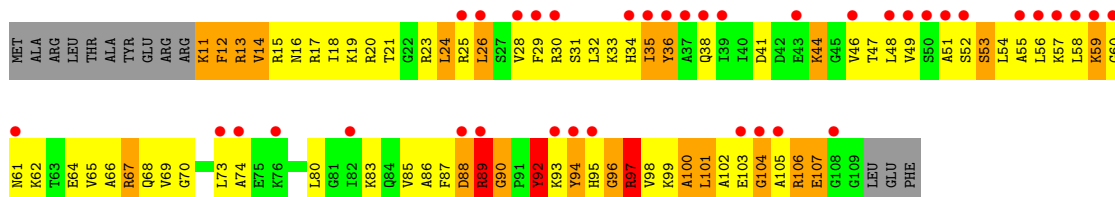
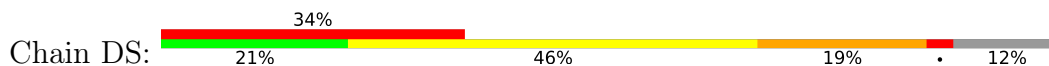


- Molecule 50: 50S RIBOSOMAL PROTEIN L18

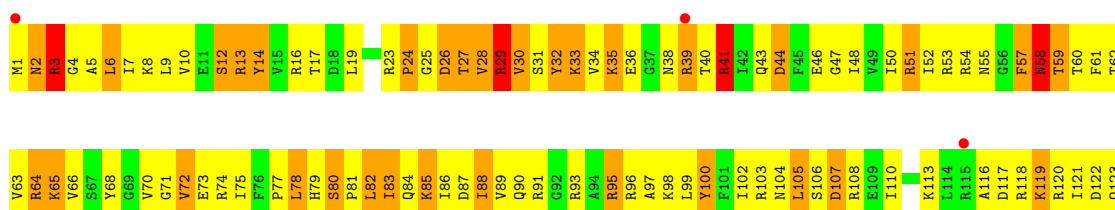
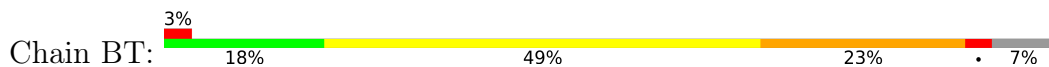




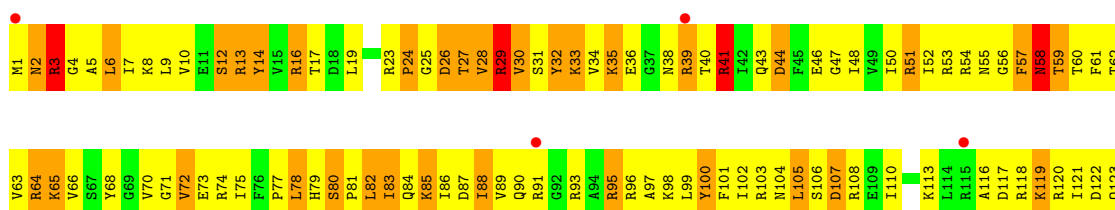
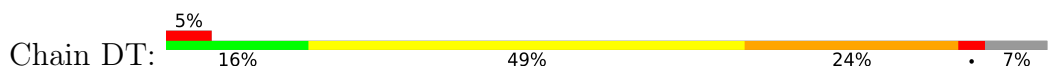
● Molecule 50: 50S RIBOSOMAL PROTEIN L18



● Molecule 51: 50S RIBOSOMAL PROTEIN L19

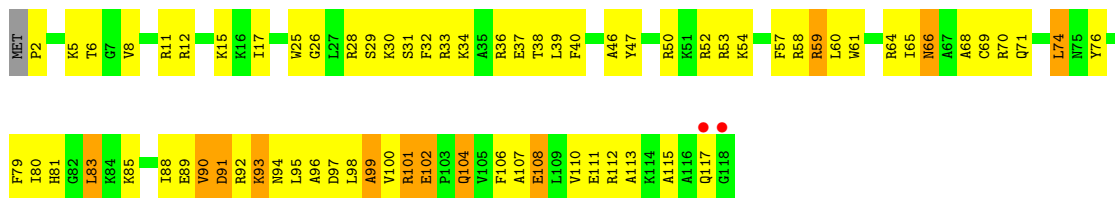


● Molecule 51: 50S RIBOSOMAL PROTEIN L19

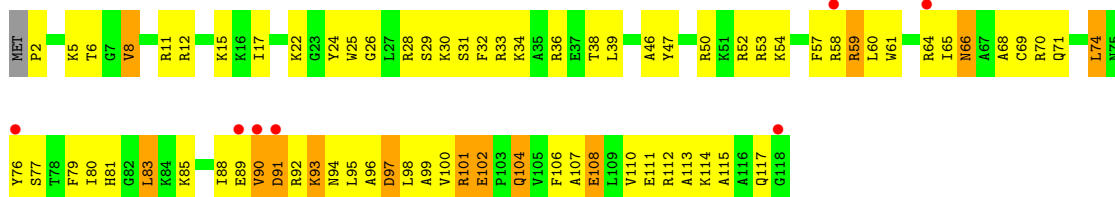


● Molecule 52: 50S RIBOSOMAL PROTEIN L20

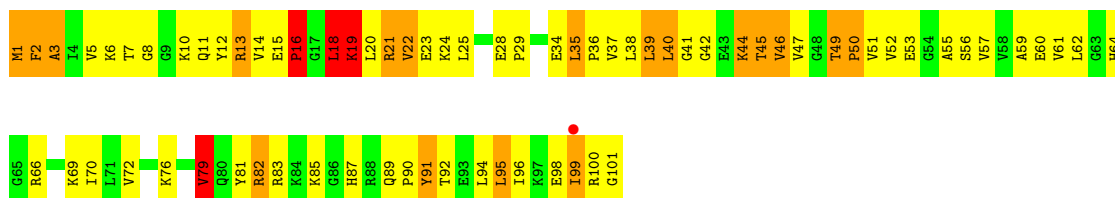




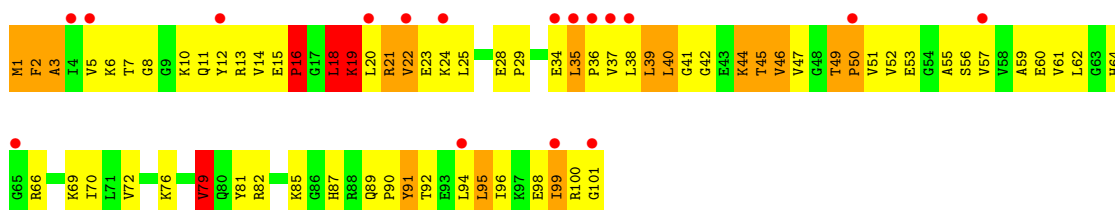
● Molecule 52: 50S RIBOSOMAL PROTEIN L20



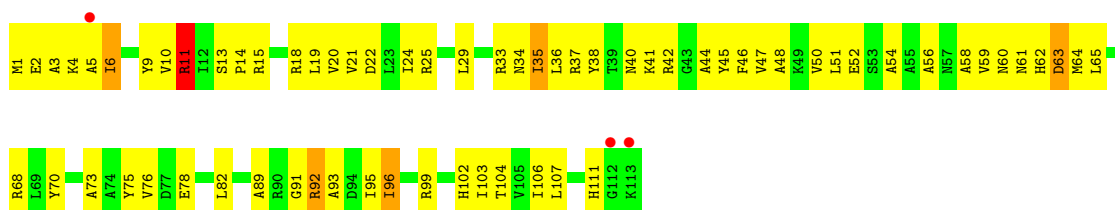
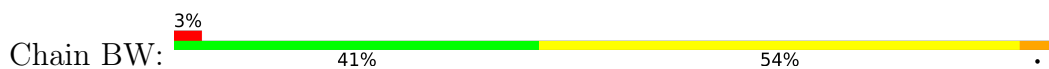
● Molecule 53: 50S RIBOSOMAL PROTEIN L21



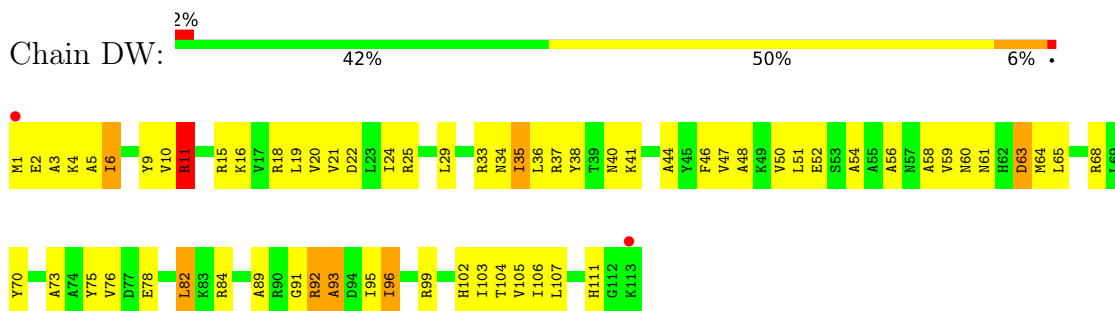
● Molecule 53: 50S RIBOSOMAL PROTEIN L21



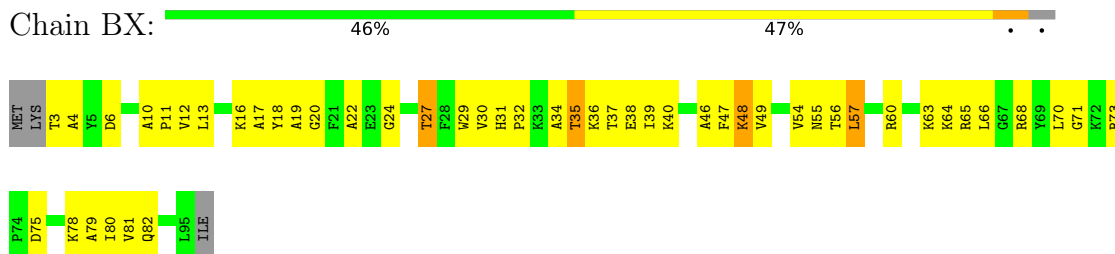
● Molecule 54: 50S RIBOSOMAL PROTEIN L22



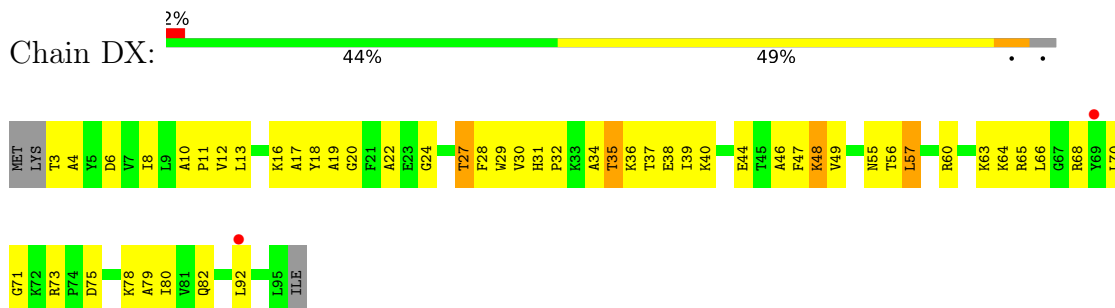
● Molecule 54: 50S RIBOSOMAL PROTEIN L22



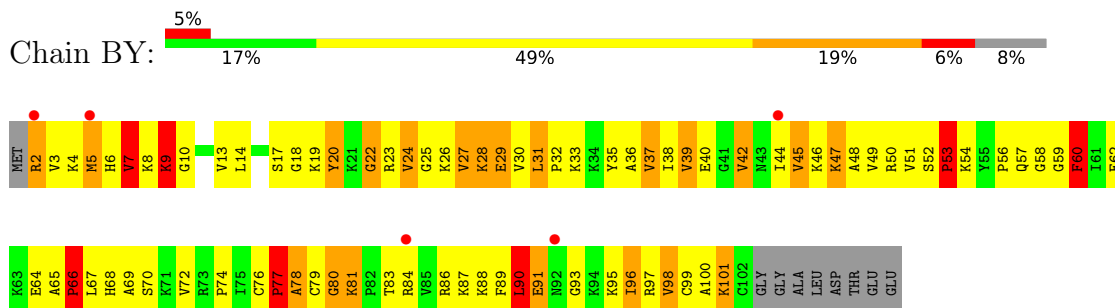
• Molecule 55: 50S RIBOSOMAL PROTEIN L23



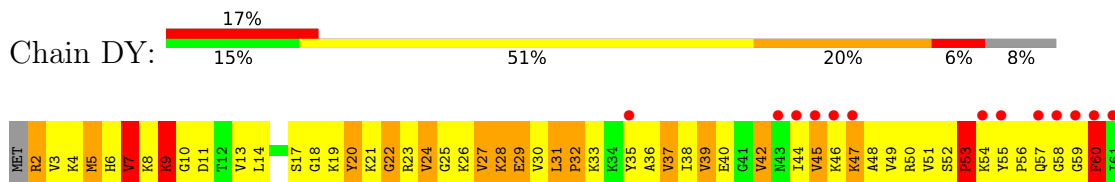
• Molecule 55: 50S RIBOSOMAL PROTEIN L23



• Molecule 56: 50S RIBOSOMAL PROTEIN L24

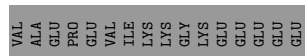
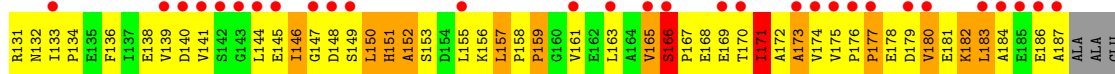
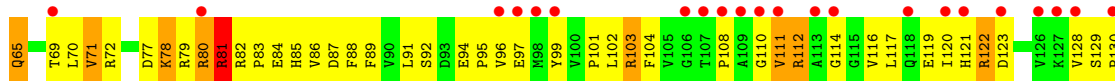
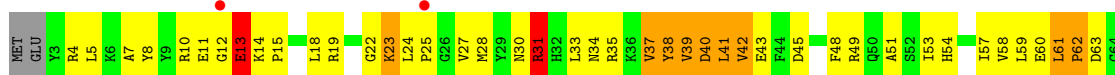


• Molecule 56: 50S RIBOSOMAL PROTEIN L24

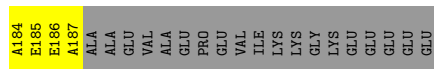
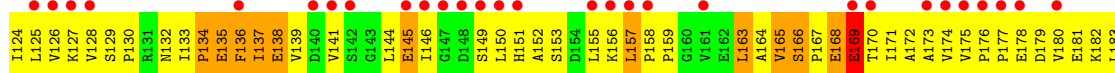
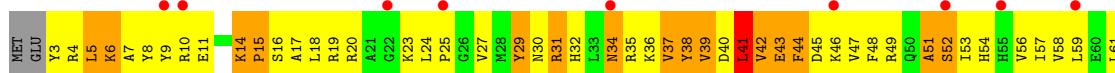
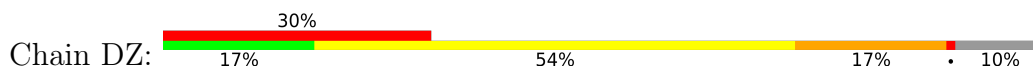




• Molecule 57: 50S RIBOSOMAL PROTEIN L25



• Molecule 57: 50S RIBOSOMAL PROTEIN L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.90Å 450.79Å 625.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.95 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-3.10) 97.6 (49.95-3.10)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.12Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.250 , 0.280 0.273 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtrriage
Anisotropy	0.237	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 91.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	298096	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AG9, ZN

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	0.44	0/36190	0.70	7/56486 (0.0%)
1	CA	0.42	0/36190	0.70	7/56486 (0.0%)
2	AB	0.30	0/1936	0.58	0/2611
2	CB	0.31	0/1936	0.58	0/2611
3	AC	0.31	0/1637	0.56	0/2207
3	CC	0.31	0/1637	0.56	0/2207
4	AD	0.37	0/1733	0.61	0/2318
4	CD	0.36	0/1733	0.60	0/2318
5	AE	0.36	0/1163	0.62	0/1566
5	CE	0.36	0/1163	0.63	0/1566
6	AF	0.34	0/856	0.59	0/1154
6	CF	0.34	0/856	0.59	0/1154
7	AG	0.29	0/1276	0.52	0/1709
7	CG	0.30	0/1276	0.52	0/1709
8	AH	0.32	0/1136	0.60	0/1527
8	CH	0.33	0/1136	0.60	0/1527
9	AI	0.31	0/1027	0.54	0/1373
9	CI	0.31	0/1027	0.55	0/1373
10	AJ	0.33	0/808	0.58	0/1087
10	CJ	0.33	0/808	0.57	0/1087
11	AK	0.33	0/900	0.60	0/1213
11	CK	0.33	0/900	0.60	0/1213
12	AL	0.46	0/987	0.79	0/1322
12	CL	0.43	0/987	0.78	0/1322
13	AM	0.32	0/943	0.61	0/1256
13	CM	0.33	0/943	0.61	0/1256
14	AN	0.31	0/501	0.51	0/664
14	CN	0.33	0/501	0.51	0/664
15	AO	0.33	0/745	0.58	0/992
15	CO	0.35	0/745	0.58	0/992
16	AP	0.38	0/717	0.61	0/965
16	CP	0.37	0/717	0.60	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.39	0/837	0.63	0/1119
17	CQ	0.37	0/837	0.62	0/1119
18	AR	0.33	0/579	0.64	0/768
18	CR	0.32	0/579	0.64	0/768
19	AS	0.36	0/643	0.58	0/867
19	CS	0.37	0/643	0.58	0/867
20	AT	0.32	0/765	0.54	0/1007
20	CT	0.31	0/765	0.54	0/1007
21	AU	0.42	0/213	0.53	0/279
21	CU	0.43	0/213	0.53	0/279
22	AV	1.84	39/1830 (2.1%)	0.95	3/2849 (0.1%)
22	AY	1.92	52/1830 (2.8%)	0.98	2/2849 (0.1%)
22	CV	0.88	0/1830	0.88	3/2849 (0.1%)
22	CY	1.56	22/1830 (1.2%)	1.25	27/2849 (0.9%)
23	AW	2.12	62/1853 (3.3%)	1.06	9/2887 (0.3%)
23	CW	0.83	0/1853	0.99	8/2887 (0.3%)
24	AX	0.55	0/290	0.83	0/450
24	CX	0.81	0/290	0.81	0/450
25	B0	0.42	0/671	0.62	0/892
25	D0	0.38	0/671	0.62	0/892
26	B1	0.48	0/741	0.78	2/986 (0.2%)
26	D1	0.44	0/741	0.76	0/986
27	B2	0.43	0/600	0.74	0/793
27	D2	0.34	0/600	0.59	0/793
28	B3	0.43	0/473	0.66	1/636 (0.2%)
28	D3	0.40	0/473	0.67	0/636
29	B4	0.38	0/461	0.64	0/623
29	D4	0.38	0/461	0.64	0/623
30	B5	0.56	0/442	0.73	0/598
30	D5	0.48	0/442	0.72	0/598
31	B6	0.37	0/440	0.72	1/586 (0.2%)
31	D6	0.37	0/440	0.72	1/586 (0.2%)
32	B7	0.54	0/418	0.65	0/552
32	D7	0.51	0/418	0.66	0/552
33	B8	0.59	0/516	0.84	0/681
33	D8	0.52	0/516	0.84	0/681
34	B9	0.31	0/310	0.59	0/407
34	D9	0.32	0/310	0.58	0/407
35	BA	0.60	1/68704 (0.0%)	0.73	42/107260 (0.0%)
35	DA	0.51	0/68704	0.73	35/107260 (0.0%)
36	BB	0.41	0/2853	0.69	0/4451
36	DB	0.38	0/2853	0.69	0/4451
37	BC	0.30	0/956	0.53	0/1288

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.31	0/956	0.53	0/1288
38	BD	0.50	0/2155	0.78	2/2907 (0.1%)
38	DD	0.46	0/2155	0.78	3/2907 (0.1%)
39	BE	0.50	0/1597	0.74	0/2155
39	DE	0.45	0/1597	0.74	0/2155
40	BF	0.46	0/1659	0.69	0/2246
40	DF	0.42	0/1659	0.68	0/2246
41	BG	0.35	0/1498	0.67	0/2013
41	DG	0.34	0/1498	0.67	0/2013
42	BH	0.36	0/1285	0.70	1/1741 (0.1%)
42	DH	0.37	0/1285	0.69	1/1741 (0.1%)
43	BI	0.36	0/1147	0.86	3/1553 (0.2%)
43	DI	0.35	0/1147	0.85	3/1553 (0.2%)
45	BN	0.43	0/1132	0.70	0/1527
45	DN	0.41	0/1132	0.69	0/1527
46	BO	0.46	0/943	0.67	0/1269
46	DO	0.45	0/943	0.69	0/1269
47	BP	0.47	0/1131	0.93	5/1504 (0.3%)
47	DP	0.42	0/1131	0.92	4/1504 (0.3%)
48	BQ	0.43	0/1134	0.59	0/1517
48	DQ	0.42	0/1134	0.59	0/1517
49	BR	0.45	0/974	0.78	2/1302 (0.2%)
49	DR	0.42	0/974	0.78	2/1302 (0.2%)
50	BS	0.36	0/779	0.63	0/1038
50	DS	0.36	0/779	0.64	0/1038
51	BT	0.44	0/1138	0.76	1/1521 (0.1%)
51	DT	0.44	0/1138	0.76	1/1521 (0.1%)
52	BU	0.50	0/975	0.69	0/1297
52	DU	0.45	0/975	0.67	0/1297
53	BV	0.40	0/790	0.70	0/1057
53	DV	0.38	0/790	0.69	0/1057
54	BW	0.52	0/907	0.73	0/1216
54	DW	0.45	0/907	0.73	0/1216
55	BX	0.46	0/740	0.69	0/995
55	DX	0.45	0/740	0.69	0/995
56	BY	0.46	0/789	0.72	1/1053 (0.1%)
56	DY	0.42	0/789	0.71	1/1053 (0.1%)
57	BZ	0.44	0/1500	0.68	0/2037
57	DZ	0.38	0/1500	0.64	0/2037
All	All	0.56	176/322506 (0.1%)	0.72	178/482452 (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	18
1	CA	0	19
22	AV	1	17
22	AY	1	19
22	CV	1	10
22	CY	1	17
23	AW	0	21
23	CW	0	11
35	BA	5	46
35	DA	4	41
All	All	13	219

The worst 5 of 176 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CY	56	U	C2-N3	28.94	1.58	1.37
22	CY	57	U	C3'-O3'	17.68	1.67	1.42
22	CY	56	U	N3-C4	14.74	1.51	1.38
22	CY	56	U	N1-C2	13.32	1.50	1.38
22	CY	58	C	P-O5'	12.55	1.72	1.59

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CY	56	U	C5-C6-N1	16.14	130.77	122.70
43	BI	50	ARG	NE-CZ-NH1	13.96	127.28	120.30
43	BI	50	ARG	NE-CZ-NH2	-13.50	113.55	120.30
43	DI	50	ARG	NE-CZ-NH2	-13.46	113.57	120.30
43	DI	50	ARG	NE-CZ-NH1	13.32	126.96	120.30

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	AV	36	AG9	C4
22	AY	36	AG9	C4
35	BA	752	A	C3'
35	BA	790	C	C3'
35	BA	1799	G	C3'

5 of 219 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	265	G	Sidechain
1	AA	292	G	Sidechain
1	AA	387	U	Sidechain
1	AA	436	C	Sidechain
1	AA	97	G	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1334	0
1	CA	32329	0	16318	1413	0
2	AB	1901	0	1951	265	0
2	CB	1901	0	1951	274	0
3	AC	1613	0	1677	225	0
3	CC	1613	0	1677	239	0
4	AD	1703	0	1765	229	1
4	CD	1703	0	1766	226	0
5	AE	1147	0	1207	149	0
5	CE	1147	0	1207	155	0
6	AF	843	0	857	81	0
6	CF	843	0	857	81	1
7	AG	1257	0	1296	124	0
7	CG	1257	0	1296	123	0
8	AH	1116	0	1177	123	0
8	CH	1116	0	1177	126	0
9	AI	1010	0	1035	154	0
9	CI	1010	0	1035	159	0
10	AJ	795	0	840	181	0
10	CJ	795	0	840	178	0
11	AK	885	0	904	85	0
11	CK	885	0	904	85	0
12	AL	971	0	1057	215	0
12	CL	971	0	1057	213	0
13	AM	938	0	991	131	0
13	CM	938	0	991	131	0
14	AN	492	0	531	49	0
14	CN	492	0	532	54	0
15	AO	734	0	771	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	734	0	771	62	0
16	AP	701	0	720	83	0
16	CP	701	0	720	82	0
17	AQ	824	0	891	83	0
17	CQ	824	0	891	79	0
18	AR	574	0	644	72	0
18	CR	574	0	644	73	0
19	AS	630	0	652	87	0
19	CS	630	0	652	79	0
20	AT	763	0	861	90	0
20	CT	763	0	861	85	0
21	AU	209	0	221	22	0
21	CU	209	0	221	24	0
22	AV	1667	0	857	264	0
22	AY	1667	0	857	326	0
22	CV	1667	0	857	235	0
22	CY	1667	0	854	329	0
23	AW	1659	0	843	396	0
23	CW	1659	0	843	323	0
24	AX	257	0	132	12	0
24	CX	257	0	132	35	0
25	B0	662	0	688	69	0
25	D0	662	0	688	72	0
26	B1	734	0	808	71	0
26	D1	734	0	808	87	0
27	B2	598	0	653	72	0
27	D2	598	0	653	70	0
28	B3	468	0	523	35	0
28	D3	468	0	523	37	0
29	B4	451	0	449	97	0
29	D4	451	0	449	82	0
30	B5	428	0	445	73	0
30	D5	428	0	445	72	0
31	B6	433	0	461	85	0
31	D6	433	0	461	86	0
32	B7	410	0	454	23	0
32	D7	410	0	454	24	0
33	B8	508	0	576	110	0
33	D8	508	0	576	110	0
34	B9	307	0	338	28	0
34	D9	307	0	338	32	0
35	BA	61341	0	30928	1763	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	DA	61341	0	30928	1842	0
36	BB	2551	0	1295	93	0
36	DB	2551	0	1295	112	0
37	BC	937	0	957	113	0
37	DC	937	0	957	112	0
38	BD	2105	0	2182	267	0
38	DD	2105	0	2182	278	0
39	BE	1564	0	1629	236	0
39	DE	1564	0	1629	240	0
40	BF	1624	0	1677	169	0
40	DF	1624	0	1677	173	0
41	BG	1474	0	1534	248	0
41	DG	1474	0	1534	305	0
42	BH	1260	0	1326	154	0
42	DH	1260	0	1326	157	0
43	BI	1132	0	1218	204	0
43	DI	1132	0	1218	196	0
44	BJ	651	0	166	32	0
44	DJ	651	0	170	17	0
45	BN	1105	0	1180	145	0
45	DN	1105	0	1180	150	0
46	BO	933	0	996	116	0
46	DO	933	0	996	112	0
47	BP	1114	0	1187	284	0
47	DP	1114	0	1187	288	0
48	BQ	1113	0	1171	132	0
48	DQ	1113	0	1171	140	0
49	BR	960	0	1021	124	0
49	DR	960	0	1021	126	0
50	BS	771	0	832	153	0
50	DS	771	0	832	146	0
51	BT	1124	0	1181	251	0
51	DT	1124	0	1181	242	0
52	BU	958	0	1015	138	0
52	DU	958	0	1015	132	0
53	BV	779	0	852	151	0
53	DV	779	0	852	149	0
54	BW	896	0	953	70	0
54	DW	896	0	953	75	0
55	BX	726	0	778	52	0
55	DX	726	0	778	60	0
56	BY	776	0	870	175	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DY	776	0	870	175	0
57	BZ	1468	0	1492	265	0
57	DZ	1468	0	1491	341	0
58	AD	1	0	0	4	0
58	AN	1	0	0	3	0
58	CD	1	0	0	5	0
58	CN	1	0	0	3	0
All	All	298096	0	201782	19809	1

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 40.

The worst 5 of 19809 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)
22:CY:57:U:C6	57:DZ:182:LYS:HA	1.08	1.58
1:CA:1196:U:C4	24:CX:23:A:C5	1.96	1.53
22:CY:57:U:H6	57:DZ:182:LYS:CA	1.20	1.50
1:CA:1196:U:O4	24:CX:23:A:C4	1.70	1.45
22:CY:62:U:O2'	57:DZ:186:GLU:CB	1.68	1.39

All (1) 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)
4:AD:27:TYR:OH	6:CF:15:ASP:OD2[4_455]	2.05	0.15

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%)	153 (66%)	55 (24%)	25 (11%)	0	2
2	CB	233/256 (91%)	152 (65%)	57 (24%)	24 (10%)	0	3
3	AC	205/239 (86%)	141 (69%)	43 (21%)	21 (10%)	0	3
3	CC	205/239 (86%)	142 (69%)	40 (20%)	23 (11%)	0	2
4	AD	206/209 (99%)	133 (65%)	46 (22%)	27 (13%)	0	1
4	CD	206/209 (99%)	135 (66%)	44 (21%)	27 (13%)	0	1
5	AE	149/162 (92%)	111 (74%)	24 (16%)	14 (9%)	0	3
5	CE	149/162 (92%)	110 (74%)	25 (17%)	14 (9%)	0	3
6	AF	99/101 (98%)	77 (78%)	15 (15%)	7 (7%)	1	6
6	CF	99/101 (98%)	76 (77%)	17 (17%)	6 (6%)	1	9
7	AG	153/156 (98%)	108 (71%)	41 (27%)	4 (3%)	5	26
7	CG	153/156 (98%)	110 (72%)	39 (26%)	4 (3%)	5	26
8	AH	136/138 (99%)	100 (74%)	29 (21%)	7 (5%)	2	13
8	CH	136/138 (99%)	99 (73%)	29 (21%)	8 (6%)	1	10
9	AI	121/128 (94%)	90 (74%)	22 (18%)	9 (7%)	1	6
9	CI	121/128 (94%)	91 (75%)	20 (16%)	10 (8%)	1	5
10	AJ	97/105 (92%)	76 (78%)	17 (18%)	4 (4%)	3	16
10	CJ	97/105 (92%)	76 (78%)	17 (18%)	4 (4%)	3	16
11	AK	117/129 (91%)	83 (71%)	26 (22%)	8 (7%)	1	7
11	CK	117/129 (91%)	83 (71%)	26 (22%)	8 (7%)	1	7
12	AL	123/135 (91%)	75 (61%)	28 (23%)	20 (16%)	0	0
12	CL	123/135 (91%)	75 (61%)	28 (23%)	20 (16%)	0	0
13	AM	107/126 (85%)	67 (63%)	25 (23%)	15 (14%)	0	1
13	CM	107/126 (85%)	66 (62%)	26 (24%)	15 (14%)	0	1
14	AN	58/61 (95%)	41 (71%)	9 (16%)	8 (14%)	0	1
14	CN	58/61 (95%)	40 (69%)	9 (16%)	9 (16%)	0	0
15	AO	86/89 (97%)	52 (60%)	25 (29%)	9 (10%)	0	3
15	CO	86/89 (97%)	50 (58%)	27 (31%)	9 (10%)	0	3
16	AP	82/88 (93%)	48 (58%)	24 (29%)	10 (12%)	0	1
16	CP	82/88 (93%)	49 (60%)	24 (29%)	9 (11%)	0	2
17	AQ	98/105 (93%)	70 (71%)	22 (22%)	6 (6%)	1	9
17	CQ	98/105 (93%)	71 (72%)	20 (20%)	7 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	68/88 (77%)	44 (65%)	18 (26%)	6 (9%)	1	4
18	CR	68/88 (77%)	44 (65%)	18 (26%)	6 (9%)	1	4
19	AS	77/93 (83%)	47 (61%)	17 (22%)	13 (17%)	0	0
19	CS	77/93 (83%)	48 (62%)	16 (21%)	13 (17%)	0	0
20	AT	97/106 (92%)	67 (69%)	17 (18%)	13 (13%)	0	1
20	CT	97/106 (92%)	67 (69%)	18 (19%)	12 (12%)	0	1
21	AU	23/27 (85%)	14 (61%)	6 (26%)	3 (13%)	0	1
21	CU	23/27 (85%)	13 (56%)	7 (30%)	3 (13%)	0	1
25	B0	82/85 (96%)	67 (82%)	12 (15%)	3 (4%)	3	19
25	D0	82/85 (96%)	66 (80%)	13 (16%)	3 (4%)	3	19
26	B1	92/98 (94%)	68 (74%)	13 (14%)	11 (12%)	0	1
26	D1	92/98 (94%)	71 (77%)	9 (10%)	12 (13%)	0	1
27	B2	69/72 (96%)	50 (72%)	14 (20%)	5 (7%)	1	6
27	D2	69/72 (96%)	45 (65%)	16 (23%)	8 (12%)	0	2
28	B3	58/60 (97%)	44 (76%)	9 (16%)	5 (9%)	1	4
28	D3	58/60 (97%)	44 (76%)	9 (16%)	5 (9%)	1	4
29	B4	56/71 (79%)	26 (46%)	15 (27%)	15 (27%)	0	0
29	D4	56/71 (79%)	26 (46%)	16 (29%)	14 (25%)	0	0
30	B5	54/60 (90%)	43 (80%)	3 (6%)	8 (15%)	0	0
30	D5	54/60 (90%)	43 (80%)	3 (6%)	8 (15%)	0	0
31	B6	48/54 (89%)	22 (46%)	12 (25%)	14 (29%)	0	0
31	D6	48/54 (89%)	22 (46%)	12 (25%)	14 (29%)	0	0
32	B7	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
32	D7	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
33	B8	62/65 (95%)	41 (66%)	13 (21%)	8 (13%)	0	1
33	D8	62/65 (95%)	41 (66%)	13 (21%)	8 (13%)	0	1
34	B9	35/37 (95%)	28 (80%)	7 (20%)	0	100	100
34	D9	35/37 (95%)	28 (80%)	7 (20%)	0	100	100
37	BC	116/229 (51%)	94 (81%)	19 (16%)	3 (3%)	5	26
37	DC	116/229 (51%)	94 (81%)	19 (16%)	3 (3%)	5	26
38	BD	270/276 (98%)	209 (77%)	32 (12%)	29 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DD	270/276 (98%)	207 (77%)	34 (13%)	29 (11%)	0	2
39	BE	203/206 (98%)	134 (66%)	36 (18%)	33 (16%)	0	0
39	DE	203/206 (98%)	134 (66%)	37 (18%)	32 (16%)	0	0
40	BF	206/210 (98%)	149 (72%)	31 (15%)	26 (13%)	0	1
40	DF	206/210 (98%)	148 (72%)	32 (16%)	26 (13%)	0	1
41	BG	177/182 (97%)	112 (63%)	39 (22%)	26 (15%)	0	0
41	DG	177/182 (97%)	93 (52%)	57 (32%)	27 (15%)	0	0
42	BH	163/180 (91%)	110 (68%)	29 (18%)	24 (15%)	0	0
42	DH	163/180 (91%)	110 (68%)	28 (17%)	25 (15%)	0	0
43	BI	144/148 (97%)	84 (58%)	37 (26%)	23 (16%)	0	0
43	DI	144/148 (97%)	85 (59%)	36 (25%)	23 (16%)	0	0
45	BN	137/140 (98%)	99 (72%)	22 (16%)	16 (12%)	0	1
45	DN	137/140 (98%)	101 (74%)	20 (15%)	16 (12%)	0	1
46	BO	120/122 (98%)	99 (82%)	14 (12%)	7 (6%)	1	10
46	DO	120/122 (98%)	96 (80%)	16 (13%)	8 (7%)	1	7
47	BP	144/150 (96%)	69 (48%)	43 (30%)	32 (22%)	0	0
47	DP	144/150 (96%)	69 (48%)	43 (30%)	32 (22%)	0	0
48	BQ	139/141 (99%)	100 (72%)	27 (19%)	12 (9%)	1	4
48	DQ	139/141 (99%)	99 (71%)	28 (20%)	12 (9%)	1	4
49	BR	115/118 (98%)	88 (76%)	13 (11%)	14 (12%)	0	1
49	DR	115/118 (98%)	87 (76%)	14 (12%)	14 (12%)	0	1
50	BS	97/112 (87%)	54 (56%)	24 (25%)	19 (20%)	0	0
50	DS	97/112 (87%)	52 (54%)	26 (27%)	19 (20%)	0	0
51	BT	134/146 (92%)	85 (63%)	19 (14%)	30 (22%)	0	0
51	DT	134/146 (92%)	86 (64%)	18 (13%)	30 (22%)	0	0
52	BU	115/118 (98%)	90 (78%)	19 (16%)	6 (5%)	2	12
52	DU	115/118 (98%)	88 (76%)	20 (17%)	7 (6%)	1	9
53	BV	99/101 (98%)	64 (65%)	22 (22%)	13 (13%)	0	1
53	DV	99/101 (98%)	64 (65%)	22 (22%)	13 (13%)	0	1
54	BW	111/113 (98%)	91 (82%)	12 (11%)	8 (7%)	1	6
54	DW	111/113 (98%)	91 (82%)	13 (12%)	7 (6%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BX	91/96 (95%)	71 (78%)	15 (16%)	5 (6%)	2	11
55	DX	91/96 (95%)	67 (74%)	19 (21%)	5 (6%)	2	11
56	BY	99/110 (90%)	48 (48%)	26 (26%)	25 (25%)	0	0
56	DY	99/110 (90%)	48 (48%)	26 (26%)	25 (25%)	0	0
57	BZ	183/206 (89%)	111 (61%)	45 (25%)	27 (15%)	0	0
57	DZ	183/206 (89%)	111 (61%)	42 (23%)	30 (16%)	0	0
All	All	11600/12592 (92%)	7946 (68%)	2292 (20%)	1362 (12%)	0	1

5 of 1362 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	75	LYS
2	AB	101	MET
2	AB	123	ALA
2	AB	165	VAL

5.3.2 Protein sidechains [i](#)

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%)	186 (92%)	16 (8%)	12	40
2	CB	202/220 (92%)	187 (93%)	15 (7%)	13	42
3	AC	160/188 (85%)	145 (91%)	15 (9%)	8	32
3	CC	160/188 (85%)	146 (91%)	14 (9%)	10	36
4	AD	180/181 (99%)	162 (90%)	18 (10%)	7	28
4	CD	180/181 (99%)	162 (90%)	18 (10%)	7	28
5	AE	115/123 (94%)	107 (93%)	8 (7%)	15	45
5	CE	115/123 (94%)	107 (93%)	8 (7%)	15	45
6	AF	90/90 (100%)	87 (97%)	3 (3%)	38	69
6	CF	90/90 (100%)	87 (97%)	3 (3%)	38	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	126/127 (99%)	121 (96%)	5 (4%)	31	65
7	CG	126/127 (99%)	121 (96%)	5 (4%)	31	65
8	AH	119/119 (100%)	109 (92%)	10 (8%)	11	38
8	CH	119/119 (100%)	109 (92%)	10 (8%)	11	38
9	AI	98/99 (99%)	90 (92%)	8 (8%)	11	38
9	CI	98/99 (99%)	90 (92%)	8 (8%)	11	38
10	AJ	88/92 (96%)	83 (94%)	5 (6%)	20	52
10	CJ	88/92 (96%)	83 (94%)	5 (6%)	20	52
11	AK	90/99 (91%)	85 (94%)	5 (6%)	21	52
11	CK	90/99 (91%)	85 (94%)	5 (6%)	21	52
12	AL	104/111 (94%)	85 (82%)	19 (18%)	1	7
12	CL	104/111 (94%)	84 (81%)	20 (19%)	1	6
13	AM	94/101 (93%)	84 (89%)	10 (11%)	6	26
13	CM	94/101 (93%)	84 (89%)	10 (11%)	6	26
14	AN	49/50 (98%)	47 (96%)	2 (4%)	30	64
14	CN	49/50 (98%)	47 (96%)	2 (4%)	30	64
15	AO	79/80 (99%)	75 (95%)	4 (5%)	24	56
15	CO	79/80 (99%)	75 (95%)	4 (5%)	24	56
16	AP	72/74 (97%)	66 (92%)	6 (8%)	11	38
16	CP	72/74 (97%)	66 (92%)	6 (8%)	11	38
17	AQ	94/97 (97%)	90 (96%)	4 (4%)	29	62
17	CQ	94/97 (97%)	90 (96%)	4 (4%)	29	62
18	AR	61/77 (79%)	59 (97%)	2 (3%)	38	69
18	CR	61/77 (79%)	59 (97%)	2 (3%)	38	69
19	AS	69/80 (86%)	62 (90%)	7 (10%)	7	28
19	CS	69/80 (86%)	61 (88%)	8 (12%)	5	22
20	AT	76/82 (93%)	71 (93%)	5 (7%)	16	47
20	CT	76/82 (93%)	71 (93%)	5 (7%)	16	47
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	26
21	CU	19/22 (86%)	18 (95%)	1 (5%)	22	54
25	B0	66/67 (98%)	59 (89%)	7 (11%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	D0	66/67 (98%)	59 (89%)	7 (11%)	6	26
26	B1	78/83 (94%)	70 (90%)	8 (10%)	7	27
26	D1	78/83 (94%)	68 (87%)	10 (13%)	4	18
27	B2	66/67 (98%)	57 (86%)	9 (14%)	3	16
27	D2	66/67 (98%)	60 (91%)	6 (9%)	9	33
28	B3	51/52 (98%)	48 (94%)	3 (6%)	19	50
28	D3	51/52 (98%)	48 (94%)	3 (6%)	19	50
29	B4	51/63 (81%)	42 (82%)	9 (18%)	2	8
29	D4	51/63 (81%)	42 (82%)	9 (18%)	2	8
30	B5	47/52 (90%)	42 (89%)	5 (11%)	6	26
30	D5	47/52 (90%)	42 (89%)	5 (11%)	6	26
31	B6	49/52 (94%)	43 (88%)	6 (12%)	5	19
31	D6	49/52 (94%)	43 (88%)	6 (12%)	5	19
32	B7	40/42 (95%)	35 (88%)	5 (12%)	4	18
32	D7	40/42 (95%)	36 (90%)	4 (10%)	7	28
33	B8	53/55 (96%)	44 (83%)	9 (17%)	2	9
33	D8	53/55 (96%)	44 (83%)	9 (17%)	2	9
34	B9	34/34 (100%)	33 (97%)	1 (3%)	42	72
34	D9	34/34 (100%)	33 (97%)	1 (3%)	42	72
37	BC	99/181 (55%)	94 (95%)	5 (5%)	24	56
37	DC	99/181 (55%)	94 (95%)	5 (5%)	24	56
38	BD	213/218 (98%)	185 (87%)	28 (13%)	4	17
38	DD	213/218 (98%)	187 (88%)	26 (12%)	5	19
39	BE	165/166 (99%)	144 (87%)	21 (13%)	4	18
39	DE	165/166 (99%)	143 (87%)	22 (13%)	4	16
40	BF	165/166 (99%)	149 (90%)	16 (10%)	8	30
40	DF	165/166 (99%)	149 (90%)	16 (10%)	8	30
41	BG	155/156 (99%)	140 (90%)	15 (10%)	8	30
41	DG	155/156 (99%)	140 (90%)	15 (10%)	8	30
42	BH	137/148 (93%)	121 (88%)	16 (12%)	5	22
42	DH	137/148 (93%)	121 (88%)	16 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BI	122/124 (98%)	112 (92%)	10 (8%)	11	38
43	DI	122/124 (98%)	112 (92%)	10 (8%)	11	38
45	BN	117/119 (98%)	101 (86%)	16 (14%)	3	16
45	DN	117/119 (98%)	101 (86%)	16 (14%)	3	16
46	BO	100/100 (100%)	94 (94%)	6 (6%)	19	49
46	DO	100/100 (100%)	94 (94%)	6 (6%)	19	49
47	BP	112/116 (97%)	93 (83%)	19 (17%)	2	9
47	DP	112/116 (97%)	93 (83%)	19 (17%)	2	9
48	BQ	110/111 (99%)	100 (91%)	10 (9%)	9	33
48	DQ	110/111 (99%)	101 (92%)	9 (8%)	11	38
49	BR	100/101 (99%)	87 (87%)	13 (13%)	4	18
49	DR	100/101 (99%)	86 (86%)	14 (14%)	3	15
50	BS	77/88 (88%)	64 (83%)	13 (17%)	2	9
50	DS	77/88 (88%)	64 (83%)	13 (17%)	2	9
51	BT	118/127 (93%)	96 (81%)	22 (19%)	1	7
51	DT	118/127 (93%)	95 (80%)	23 (20%)	1	6
52	BU	92/94 (98%)	83 (90%)	9 (10%)	8	29
52	DU	92/94 (98%)	81 (88%)	11 (12%)	5	20
53	BV	82/82 (100%)	67 (82%)	15 (18%)	1	7
53	DV	82/82 (100%)	68 (83%)	14 (17%)	2	9
54	BW	91/92 (99%)	81 (89%)	10 (11%)	6	25
54	DW	91/92 (99%)	81 (89%)	10 (11%)	6	25
55	BX	74/78 (95%)	69 (93%)	5 (7%)	16	45
55	DX	74/78 (95%)	69 (93%)	5 (7%)	16	45
56	BY	84/91 (92%)	70 (83%)	14 (17%)	2	9
56	DY	84/91 (92%)	69 (82%)	15 (18%)	2	8
57	BZ	162/179 (90%)	140 (86%)	22 (14%)	3	16
57	DZ	162/179 (90%)	145 (90%)	17 (10%)	7	26
All	All	9790/10432 (94%)	8794 (90%)	996 (10%)	7	27

5 of 996 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	BX	68	ARG
49	DR	100	LEU
8	CH	115	SER
49	DR	54	LEU
53	DV	91	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 311 such sidechains are listed below:

Mol	Chain	Res	Type
27	D2	70	GLN
48	DQ	45	GLN
30	D5	4	HIS
39	DE	192	ASN
53	DV	80	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	215 (14%)	29 (1%)
1	CA	1503/1522 (98%)	218 (14%)	31 (2%)
22	AV	76/78 (97%)	25 (32%)	0
22	AY	76/78 (97%)	24 (31%)	2 (2%)
22	CV	76/78 (97%)	24 (31%)	0
22	CY	76/78 (97%)	23 (30%)	2 (2%)
23	AW	77/78 (98%)	41 (53%)	4 (5%)
23	CW	77/78 (98%)	39 (50%)	3 (3%)
24	AX	11/24 (45%)	2 (18%)	0
24	CX	11/24 (45%)	2 (18%)	0
35	BA	2847/2915 (97%)	498 (17%)	49 (1%)
35	DA	2847/2915 (97%)	498 (17%)	49 (1%)
36	BB	118/122 (96%)	18 (15%)	1 (0%)
36	DB	118/122 (96%)	17 (14%)	1 (0%)
All	All	9416/9634 (97%)	1644 (17%)	171 (1%)

5 of 1644 RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
1	AA	47	C

5 of 171 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	1504	G
35	DA	1395	A
22	CY	4	C
35	DA	474	G
35	DA	1819	A

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

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	AG9	AV	36	22	22,29,30	0.76	1 (4%)	25,39,42	1.05	2 (8%)
22	AG9	AY	36	22	22,29,30	1.36	2 (9%)	25,39,42	1.21	3 (12%)
22	AG9	CY	36	22	22,29,30	1.86	4 (18%)	25,39,42	1.09	2 (8%)
22	AG9	CV	36	22	22,29,30	1.53	2 (9%)	25,39,42	1.04	2 (8%)

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	AG9	AV	36	22	1/1/9/13	3/14/47/48	0/2/2/2
22	AG9	AY	36	22	1/1/9/13	7/14/47/48	0/2/2/2
22	AG9	CY	36	22	1/1/9/13	7/14/47/48	0/2/2/2
22	AG9	CV	36	22	1/1/9/13	3/14/47/48	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CY	36	AG9	C2-N1	6.08	1.43	1.38
22	CV	36	AG9	C2-N1	5.59	1.43	1.38
22	AY	36	AG9	C2-N1	5.10	1.42	1.38
22	CV	36	AG9	C2-N3	3.89	1.37	1.30
22	CY	36	AG9	C2-N3	3.43	1.36	1.30

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AY	36	AG9	N2-C2-N1	3.73	119.71	117.34
22	AV	36	AG9	N2-C2-N1	3.49	119.56	117.34
22	CV	36	AG9	N2-C2-N1	3.47	119.54	117.34
22	AY	36	AG9	CD-NE-CZ	3.09	124.72	114.64
22	CV	36	AG9	CD-NE-CZ	3.01	124.45	114.64

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	AV	36	AG9	C4
22	AY	36	AG9	C4
22	CV	36	AG9	C4
22	CY	36	AG9	C4

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	AV	36	AG9	N1-C2-N2-CA
22	AV	36	AG9	N3-C2-N2-CA
22	AY	36	AG9	N1-C2-N2-CA
22	AY	36	AG9	N3-C2-N2-CA
22	CV	36	AG9	N1-C2-N2-CA

There are no ring outliers.

4 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AV	36	AG9	6	0
22	AY	36	AG9	11	0
22	CY	36	AG9	7	0
22	CV	36	AG9	12	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	AM	5
13	CM	5
9	AI	2
9	CI	2
41	DG	1
41	BG	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AM	112:GLY	C	113:PRO	N	4.84
1	CM	112:GLY	C	113:PRO	N	4.84
1	AM	69:GLU	C	70:LEU	N	4.24
1	CM	69:GLU	C	70:LEU	N	4.23
1	DG	112:PRO	C	113:ARG	N	4.14

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.58	95 (6%) 20 8	44, 101, 184, 200	0
1	CA	1504/1522 (98%)	0.57	103 (6%) 17 7	55, 115, 186, 200	0
2	AB	235/256 (91%)	0.69	30 (12%) 3 1	75, 134, 176, 198	0
2	CB	235/256 (91%)	1.22	55 (23%) 0 0	94, 148, 183, 200	0
3	AC	207/239 (86%)	0.80	28 (13%) 3 1	82, 127, 157, 179	0
3	CC	207/239 (86%)	1.21	51 (24%) 0 0	92, 141, 170, 185	0
4	AD	208/209 (99%)	0.63	17 (8%) 11 4	64, 112, 142, 179	0
4	CD	208/209 (99%)	0.27	7 (3%) 45 24	56, 99, 135, 157	0
5	AE	151/162 (93%)	0.42	6 (3%) 38 19	65, 95, 142, 167	0
5	CE	151/162 (93%)	0.95	26 (17%) 1 0	69, 119, 151, 160	0
6	AF	101/101 (100%)	0.10	0 100 100	59, 98, 138, 173	0
6	CF	101/101 (100%)	0.10	3 (2%) 50 27	64, 110, 133, 173	0
7	AG	155/156 (99%)	1.21	35 (22%) 0 0	76, 123, 155, 198	0
7	CG	155/156 (99%)	1.14	33 (21%) 0 0	94, 131, 160, 194	0
8	AH	138/138 (100%)	0.35	7 (5%) 28 13	61, 101, 128, 144	0
8	CH	138/138 (100%)	0.73	14 (10%) 7 2	83, 121, 148, 166	0
9	AI	127/128 (99%)	1.66	39 (30%) 0 0	81, 148, 176, 191	0
9	CI	127/128 (99%)	2.05	61 (48%) 0 0	99, 153, 181, 193	0
10	AJ	99/105 (94%)	1.82	41 (41%) 0 0	71, 149, 177, 185	0
10	CJ	99/105 (94%)	2.37	54 (54%) 0 0	97, 159, 182, 189	0
11	AK	119/129 (92%)	0.52	9 (7%) 13 5	63, 94, 136, 187	0
11	CK	119/129 (92%)	0.57	12 (10%) 7 2	78, 108, 141, 176	0
12	AL	125/135 (92%)	1.05	22 (17%) 1 0	53, 93, 146, 180	0
12	CL	125/135 (92%)	1.11	27 (21%) 0 0	63, 111, 149, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	119/126 (94%)	1.32	33 (27%)	0	0	75, 129, 161, 178	0
13	CM	119/126 (94%)	1.99	49 (41%)	0	0	96, 150, 169, 186	0
14	AN	60/61 (98%)	1.37	16 (26%)	0	0	71, 118, 145, 157	0
14	CN	60/61 (98%)	1.53	21 (35%)	0	0	108, 143, 166, 187	0
15	AO	88/89 (98%)	0.41	4 (4%)	33	16	60, 97, 130, 148	0
15	CO	88/89 (98%)	0.65	8 (9%)	9	3	67, 110, 138, 146	0
16	AP	84/88 (95%)	1.07	14 (16%)	1	1	67, 112, 156, 178	0
16	CP	84/88 (95%)	0.48	3 (3%)	42	22	60, 87, 137, 157	0
17	AQ	100/105 (95%)	0.63	9 (9%)	9	3	74, 109, 138, 151	0
17	CQ	100/105 (95%)	0.77	12 (12%)	4	2	70, 109, 139, 165	0
18	AR	70/88 (79%)	0.58	5 (7%)	16	6	69, 98, 139, 157	0
18	CR	70/88 (79%)	0.78	7 (10%)	7	2	77, 111, 148, 156	0
19	AS	79/93 (84%)	1.90	28 (35%)	0	0	89, 137, 171, 185	0
19	CS	79/93 (84%)	2.41	38 (48%)	0	0	112, 154, 178, 200	0
20	AT	99/106 (93%)	1.11	16 (16%)	1	1	65, 117, 160, 167	0
20	CT	99/106 (93%)	0.89	11 (11%)	5	2	66, 107, 151, 163	0
21	AU	25/27 (92%)	2.10	13 (52%)	0	0	84, 120, 146, 156	0
21	CU	25/27 (92%)	3.92	19 (76%)	0	0	91, 135, 171, 188	0
22	AV	77/78 (98%)	1.44	22 (28%)	0	0	65, 141, 179, 199	0
22	AY	77/78 (98%)	1.56	23 (29%)	0	0	90, 140, 185, 189	0
22	CV	77/78 (98%)	2.17	34 (44%)	0	0	94, 175, 196, 200	0
22	CY	77/78 (98%)	2.82	46 (59%)	0	0	138, 176, 197, 200	0
23	AW	78/78 (100%)	2.19	38 (48%)	0	0	70, 173, 191, 199	0
23	CW	78/78 (100%)	3.28	55 (70%)	0	0	99, 188, 200, 200	0
24	AX	12/24 (50%)	1.04	1 (8%)	11	4	59, 88, 157, 160	0
24	CX	12/24 (50%)	1.89	4 (33%)	0	0	92, 163, 185, 185	0
25	B0	84/85 (98%)	0.75	7 (8%)	11	4	39, 66, 124, 167	0
25	D0	84/85 (98%)	1.26	19 (22%)	0	0	71, 105, 146, 165	0
26	B1	94/98 (95%)	0.07	0	100	100	33, 61, 114, 141	0
26	D1	94/98 (95%)	0.22	2 (2%)	63	43	43, 74, 127, 149	0
27	B2	71/72 (98%)	-0.09	1 (1%)	75	56	41, 70, 122, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	0.24	4 (5%) 24 11	57, 97, 139, 178	0
28	B3	60/60 (100%)	0.39	2 (3%) 46 24	42, 63, 108, 167	0
28	D3	60/60 (100%)	1.31	15 (25%) 0 0	65, 109, 149, 175	0
29	B4	58/71 (81%)	1.32	12 (20%) 1 0	96, 144, 171, 187	0
29	D4	58/71 (81%)	1.32	14 (24%) 0 0	86, 165, 194, 200	0
30	B5	56/60 (93%)	-0.11	0 100 100	25, 63, 126, 148	0
30	D5	56/60 (93%)	0.17	1 (1%) 68 47	48, 80, 128, 146	0
31	B6	50/54 (92%)	3.53	39 (78%) 0 0	99, 140, 171, 180	0
31	D6	50/54 (92%)	4.67	41 (82%) 0 0	113, 150, 174, 191	0
32	B7	48/49 (97%)	0.14	1 (2%) 63 43	23, 42, 83, 129	0
32	D7	48/49 (97%)	0.31	1 (2%) 63 43	35, 54, 98, 131	0
33	B8	64/65 (98%)	0.39	2 (3%) 49 26	30, 61, 107, 123	0
33	D8	64/65 (98%)	0.70	7 (10%) 5 2	46, 88, 134, 177	0
34	B9	37/37 (100%)	5.29	35 (94%) 0 0	91, 136, 157, 159	0
34	D9	37/37 (100%)	6.00	36 (97%) 0 0	126, 149, 172, 183	0
35	BA	2848/2915 (97%)	0.34	124 (4%) 34 17	20, 56, 184, 200	0
35	DA	2848/2915 (97%)	0.40	150 (5%) 26 12	39, 82, 186, 200	0
36	BB	119/122 (97%)	0.63	1 (0%) 86 72	52, 81, 149, 178	0
36	DB	119/122 (97%)	0.87	9 (7%) 13 5	102, 151, 183, 195	0
37	BC	120/229 (52%)	3.70	85 (70%) 0 0	119, 168, 189, 200	0
37	DC	120/229 (52%)	3.45	81 (67%) 0 0	132, 170, 187, 199	0
38	BD	272/276 (98%)	-0.02	4 (1%) 73 54	24, 55, 93, 150	0
38	DD	272/276 (98%)	0.11	2 (0%) 87 75	37, 73, 110, 144	0
39	BE	205/206 (99%)	0.17	7 (3%) 45 24	20, 62, 129, 165	0
39	DE	205/206 (99%)	0.31	6 (2%) 51 28	41, 82, 136, 159	0
40	BF	208/210 (99%)	0.28	12 (5%) 23 10	22, 63, 144, 195	0
40	DF	208/210 (99%)	0.23	7 (3%) 45 24	38, 90, 145, 184	0
41	BG	181/182 (99%)	1.00	28 (15%) 2 1	51, 103, 155, 182	0
41	DG	181/182 (99%)	1.30	47 (25%) 0 0	102, 141, 167, 183	0
42	BH	165/180 (91%)	0.61	14 (8%) 10 4	49, 86, 136, 174	0
42	DH	165/180 (91%)	1.99	68 (41%) 0 0	102, 139, 167, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BI	146/148 (98%)	1.76	49 (33%) 0 0	55, 147, 187, 200	0
43	DI	146/148 (98%)	1.65	45 (30%) 0 0	59, 139, 183, 200	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BN	139/140 (99%)	0.02	2 (1%) 75 56	36, 64, 118, 147	0
45	DN	139/140 (99%)	0.39	3 (2%) 62 41	69, 104, 136, 155	0
46	BO	122/122 (100%)	-0.11	0 100 100	33, 60, 94, 116	0
46	DO	122/122 (100%)	0.07	0 100 100	54, 83, 110, 141	0
47	BP	146/150 (97%)	0.51	5 (3%) 45 24	28, 74, 128, 189	0
47	DP	146/150 (97%)	0.68	10 (6%) 17 7	41, 98, 144, 173	0
48	BQ	141/141 (100%)	0.29	2 (1%) 75 56	38, 67, 109, 143	0
48	DQ	141/141 (100%)	0.81	15 (10%) 6 2	63, 113, 153, 178	0
49	BR	117/118 (99%)	0.09	0 100 100	36, 62, 103, 136	0
49	DR	117/118 (99%)	0.17	2 (1%) 70 49	42, 76, 118, 151	0
50	BS	99/112 (88%)	1.21	22 (22%) 0 0	52, 95, 141, 160	0
50	DS	99/112 (88%)	1.93	38 (38%) 0 0	101, 137, 163, 186	0
51	BT	136/146 (93%)	0.06	4 (2%) 51 28	47, 78, 140, 181	0
51	DT	136/146 (93%)	0.31	7 (5%) 28 13	58, 92, 151, 176	0
52	BU	117/118 (99%)	0.03	2 (1%) 70 49	27, 53, 102, 144	0
52	DU	117/118 (99%)	0.45	7 (5%) 21 10	46, 97, 137, 163	0
53	BV	101/101 (100%)	0.03	1 (0%) 82 67	24, 72, 124, 168	0
53	DV	101/101 (100%)	0.98	17 (16%) 1 0	53, 116, 146, 171	0
54	BW	113/113 (100%)	0.05	3 (2%) 54 31	28, 52, 105, 180	0
54	DW	113/113 (100%)	0.07	2 (1%) 68 47	49, 71, 119, 165	0
55	BX	93/96 (96%)	-0.15	0 100 100	29, 63, 100, 141	0
55	DX	93/96 (96%)	0.16	2 (2%) 62 41	55, 83, 115, 138	0
56	BY	101/110 (91%)	0.35	5 (4%) 28 13	47, 89, 131, 157	0
56	DY	101/110 (91%)	1.03	19 (18%) 1 0	60, 106, 149, 164	0
57	BZ	185/206 (89%)	1.59	54 (29%) 0 0	51, 113, 163, 188	0
57	DZ	185/206 (89%)	1.74	62 (33%) 0 0	99, 144, 171, 189	0
All	All	21266/22572 (94%)	0.72	2566 (12%) 4 1	20, 98, 177, 200	0

The worst 5 of 2566 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	BI	88	ILE	22.2
37	BC	171	ALA	19.2
35	BA	277	C	18.4
34	D9	34	GLN	17.3
48	DQ	141	GLN	15.8

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. 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	B-factors(Å ²)	Q<0.9
22	AG9	CY	36	28/29	0.75	0.51	33,49,70,70	0
22	AG9	CV	36	28/29	0.81	0.42	33,49,70,70	0
22	AG9	AY	36	28/29	0.88	0.34	43,59,79,79	0
22	AG9	AV	36	28/29	0.90	0.26	43,59,79,79	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors(Å ²)	Q<0.9
58	ZN	AD	1000	1/1	0.84	0.25	165,165,165,165	0
58	ZN	CN	1000	1/1	0.84	0.07	178,178,178,178	0
58	ZN	CD	1000	1/1	0.95	0.29	200,200,200,200	0
58	ZN	AN	1000	1/1	0.95	0.08	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.