



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:57 PM UTC

PDB ID : 4V8N / pdb_00004v8n
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

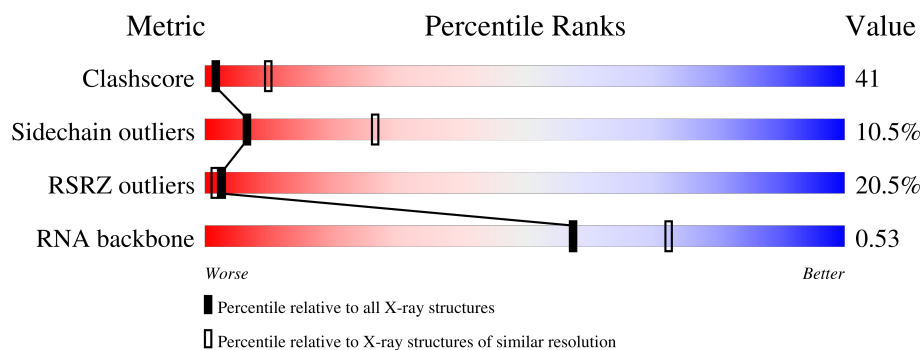
1 Overall quality at a glance

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	190562	1539 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	26% 24% 63% 10% ..
1	CA	1522	24% 23% 64% 10% ..
2	AB	256	17% 19% 65% 8% 8%
2	CB	256	23% 18% 65% 8% 8%
3	AC	239	21% 24% 56% 6% 13%
3	CC	239	20% 22% 59% 6% 13%

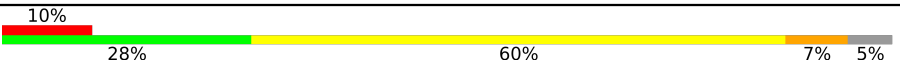
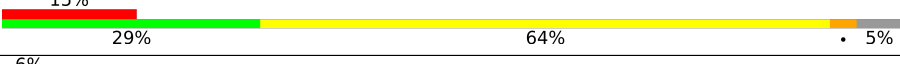
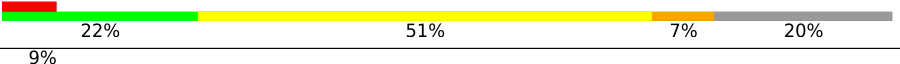
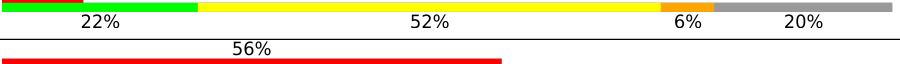
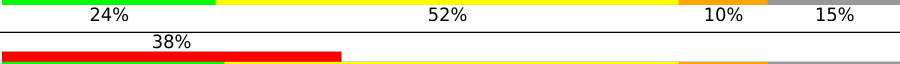
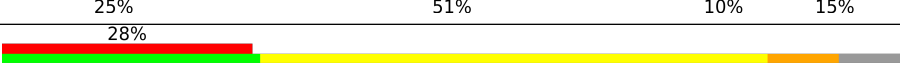
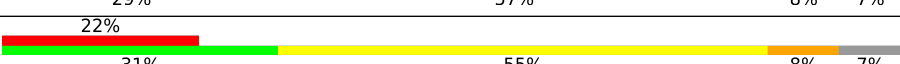
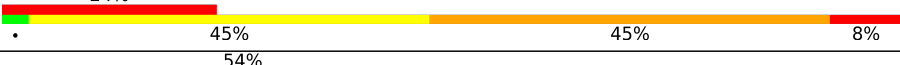
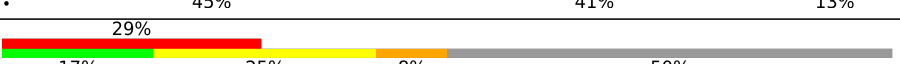
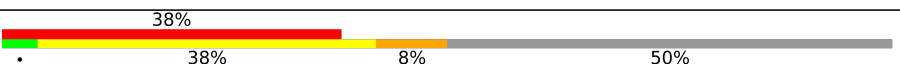
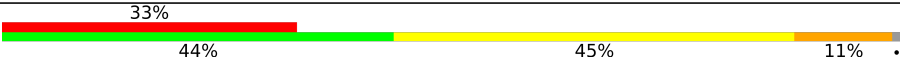
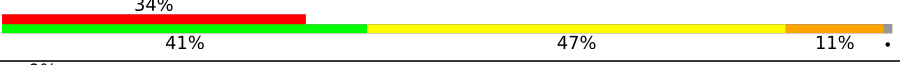
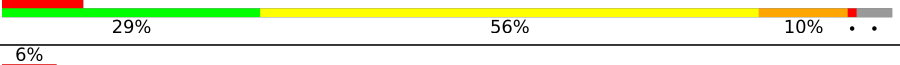
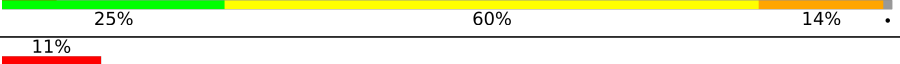
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Mol	Chain	Length	Quality of chain
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	

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Mol	Chain	Length	Quality of chain
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	
27	D2	72	

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Mol	Chain	Length	Quality of chain
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2915	
35	DA	2915	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	
39	DE	206	
40	BF	210	

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Mol	Chain	Length	Quality of chain
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	
52	DU	118	

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Mol	Chain	Length	Quality of chain
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	-	-	-
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
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
13	AM	119	Total	C	N	O	S	0	0	1
			938	579	194	163	2			
13	CM	119	Total	C	N	O	S	0	0	1
			938	579	194	163	2			

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

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

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

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

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

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

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

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

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

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

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

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

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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
45	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
45	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

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

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

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

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

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

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

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

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

- 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
55	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

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

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

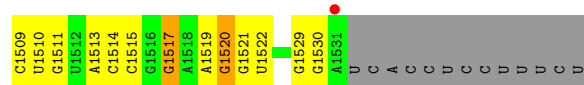
- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

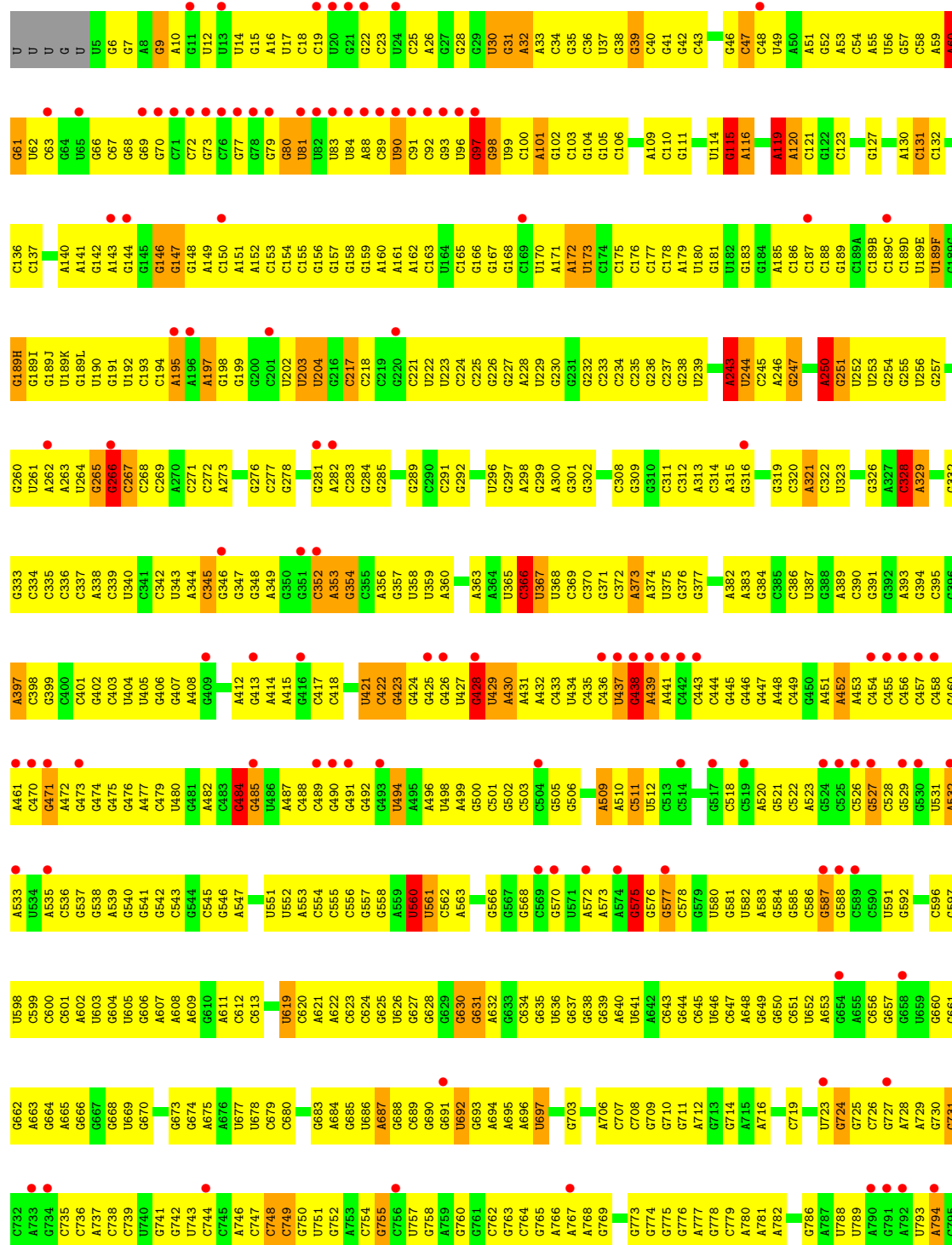
- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

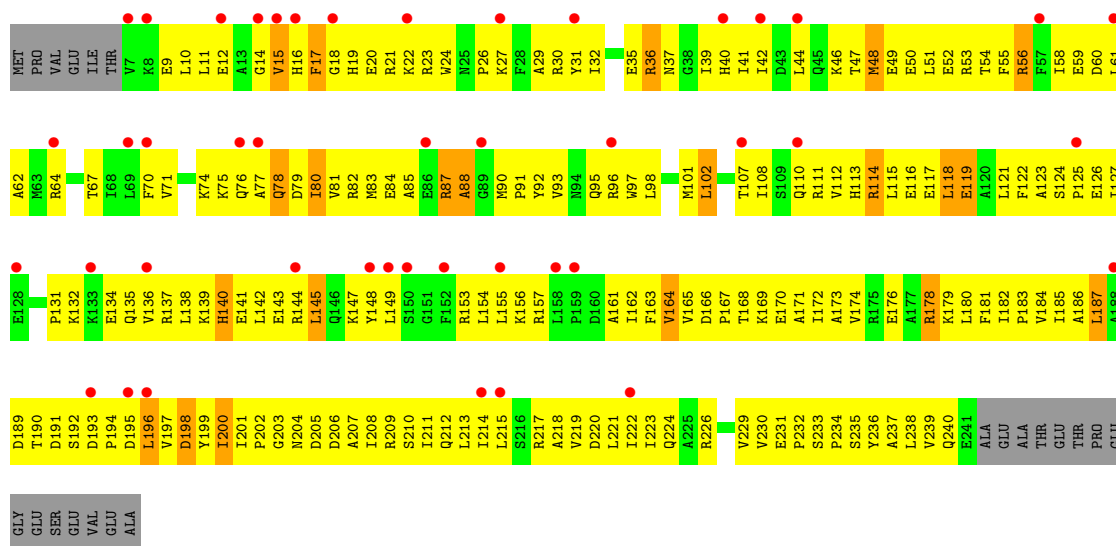
A1483	C1363	G1174	C1112	C1051	U997	C931	G858	A780	G713	G644
A1484	A1363A	G1175	C1113	U1052	G993	C932	A859	A781	G714	C645
G1435	U1364	A1176	C1114	G1054	A994	G933	A860	A782	A715	U646
C1437	C1366	A1179	C1115	A1055	U997	A935	C962	C783	A716	C647
G1438	C1367	A1180	G1117	U1056	G998	C936	U863	C784	C719	A648
A1439	G1368	G1181	C1118	G1057	C999	A937	A864	U788	U723	G649
C1440	C1369	G1182	G1119	G1058	U1000	A938	A865	U789	U724	G650
G1441	G1370	A1183	C1120	U1059	A1001	G939	C966	U790	G725	C651
A1442	A1371	G1184	U1121	C1060	G1001A	C940	G867	A792	G726	A653
G1442A	C1372	G1185	U1122	U1061	G1002	G941	C968	U793	G727	C656
A1442B	G1373	G1186	A1123	U1062	G1003	G942	G869	A794	A728	G657
A147	A1374	A1187	G1124	C1063	A1004	A943	U870	C795	U729	G660
G1452	A1375	A1188	U1125	G1064	A1005	G944	G874	C797	G730	G662
C1456	U1376	C1189	U1126	U1065	C1006	G945	C875	G797	G731	A663
G1457	A1377	G1190	G1127	A1066	C1007	G947	C876	G798	U732	G664
G1458	C1381	A1191	C1128	A1067	G1008	G948	G878	G799	C735	A665
C1459	U1382	C1192	G1129	G1068	G1009	U949	C879	U801	C736	G666
A1460	C1383	G1193	A1130	U1069	G1010	U950	C880	A802	A737	G667
G1461	U1384	U1194	G1131	C1070	G1011	G951	G881	C741	G742	U669
C1462	G1385	C1195	C1132	G1071	A1014	U952	C882	U813	U743	G673
G1463	U1386	U1196	G1133	U1072	A1015	G953	C883	A814	C744	G674
G1464	C1387	G1197	C1134	U1073	A1016	U954	G887	A815	G745	A675
A1468	U1389	U1198	U1135	G1074	G1017	U955	U887	A816	A746	A676
G1469	C1390	C1200	C1137	G1077	C1018	U956	G888	U820	C747	U678
G1470	U1391	A1201	G1138	U1078	C1019	U957	A892	C821	U748	C679
G1471	C1392	C1202	C1139	G1079	U1020	A958	C893	C822	C749	C680
U1472	U1393	C1203	C1140	A1080	G1021	A959	C894	C823	G750	C681
A1473	C1398	U1205	C1141	G1081	G1022	U960	G895	C824	U751	G682
G1486	U1399	G1206	G1142	U1082	G1023	U961	C896	C825	A753	G683
C1487	C1400	G1207	G1143	U1083	U1024	C962	C897	C826	C754	A684
A1488	U1401	C1208	C1144	G1084	G1025	G963	C898	U827	G755	G685
G1489	A1406	C1209	U1145	U1085	C1026	G966	G901	A828	G756	U686
C1490	C1407	C1210	C1146	U1086	G1027	A968	A902	C829	U757	A687
A1492	A1408	U1211	U1147	G1087	C1028	U969	A908	C830	G758	G688
G1493	U1409	U1212	C1148	U1088	U1029	A970	A909	C831	A759	G689
C1494	G1412	A1213	U1149	G1089	C1030B	C971	C910	U832	G760	G690
U1495	A1413	G1214	C1152	A1092	A1030D	C972	U911	C833	C761	U692
G1496	U1414	G1215	A1153	G1093	G1031	C973	C912	U834	G762	G693
C1497	G1415	C1216	G1154	U1094	G1032	A974	A913	C835	C763	A694
U1488	A1418	U1217	G1155	G1095	G1033	A975	A914	U836	C764	A695
A1502	C1419	U1218	G1156	C1096	G1034	C976	A915	C837	G765	A696
G1503	U1422	G1219	C1157	U1097	G1035	A977	A918	C838	A766	U697
A1504	G1423	C1220	U1158	C1098	G1036	A978	A919	U839	A767	G703
G1505	U1424	U1221	U1159	U1099	C1037	C979	U920	C840	G769	A706
U1506	C1425	G1222	G1160	C1100	C1038	C980	U921	U841	G773	C707
A1507	A1426	C1223	C1161	A1101	U1039	U981	G922	C848	G774	C708
G1508	U1427	U1224	C1162	U1102	U1040	U982	A923	G851	G775	G709
	G1428	A1225	G1163	A1103	A1041	C983	G924	G852	G776	G710
	C1429	C1226	C1164	G1104	G1042	C984	G925	G853	A777	G711
	A1430	U1227	G1165	A1105	C1043	C985	G926	G854	G778	C779
	U1431	C1228	U1166	G1106	A1044	A986	G927			
	C1432	A1229	A1167	C1107	G1047	G988	G928			
		U1230	U1168	G1108	G1048	C989	C930			
		G1231	A1169	G1109	U1049	C990				
		U1232	G1170	A1110	G1050	U991				
		C1233	C1171	A1111						
		G1234	G1172	A1111						



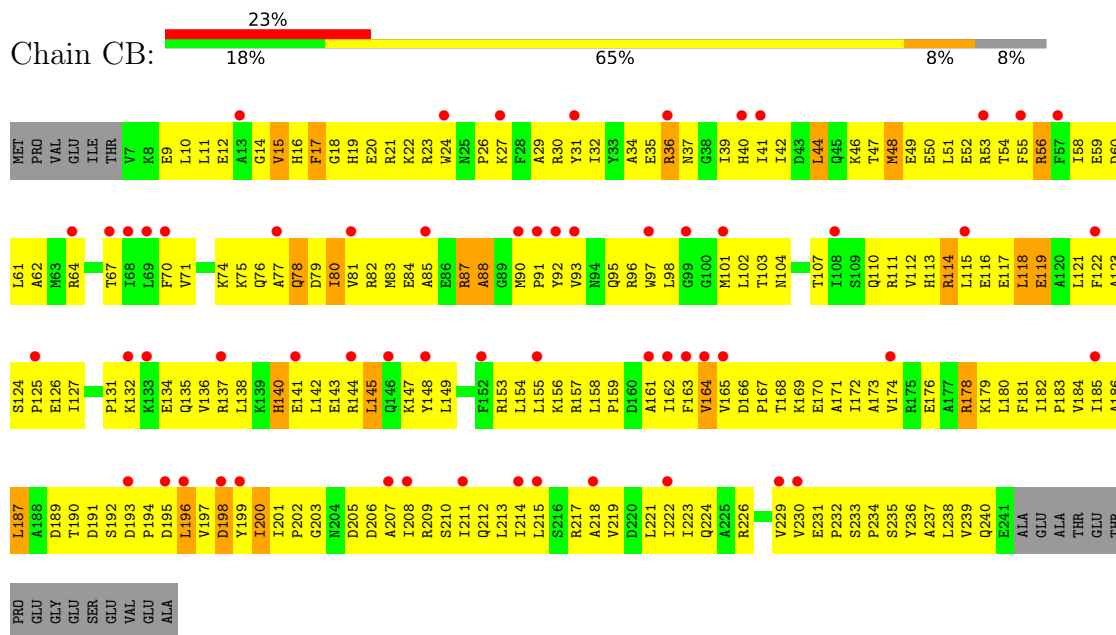
● Molecule 1: 16S rRNA



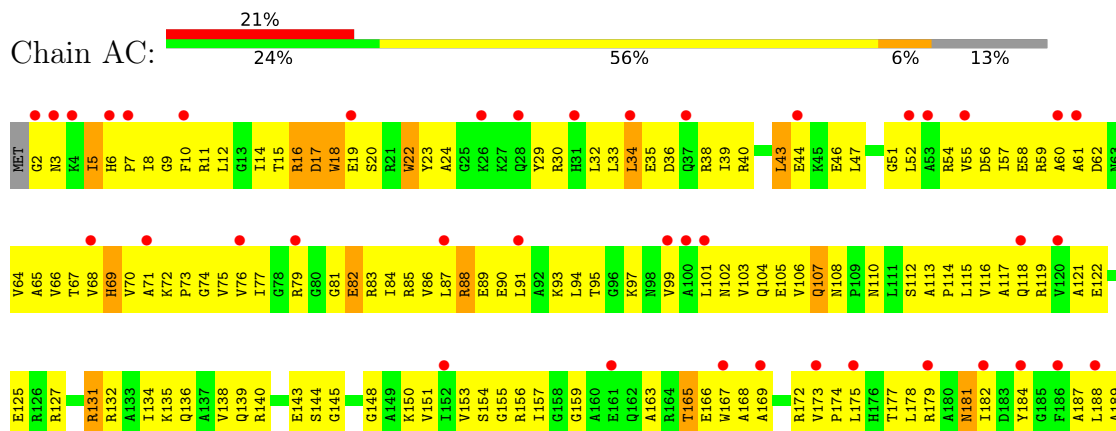


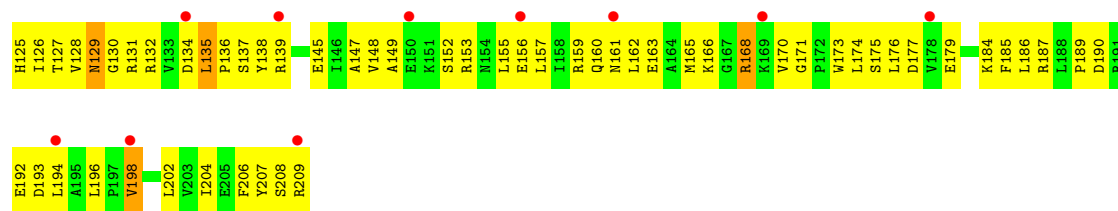


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

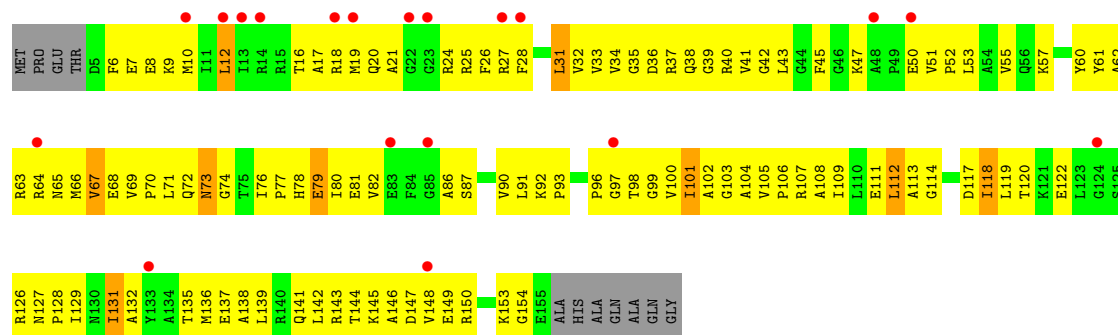


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

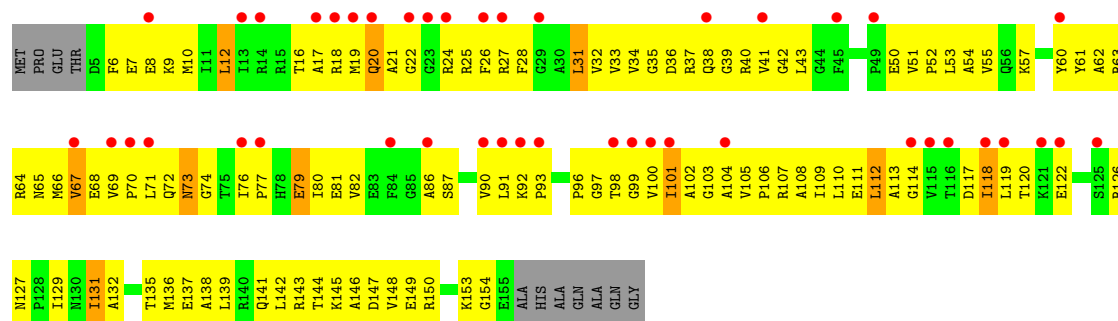




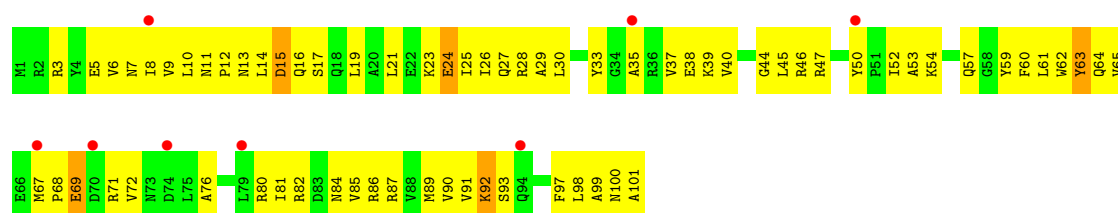
● Molecule 5: 30S RIBOSOMAL PROTEIN S5



● Molecule 5: 30S RIBOSOMAL PROTEIN S5

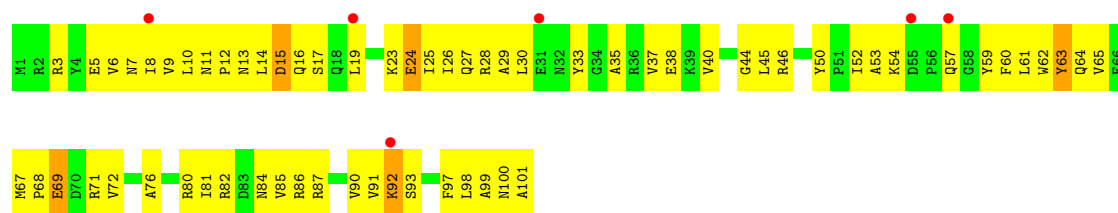


● Molecule 6: 30S RIBOSOMAL PROTEIN S6

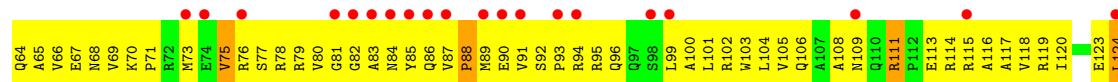
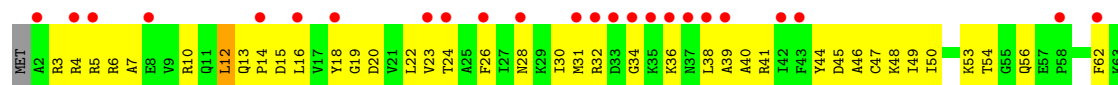


● Molecule 6: 30S RIBOSOMAL PROTEIN S6

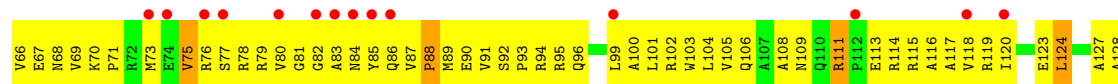
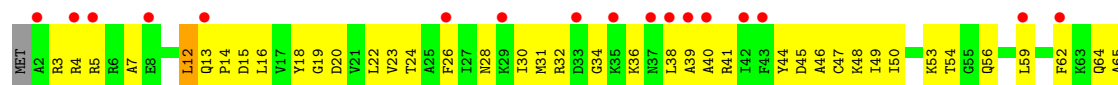




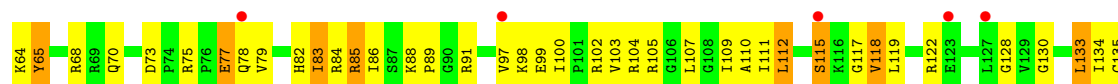
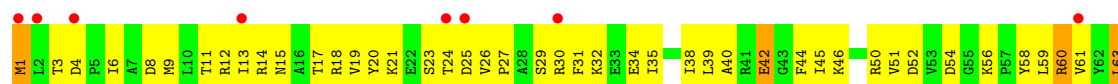
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



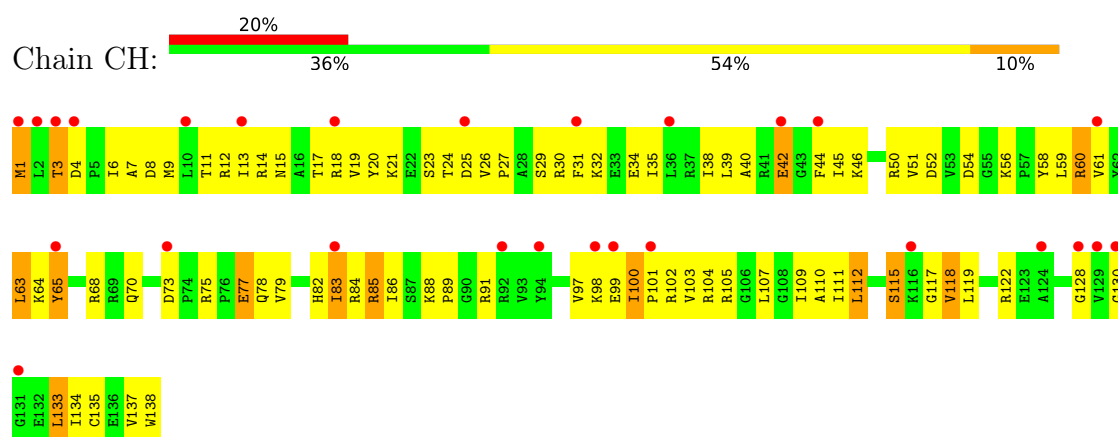
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



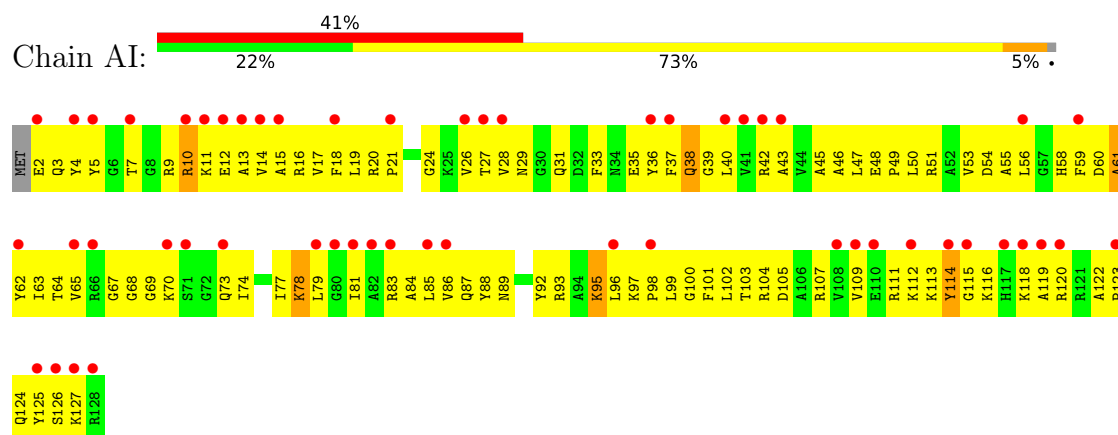
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



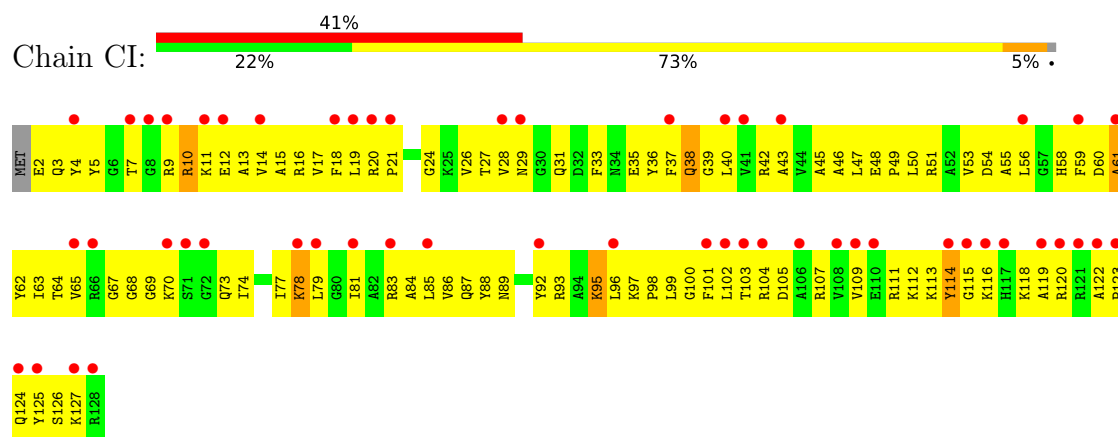
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



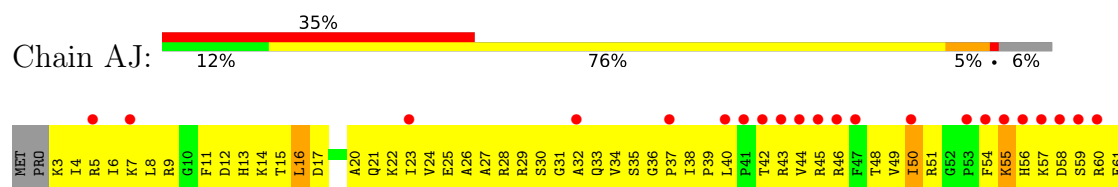
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

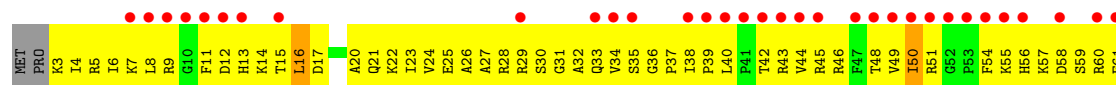


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

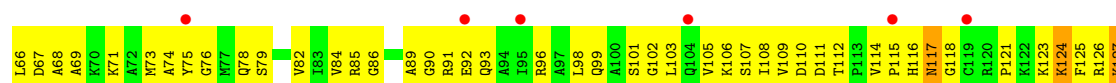
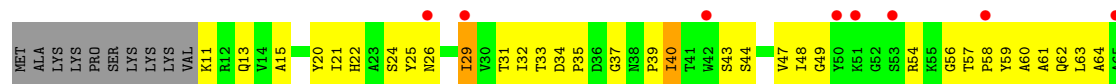




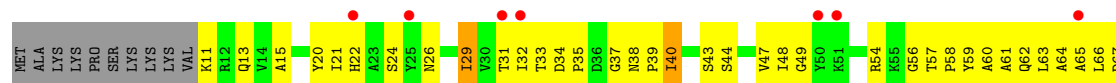
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



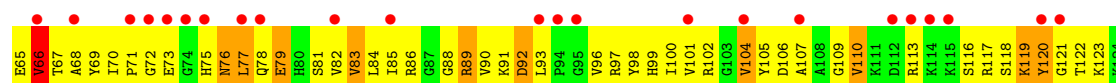
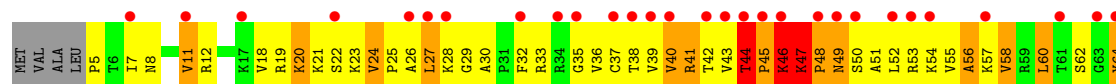
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

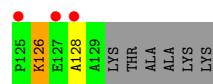


• Molecule 11: 30S RIBOSOMAL PROTEIN S11



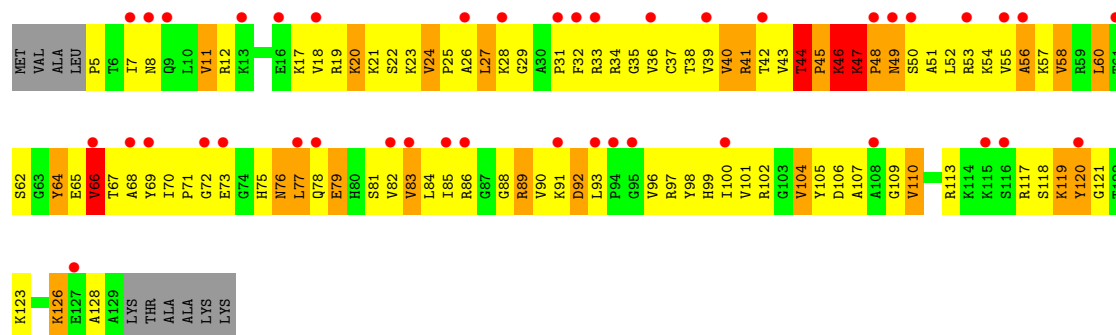
• Molecule 12: 30S RIBOSOMAL PROTEIN S12





• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL: 31% 21% 51% 18% 7%



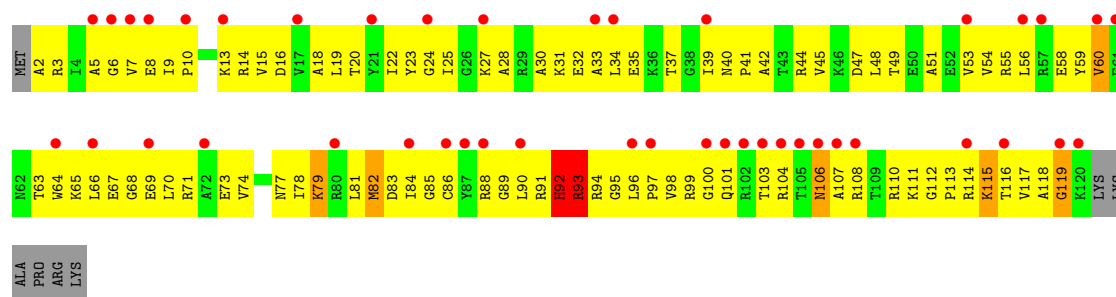
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM: 44% 22% 66% 5% 6%



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

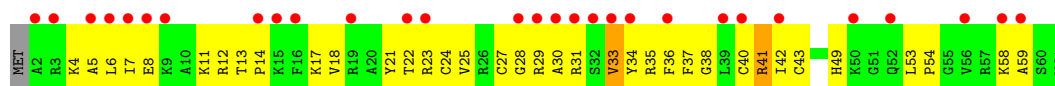
Chain CM: 34% 20% 68% 5% 6%



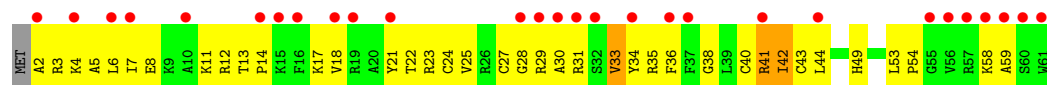
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN: 48% 39% 56% 2%

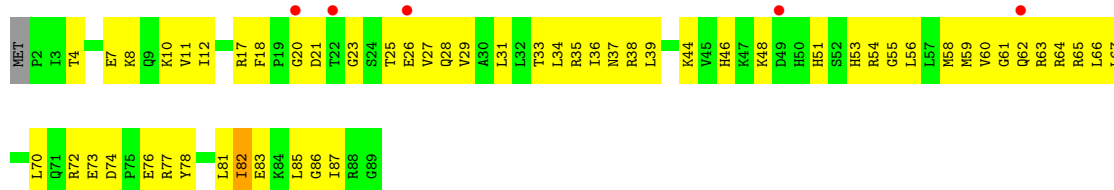




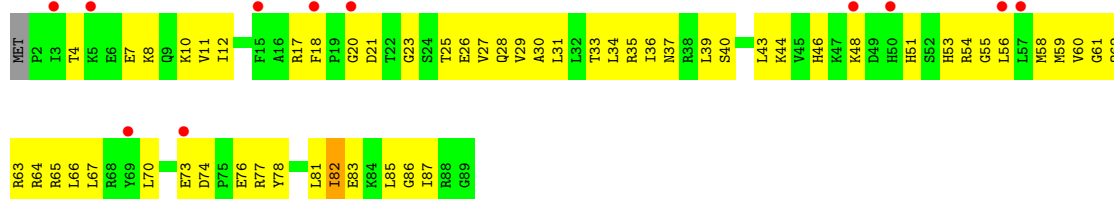
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



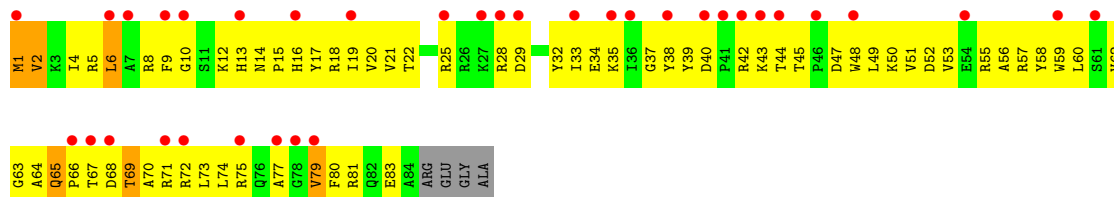
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

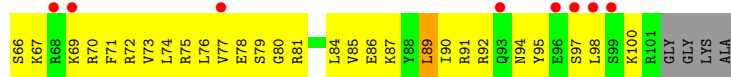
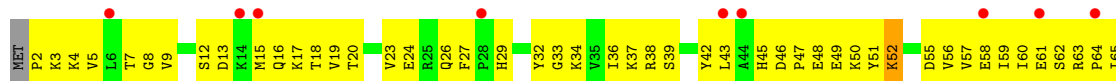


• Molecule 16: 30S RIBOSOMAL PROTEIN S16





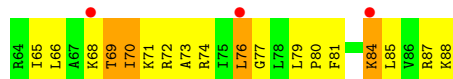
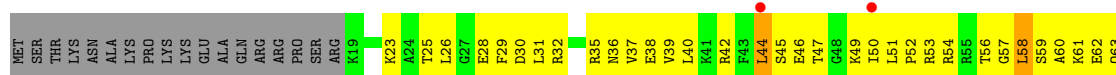
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



• Molecule 17: 30S RIBOSOMAL PROTEIN S17



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

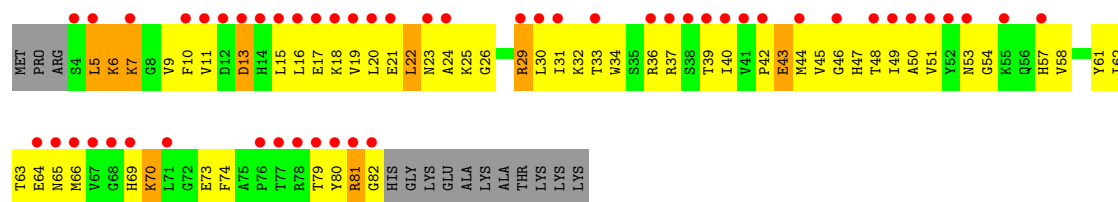


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

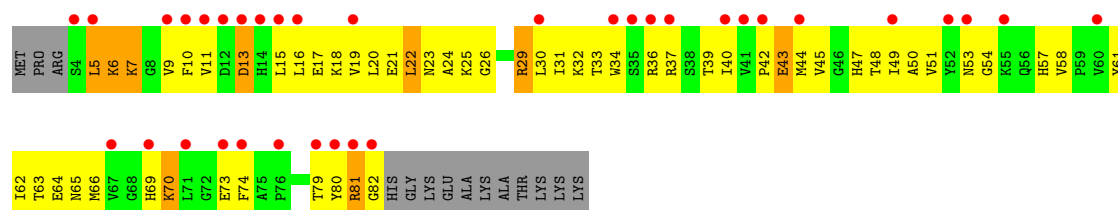


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

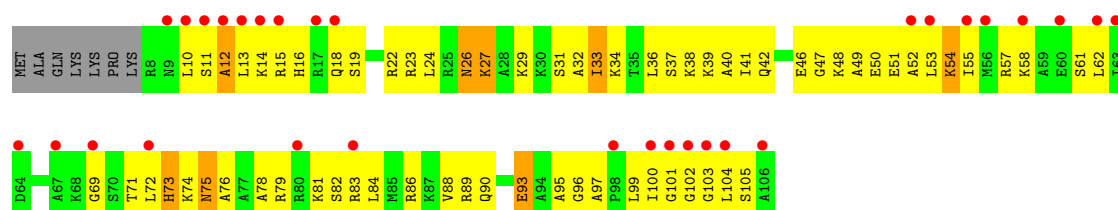




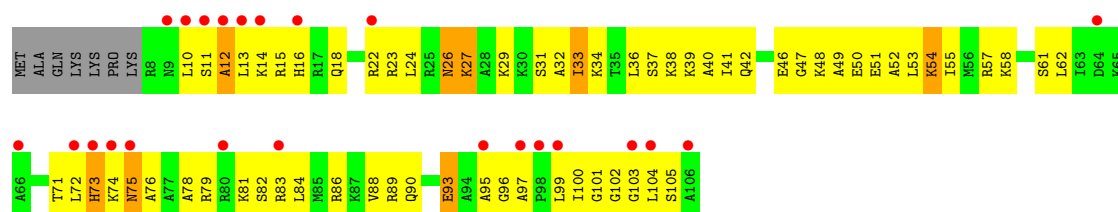
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



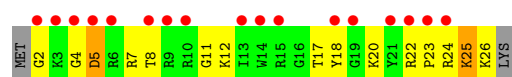
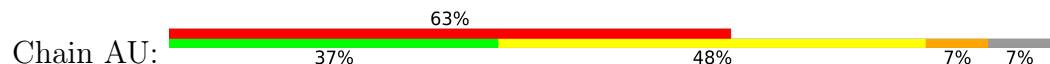
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

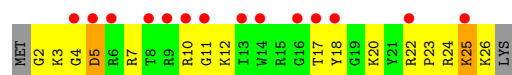


• Molecule 21: 30S RIBOSOMAL PROTEIN THX

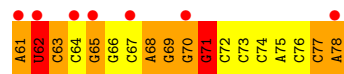
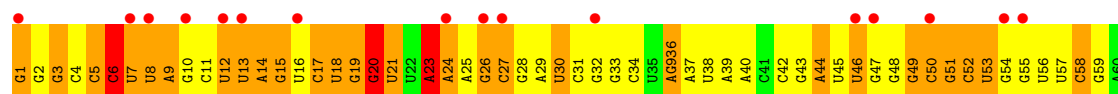


• Molecule 21: 30S RIBOSOMAL PROTEIN THX

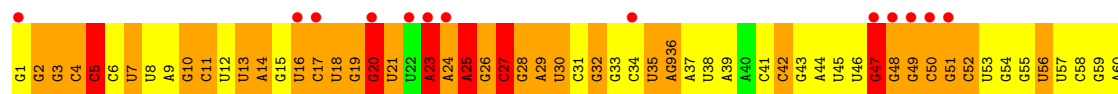




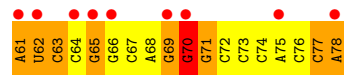
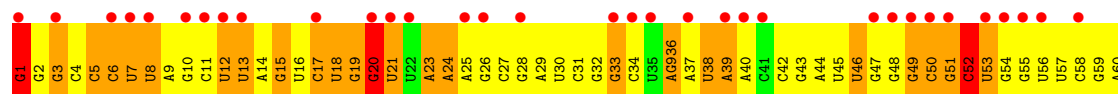
- Molecule 22: E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE



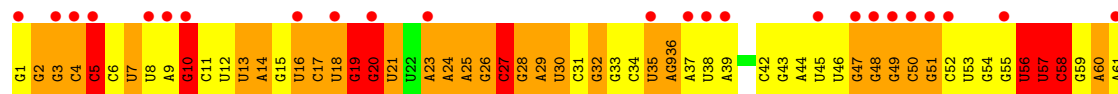
- Molecule 22: E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE



- 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

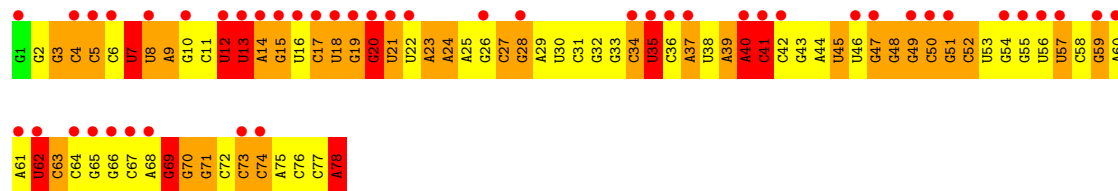


- Molecule 23: A-SITE TRNA ILE2 AGMATIDINE

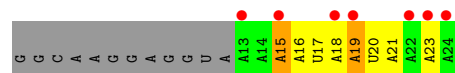




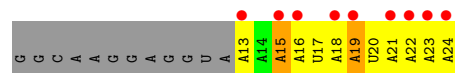
• Molecule 23: A-SITE TRNA ILE2 AGMATIDINE



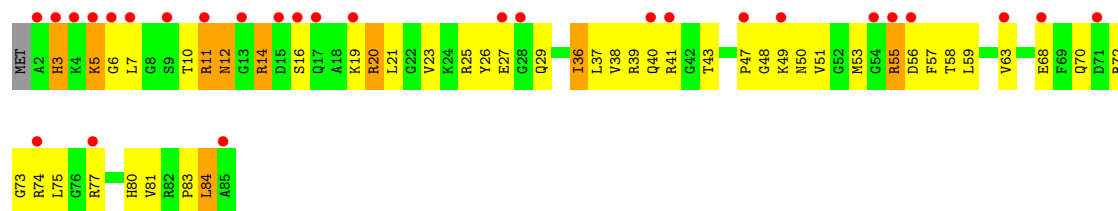
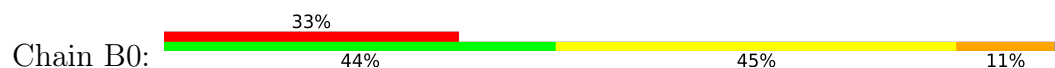
• Molecule 24: MRNA



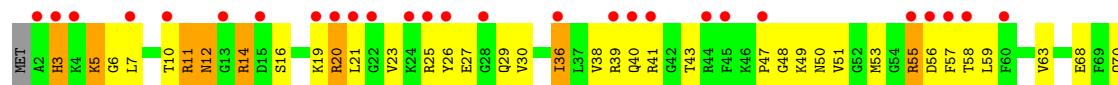
• Molecule 24: MRNA



• Molecule 25: 50S RIBOSOMAL PROTEIN L27

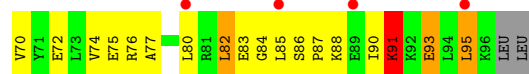
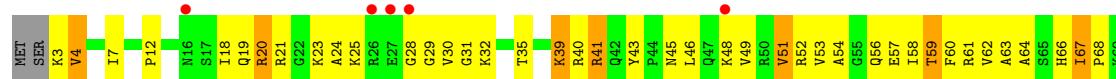


• Molecule 25: 50S RIBOSOMAL PROTEIN L27

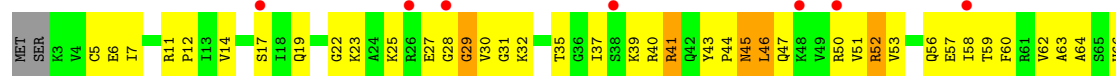




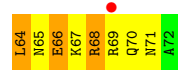
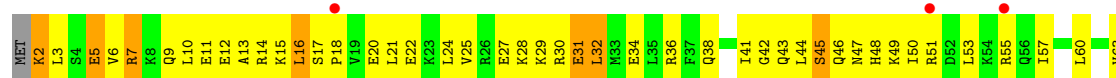
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



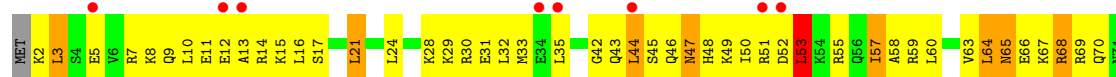
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



• Molecule 27: 50S RIBOSOMAL PROTEIN L29

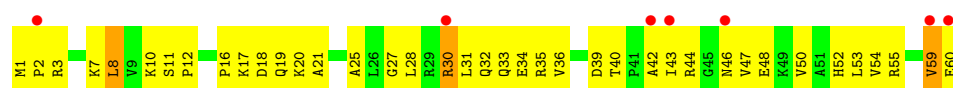


• Molecule 27: 50S RIBOSOMAL PROTEIN L29

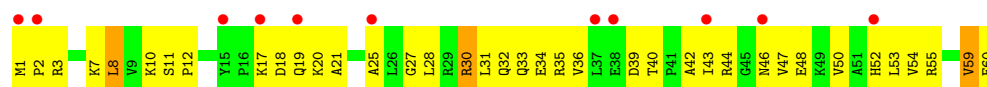


• Molecule 28: 50S RIBOSOMAL PROTEIN L30

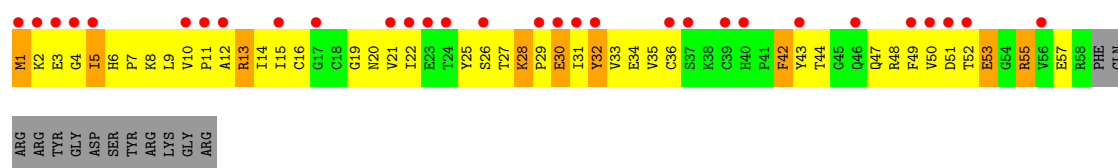
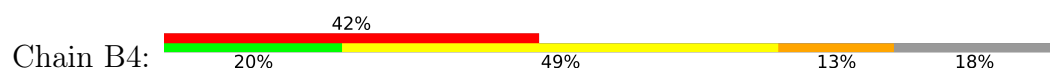




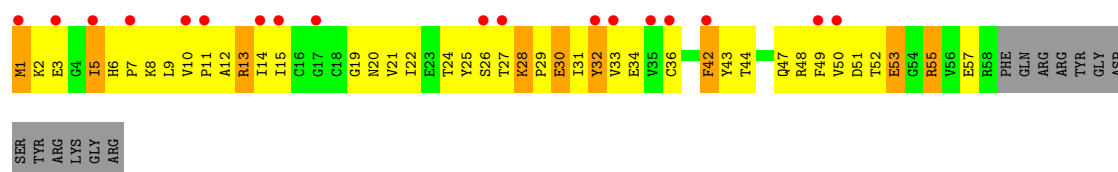
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



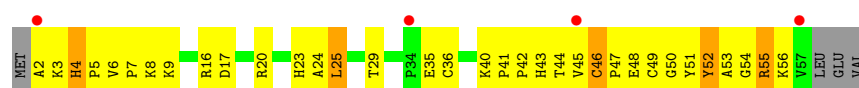
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



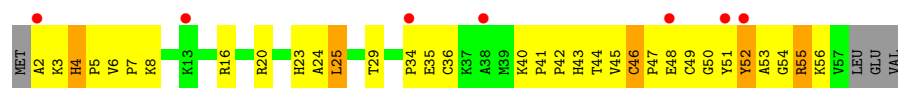
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



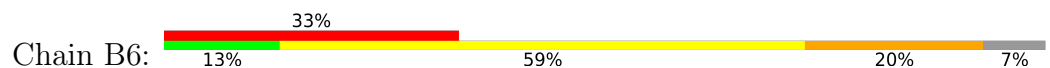
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



• Molecule 30: 50S RIBOSOMAL PROTEIN L32

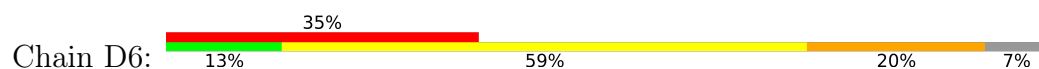


• Molecule 31: 50S RIBOSOMAL PROTEIN L33

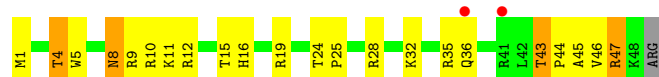




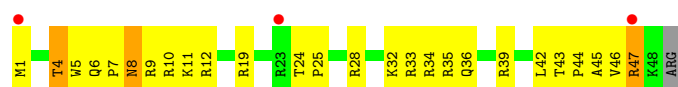
● Molecule 31: 50S RIBOSOMAL PROTEIN L33



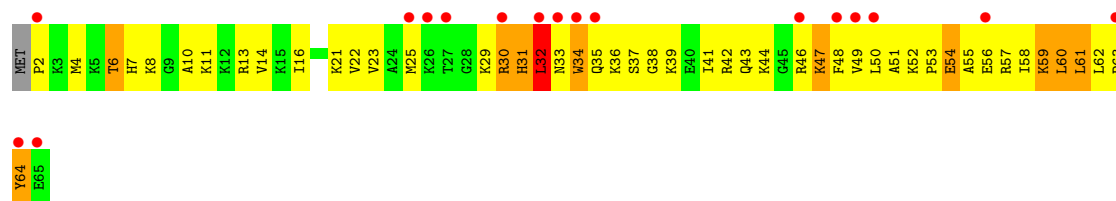
● Molecule 32: 50S RIBOSOMAL PROTEIN L34



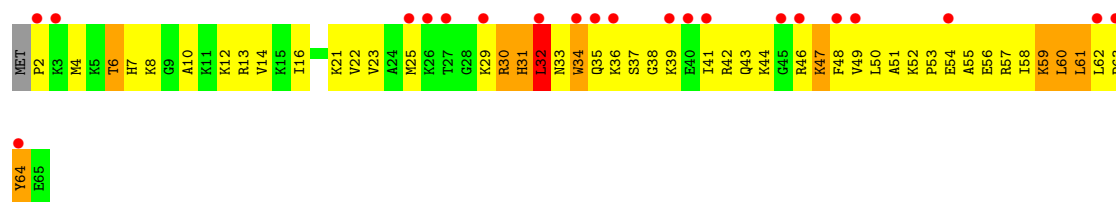
● Molecule 32: 50S RIBOSOMAL PROTEIN L34



● Molecule 33: 50S RIBOSOMAL PROTEIN L35



● Molecule 33: 50S RIBOSOMAL PROTEIN L35

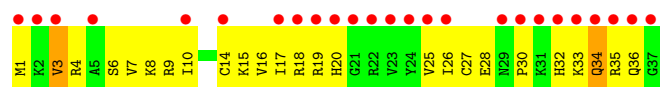


● Molecule 34: 50S RIBOSOMAL PROTEIN L36

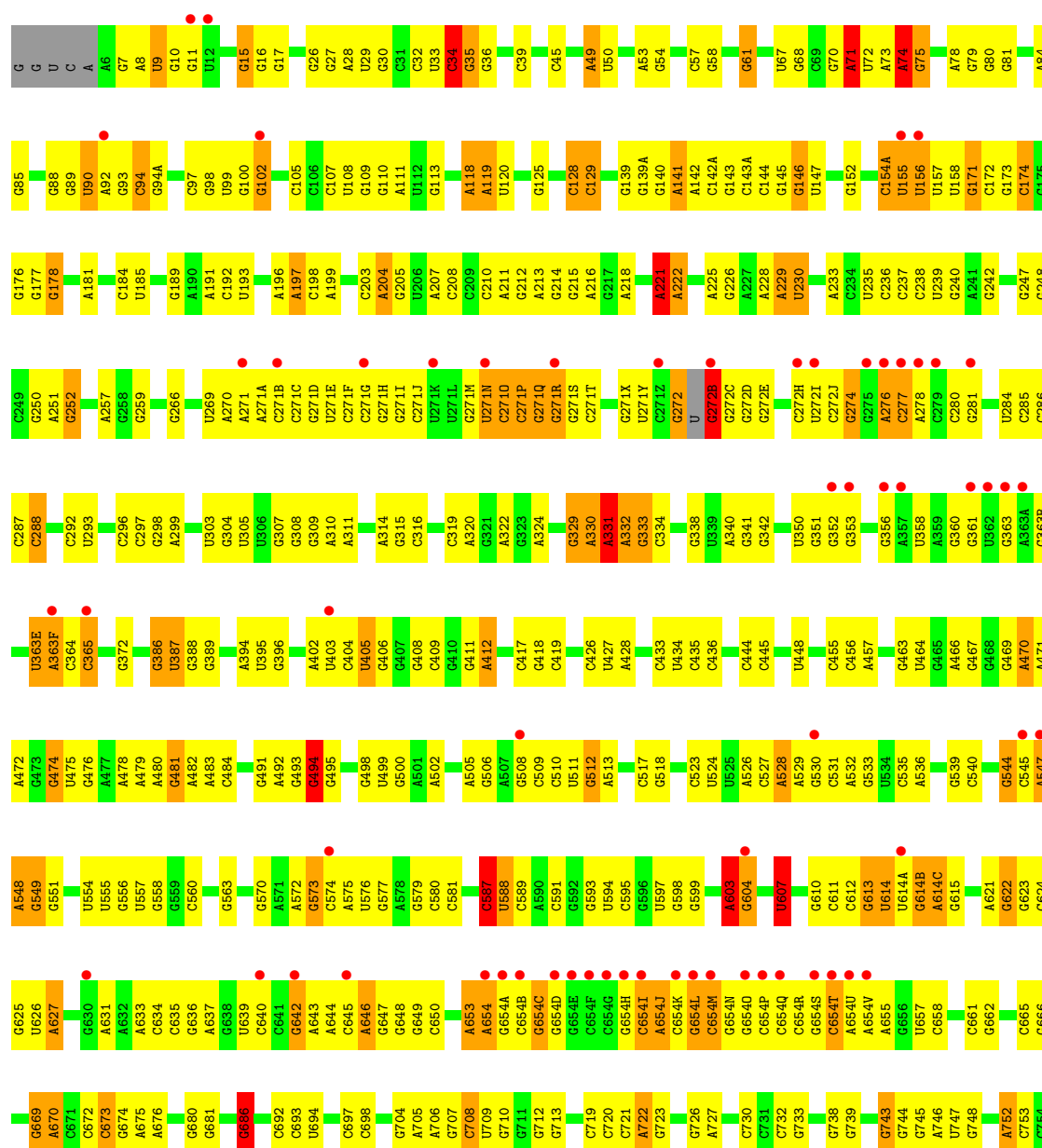




• Molecule 34: 50S RIBOSOMAL PROTEIN L36



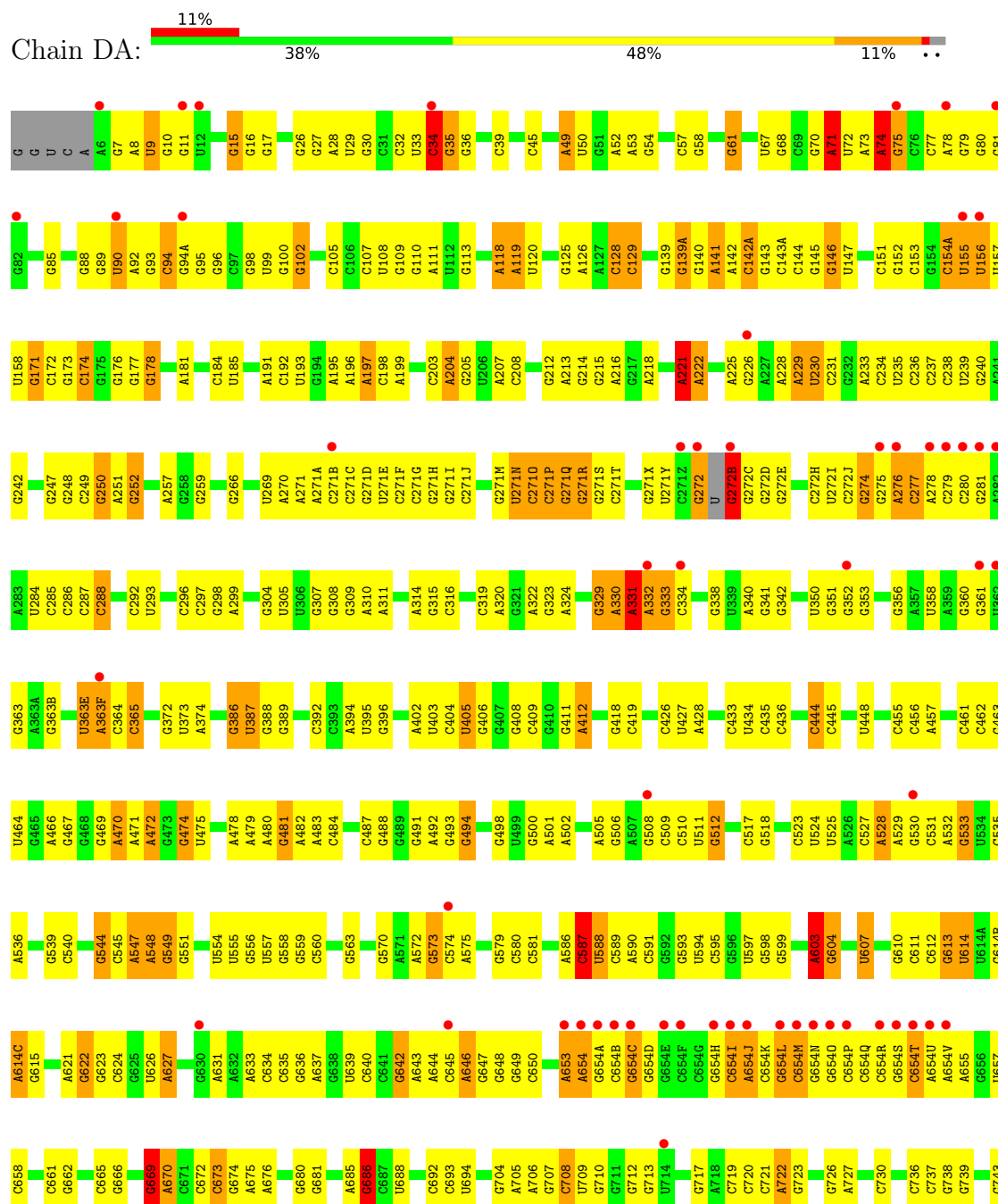
• Molecule 35: 23S RIBOSOMAL RNA



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C1682	A1509A	A1509B	U1433	A1354	U1249	U1165	C	G1030	U963	G892	C756
C1683	A1586	G1510	A1434	G1355	G1250	C1166	G	U1033	C964	C893	C758
U1688	A1587	C1511	G1440	G1358	G1251	U1167	A	G1034	C965	C894	
A1689	C1588		G1441	G1359	A1253	G1168	A		U969	U895	A764
	U1590	C1515	G1442	A1359		G1169	U	G1037	C970	A829	C765
U1693	C1516	C1517	A1445	A1360	G1256	G1170	A	A1038	C971	G830	C766
C1694	U1517	U1518	G1361	A1361	A1265	G1171	C	G1039	C972	G831	C767
G1695	C1519	U1519	G1362	C1363	G1266	G1173	G	C1040	A999	G832	G768
C1697	G1520	G1520	G1448	G1364		A1174	U	C1041	A901	U833	G769
	U1523	G1523	A1449	G1365	C1270	U1175	C	G1042	C975	C834	
C1698	G1524		G1450	A1365		G1176	A	C1043	C975	C902	G770
	A1528		U1453	G1368	A1271	G1177	C	A1044	G979	C903	G771
U1602	A1528A		G1459	G1369	A1272	C1178	U	A1045	A980	C904	G772
A1603	G1529		A1460		U1273	C1179	G	A1046	C908	U909	A774
C1607	C1530		G1461	U1372	A1275	U1180	U1108	G1047	A841	A842	G775
A1608	C1531		A1373	A1373		A1182	C1109	A1048	A843	G843	G776
A1609	G1532		C1375	C1375	A1278		G1110	C1049	A911	C844	A777
A1610	C1533		C1464	C1376	G1279	G1186	A111	G1051	C912	G845	G778
	U1534		C1467	G1377	G1280	G1187	C	G1052	U913	U846	G779
U1614	A1535		C1468	A1378	G1281	U1188	C1063	C1053	C914	U847	G780
	C1536		A1469	A1379	A1286	U1189	A1054	C1054	C915	G848	A781
C1617	G1537		A1470	G1380	A1287	G1190	G		C916	A849	A782
A1618	A1538		A1471	C1380	U1288	G1191	A	A	G993	C850	A783
G1620	C1539		A1472	G1381	C1289	G1192	C	A	C994	U851	G784
U1621	U1540		A1473	G1385	G1290	A1194	G	C	A996	G852	C786
	G1541		C1474	C1386	C1291	G1195	U	C	G997	G853	G787
	A1542		G1475	C1387	C1292			C	C998	U854	C788
G1628	C1543		G1478	C1388	U1292			U	U999	G855	A788
U1720	A1544			G1389	C1293	G1203		G	C924	C856	A789
C1638	A1545		U1481	A1395	U1300	U1205	A1129	G	U999	C925	C790
U1739	C1546		G1482	U1396	A1301	U1206	U1130	C	A1001	U858	G791
C1640	C1547		G1484	U1406	A1302	C1208	G1131	A	C1002	G859	C792
A1641	C1548		A1485	U1407	C1403	G1209	U1132	C	C1005	U860	A793
G1642	C1549		G1486	C1408	C1305	A1210	U1133	G	A933	G861	C796
	A1554		A1487	U1409	C1404	U1211	C1135	C	C1006	G862	C797
C1648			C1488	U1412	C1406	G1212	G1136	A	C1007	G864	G798
U1745A			U1489	A1412	G1311		G1137	C	G1008	C865	
C1746	A1558		A1490	G1413	U1312	G1216	G1138	C	A1009	A941	A802
C1747	G1559		A1491	C1416	U1313		G1139	U	A1010	C942	U803
C1748	C1564		G1492	G1417	C1314		U1139	C	G1011	G943	U804
A1749	C1565		C1493	A1418	C1315	A1220	C1140	G	U1012	U944	G805
C1657	U1659		A1494	G1419	C1316	C1221	U1141	C	G1013	G945	C906
			A1495	A1419	A1317	C1221A	U1142	C	U1014	G946	U807
C1751	G1568		A1496	G1413	C1318	G1231	A1142A	A	G1015	G947	G808
	A1569		A1497	C1417	G1319	U1232	A1143	U	G1016		
U1754	C1666		U1503	G1416	C1319	C1233	C1147	C	G1017	G950	C812
C1755	A1667		C1504	A1570	A1320	U1234	A1148	U	C1018	C951	U813
U1757	A1669		G1572	G1418	A1321	G1417	G1149	U	U1019	G952	C814
G1758	C1670		C1574	A1419	A1331	U1240	C1150	U	A1020	A953	C815
	U1671		C1575	U1420	G1332	A1241	G1151	A	U1021	G954	C816
C1761	C1672		C1577	U1503	A1331	A1242	C1152	C	G1022	C955	C817
A1762	U1673		C1578	C1504	G1339	G1243	C1153	A	U1023	C956	G818
G1763	G1674		A1579	C1505	U1427	A1248	G1154	A	G1024	C884	A819
G1764			C1506	G1429	G1345	G1245	A1155	G	U1025	U958	A820
			A1507	C1430	C1348	A1246	A1156	A	U1026	A877	A821
	G1678		U1508	A1507	C1349	A1247	C1157	U	A1027	C960	C822
			A1509	U1508	C1348	A1247	C1158	C	U1028	U961	C823

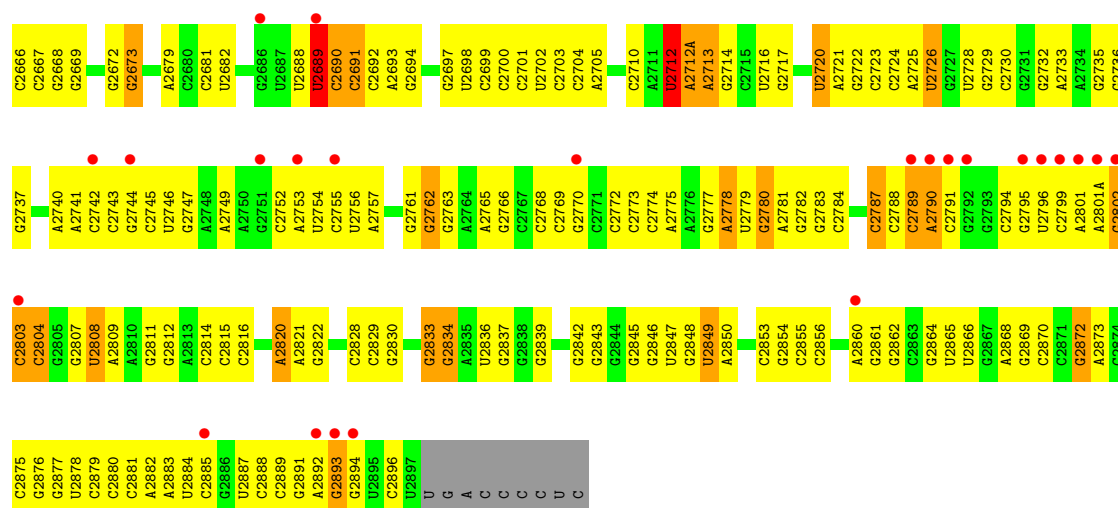


- Molecule 35: 23S RIBOSOMAL RNA

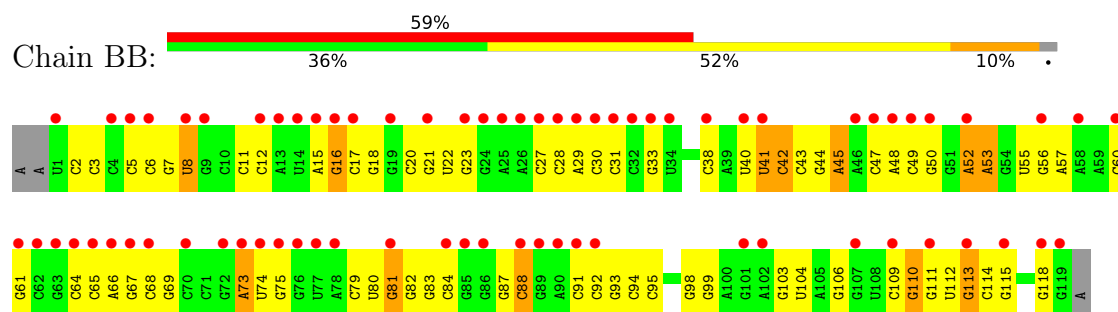


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C1598	U1523	C1376	C1291	A1210	U1133	A	A1010	A945	C815	G745
U1602	G1524	G1377	U1292	G1212	C1135	G	G1011	G946	C816	A746
A1603	G1527	A1378	C1293	G1215	G1137	C	U1012	G947	C817	U747
C1607	A1528	G1379	U1300	G1216	G1138	G	U1013	G948	C818	G748
A1608	A1528A	G1380	A1301	G1220	G1139	C	G1014	C949	A819	A752
A1609	G1529	C1381	A1302	A1221	U1141	C	G1015	G950	A820	A753
A1610	C1530	C1382	C1305	C1221A	U1142	A	G1016	C951	A821	C754
A1614	G1531	C1383	C1306	C1221A	A1142A	C	G1017	G952	U822	G755
A1618	G1532	C1384	C1307	G1231	A1143	C	U1018	A953	C823	C756
A1619	C1533	C1385	C1308	G1232	G1144	C	U1019	G954	C824	C757
A1628	U1534	C1386	G1311	G1233	A1145	C	A1020	G955	U825	U757
C1638	A1535	C1387	U1312	C1234	G1149	U	G1021	G956	U826	C758
C1639	G1536	C1388	U1313	C1235	U1150	U	U1022	A957	U827	G759
C1640	U1537	C1389	C1314	U1240	C1151	A	G1023	U958	A828	G760
C1641	C1538	C1390	C1315	U1241	G1152	A	U1024	A959	A829	A764
C1642	G1539	C1391	U1316	A1242	U1153	A	G1025	A960	A830	G765
C1648	U1540	C1392	U1317	G1243	G1154	G	U1026	C961	G831	
A1652	G1541	C1393	A1318	G1244	A1155	A	A1027	U962	G832	
G1653	A1542	C1394	C1319	G1245	A1156	G	U1028	U963	U833	
A1654	C1543	C1395	G1320	A1246	U1157	C	G1029	C964	C834	G768
A1655	U1544	C1396	A1321	A1247	G1161	C	U1030	C965	A835	G769
A1656	A1545	C1397	U1322	G1248	G1162	G	U1031	U969	G770	G771
C1657	C1546	C1398	G1323	U1249	U1165	A	G1032	C970	U772	C772
C1658	U1547	C1399	U1324	G1250	C1166	A	U1033	C971	U773	U773
C1659	C1548	C1400	U1325	G1251	U1167	A	G1034	G972	G775	G775
A1662	G1549	C1401	U1326	G1252	U1168	U	U1035	A973	C840	G776
G1663	A1550	C1402	U1327	A1253	U1169	U	G1036	G974	A841	G777
A1664	U1551	C1403	U1328	G1256	G1170	C	U1037	C975	G842	A777
A1665	C1552	C1404	U1329	G1257	G1171	C	G1038	G976	G843	G778
A1666	A1553	C1405	U1330	G1258	G1172	U	U1039	G977	C844	U779
A1667	G1554	C1406	U1331	G1259	U1173	G	C1040	U979	G845	G780
C1668	U1555	C1407	U1332	G1260	A1174	C	U1041	A980	C846	A781
A1669	A1556	C1408	U1333	G1261	U1175	C	G1042	A983	U847	A782
C1670	C1557	C1409	U1334	A1262	U1176	U	U1043	C984	G848	A783
U1671	G1558	C1410	U1335	G1263	U1177	U	A1044	A984	A849	A784
C1672	A1559	C1411	U1336	G1264	C1178	G	A1045	C985	G852	C786
G1666	G1560	C1412	U1337	G1265	C1179	U	A1046	C986	G853	U787
A1668	U1561	C1413	U1338	G1266	U1180	U	U1047	G987	G854	A788
A1669	C1562	C1414	U1339	G1267	C1181	G	A1048	U989	G855	A789
C1673	A1563	C1415	U1340	G1268	U1182	U	G1049	A990	C857	C791
C1674	G1564	C1416	U1341	G1269	G1186	G	U1050	C991	U858	G792
C1675	U1565	C1417	U1342	G1270	U1187	U	C1051	G992	C859	A793
G1668	A1566	C1418	U1343	G1271	G1188	G	C1052	G993	U860	C796
A1669	C1567	C1419	U1344	U1272	U1189	U	C1053	C994	A861	C797
U1673	U1568	C1420	U1345	U1273	A1189	A	U1054	A995	G862	G798
C1674	A1569	C1421	U1346	U1274	G1190	G	G	G996	A863	
C1675	U1570	C1422	U1347	A1275	G1191	G	A	C997	C864	A802
C1676	C1571	C1423	U1348	G1276	U1192	U	G	U998	C865	U803
C1677	G1572	C1424	U1349	G1277	G1193	U	G	U999	A866	A804
C1678	U1573	C1425	U1350	U1278	U1194	U	U1055	A1000	C867	G805
C1679	C1574	C1426	U1351	U1279	G1195	U	C1056	A1001	A870	C806
C1680	U1575	C1427	U1352	G1280	U1196	G	C1057	U1002	U871	U807
C1681	G1576	C1428	U1353	U1281	G1197	C	C1058	C1003	G808	
C1682	C1577	C1429	U1354	U1282	U1198	U	C1059	C1004		
C1683	U1578	C1430	U1355	U1283	G1199	U	C1060	C1005	G874	C812
C1684	C1579	C1431	U1356	U1284	U1200	U	C1061	C1006	U877	U813
C1685	A1580	C1432	U1357	U1285	A1204	A	C1062	C1007		
C1686	U1581	C1433	U1358	U1286	U1205	G	C1063	C1008		
C1687	A1582	C1434	U1359	U1287	C1208	G	C1064			
C1688	C1583	C1435	U1360	U1288			C1065			
C1689	U1584	C1436	U1361	U1289			C1066			
C1690	A1585	C1437	U1362	U1290			C1067			
C1691	C1586	C1438	U1363	U1291			C1068			
C1692	U1587	C1439	U1364	U1292			C1069			
C1693	A1588	C1440	U1365	U1293			C1070			
C1694	C1589	C1441	U1366	U1294			C1071			
C1695	U1589	C1442	U1367	U1295			C1072			
C1696	A1590	C1443	U1368	U1296			C1073			
C1697	C1591	C1444	U1369	U1297			C1074			
C1698	U1592	C1445	U1370	U1298			C1075			
C1699	A1593	C1446	U1371	U1299			C1076			
C1700	C1594	C1447	U1372	U1300			C1077			
C1701	U1595	C1448	U1373	U1301			C1078			
C1702	A1596	C1449	U1374	U1302			C1079			
C1703	C1597	C1450					C1080			

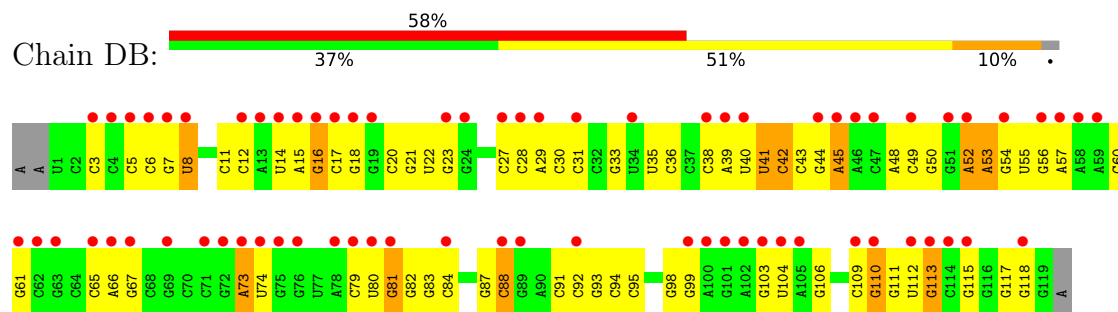




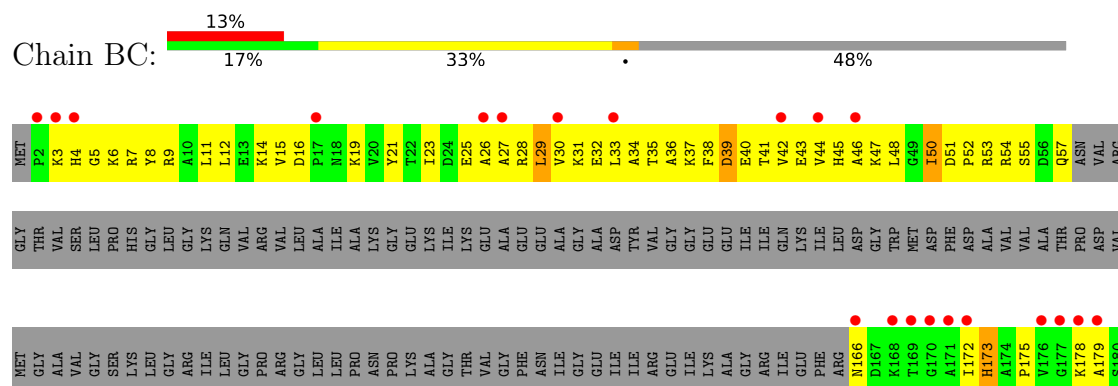
• Molecule 36: 5S RIBOSOMAL RNA



• Molecule 36: 5S RIBOSOMAL RNA

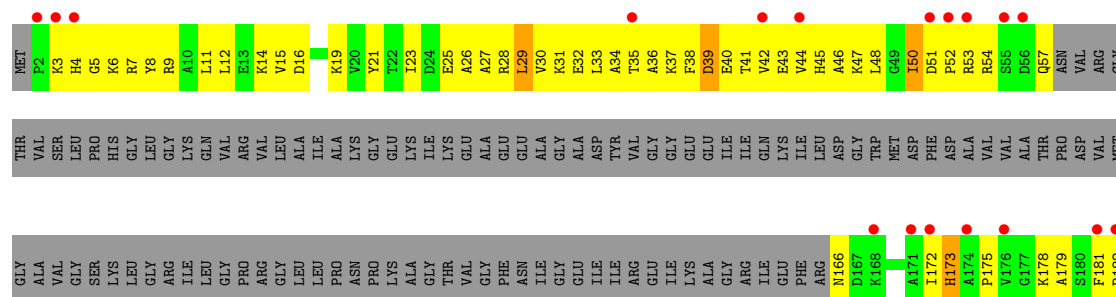


• Molecule 37: 50S RIBOSOMAL PROTEIN L1

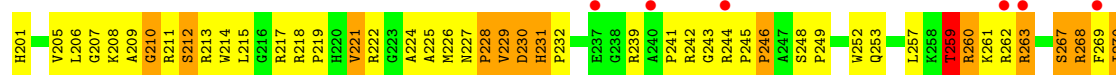
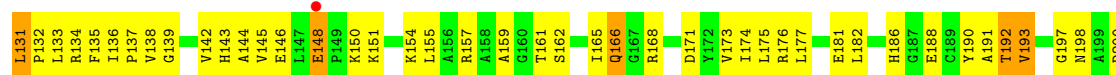
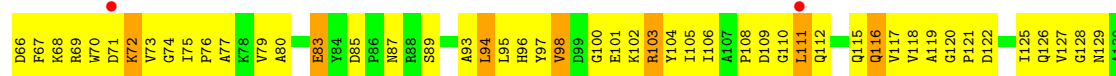
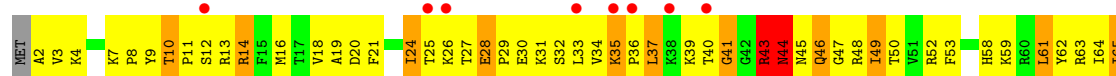




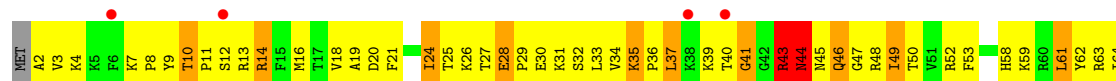
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

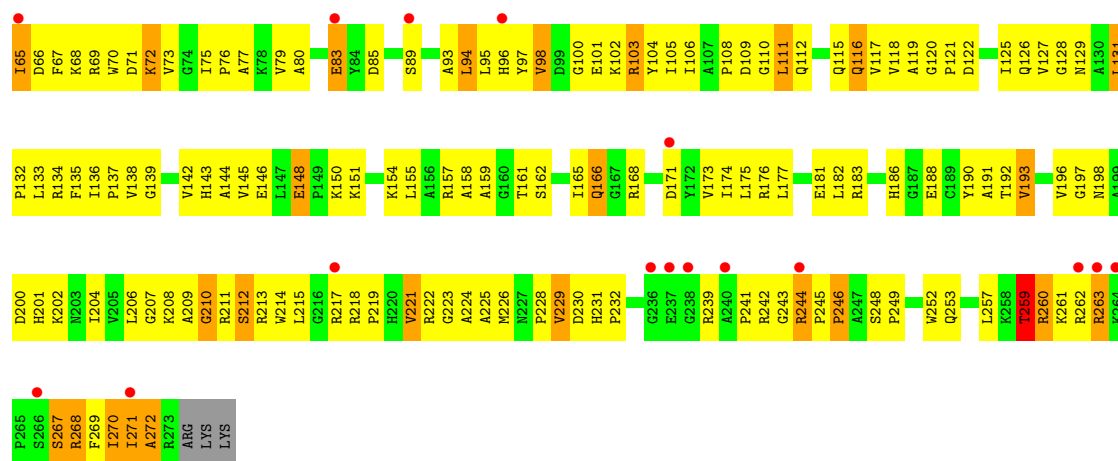


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

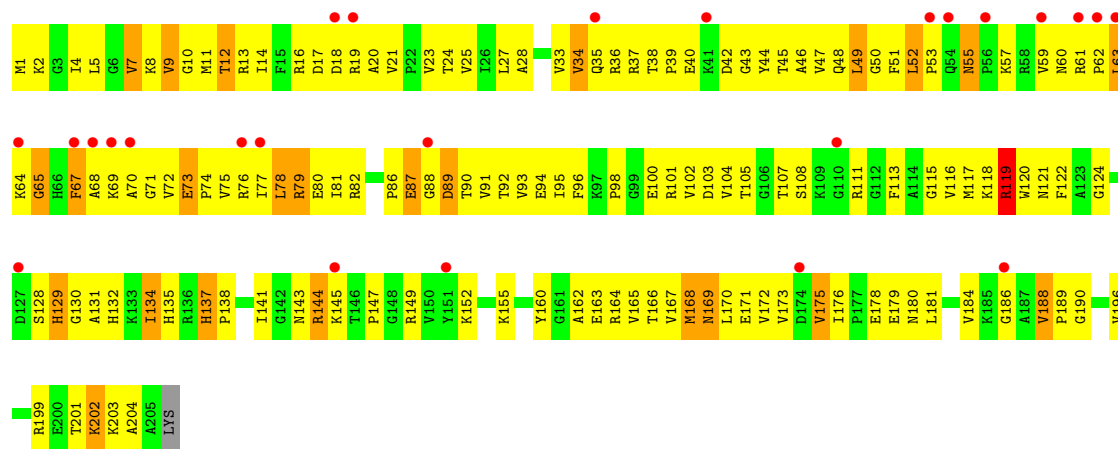


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

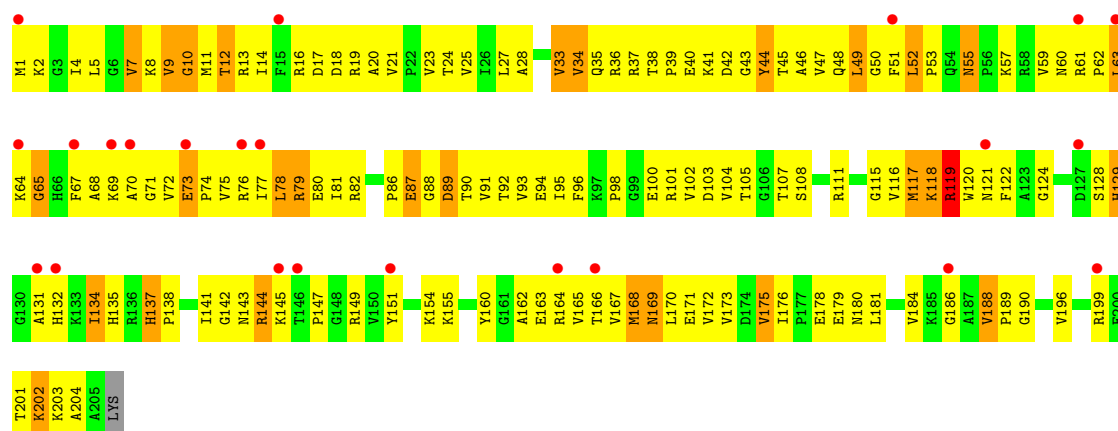




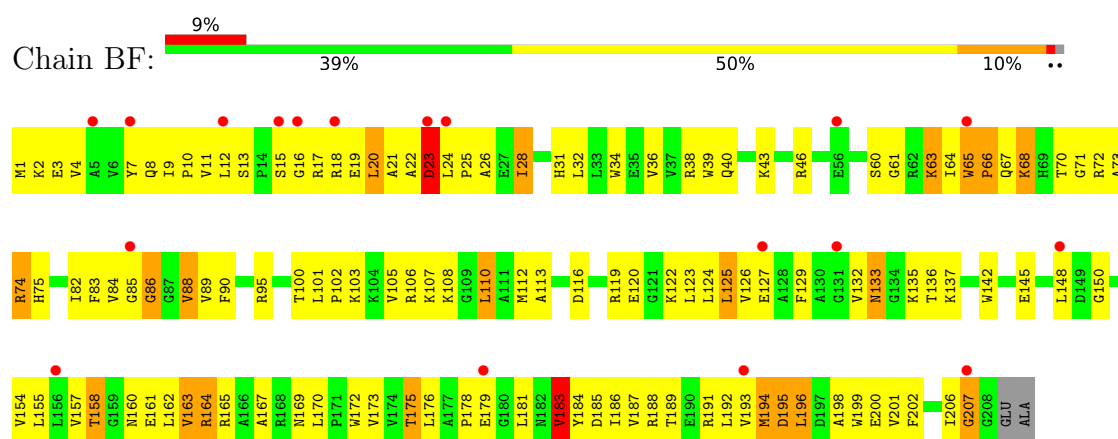
• Molecule 39: 50S RIBOSOMAL PROTEIN L3



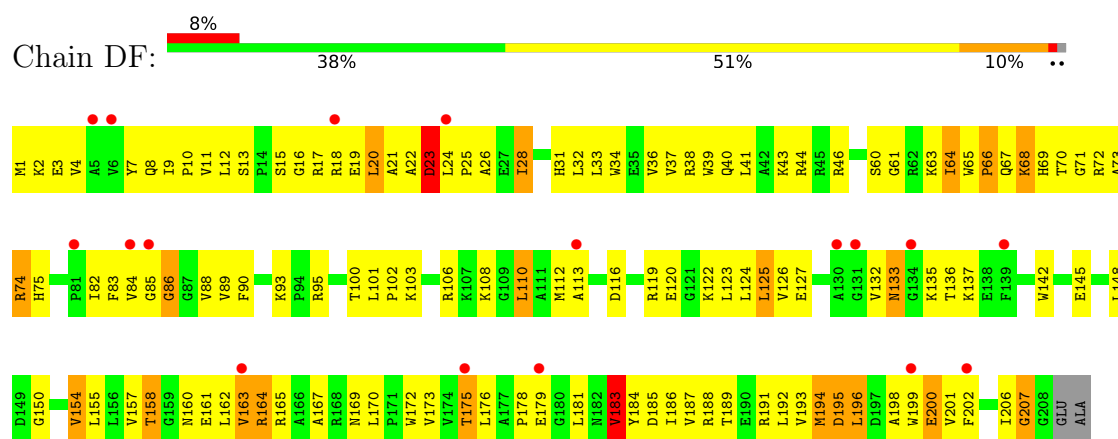
• Molecule 39: 50S RIBOSOMAL PROTEIN L3



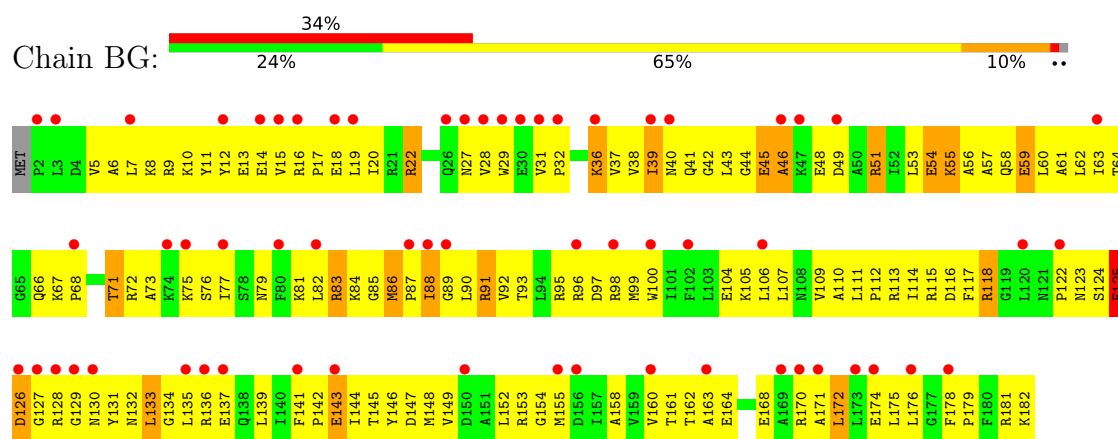
• Molecule 40: 50S RIBOSOMAL PROTEIN L4



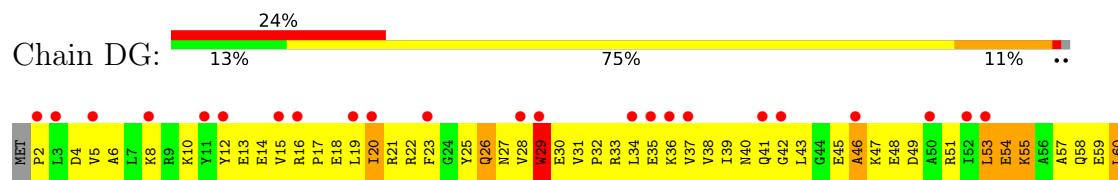
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

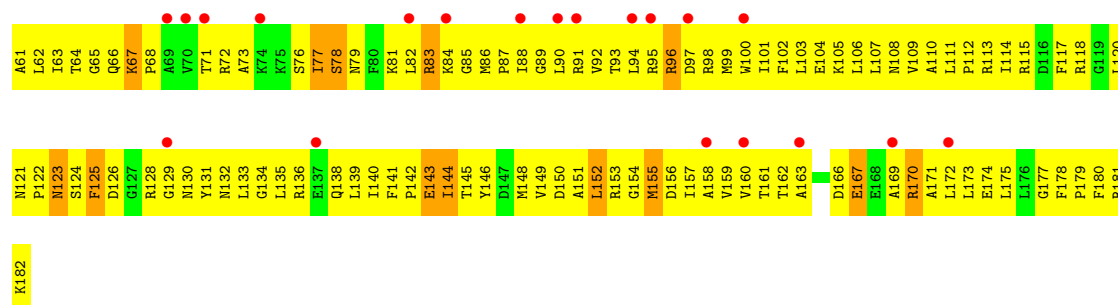


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

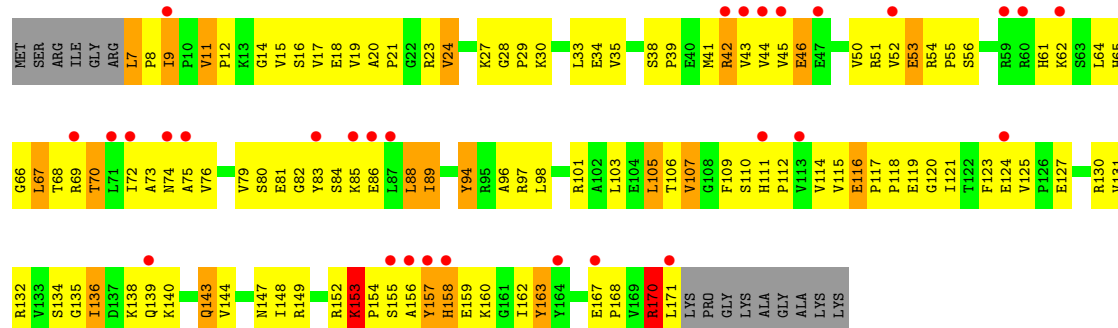


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

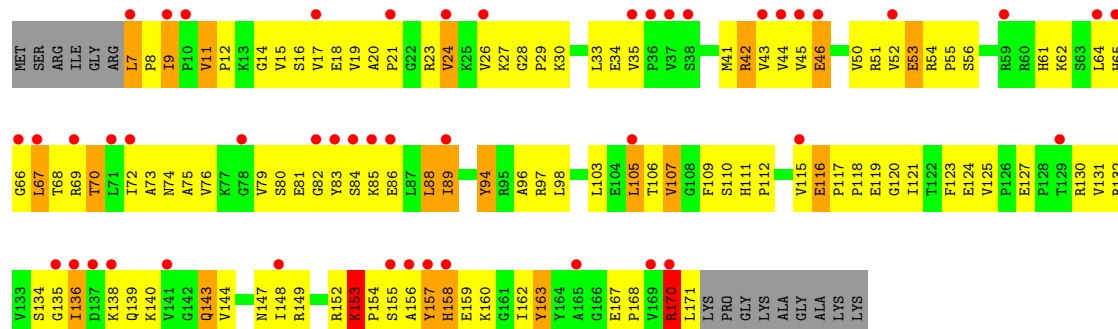




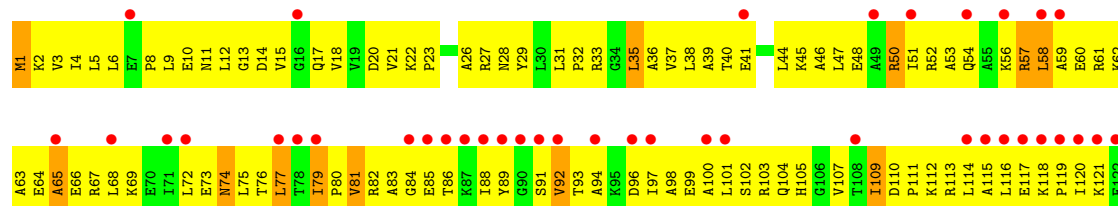
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

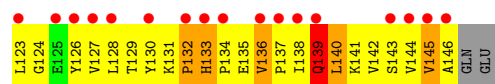


• Molecule 42: 50S RIBOSOMAL PROTEIN L6

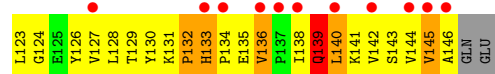
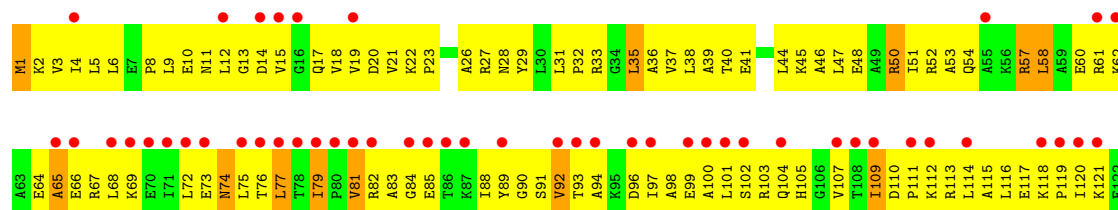


• Molecule 43: 50S RIBOSOMAL PROTEIN L9

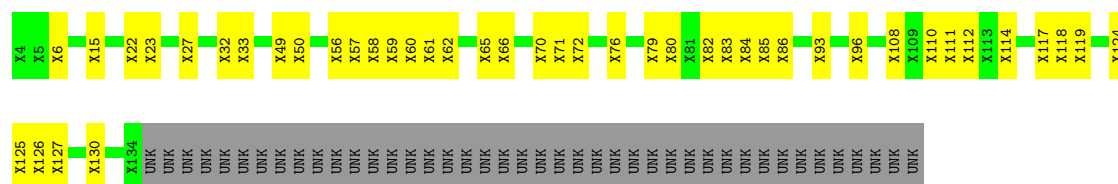




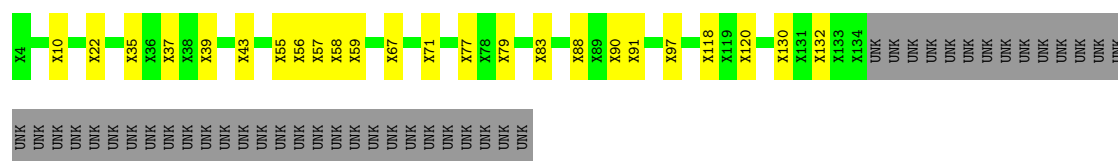
• Molecule 43: 50S RIBOSOMAL PROTEIN L9



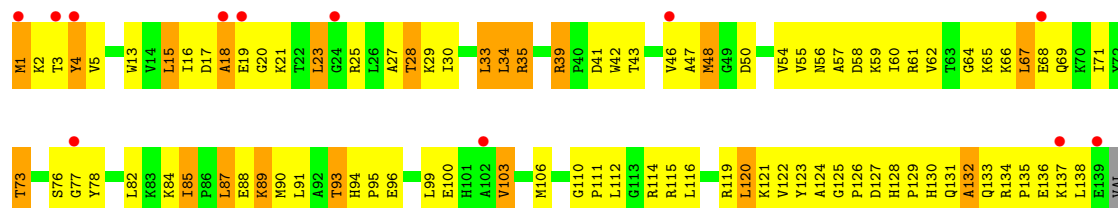
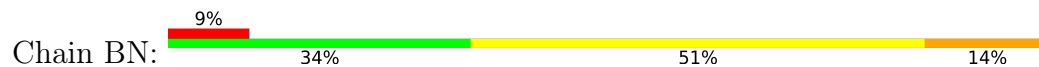
• Molecule 44: 50S RIBOSOMAL PROTEIN L10



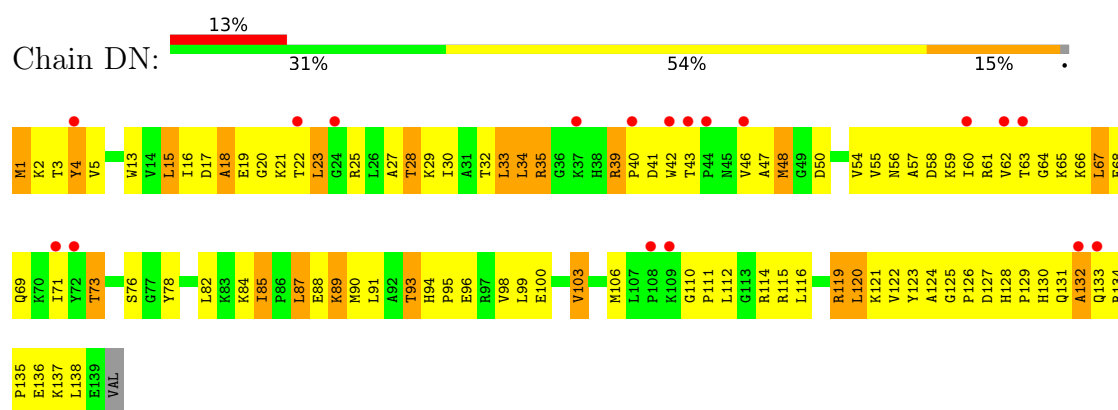
• Molecule 44: 50S RIBOSOMAL PROTEIN L10



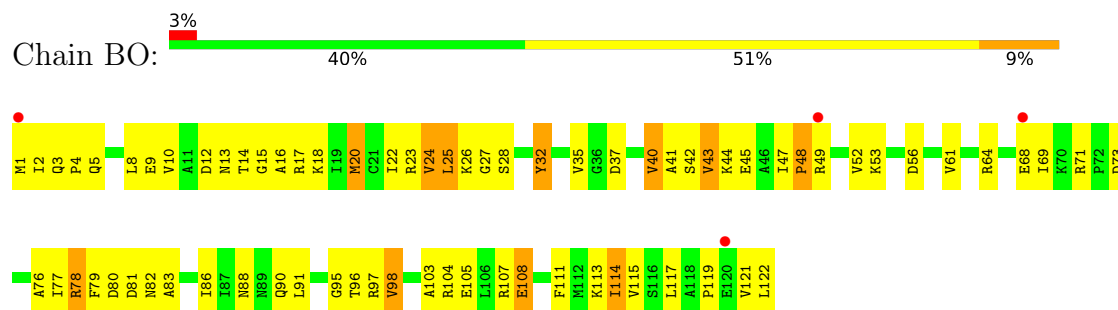
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



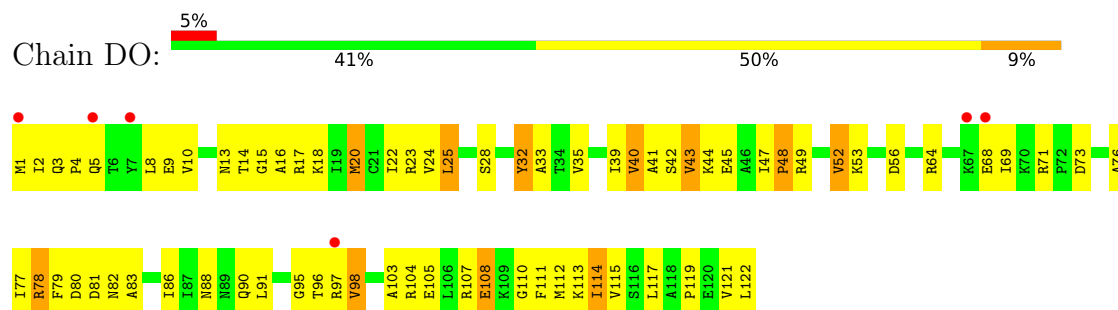
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



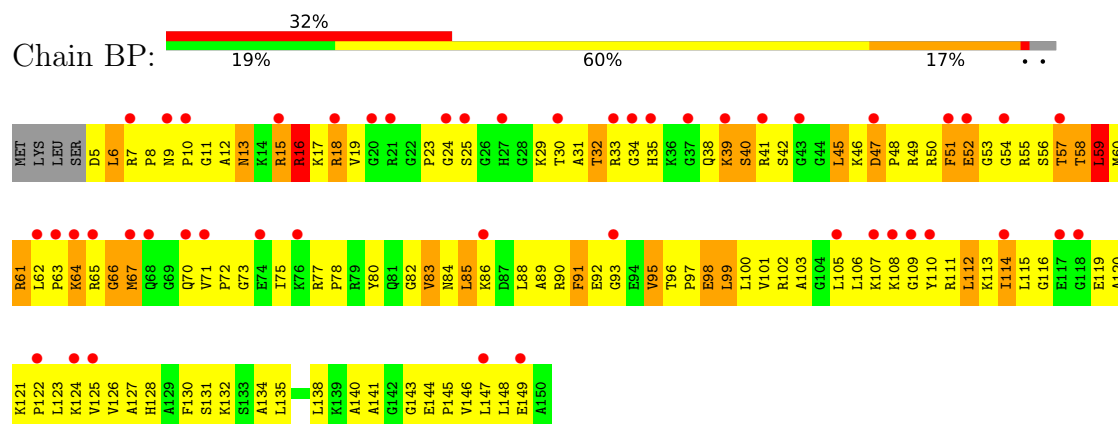
• Molecule 46: 50S RIBOSOMAL PROTEIN L14



• Molecule 46: 50S RIBOSOMAL PROTEIN L14

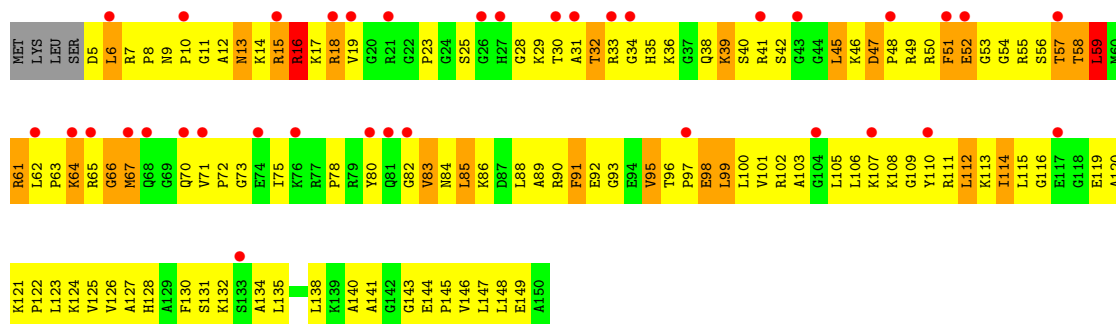


• Molecule 47: 50S RIBOSOMAL PROTEIN L15

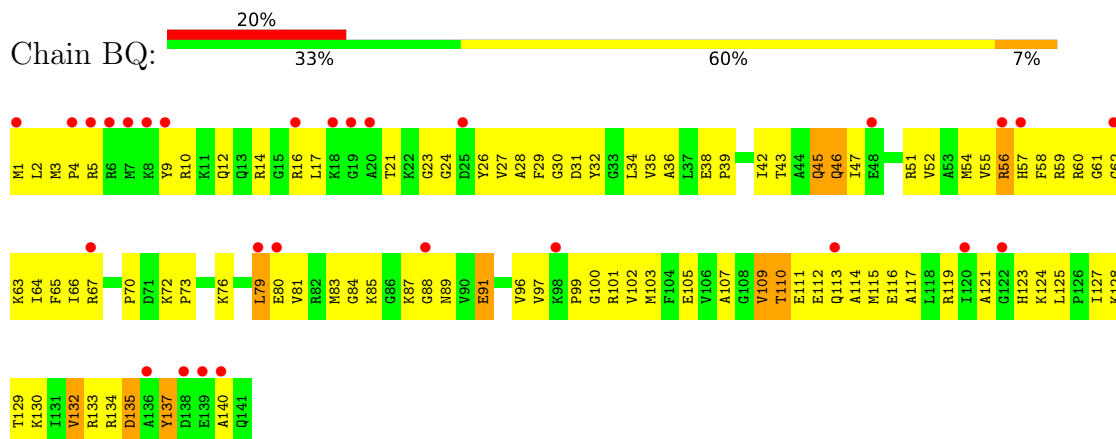


• Molecule 47: 50S RIBOSOMAL PROTEIN L15

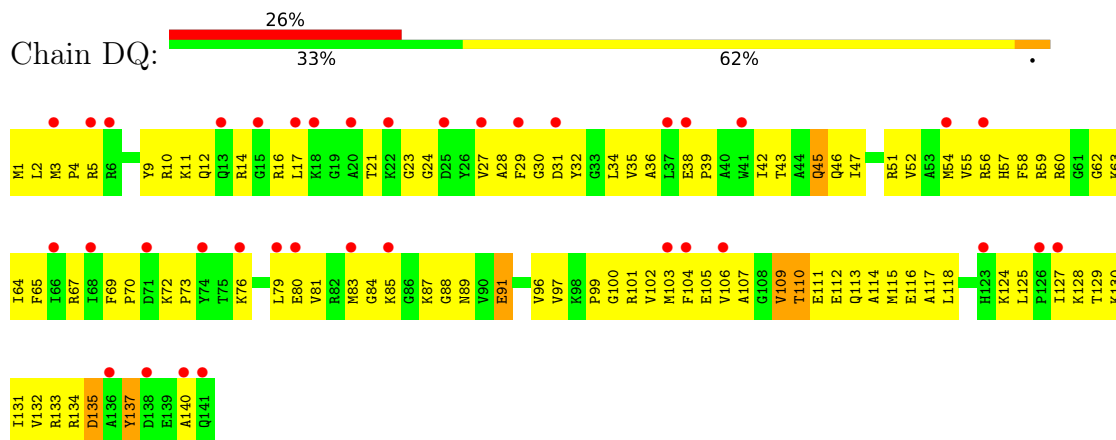




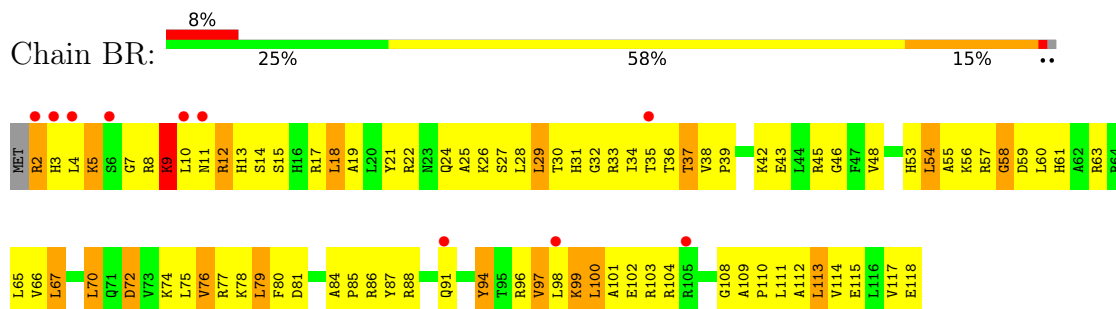
● Molecule 48: 50S RIBOSOMAL PROTEIN L16



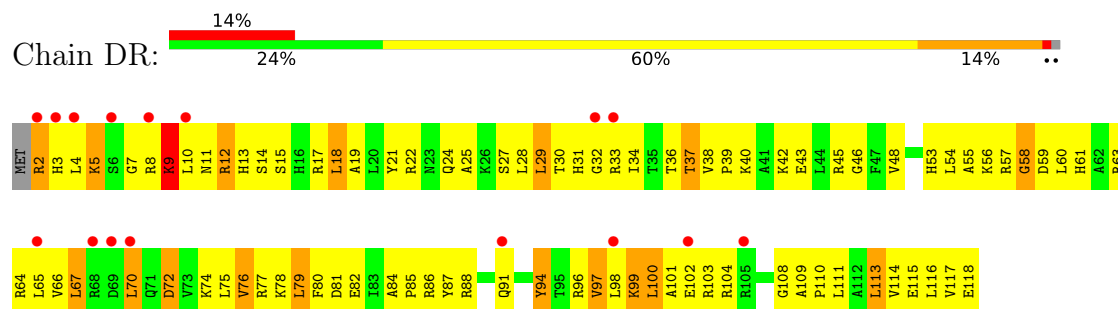
● Molecule 48: 50S RIBOSOMAL PROTEIN L16



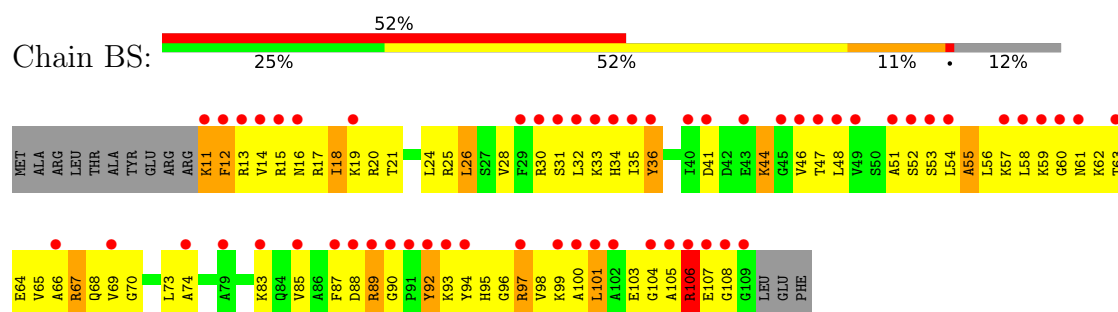
● Molecule 49: 50S RIBOSOMAL PROTEIN L17



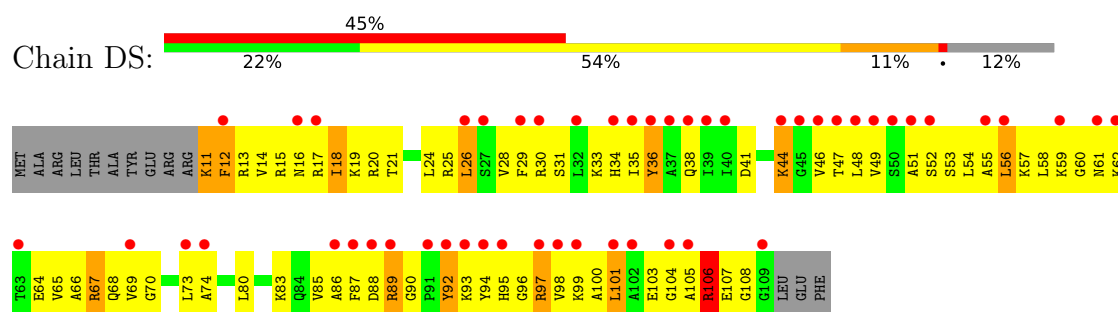
● Molecule 49: 50S RIBOSOMAL PROTEIN L17



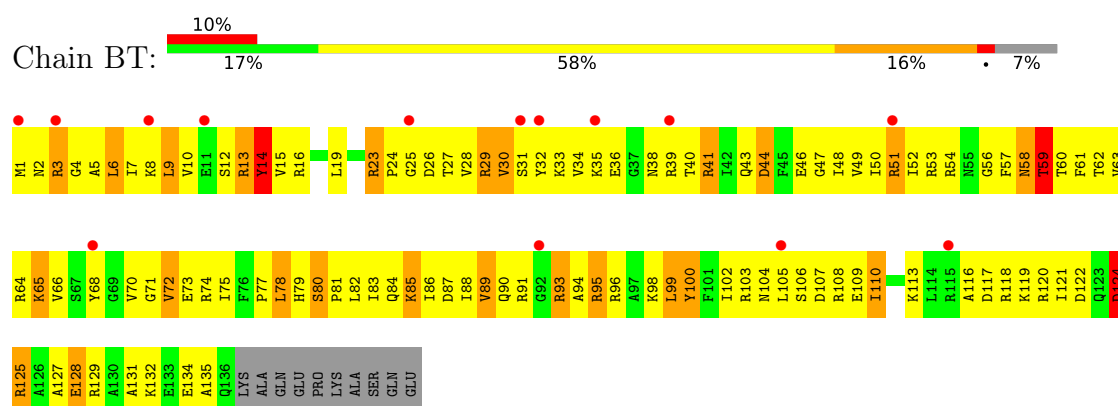
● Molecule 50: 50S RIBOSOMAL PROTEIN L18



● Molecule 50: 50S RIBOSOMAL PROTEIN L18

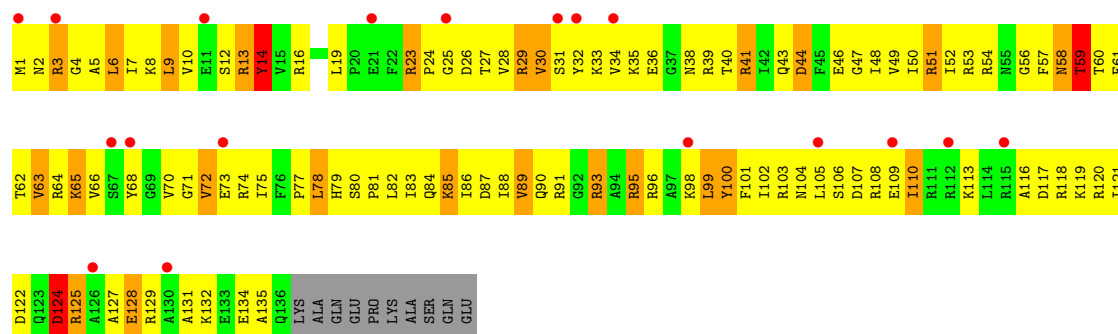


● Molecule 51: 50S RIBOSOMAL PROTEIN L19

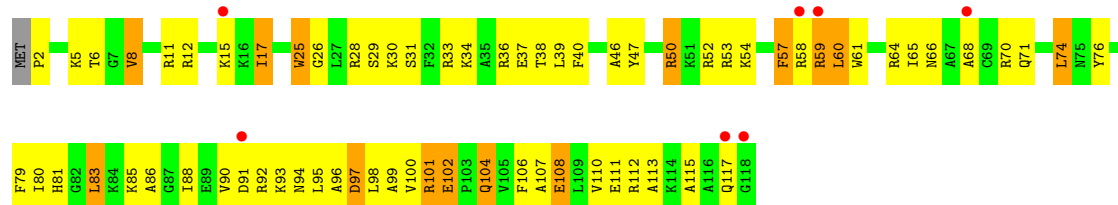


● Molecule 51: 50S RIBOSOMAL PROTEIN L19

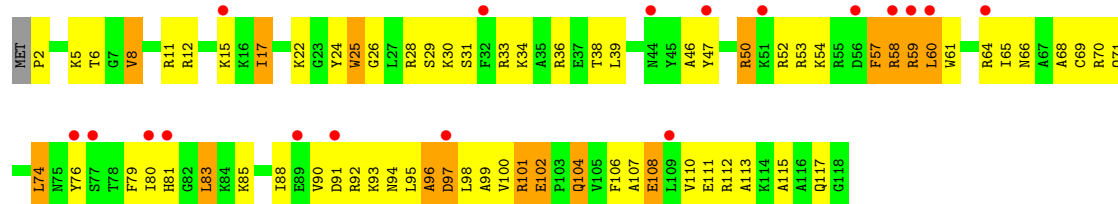




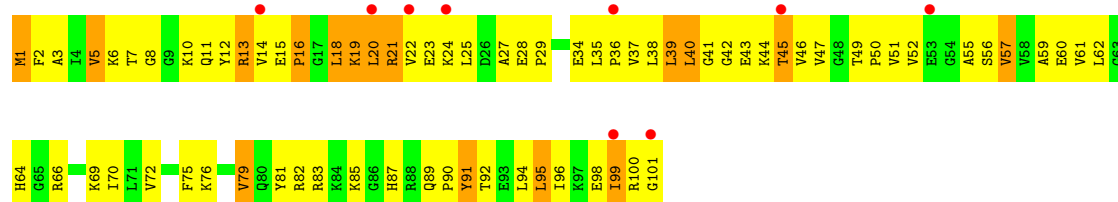
• Molecule 52: 50S RIBOSOMAL PROTEIN L20



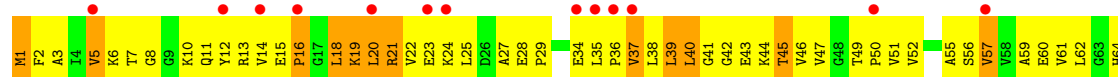
• Molecule 52: 50S RIBOSOMAL PROTEIN L20

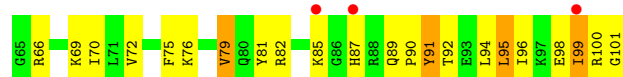


• Molecule 53: 50S RIBOSOMAL PROTEIN L21

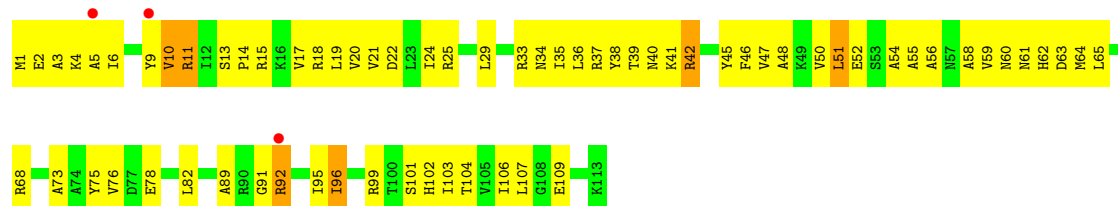


• Molecule 53: 50S RIBOSOMAL PROTEIN L21

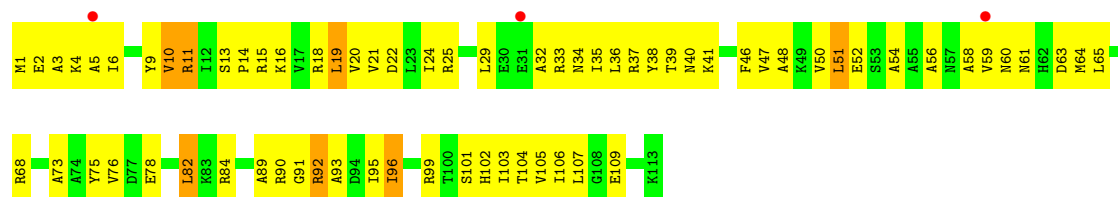




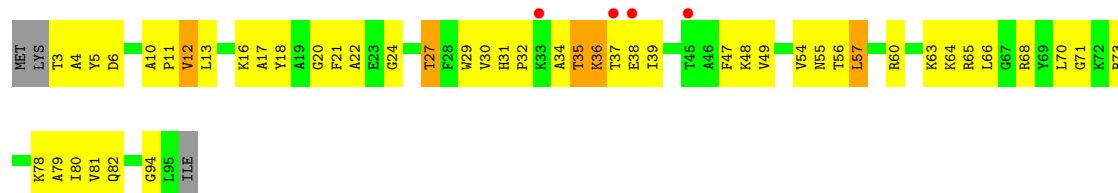
• Molecule 54: 50S RIBOSOMAL PROTEIN L22



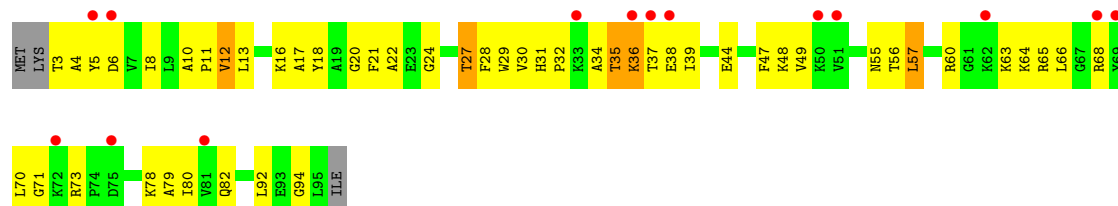
• Molecule 54: 50S RIBOSOMAL PROTEIN L22



• Molecule 55: 50S RIBOSOMAL PROTEIN L23

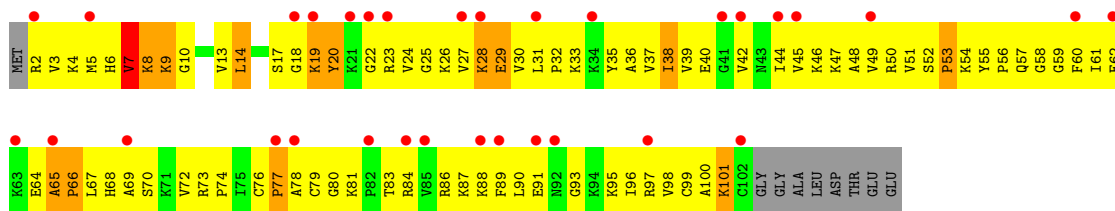


• Molecule 55: 50S RIBOSOMAL PROTEIN L23

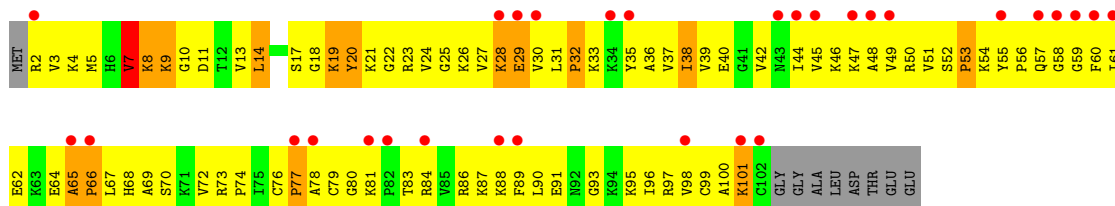


• Molecule 56: 50S RIBOSOMAL PROTEIN L24

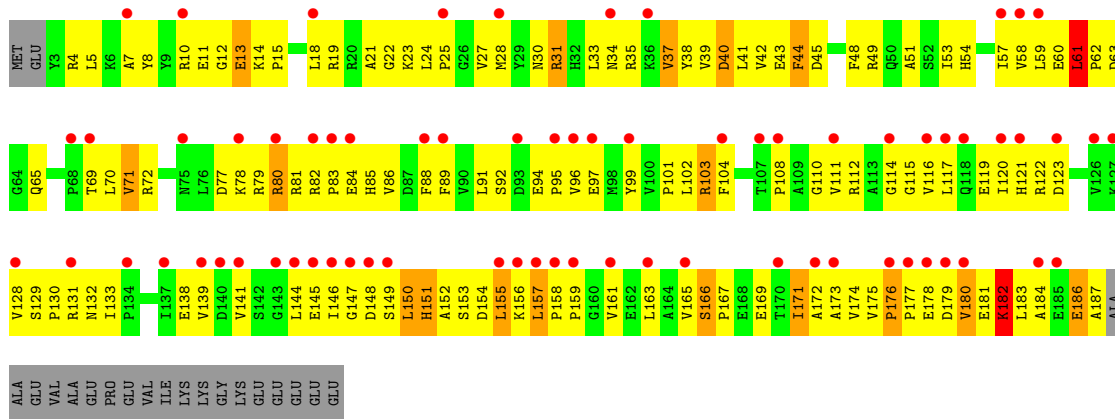




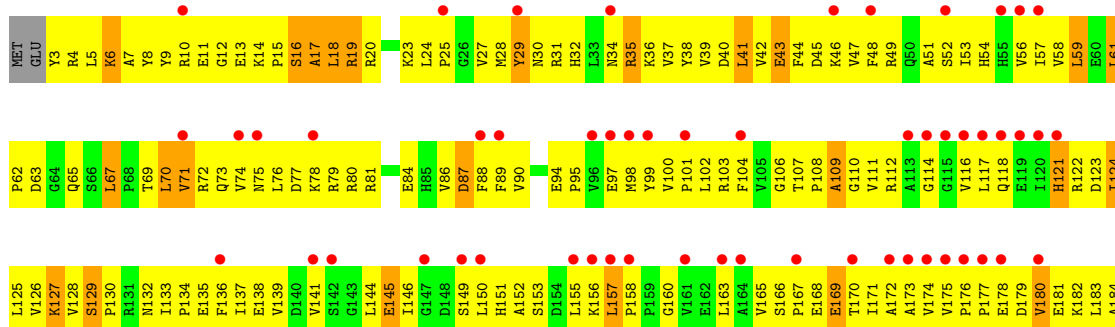
• Molecule 56: 50S RIBOSOMAL PROTEIN L24



• Molecule 57: 50S RIBOSOMAL PROTEIN L25



• Molecule 57: 50S RIBOSOMAL PROTEIN L25



E185	
E186	
A187	
ALA	
ALA	
GLU	
VAL	
ALA	
GLU	
PRO	
GLU	
VAL	
ILE	
LYS	
LYS	
GLY	
LYS	
GLU	
GLU	
GLU	
GLU	
GLU	

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 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-3.10) 97.6 (50.00-3.10)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.12Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.250 , 0.280 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 87.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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: ZN, AG9

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	0.43	0/36190	0.62	28/56486 (0.0%)
1	CA	0.43	0/36190	0.63	28/56486 (0.0%)
2	AB	0.38	1/1936 (0.1%)	0.97	13/2611 (0.5%)
2	CB	0.37	1/1936 (0.1%)	0.97	12/2611 (0.5%)
3	AC	0.41	1/1637 (0.1%)	0.88	2/2207 (0.1%)
3	CC	0.40	1/1637 (0.1%)	0.88	4/2207 (0.2%)
4	AD	0.44	0/1733	0.94	6/2318 (0.3%)
4	CD	0.44	0/1733	0.93	6/2318 (0.3%)
5	AE	0.47	1/1163 (0.1%)	0.92	3/1566 (0.2%)
5	CE	0.45	1/1163 (0.1%)	0.92	3/1566 (0.2%)
6	AF	0.43	0/856	0.88	2/1154 (0.2%)
6	CF	0.41	0/856	0.87	2/1154 (0.2%)
7	AG	0.37	0/1276	0.92	5/1709 (0.3%)
7	CG	0.37	0/1276	0.92	5/1709 (0.3%)
8	AH	0.41	0/1136	0.97	5/1527 (0.3%)
8	CH	0.40	0/1136	0.96	6/1527 (0.4%)
9	AI	0.35	0/1027	0.86	2/1373 (0.1%)
9	CI	0.35	0/1027	0.87	2/1373 (0.1%)
10	AJ	0.44	1/808 (0.1%)	0.92	2/1087 (0.2%)
10	CJ	0.43	1/808 (0.1%)	0.92	1/1087 (0.1%)
11	AK	0.43	0/900	0.93	3/1213 (0.2%)
11	CK	0.41	0/900	0.93	3/1213 (0.2%)
12	AL	0.61	1/987 (0.1%)	1.33	13/1322 (1.0%)
12	CL	0.57	1/987 (0.1%)	1.30	13/1322 (1.0%)
13	AM	0.43	1/943 (0.1%)	0.95	3/1256 (0.2%)
13	CM	0.42	1/943 (0.1%)	0.94	3/1256 (0.2%)
14	AN	0.37	0/501	0.82	0/664
14	CN	0.36	0/501	0.82	0/664
15	AO	0.41	0/745	0.84	0/992
15	CO	0.39	0/745	0.84	0/992
16	AP	0.49	1/717 (0.1%)	0.97	4/965 (0.4%)
16	CP	0.50	1/717 (0.1%)	0.97	5/965 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.45	1/837 (0.1%)	0.93	4/1119 (0.4%)
17	CQ	0.44	1/837 (0.1%)	0.93	3/1119 (0.3%)
18	AR	0.42	0/579	1.08	6/768 (0.8%)
18	CR	0.38	0/579	1.09	6/768 (0.8%)
19	AS	0.47	1/643 (0.2%)	0.95	1/867 (0.1%)
19	CS	0.48	1/643 (0.2%)	0.93	1/867 (0.1%)
20	AT	0.39	0/765	0.89	3/1007 (0.3%)
20	CT	0.40	0/765	0.90	3/1007 (0.3%)
21	AU	0.54	1/213 (0.5%)	0.79	1/279 (0.4%)
21	CU	0.55	1/213 (0.5%)	0.79	0/279
22	AV	1.06	0/1830	0.90	3/2849 (0.1%)
22	AY	1.11	0/1830	0.90	4/2849 (0.1%)
22	CV	0.61	0/1830	0.84	5/2849 (0.2%)
22	CY	1.00	10/1830 (0.5%)	1.01	16/2849 (0.6%)
23	AW	1.28	3/1853 (0.2%)	1.02	11/2887 (0.4%)
23	CW	0.62	0/1853	0.91	9/2887 (0.3%)
24	AX	0.47	0/290	0.82	0/450
24	CX	0.63	0/290	0.89	0/450
25	B0	0.54	0/671	0.94	1/892 (0.1%)
25	D0	0.45	0/671	0.93	1/892 (0.1%)
26	B1	0.63	1/741 (0.1%)	1.11	4/986 (0.4%)
26	D1	0.57	0/741	1.16	7/986 (0.7%)
27	B2	0.57	0/600	1.12	4/793 (0.5%)
27	D2	0.43	0/600	0.91	1/793 (0.1%)
28	B3	0.58	1/473 (0.2%)	1.01	3/636 (0.5%)
28	D3	0.51	1/473 (0.2%)	1.03	3/636 (0.5%)
29	B4	0.50	1/461 (0.2%)	0.97	1/623 (0.2%)
29	D4	0.50	1/461 (0.2%)	0.96	1/623 (0.2%)
30	B5	0.70	1/442 (0.2%)	1.03	2/598 (0.3%)
30	D5	0.62	1/442 (0.2%)	1.01	2/598 (0.3%)
31	B6	0.51	0/440	1.12	5/586 (0.9%)
31	D6	0.53	0/440	1.12	5/586 (0.9%)
32	B7	0.76	1/418 (0.2%)	1.10	1/552 (0.2%)
32	D7	0.72	1/418 (0.2%)	1.10	4/552 (0.7%)
33	B8	0.75	1/516 (0.2%)	1.21	3/681 (0.4%)
33	D8	0.64	1/516 (0.2%)	1.20	3/681 (0.4%)
34	B9	0.44	0/310	0.94	2/407 (0.5%)
34	D9	0.45	0/310	0.94	2/407 (0.5%)
35	BA	0.47	1/68704 (0.0%)	0.68	59/107260 (0.1%)
35	DA	0.44	1/68704 (0.0%)	0.68	60/107260 (0.1%)
36	BB	0.40	0/2853	0.60	0/4451
36	DB	0.40	0/2853	0.61	0/4451
37	BC	0.41	0/956	0.90	3/1288 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.42	0/956	0.90	3/1288 (0.2%)
38	BD	0.65	1/2155 (0.0%)	1.17	18/2907 (0.6%)
38	DD	0.57	1/2155 (0.0%)	1.15	17/2907 (0.6%)
39	BE	0.66	1/1597 (0.1%)	1.10	9/2155 (0.4%)
39	DE	0.57	1/1597 (0.1%)	1.10	13/2155 (0.6%)
40	BF	0.60	2/1659 (0.1%)	1.08	14/2246 (0.6%)
40	DF	0.51	1/1659 (0.1%)	1.08	13/2246 (0.6%)
41	BG	0.46	0/1498	1.01	9/2013 (0.4%)
41	DG	0.41	0/1498	1.03	10/2013 (0.5%)
42	BH	0.50	1/1285 (0.1%)	1.11	14/1741 (0.8%)
42	DH	0.50	1/1285 (0.1%)	1.10	12/1741 (0.7%)
43	BI	0.51	1/1147 (0.1%)	1.14	14/1553 (0.9%)
43	DI	0.48	1/1147 (0.1%)	1.13	13/1553 (0.8%)
45	BN	0.57	1/1132 (0.1%)	1.13	9/1527 (0.6%)
45	DN	0.49	1/1132 (0.1%)	1.10	9/1527 (0.6%)
46	BO	0.60	0/943	0.98	2/1269 (0.2%)
46	DO	0.55	0/943	0.97	2/1269 (0.2%)
47	BP	0.63	0/1131	1.33	14/1504 (0.9%)
47	DP	0.52	0/1131	1.31	13/1504 (0.9%)
48	BQ	0.57	1/1134 (0.1%)	0.94	5/1517 (0.3%)
48	DQ	0.49	1/1134 (0.1%)	0.92	3/1517 (0.2%)
49	BR	0.62	0/974	1.12	7/1302 (0.5%)
49	DR	0.56	0/974	1.11	7/1302 (0.5%)
50	BS	0.48	1/779 (0.1%)	1.00	3/1038 (0.3%)
50	DS	0.44	1/779 (0.1%)	1.00	3/1038 (0.3%)
51	BT	0.60	1/1138 (0.1%)	1.20	16/1521 (1.1%)
51	DT	0.55	1/1138 (0.1%)	1.19	13/1521 (0.9%)
52	BU	0.65	0/975	1.03	5/1297 (0.4%)
52	DU	0.52	0/975	1.06	6/1297 (0.5%)
53	BV	0.53	0/790	0.99	2/1057 (0.2%)
53	DV	0.46	0/790	0.97	2/1057 (0.2%)
54	BW	0.66	0/907	1.03	5/1216 (0.4%)
54	DW	0.56	0/907	1.03	4/1216 (0.3%)
55	BX	0.62	1/740 (0.1%)	1.11	3/995 (0.3%)
55	DX	0.55	1/740 (0.1%)	1.09	3/995 (0.3%)
56	BY	0.62	1/789 (0.1%)	1.13	5/1053 (0.5%)
56	DY	0.55	1/789 (0.1%)	1.11	5/1053 (0.5%)
57	BZ	0.57	1/1500 (0.1%)	1.03	8/2037 (0.4%)
57	DZ	0.47	1/1500 (0.1%)	1.04	15/2037 (0.7%)
All	All	0.49	71/322506 (0.0%)	0.79	765/482452 (0.2%)

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 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CY	57	U	C3'-O3'	16.50	1.67	1.42
22	CY	56	U	C2-N3	10.13	1.58	1.37
22	CY	57	U	O3'-P	9.24	1.75	1.61
22	CY	58	C	P-O5'	8.37	1.72	1.59
57	BZ	186	GLU	C-N	-7.08	1.23	1.33

The worst 5 of 765 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	1992	G	C2'-C3'-O3'	14.71	131.57	109.50
35	DA	1992	G	C2'-C3'-O3'	14.61	131.42	109.50
35	DA	331	A	C2'-C3'-O3'	14.12	130.68	109.50
35	BA	790	C	C2'-C3'-O3'	13.91	130.36	109.50
35	BA	331	A	C2'-C3'-O3'	13.82	130.23	109.50

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

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	1336	0
1	CA	32329	0	16318	1414	0
2	AB	1901	0	1951	282	0
2	CB	1901	0	1951	288	0
3	AC	1613	0	1677	232	0
3	CC	1613	0	1677	248	0
4	AD	1703	0	1765	251	1
4	CD	1703	0	1766	247	0
5	AE	1147	0	1207	155	0
5	CE	1147	0	1207	160	0
6	AF	843	0	857	85	0
6	CF	843	0	857	84	1
7	AG	1257	0	1296	133	0
7	CG	1257	0	1296	134	0
8	AH	1116	0	1177	130	0
8	CH	1116	0	1177	135	0
9	AI	1010	0	1035	161	0
9	CI	1010	0	1035	166	0
10	AJ	795	0	840	184	0
10	CJ	795	0	840	181	0
11	AK	885	0	904	91	0
11	CK	885	0	904	91	0
12	AL	971	0	1057	217	0
12	CL	971	0	1057	219	0
13	AM	938	0	991	139	0
13	CM	938	0	991	138	0
14	AN	492	0	531	52	0
14	CN	492	0	532	56	0
15	AO	734	0	771	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	734	0	771	67	0
16	AP	701	0	720	91	0
16	CP	701	0	720	89	0
17	AQ	824	0	891	88	0
17	CQ	824	0	891	83	0
18	AR	574	0	644	76	0
18	CR	574	0	644	78	0
19	AS	630	0	652	91	0
19	CS	630	0	652	85	0
20	AT	763	0	861	92	0
20	CT	763	0	861	87	0
21	AU	209	0	221	22	0
21	CU	209	0	221	23	0
22	AV	1667	0	857	264	0
22	AY	1667	0	857	327	0
22	CV	1667	0	857	236	0
22	CY	1667	0	854	330	0
23	AW	1659	0	843	397	0
23	CW	1659	0	843	323	0
24	AX	257	0	132	11	0
24	CX	257	0	132	35	0
25	B0	662	0	688	71	0
25	D0	662	0	688	73	0
26	B1	734	0	808	78	0
26	D1	734	0	808	90	0
27	B2	598	0	653	74	0
27	D2	598	0	653	82	0
28	B3	468	0	523	38	0
28	D3	468	0	523	39	0
29	B4	451	0	449	100	0
29	D4	451	0	449	83	0
30	B5	428	0	445	76	0
30	D5	428	0	445	74	0
31	B6	433	0	461	86	0
31	D6	433	0	461	89	0
32	B7	410	0	454	24	0
32	D7	410	0	454	25	0
33	B8	508	0	576	110	0
33	D8	508	0	576	113	0
34	B9	307	0	338	31	0
34	D9	307	0	338	36	0
35	BA	61341	0	30928	1760	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	DA	61341	0	30928	1847	0
36	BB	2551	0	1295	93	0
36	DB	2551	0	1295	109	0
37	BC	937	0	957	116	0
37	DC	937	0	957	116	0
38	BD	2105	0	2182	273	0
38	DD	2105	0	2182	285	0
39	BE	1564	0	1629	253	0
39	DE	1564	0	1629	254	0
40	BF	1624	0	1677	180	0
40	DF	1624	0	1677	186	0
41	BG	1474	0	1534	259	0
41	DG	1474	0	1534	317	0
42	BH	1260	0	1326	158	0
42	DH	1260	0	1326	162	0
43	BI	1132	0	1218	216	0
43	DI	1132	0	1218	207	0
44	BJ	651	0	166	32	0
44	DJ	651	0	170	17	0
45	BN	1105	0	1180	151	0
45	DN	1105	0	1180	151	0
46	BO	933	0	996	118	0
46	DO	933	0	996	118	0
47	BP	1114	0	1187	287	0
47	DP	1114	0	1187	293	0
48	BQ	1113	0	1171	140	0
48	DQ	1113	0	1171	149	0
49	BR	960	0	1021	131	0
49	DR	960	0	1021	130	0
50	BS	771	0	832	157	0
50	DS	771	0	832	151	0
51	BT	1124	0	1181	265	0
51	DT	1124	0	1181	252	0
52	BU	958	0	1015	138	0
52	DU	958	0	1015	136	0
53	BV	779	0	852	156	0
53	DV	779	0	852	156	0
54	BW	896	0	953	73	0
54	DW	896	0	953	79	0
55	BX	726	0	778	54	0
55	DX	726	0	778	62	0
56	BY	776	0	870	182	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DY	776	0	870	188	0
57	BZ	1468	0	1492	273	0
57	DZ	1468	0	1491	349	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	20387	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 41.

The worst 5 of 20387 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](#)

There are no protein backbone outliers to report in this entry.

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%)	187 (93%)	15 (7%)	13	40
2	CB	202/220 (92%)	187 (93%)	15 (7%)	13	40
3	AC	160/188 (85%)	146 (91%)	14 (9%)	9	33
3	CC	160/188 (85%)	148 (92%)	12 (8%)	12	39
4	AD	180/181 (99%)	167 (93%)	13 (7%)	13	40
4	CD	180/181 (99%)	167 (93%)	13 (7%)	13	40
5	AE	115/123 (94%)	109 (95%)	6 (5%)	21	51
5	CE	115/123 (94%)	108 (94%)	7 (6%)	17	46
6	AF	90/90 (100%)	86 (96%)	4 (4%)	25	56
6	CF	90/90 (100%)	86 (96%)	4 (4%)	25	56
7	AG	126/127 (99%)	119 (94%)	7 (6%)	19	49
7	CG	126/127 (99%)	119 (94%)	7 (6%)	19	49
8	AH	119/119 (100%)	108 (91%)	11 (9%)	8	31
8	CH	119/119 (100%)	108 (91%)	11 (9%)	8	31
9	AI	98/99 (99%)	93 (95%)	5 (5%)	21	52
9	CI	98/99 (99%)	93 (95%)	5 (5%)	21	52
10	AJ	88/92 (96%)	84 (96%)	4 (4%)	24	56
10	CJ	88/92 (96%)	84 (96%)	4 (4%)	24	56
11	AK	90/99 (91%)	85 (94%)	5 (6%)	19	49
11	CK	90/99 (91%)	85 (94%)	5 (6%)	19	49
12	AL	104/111 (94%)	81 (78%)	23 (22%)	1	4
12	CL	104/111 (94%)	81 (78%)	23 (22%)	1	4
13	AM	94/101 (93%)	87 (93%)	7 (7%)	13	40
13	CM	94/101 (93%)	87 (93%)	7 (7%)	13	40
14	AN	49/50 (98%)	47 (96%)	2 (4%)	27	59
14	CN	49/50 (98%)	46 (94%)	3 (6%)	17	46
15	AO	79/80 (99%)	77 (98%)	2 (2%)	42	69
15	CO	79/80 (99%)	77 (98%)	2 (2%)	42	69
16	AP	72/74 (97%)	66 (92%)	6 (8%)	10	35
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AQ	94/97 (97%)	90 (96%)	4 (4%)	26	57
17	CQ	94/97 (97%)	90 (96%)	4 (4%)	26	57
18	AR	61/77 (79%)	58 (95%)	3 (5%)	22	53
18	CR	61/77 (79%)	58 (95%)	3 (5%)	22	53
19	AS	69/80 (86%)	61 (88%)	8 (12%)	5	22
19	CS	69/80 (86%)	61 (88%)	8 (12%)	5	22
20	AT	76/82 (93%)	70 (92%)	6 (8%)	11	37
20	CT	76/82 (93%)	70 (92%)	6 (8%)	11	37
21	AU	19/22 (86%)	18 (95%)	1 (5%)	20	51
21	CU	19/22 (86%)	18 (95%)	1 (5%)	20	51
25	B0	66/67 (98%)	58 (88%)	8 (12%)	5	20
25	D0	66/67 (98%)	58 (88%)	8 (12%)	5	20
26	B1	78/83 (94%)	66 (85%)	12 (15%)	2	12
26	D1	78/83 (94%)	66 (85%)	12 (15%)	2	12
27	B2	66/67 (98%)	56 (85%)	10 (15%)	3	13
27	D2	66/67 (98%)	57 (86%)	9 (14%)	3	16
28	B3	51/52 (98%)	48 (94%)	3 (6%)	18	48
28	D3	51/52 (98%)	48 (94%)	3 (6%)	18	48
29	B4	51/63 (81%)	43 (84%)	8 (16%)	2	12
29	D4	51/63 (81%)	43 (84%)	8 (16%)	2	12
30	B5	47/52 (90%)	43 (92%)	4 (8%)	10	35
30	D5	47/52 (90%)	43 (92%)	4 (8%)	10	35
31	B6	49/52 (94%)	41 (84%)	8 (16%)	2	11
31	D6	49/52 (94%)	41 (84%)	8 (16%)	2	11
32	B7	40/42 (95%)	36 (90%)	4 (10%)	7	29
32	D7	40/42 (95%)	36 (90%)	4 (10%)	7	29
33	B8	53/55 (96%)	44 (83%)	9 (17%)	2	10
33	D8	53/55 (96%)	44 (83%)	9 (17%)	2	10
34	B9	34/34 (100%)	34 (100%)	0	100	100
34	D9	34/34 (100%)	34 (100%)	0	100	100
37	BC	99/181 (55%)	94 (95%)	5 (5%)	21	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DC	99/181 (55%)	94 (95%)	5 (5%)	21	52
38	BD	213/218 (98%)	182 (85%)	31 (15%)	3	14
38	DD	213/218 (98%)	183 (86%)	30 (14%)	3	15
39	BE	165/166 (99%)	142 (86%)	23 (14%)	3	15
39	DE	165/166 (99%)	143 (87%)	22 (13%)	4	17
40	BF	165/166 (99%)	148 (90%)	17 (10%)	7	27
40	DF	165/166 (99%)	148 (90%)	17 (10%)	7	27
41	BG	155/156 (99%)	141 (91%)	14 (9%)	9	33
41	DG	155/156 (99%)	141 (91%)	14 (9%)	9	33
42	BH	137/148 (93%)	119 (87%)	18 (13%)	4	17
42	DH	137/148 (93%)	119 (87%)	18 (13%)	4	17
43	BI	122/124 (98%)	110 (90%)	12 (10%)	7	29
43	DI	122/124 (98%)	110 (90%)	12 (10%)	7	29
45	BN	117/119 (98%)	100 (86%)	17 (14%)	3	14
45	DN	117/119 (98%)	98 (84%)	19 (16%)	2	11
46	BO	100/100 (100%)	90 (90%)	10 (10%)	7	29
46	DO	100/100 (100%)	90 (90%)	10 (10%)	7	29
47	BP	112/116 (97%)	91 (81%)	21 (19%)	1	7
47	DP	112/116 (97%)	92 (82%)	20 (18%)	2	9
48	BQ	110/111 (99%)	101 (92%)	9 (8%)	10	36
48	DQ	110/111 (99%)	102 (93%)	8 (7%)	13	40
49	BR	100/101 (99%)	83 (83%)	17 (17%)	2	10
49	DR	100/101 (99%)	83 (83%)	17 (17%)	2	10
50	BS	77/88 (88%)	64 (83%)	13 (17%)	2	10
50	DS	77/88 (88%)	64 (83%)	13 (17%)	2	10
51	BT	118/127 (93%)	96 (81%)	22 (19%)	1	8
51	DT	118/127 (93%)	95 (80%)	23 (20%)	1	6
52	BU	92/94 (98%)	82 (89%)	10 (11%)	6	24
52	DU	92/94 (98%)	81 (88%)	11 (12%)	5	21
53	BV	82/82 (100%)	66 (80%)	16 (20%)	1	6
53	DV	82/82 (100%)	65 (79%)	17 (21%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	BW	91/92 (99%)	81 (89%)	10 (11%)	6	24
54	DW	91/92 (99%)	80 (88%)	11 (12%)	5	20
55	BX	74/78 (95%)	70 (95%)	4 (5%)	20	50
55	DX	74/78 (95%)	70 (95%)	4 (5%)	20	50
56	BY	84/91 (92%)	70 (83%)	14 (17%)	2	10
56	DY	84/91 (92%)	70 (83%)	14 (17%)	2	10
57	BZ	162/179 (90%)	142 (88%)	20 (12%)	4	20
57	DZ	162/179 (90%)	148 (91%)	14 (9%)	10	34
All	All	9790/10432 (94%)	8764 (90%)	1026 (10%)	6	26

5 of 1026 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	DS	67	ARG
51	DT	124	ASP
50	DS	44	LYS
48	BQ	137	TYR
47	BP	119	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 339 such sidechains are listed below:

Mol	Chain	Res	Type
15	CO	37	ASN
39	DE	180	ASN
19	CS	47	HIS
29	D4	40	HIS
43	DI	74	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	218 (14%)	29 (1%)
1	CA	1503/1522 (98%)	221 (14%)	31 (2%)
22	AV	75/78 (96%)	25 (33%)	0
22	AY	75/78 (96%)	24 (32%)	2 (2%)
22	CV	75/78 (96%)	24 (32%)	0
22	CY	75/78 (96%)	23 (30%)	2 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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%)	502 (17%)	49 (1%)
35	DA	2847/2915 (97%)	501 (17%)	49 (1%)
36	BB	118/122 (96%)	18 (15%)	1 (0%)
36	DB	118/122 (96%)	17 (14%)	1 (0%)
All	All	9412/9634 (97%)	1657 (17%)	171 (1%)

5 of 1657 RNA backbone outliers are listed below:

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

5 of 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	CY	36	22	21,29,30	2.00	5 (23%)	23,39,42	1.10	2 (8%)
22	AG9	AY	36	22	21,29,30	1.51	3 (14%)	23,39,42	1.27	3 (13%)
22	AG9	CV	36	22	21,29,30	1.66	3 (14%)	23,39,42	1.08	2 (8%)
22	AG9	AV	36	22	21,29,30	1.07	2 (9%)	23,39,42	1.09	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	CY	36	22	1/1/9/13	7/14/47/48	0/2/2/2
22	AG9	AY	36	22	1/1/9/13	7/14/47/48	0/2/2/2
22	AG9	CV	36	22	1/1/9/13	3/14/47/48	0/2/2/2
22	AG9	AV	36	22	1/1/9/13	3/14/47/48	0/2/2/2

The worst 5 of 13 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	3.90	1.37	1.30
22	CY	36	AG9	C2-N3	3.44	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	3.16	124.72	114.65
22	CV	36	AG9	CD-NE-CZ	3.07	124.45	114.65

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	CY	36	AG9	7	0
22	AY	36	AG9	11	0
22	CV	36	AG9	12	0
22	AV	36	AG9	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	1.44	403 (26%) 1 1	44, 101, 184, 200	0
1	CA	1504/1522 (98%)	1.44	367 (24%) 2 1	55, 115, 186, 200	0
2	AB	235/256 (91%)	1.19	44 (18%) 3 1	75, 134, 176, 198	0
2	CB	235/256 (91%)	1.49	59 (25%) 1 1	94, 148, 183, 200	0
3	AC	207/239 (86%)	1.48	51 (24%) 2 1	82, 127, 157, 179	0
3	CC	207/239 (86%)	1.52	48 (23%) 2 1	92, 141, 170, 185	0
4	AD	208/209 (99%)	1.57	65 (31%) 1 1	64, 112, 142, 179	0
4	CD	208/209 (99%)	1.13	37 (17%) 4 2	56, 99, 135, 157	0
5	AE	151/162 (93%)	0.99	19 (12%) 8 4	65, 95, 142, 167	0
5	CE	151/162 (93%)	1.48	43 (28%) 1 1	69, 119, 151, 160	0
6	AF	101/101 (100%)	0.96	8 (7%) 18 10	59, 98, 138, 173	0
6	CF	101/101 (100%)	0.79	6 (5%) 28 15	64, 110, 133, 173	0
7	AG	155/156 (99%)	1.63	52 (33%) 1 0	76, 123, 155, 198	0
7	CG	155/156 (99%)	1.50	35 (22%) 2 1	94, 131, 160, 194	0
8	AH	138/138 (100%)	1.02	13 (9%) 14 8	61, 101, 128, 144	0
8	CH	138/138 (100%)	1.31	27 (19%) 3 1	83, 121, 148, 166	0
9	AI	127/128 (99%)	1.87	53 (41%) 0 0	81, 148, 176, 191	0
9	CI	127/128 (99%)	1.99	53 (41%) 0 0	99, 153, 181, 193	0
10	AJ	99/105 (94%)	1.88	37 (37%) 1 0	71, 149, 177, 185	0
10	CJ	99/105 (94%)	2.11	49 (49%) 0 0	97, 159, 182, 189	0
11	AK	119/129 (92%)	1.04	15 (12%) 8 4	63, 94, 136, 187	0
11	CK	119/129 (92%)	1.08	15 (12%) 8 4	78, 108, 141, 176	0
12	AL	125/135 (92%)	1.97	55 (44%) 0 0	53, 93, 146, 180	0
12	CL	125/135 (92%)	1.71	42 (33%) 1 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%)	2.15	55 (46%)	0	0	75, 129, 161, 178	0
13	CM	119/126 (94%)	1.83	43 (36%)	1	0	96, 150, 169, 186	0
14	AN	60/61 (98%)	2.25	29 (48%)	0	0	71, 118, 145, 157	0
14	CN	60/61 (98%)	1.87	28 (46%)	0	0	108, 143, 166, 187	0
15	AO	88/89 (98%)	0.79	5 (5%)	29	16	60, 97, 130, 148	0
15	CO	88/89 (98%)	1.10	11 (12%)	8	5	67, 110, 138, 146	0
16	AP	84/88 (95%)	1.81	35 (41%)	0	0	67, 112, 156, 178	0
16	CP	84/88 (95%)	1.02	9 (10%)	11	6	60, 87, 137, 157	0
17	AQ	100/105 (95%)	1.20	17 (17%)	4	2	74, 109, 138, 151	0
17	CQ	100/105 (95%)	1.18	16 (16%)	5	2	70, 109, 139, 165	0
18	AR	70/88 (79%)	0.88	5 (7%)	22	12	69, 98, 139, 157	0
18	CR	70/88 (79%)	0.92	8 (11%)	10	5	77, 111, 148, 156	0
19	AS	79/93 (84%)	2.60	52 (65%)	0	0	89, 137, 171, 185	0
19	CS	79/93 (84%)	2.10	35 (44%)	0	0	112, 154, 178, 200	0
20	AT	99/106 (93%)	1.63	30 (30%)	1	1	65, 117, 160, 167	0
20	CT	99/106 (93%)	1.38	23 (23%)	2	1	66, 107, 151, 163	0
21	AU	25/27 (92%)	2.31	17 (68%)	0	0	84, 120, 146, 156	0
21	CU	25/27 (92%)	2.46	14 (56%)	0	0	91, 135, 171, 188	0
22	AV	77/78 (98%)	1.64	23 (29%)	1	1	65, 141, 179, 199	0
22	AY	77/78 (98%)	1.52	19 (24%)	2	1	90, 140, 185, 189	0
22	CV	77/78 (98%)	2.20	42 (54%)	0	0	94, 175, 196, 200	0
22	CY	77/78 (98%)	2.04	36 (46%)	0	0	138, 176, 197, 200	0
23	AW	78/78 (100%)	1.73	27 (34%)	1	0	70, 173, 191, 199	0
23	CW	78/78 (100%)	2.36	46 (58%)	0	0	99, 188, 200, 200	0
24	AX	12/24 (50%)	2.06	7 (58%)	0	0	59, 88, 157, 160	0
24	CX	12/24 (50%)	2.88	9 (75%)	0	0	92, 163, 185, 185	0
25	B0	84/85 (98%)	1.71	28 (33%)	1	0	39, 66, 124, 167	0
25	D0	84/85 (98%)	1.82	29 (34%)	1	0	71, 105, 146, 165	0
26	B1	94/98 (95%)	0.85	9 (9%)	13	7	33, 61, 114, 141	0
26	D1	94/98 (95%)	0.66	9 (9%)	13	7	43, 74, 127, 149	0
27	B2	71/72 (98%)	0.48	4 (5%)	30	16	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%)	0.97	8 (11%)	10 5	57, 97, 139, 178	0
28	B3	60/60 (100%)	1.17	7 (11%)	9 5	42, 63, 108, 167	0
28	D3	60/60 (100%)	1.24	11 (18%)	3 1	65, 109, 149, 175	0
29	B4	58/71 (81%)	2.17	30 (51%)	0 0	96, 144, 171, 187	0
29	D4	58/71 (81%)	1.56	18 (31%)	1 1	86, 165, 194, 200	0
30	B5	56/60 (93%)	0.64	4 (7%)	22 12	25, 63, 126, 148	0
30	D5	56/60 (93%)	0.86	7 (12%)	8 5	48, 80, 128, 146	0
31	B6	50/54 (92%)	1.83	18 (36%)	1 0	99, 140, 171, 180	0
31	D6	50/54 (92%)	1.89	19 (38%)	1 0	113, 150, 174, 191	0
32	B7	48/49 (97%)	0.31	2 (4%)	40 22	23, 42, 83, 129	0
32	D7	48/49 (97%)	0.35	3 (6%)	26 14	35, 54, 98, 131	0
33	B8	64/65 (98%)	1.42	17 (26%)	1 1	30, 61, 107, 123	0
33	D8	64/65 (98%)	1.51	21 (32%)	1 0	46, 88, 134, 177	0
34	B9	37/37 (100%)	2.40	23 (62%)	0 0	91, 136, 157, 159	0
34	D9	37/37 (100%)	2.87	25 (67%)	0 0	126, 149, 172, 183	0
35	BA	2848/2915 (97%)	0.72	281 (9%)	13 7	20, 56, 184, 200	0
35	DA	2848/2915 (97%)	0.88	327 (11%)	9 5	39, 82, 186, 200	0
36	BB	119/122 (97%)	2.29	72 (60%)	0 0	52, 81, 149, 178	0
36	DB	119/122 (97%)	2.22	71 (59%)	0 0	102, 151, 183, 195	0
37	BC	120/229 (52%)	1.66	29 (24%)	2 1	119, 168, 189, 200	0
37	DC	120/229 (52%)	1.42	27 (22%)	2 1	132, 170, 187, 199	0
38	BD	272/276 (98%)	0.58	17 (6%)	26 14	24, 55, 93, 150	0
38	DD	272/276 (98%)	0.68	20 (7%)	20 11	37, 73, 110, 144	0
39	BE	205/206 (99%)	0.78	25 (12%)	8 5	20, 62, 129, 165	0
39	DE	205/206 (99%)	0.90	23 (11%)	10 5	41, 82, 136, 159	0
40	BF	208/210 (99%)	0.76	18 (8%)	16 9	22, 63, 144, 195	0
40	DF	208/210 (99%)	0.80	17 (8%)	17 10	38, 90, 145, 184	0
41	BG	181/182 (99%)	1.78	61 (33%)	1 0	51, 103, 155, 182	0
41	DG	181/182 (99%)	1.44	43 (23%)	2 1	102, 141, 167, 183	0
42	BH	165/180 (91%)	1.28	30 (18%)	3 1	49, 86, 136, 174	0
42	DH	165/180 (91%)	1.52	47 (28%)	1 1	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%)	1.96	57 (39%) 1 0	55, 147, 187, 200	0
43	DI	146/148 (98%)	2.05	61 (41%) 0 0	59, 139, 183, 200	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BN	139/140 (99%)	0.84	12 (8%) 16 9	36, 64, 118, 147	0
45	DN	139/140 (99%)	1.05	18 (12%) 7 4	69, 104, 136, 155	0
46	BO	122/122 (100%)	0.41	4 (3%) 49 29	33, 60, 94, 116	0
46	DO	122/122 (100%)	0.74	6 (4%) 35 18	54, 83, 110, 141	0
47	BP	146/150 (97%)	1.58	48 (32%) 1 0	28, 74, 128, 189	0
47	DP	146/150 (97%)	1.46	36 (24%) 2 1	41, 98, 144, 173	0
48	BQ	141/141 (100%)	1.23	28 (19%) 3 1	38, 67, 109, 143	0
48	DQ	141/141 (100%)	1.48	37 (26%) 1 1	63, 113, 153, 178	0
49	BR	117/118 (99%)	0.68	10 (8%) 16 9	36, 62, 103, 136	0
49	DR	117/118 (99%)	0.88	16 (13%) 6 4	42, 76, 118, 151	0
50	BS	99/112 (88%)	2.39	58 (58%) 0 0	52, 95, 141, 160	0
50	DS	99/112 (88%)	2.18	50 (50%) 0 0	101, 137, 163, 186	0
51	BT	136/146 (93%)	0.82	14 (10%) 12 6	47, 78, 140, 181	0
51	DT	136/146 (93%)	1.03	18 (13%) 7 4	58, 92, 151, 176	0
52	BU	117/118 (99%)	0.68	7 (5%) 27 15	27, 53, 102, 144	0
52	DU	117/118 (99%)	1.13	18 (15%) 5 2	46, 97, 137, 163	0
53	BV	101/101 (100%)	0.78	9 (8%) 15 8	24, 72, 124, 168	0
53	DV	101/101 (100%)	1.17	16 (15%) 5 2	53, 116, 146, 171	0
54	BW	113/113 (100%)	0.36	3 (2%) 56 35	28, 52, 105, 180	0
54	DW	113/113 (100%)	0.56	3 (2%) 56 35	49, 71, 119, 165	0
55	BX	93/96 (96%)	0.49	4 (4%) 40 22	29, 63, 100, 141	0
55	DX	93/96 (96%)	1.00	14 (15%) 5 3	55, 83, 115, 138	0
56	BY	101/110 (91%)	1.56	32 (31%) 1 1	47, 89, 131, 157	0
56	DY	101/110 (91%)	1.56	30 (29%) 1 1	60, 106, 149, 164	0
57	BZ	185/206 (89%)	1.81	70 (37%) 1 0	51, 113, 163, 188	0
57	DZ	185/206 (89%)	1.63	54 (29%) 1 1	99, 144, 171, 189	0
All	All	21266/22572 (94%)	1.21	4370 (20%) 2 1	20, 98, 177, 200	0

The worst 5 of 4370 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	BI	88	ILE	15.5
43	DI	72	LEU	14.3
35	BA	277	C	13.0
10	CJ	55	LYS	10.2
56	BY	92	ASN	9.7

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	0.72	0.30	33,49,70,70	0
22	AG9	CV	36	28/29	0.82	0.22	33,49,70,70	0
22	AG9	AY	36	28/29	0.86	0.20	43,59,79,79	0
22	AG9	AV	36	28/29	0.91	0.13	43,59,79,79	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	0.82	0.19	165,165,165,165	0
58	ZN	CD	1000	1/1	0.86	0.22	200,200,200,200	0
58	ZN	AN	1000	1/1	0.96	0.12	88,88,88,88	0
58	ZN	CN	1000	1/1	0.96	0.07	178,178,178,178	0

6.5 Other polymers [i](#)

There are no such residues in this entry.