



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:02 PM 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

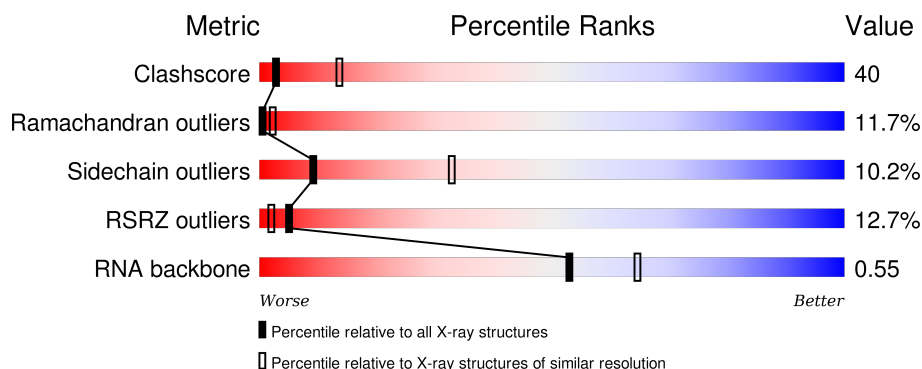
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>7%</div> <div>24%</div> <div>63%</div> <div>11%</div> <div>..</div> </div>
1	CA	1522	<div> <div>7%</div> <div>23%</div> <div>64%</div> <div>11%</div> <div>..</div> </div>
2	AB	256	<div> <div>13%</div> <div>21%</div> <div>59%</div> <div>12%</div> <div>8%</div> </div>
2	CB	256	<div> <div>22%</div> <div>20%</div> <div>59%</div> <div>13%</div> <div>8%</div> </div>
3	AC	239	<div> <div>12%</div> <div>23%</div> <div>50%</div> <div>13%</div> <div>13%</div> </div>

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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	
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	

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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	X
22	AG9	CY	36	X	-	-	X
58	ZN	AD	1000	-	-	X	-
58	ZN	CD	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			

*Continued on next page...*

*Continued from previous page...*

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			

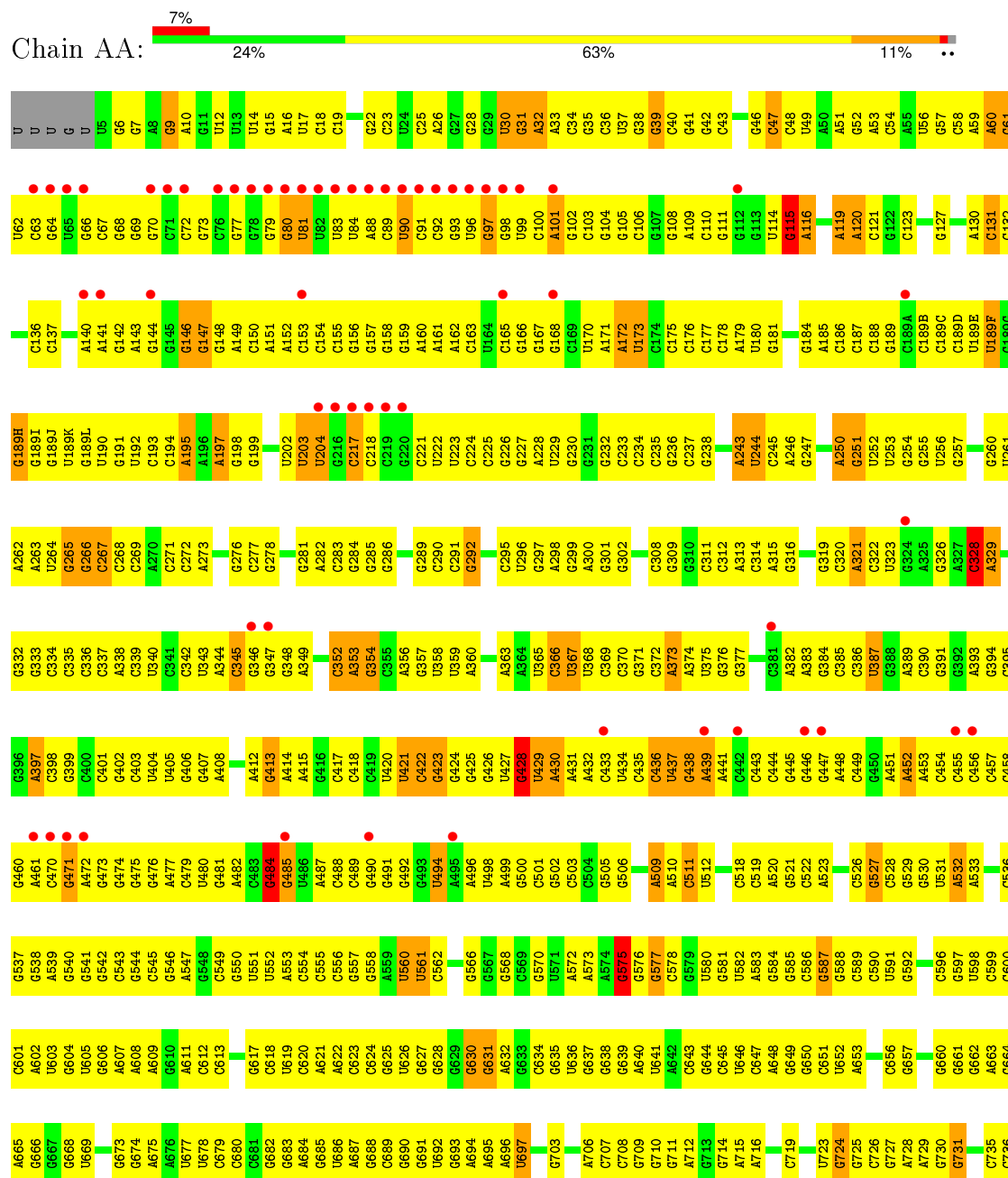
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

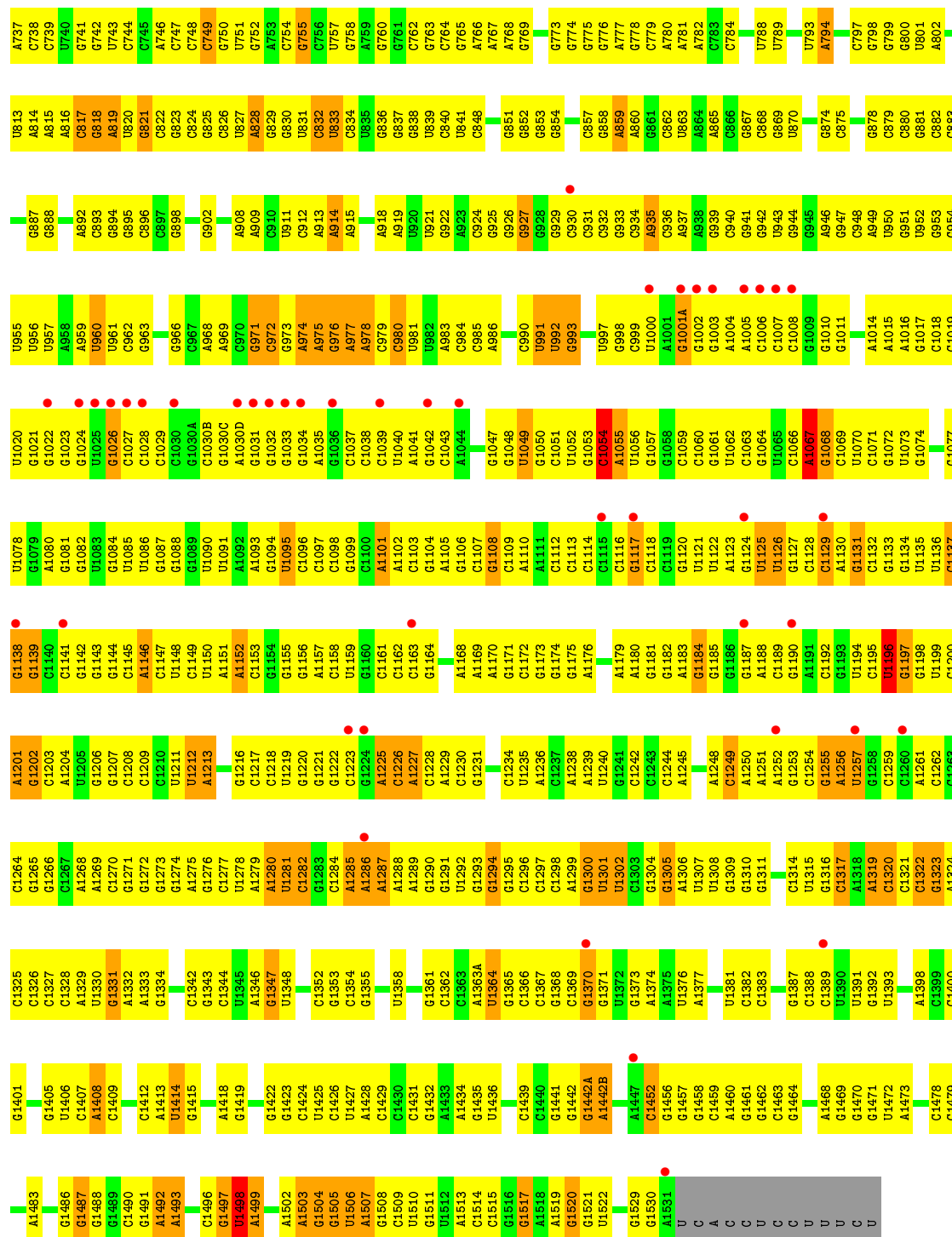
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

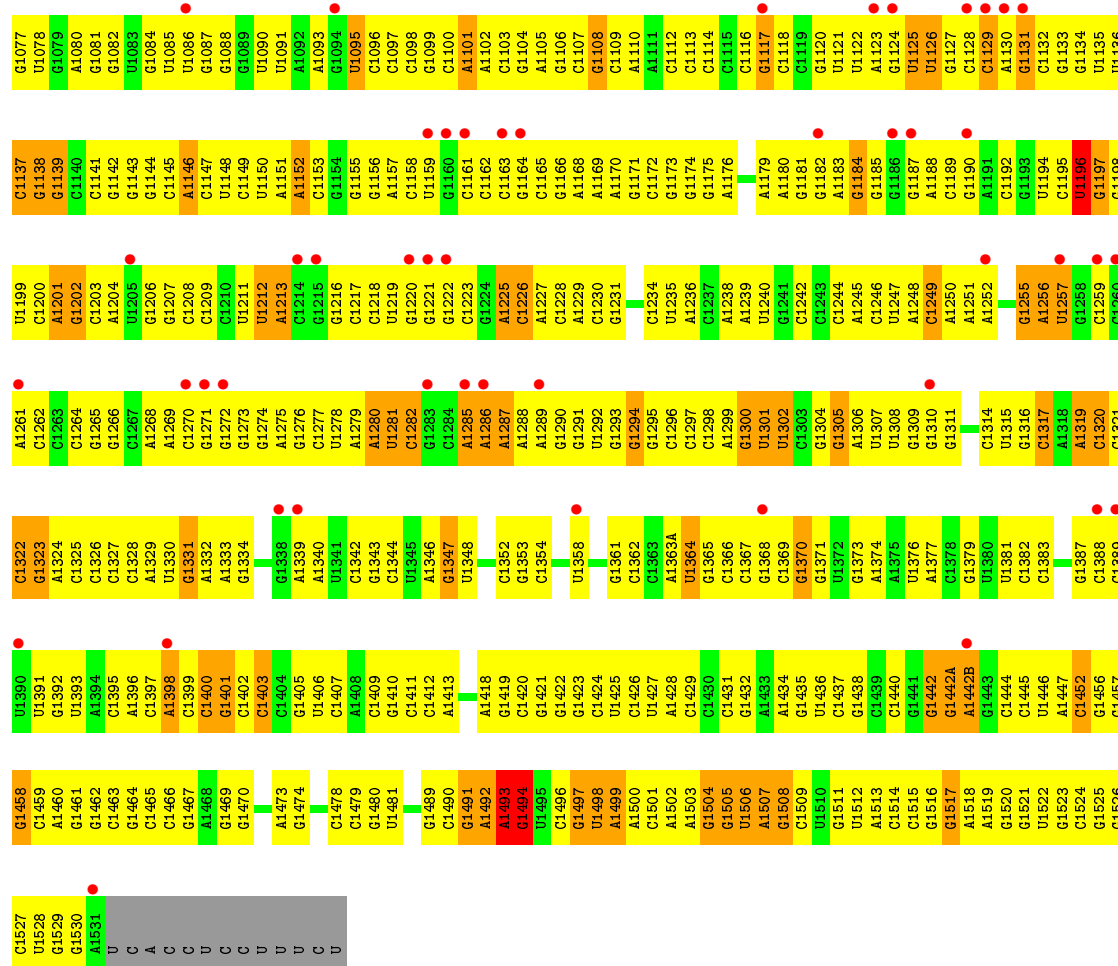
#### • Molecule 1: 16S rRNA



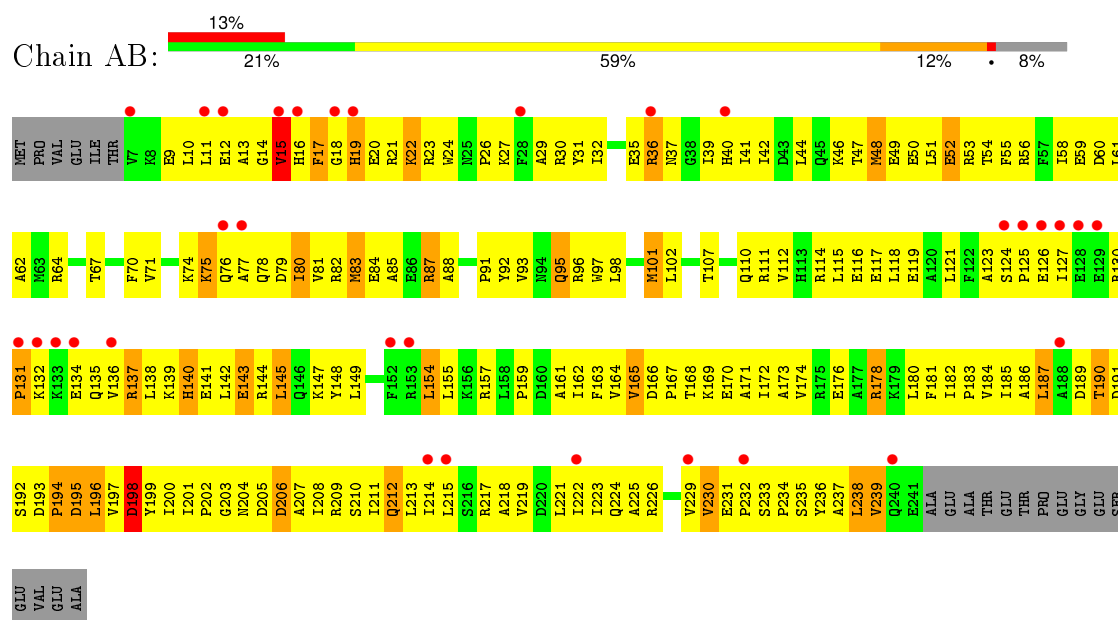




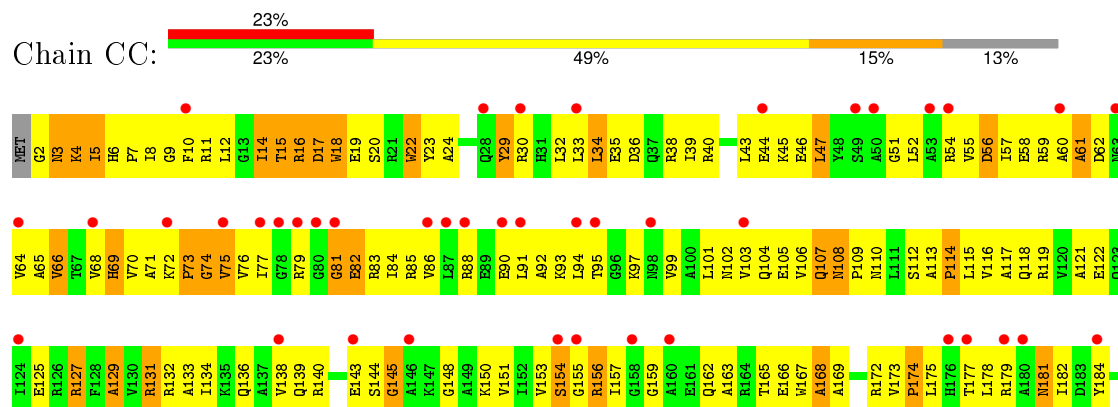
U1020	U957	A819	C748	U677	G610	C543	G475	G402	U264	G189J	U62
G1021	A958	U820	C749	U678	A611	G544	G476	C403	G265	U189K	C63
G1022	A959	G821	G750	C679	C612	G545	A477	U404	G266	U189L	
G1023	U960	C822	U751	C680	C613	G546	U480	U405	C267	U190	G66
G1024	U961	C823	G752		C614	A547	G406	G407	C268	U191	C67
U1025	C962	C924	A753		U619		G407	G408	C269	U192	G68
G1026	G963	G825	C754		C620	U551	A482	A408	A370	U193	G69
C1027	G964	G826	G755		A621	U552	C483		C271	C194	
C1028	G965	U827	C756		A622	U553	G484	A412	C345	A195	G70
C1029	A901	A828	U757		C623	U554	G485	G413	A273	A196	C72
C1030	A968	C829	G758		C624	C555	U486	A414	G347	A197	G73
G1030A	A969	G830	U759		G625	C556	A487	G415	G276	G198	
C1030B	C970	U831	G760		U626	G557	C488	A416	C277	G199	G76
G1030C	G971	C832	G761		G627	G558	C489	C417	G278		G77
A1030D	C972	U833	G762		G628	U559	G490	C418			G78
G1031	G973	C834	G763		U629	U560	G491		G281	U202	G79
G1032	A974	U835	G764		G630	U561	G492	U421	A282	U203	G80
G1033	A975	G836	G765		U631	C562	G493	C422	G355	U204	U81
G1034	G976	U837	A766		A632	G566	U494	G423	C383	G216	U82
A1035	A977	G838	A767		G633	G567	A495	G424	A356	C217	U83
G1036	A978	U839	A768		U634	G568	A496	G425	G357	C218	U84
C1037	C979	C840	G769		U635	C569	U498	G426	U358		U88
C1038	C980	U841			U636	G570	U499	U427	A360		U90
C1039	U981	C848			G637	U571	G500	G428	C291	U221	C91
U1040	U982		G773		G638	A572	U501	U429	G292	U222	C92
A1041	A983		G774		G639	A573	G502	A430		U223	G93
G1042	C984		G775		A640	A574	C503	A431	U296	U224	U96
C1043	C985		G776		U641	G575	U504	A432	G297	G227	G97
A1044	A986		G777		A642	G576	U505	C433	A298	A228	G98
G1045			G778		C643	G577	U506	U434	G299	U229	U99
U1046			G779		U644	G578		C435	A300	G230	
G1047	C990		G780		C645	C579	A509	C436	G301	G231	A101
U1048	U991		A781		U646	G579	A510	U437	G302	U170	
U1049	U992		A782		C647	U580	U511	G438	G303	A171	G102
G1050	A993		G786		A648	G581	U512	C439	U172	C103	G103
C1051	C994		G787		G649	U582		A441	G309	U173	G104
U1052	C995		U788		G650	A583		C442	U375	G174	G105
G1053	A996		U789		C651	G584		C443	G376	G175	
	U997				U652	G585		C444		C176	
C1054	C998				A653	G586		G445		C177	
A1055	C999				C656	G587		G446		C178	
U1056	U1000				U657	U588		G447		A179	
G1057	A1001				C658	G589		A448		U180	
C1058	G1001A				U591	G590		C449		U181	
G1059	U1002				G592			G450		U182	
C1060	G1003				G660			A451		G183	
U1061	A1004				G661			A452		G184	
C1062	U1005				G662			A453		A185	
G1063	C1006				A663			C454		A186	
U1064	U1007				G664			C455		C187	
U1065	C1008				A665			C456		G188	
C1066	G1009				G666			C457		G189	
A1067	U1010				U667			C458		C189A	
C1068	G1011				G668			G459		C189B	
					U669			G460		C189C	
A1014					G670			A461		U189D	
A1015					U673			C470		U189E	
A1016					A674			G471		U189F	
G1072					G675			A472		G189G	
U1070					A676			G473		G189H	
C1071					U677			A608		C136	
G1072					A678			G474		C137	
U1073					G679						

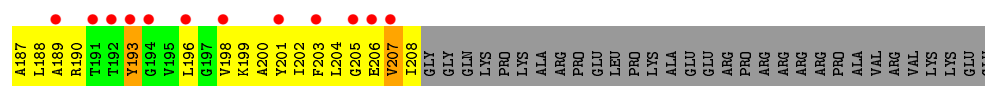


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

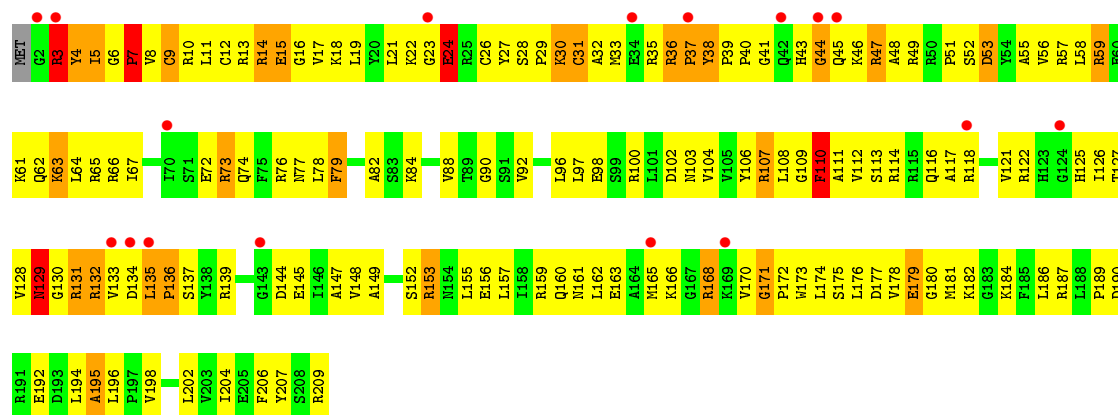


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

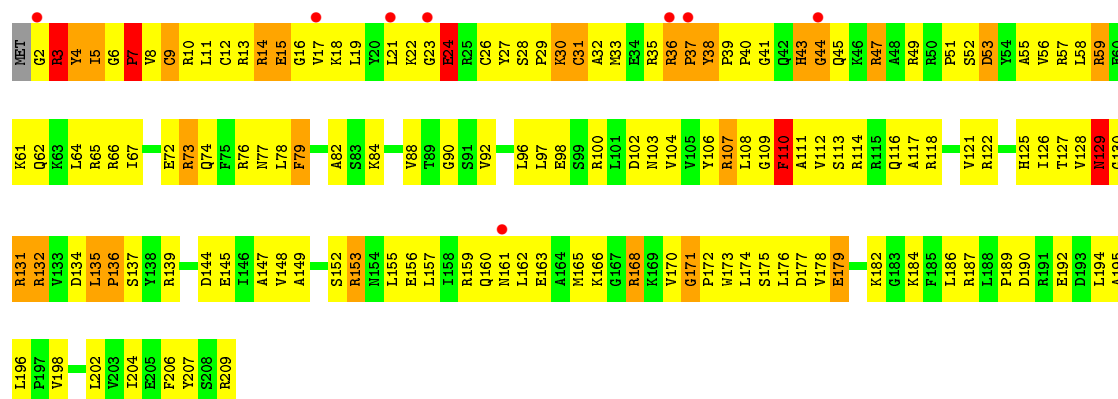




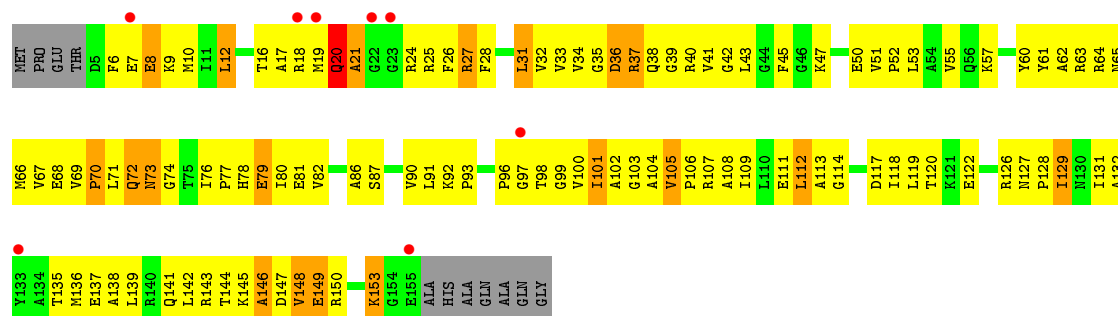
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



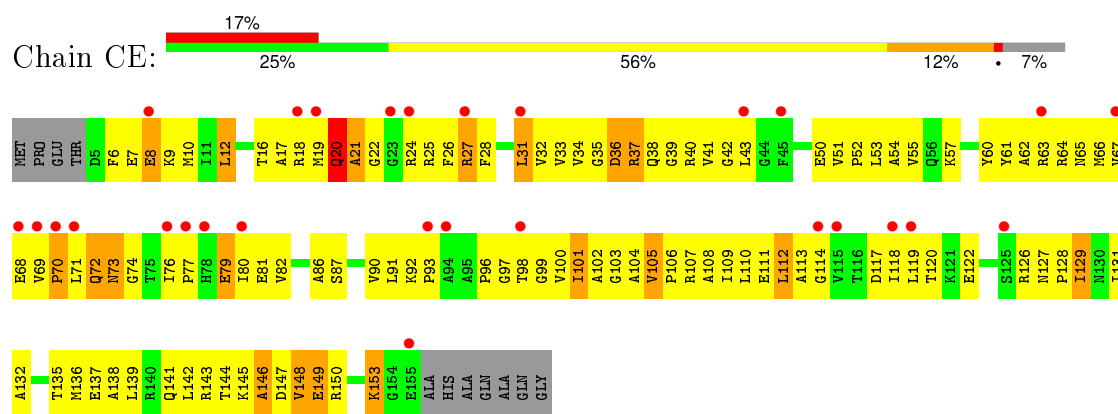
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



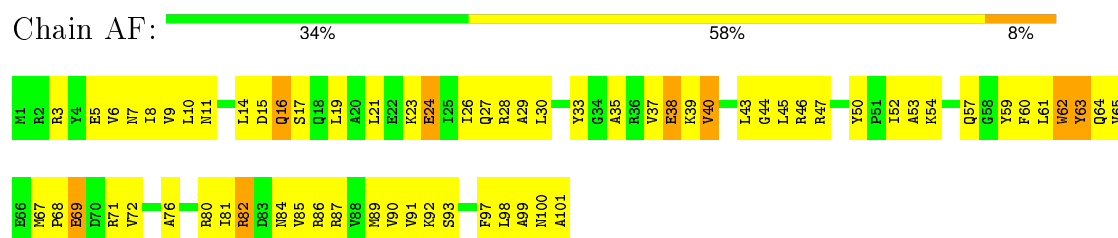
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



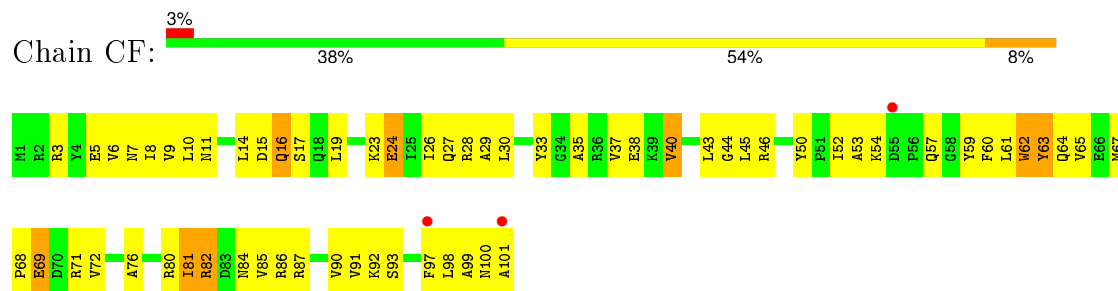
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



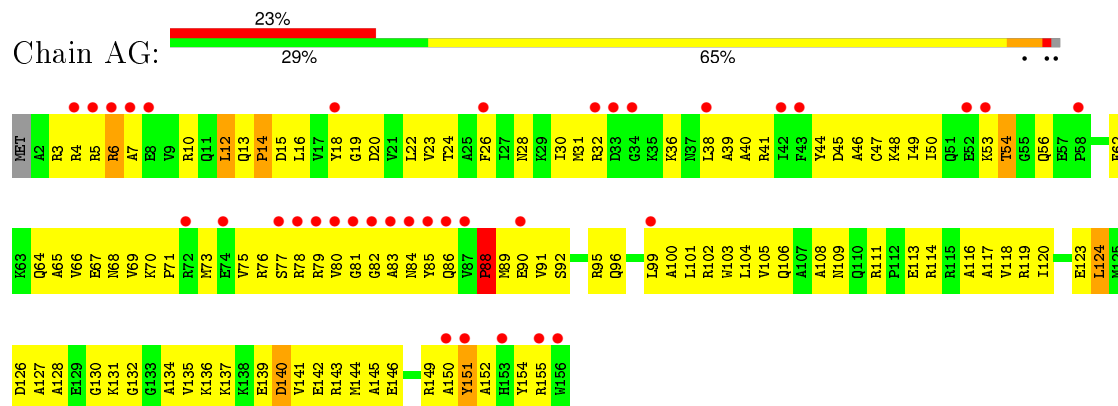
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

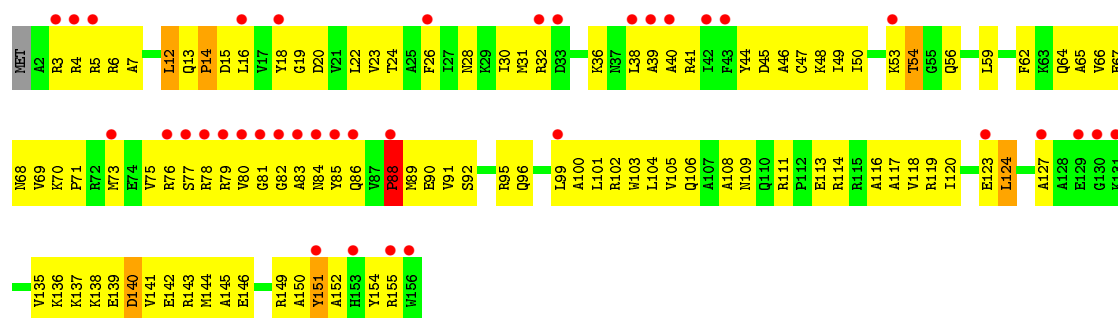


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

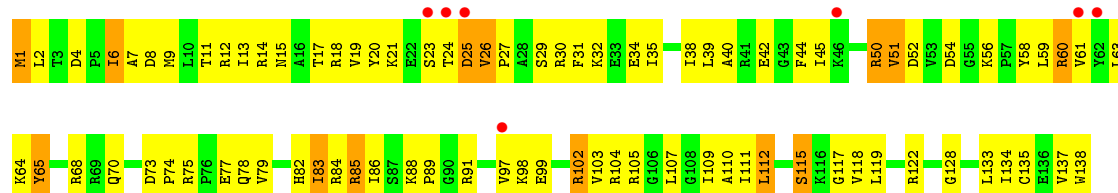


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

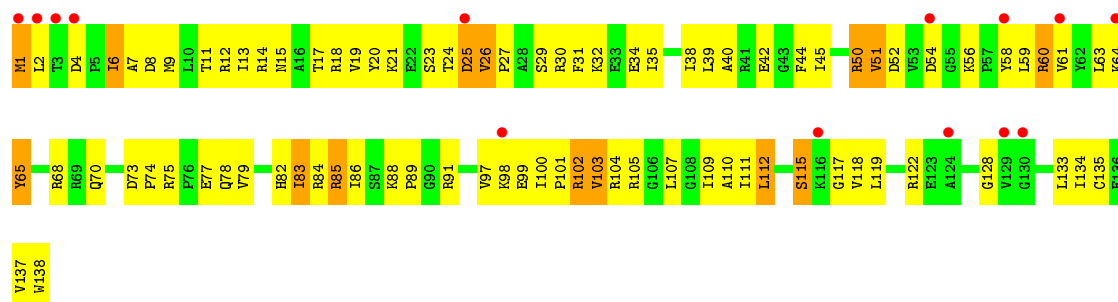




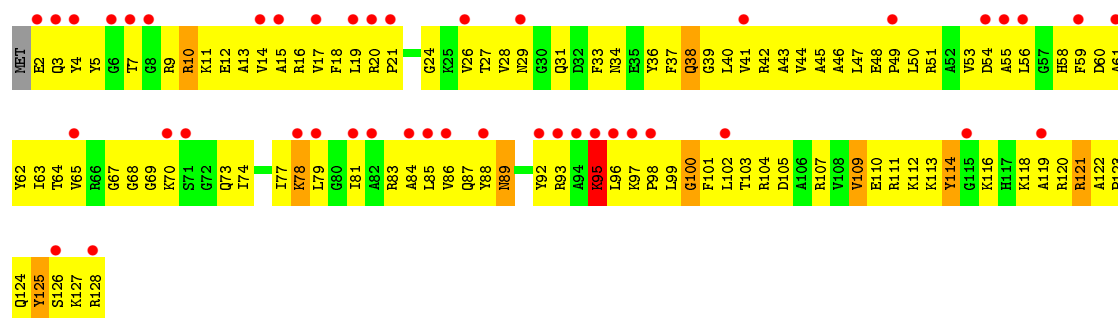
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

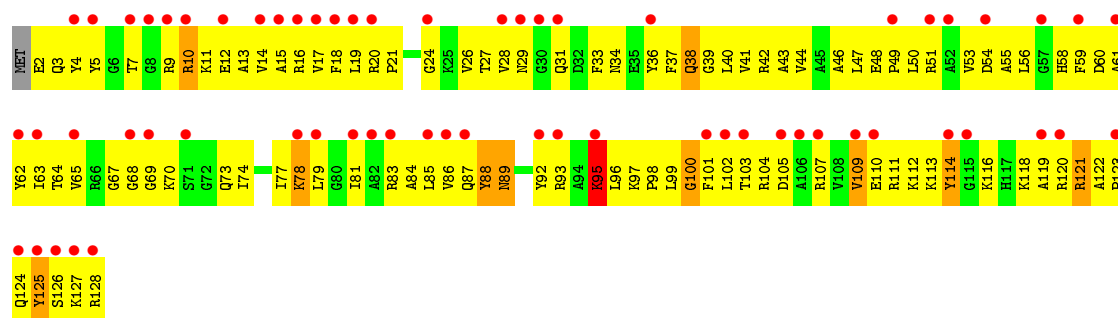


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

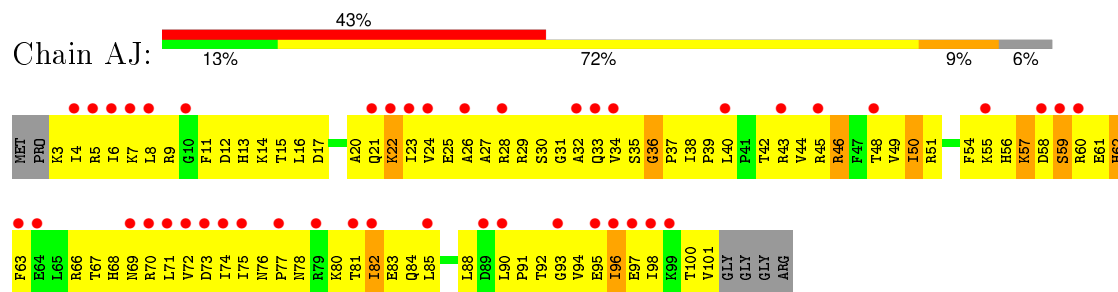


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

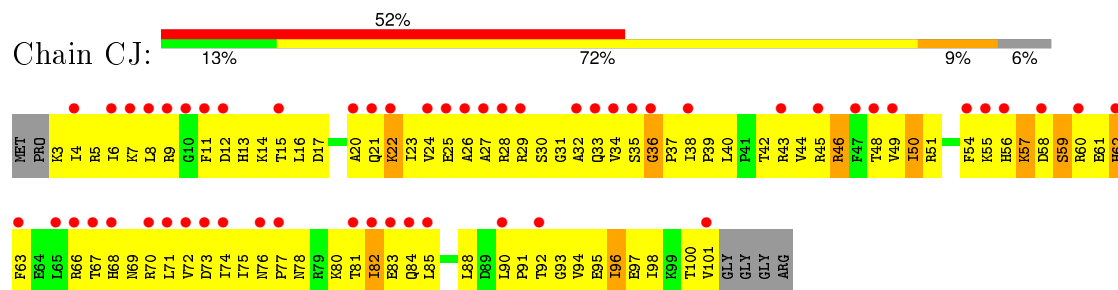




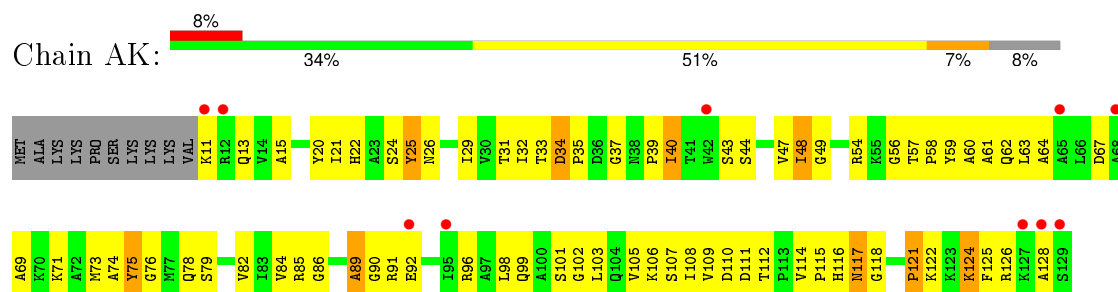
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



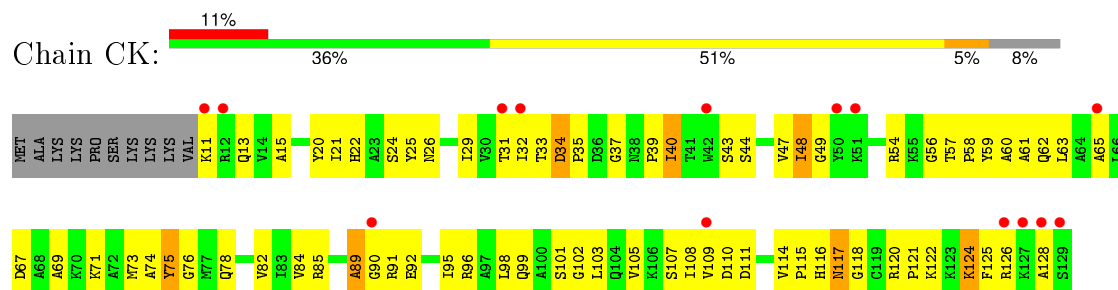
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

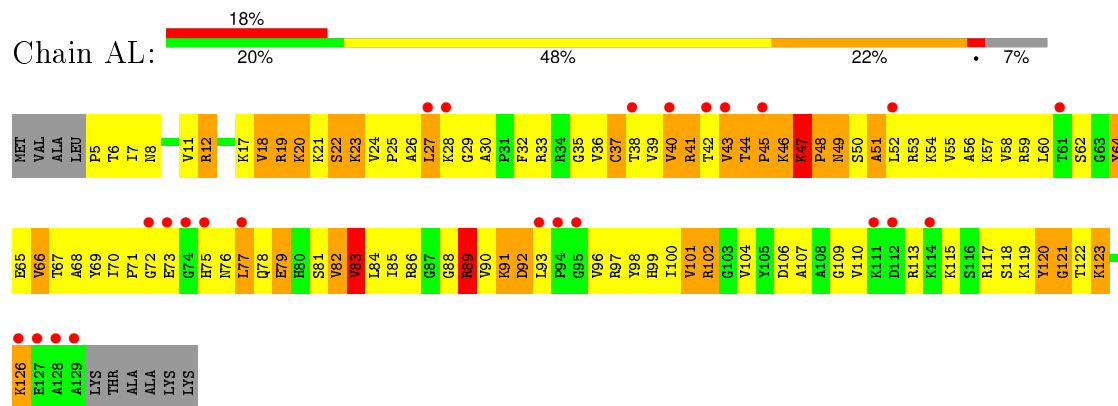


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

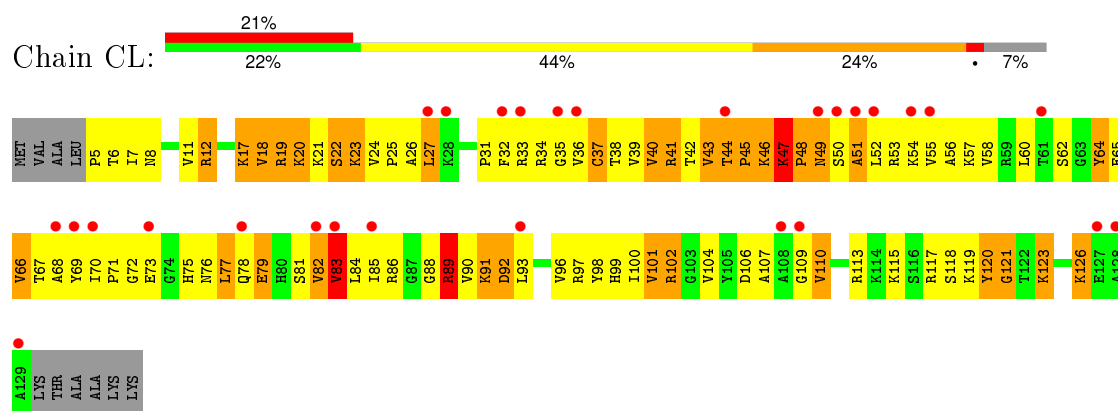




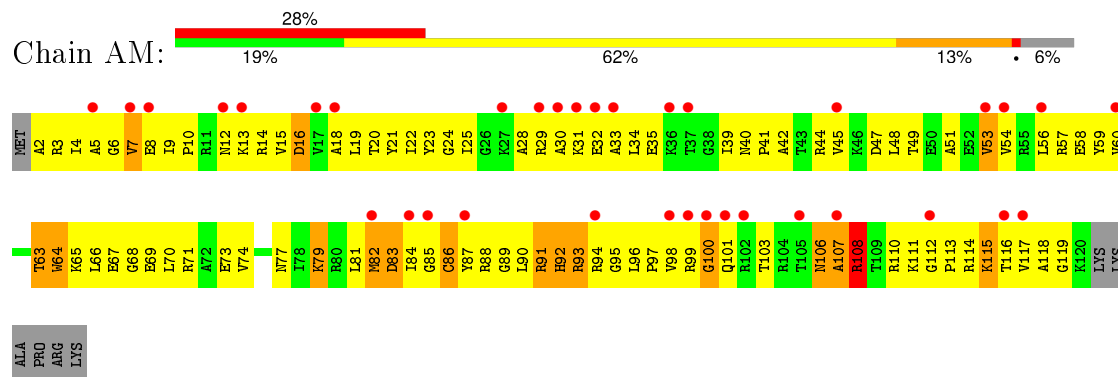
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



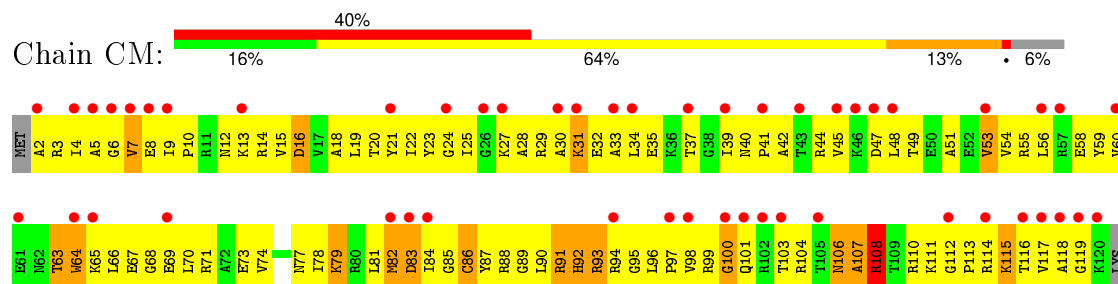
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



- Molecule 13: 30S RIBOSOMAL PROTEIN S13



- Molecule 13: 30S RIBOSOMAL PROTEIN S13



LYS  
ALA  
PRO  
ARG  
LYS

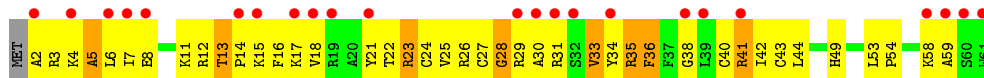
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN: 26% 41% 46% 11%



• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN: 38% 31% 54% 13%



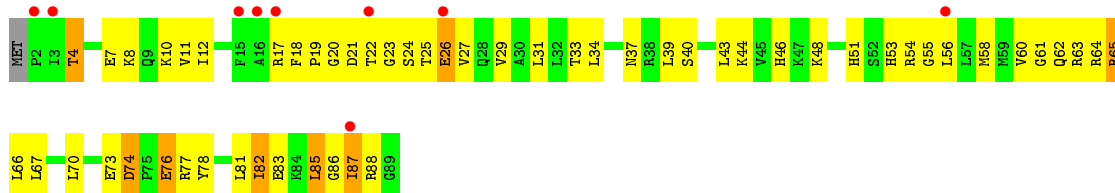
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO: 4% 37% 53% 9%



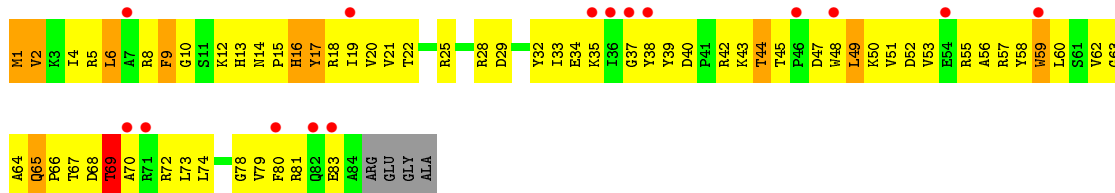
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO: 10% 37% 53% 9%



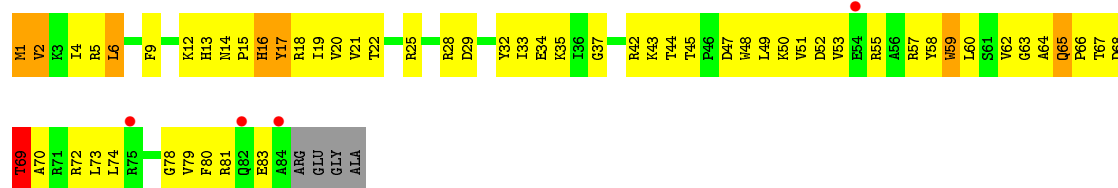
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP: 17% 23% 60% 11% 5%

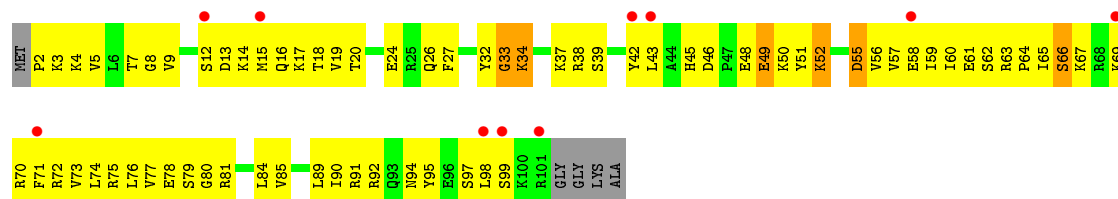


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

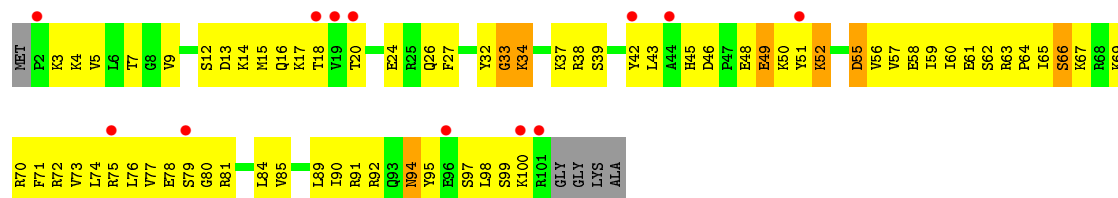
Chain CP: 5% 30% 57% 8% 5%



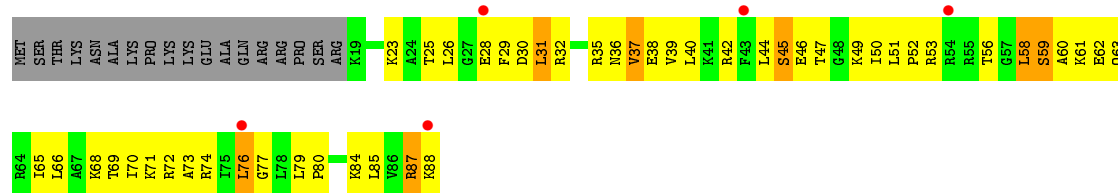
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



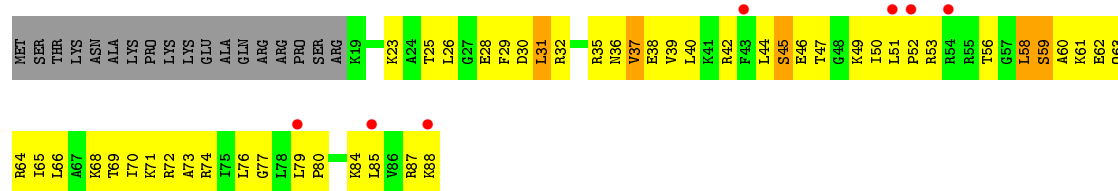
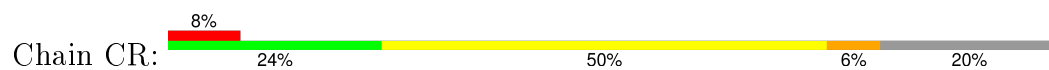
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



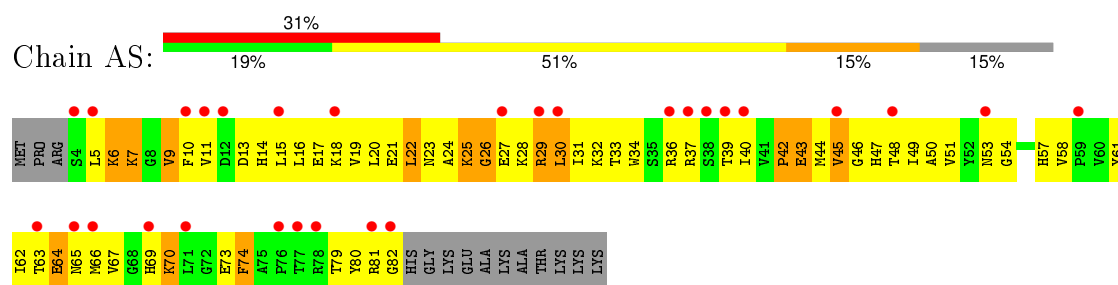
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



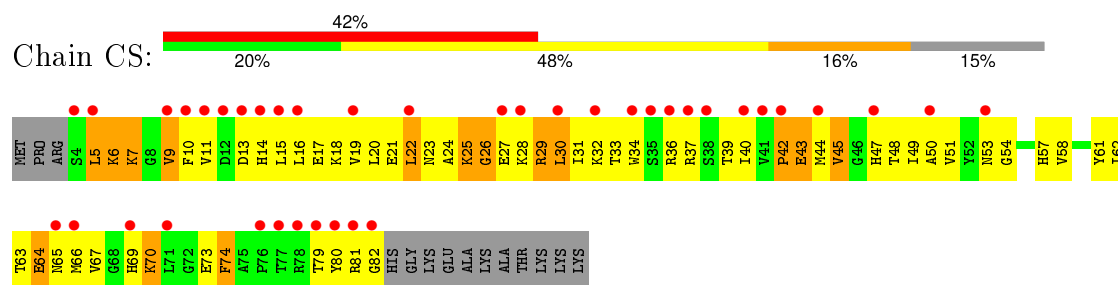
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



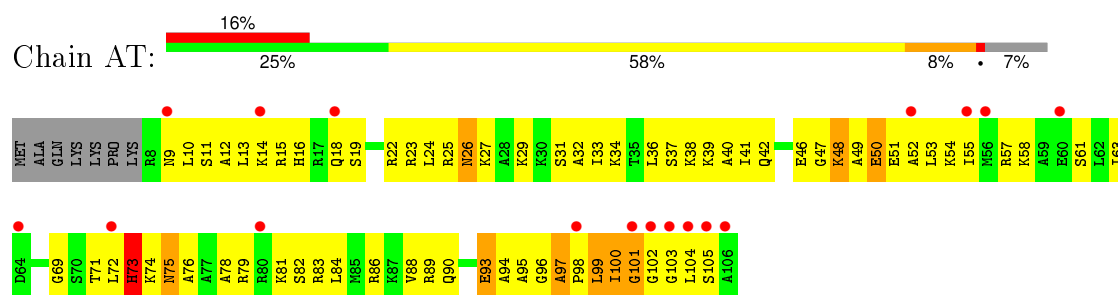
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



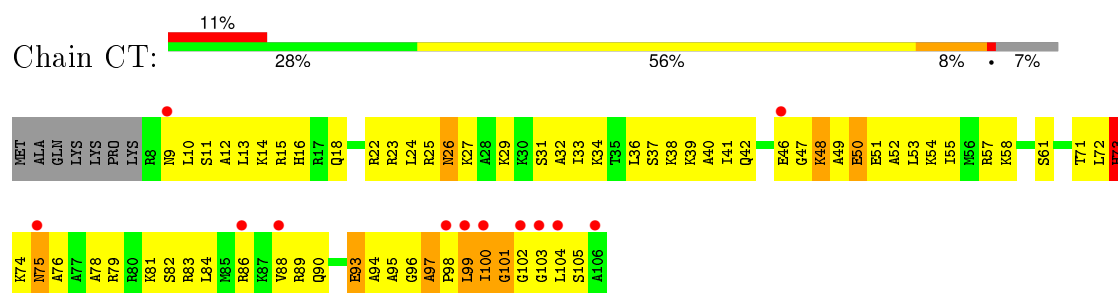
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



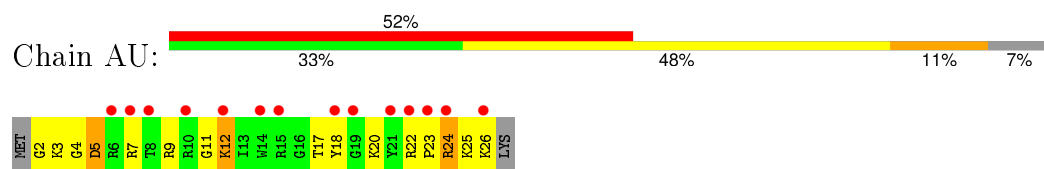
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



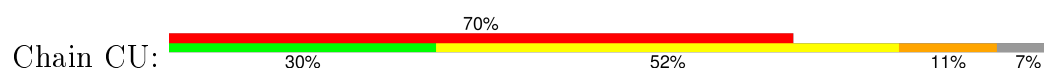
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

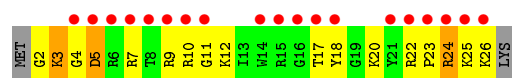


• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

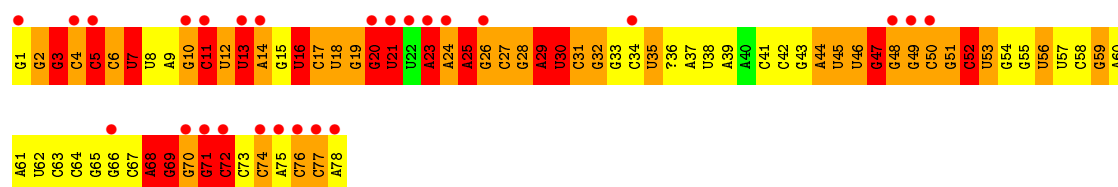




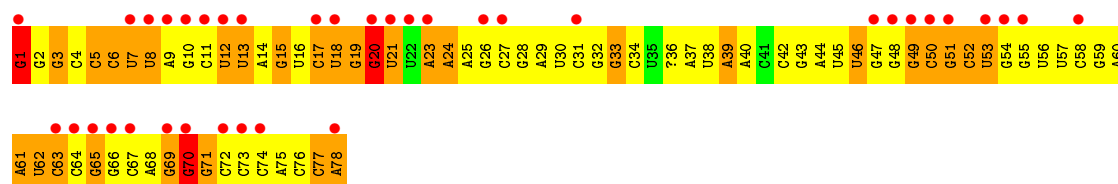
- Molecule 22: E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE



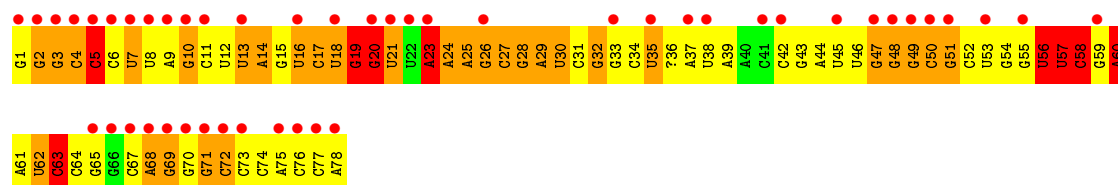
- Molecule 22: E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE



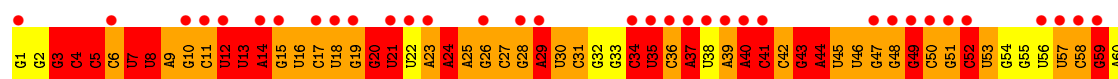
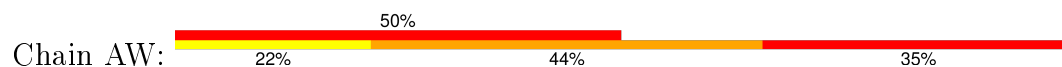
- Molecule 22: E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE



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

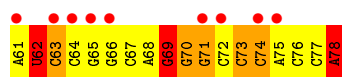
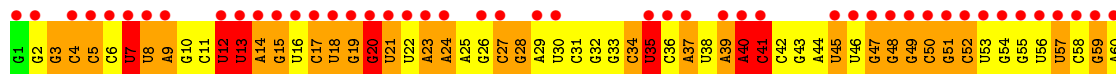
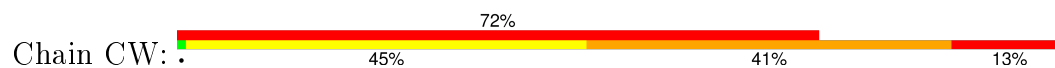


- Molecule 23: A-SITE TRNA ILE2 AGMATIDINE

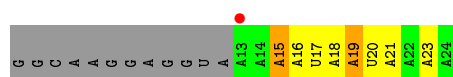




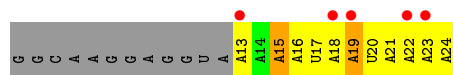
• Molecule 23: A-SITE TRNA ILE2 AGMATIDINE



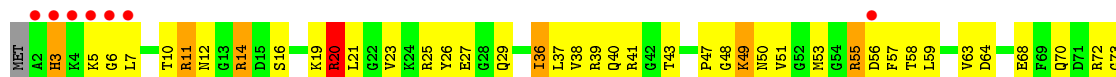
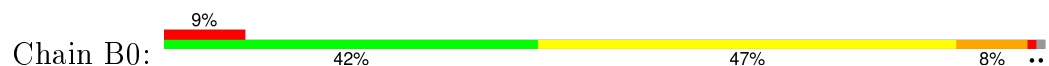
• Molecule 24: MRNA



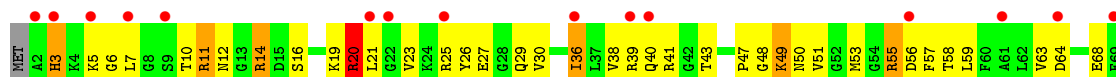
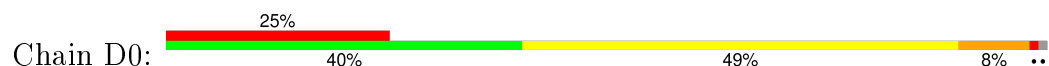
• Molecule 24: MRNA



• Molecule 25: 50S RIBOSOMAL PROTEIN L27

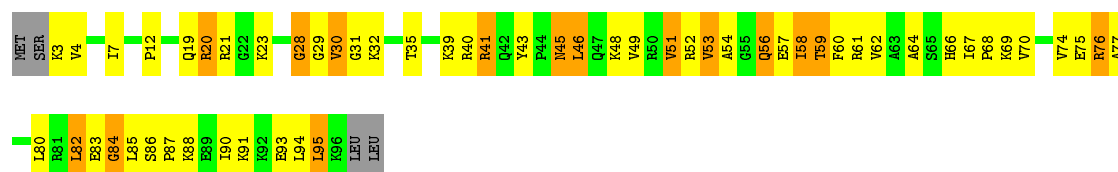


• Molecule 25: 50S RIBOSOMAL PROTEIN L27

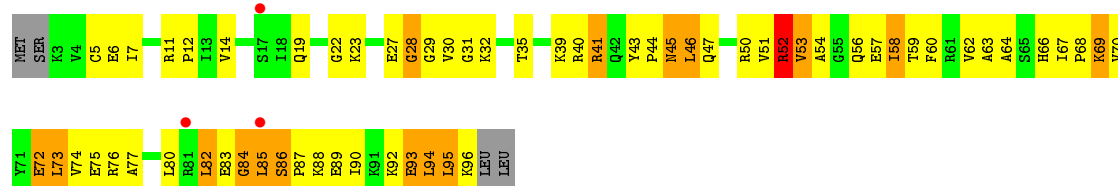


• Molecule 26: 50S RIBOSOMAL PROTEIN L28

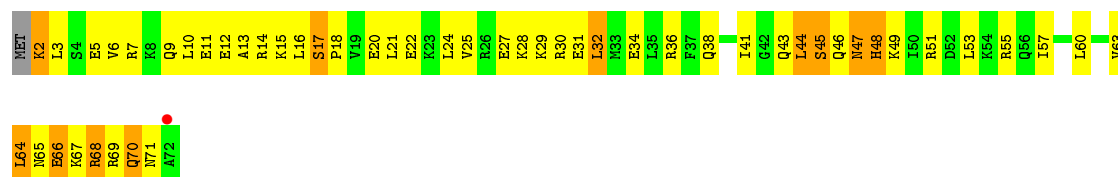




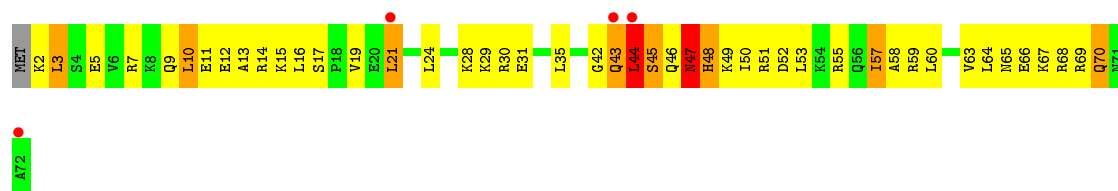
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



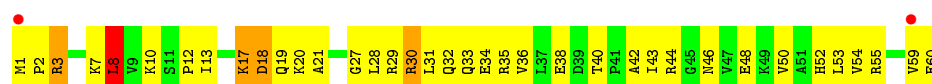
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



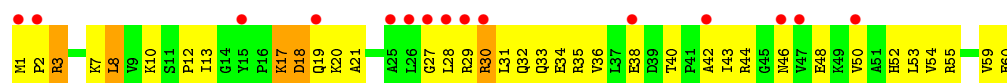
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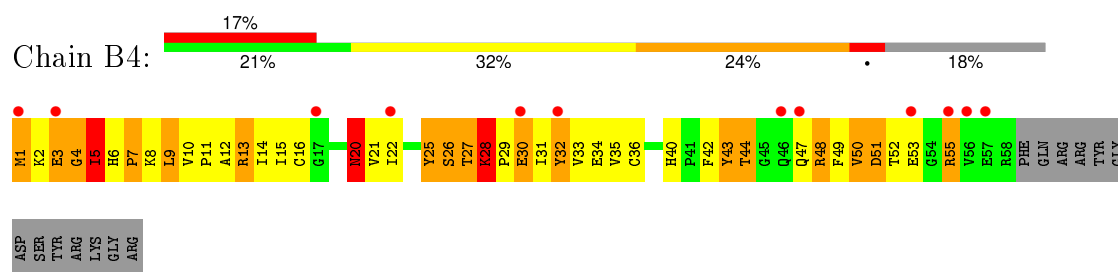
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



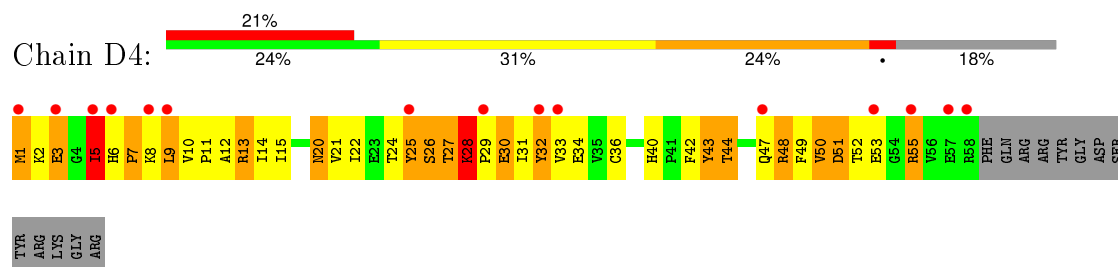
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



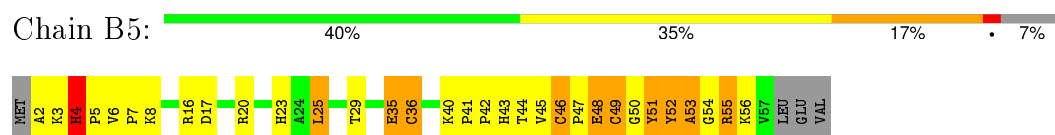
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



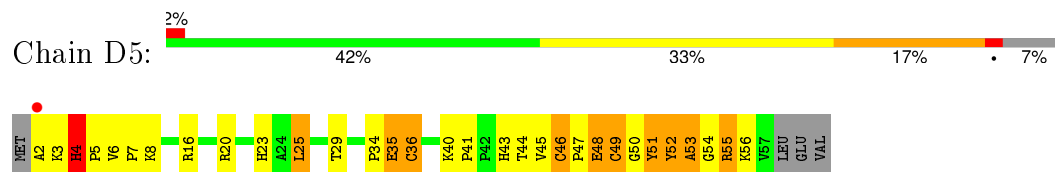
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



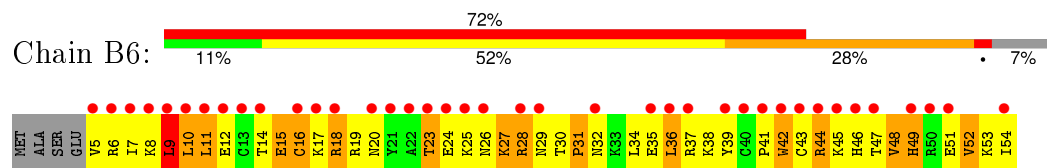
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



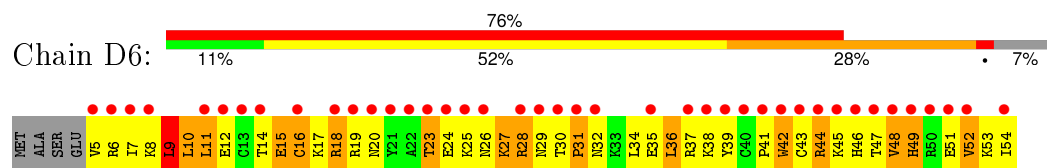
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



• Molecule 31: 50S RIBOSOMAL PROTEIN L33



• Molecule 31: 50S RIBOSOMAL PROTEIN L33



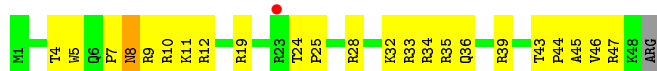
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



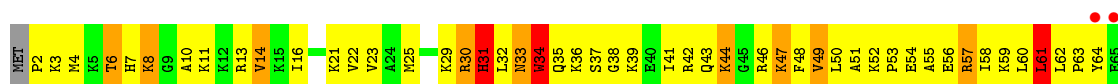




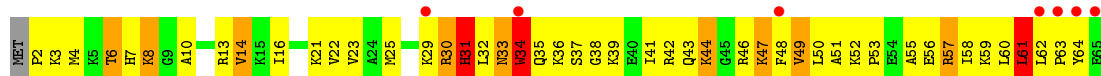
- Molecule 32: 50S RIBOSOMAL PROTEIN L34



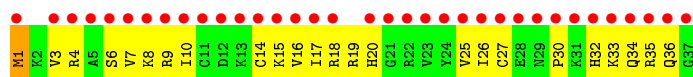
- Molecule 33: 50S RIBOSOMAL PROTEIN L35



- Molecule 33: 50S RIBOSOMAL PROTEIN L35



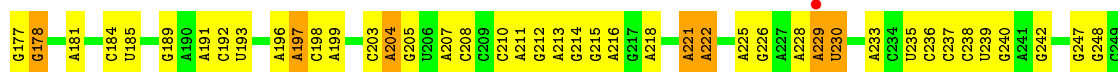
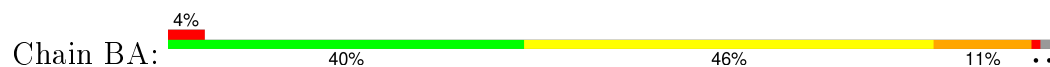
- Molecule 34: 50S RIBOSOMAL PROTEIN L36



- Molecule 34: 50S RIBOSOMAL PROTEIN L36

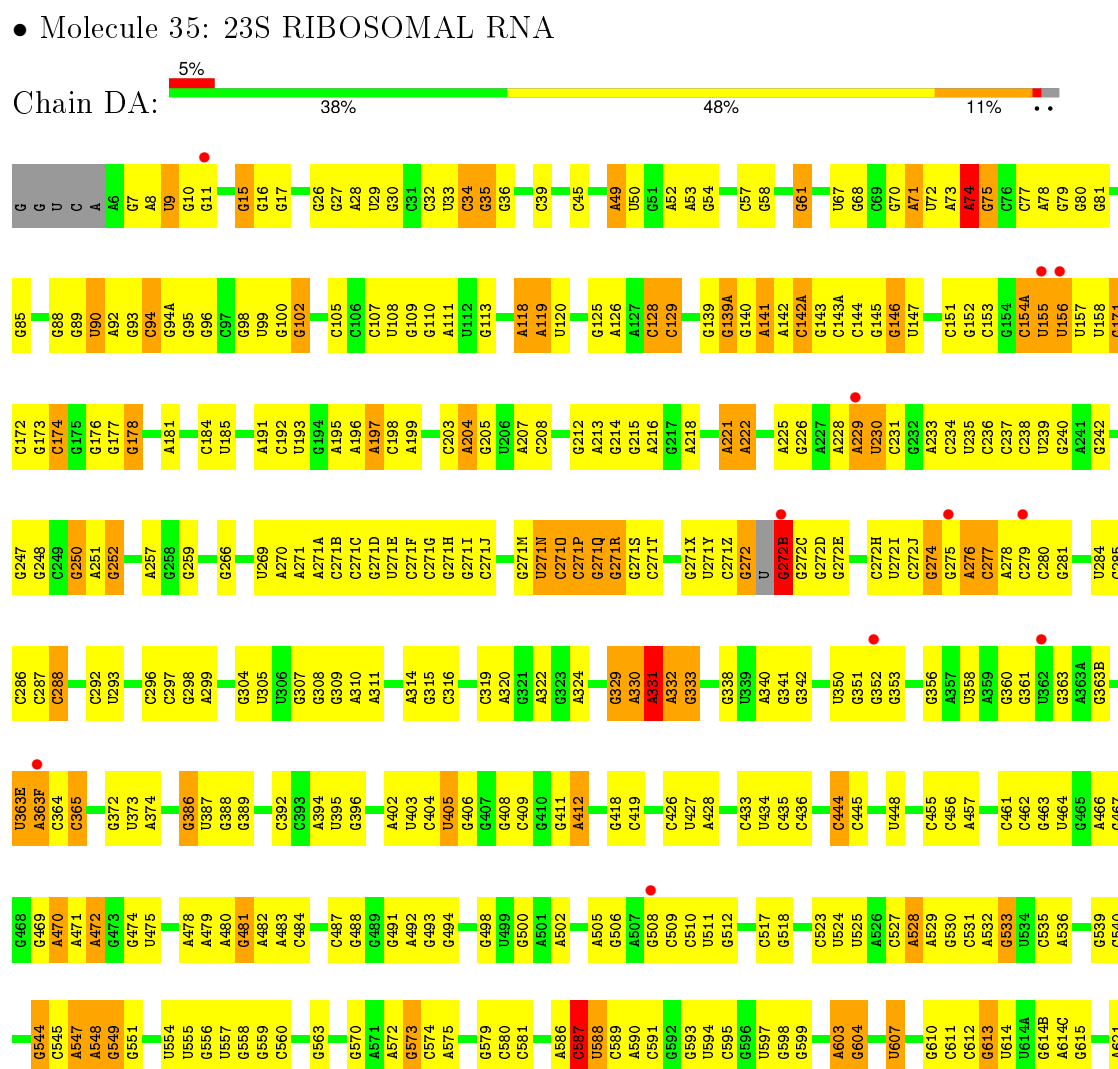
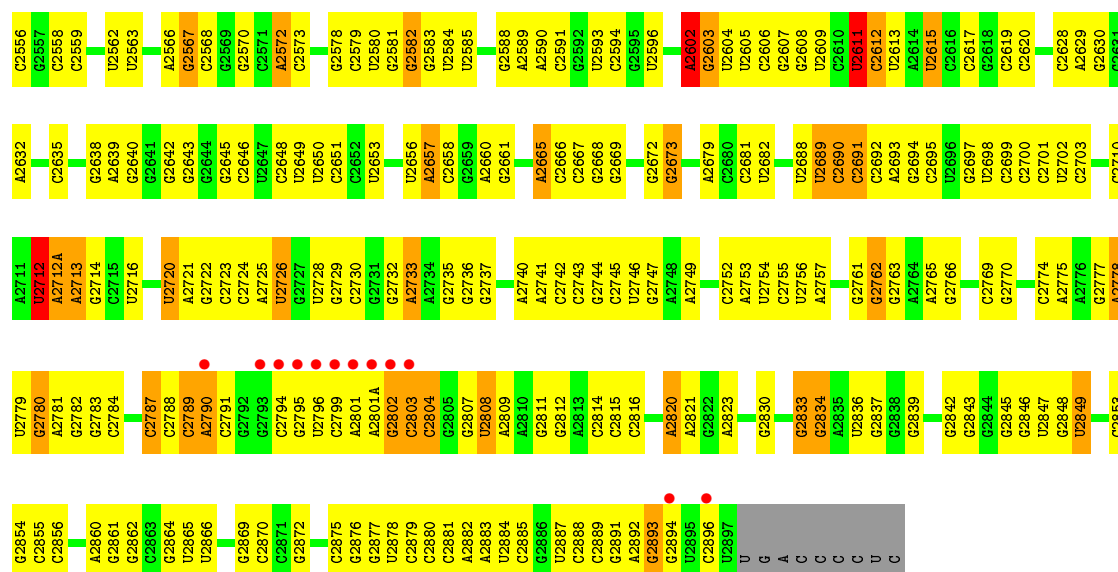


- Molecule 35: 23S RIBOSOMAL RNA



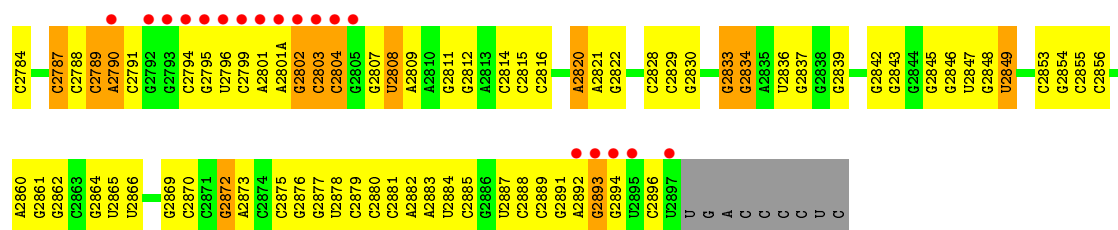






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U1639	A1542	G1475	C1398	C1314	G1235	G1151	A1020	A953	A887	G823	C754	A887	G624
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A1652	C1548	C1320	G1404	G1320	G1244	G1157	G1026	U958	C893	U828	G759	C673	A632
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G2734	A2660	U2576	G2503	G2428	C2283	C2280	C2201	C2141	G2078	G2000	U1917	G1831	A1749
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G2736	A2662	G2582	U2506	A2430	G2285	A2286	G2203	C2143	G2078	G2002	G1918	U1833	G1751
G2737	G2665	G2583	C2507	A2435	A2287	A2287	G2206	U2144	U2086	U1923	U1923	U1834	C1751
A2740	C2666	U2584	G2512	A2439	A2288	A2288	G2207	C2145	G2087	G2009	C1924	G1835	G1754
A2741	C2667	U2585	G2513	C2440	A2289	A2289	A2208	C2146	G2087	G2010	C1925	G1836	A1755
C2742	G2668	G2586	U2514	C2441	G2290	G2289	G2219	G2148	G2088	U2011	U1926	C1837	G1756
C2743	G2669	A2588	C2515	C2442	U2291	U2291	G2220	G2149	U2089	G2012	A1927	C1838	U1757
G2744	A2589	A2590	C2516	C2443	G2292	C2292	G2221	U2150	G2090	A2013	A1928	G1758	G1758
C2745	C2591	C2592	C2517	G2444	C2293	G2293	G2222	G2151	U2091	A2014	G1929	U1841	C1761
U2746	G2672	G2593	A2518	G2445	C2294	G2294	G2223	G2152	U2092	A2015	G1930	G1842	A1762
G2747	G2673	U2594	C2519	G2446	C2295	U2295	A2224	G2153	G2093	U2016	G1935	C1844	G1763
A2748	A2679	C2595	C2520	C2447	C2296	C2296	G2225	G2154	C2095	U2017	G1935	G1845	G1764
G2749	C2680	U2596	G2521	A2448	G2297	A2297	G2226	G2155	G2096	A2020	A1938	G1846	G1769
C2752	U2682	G2597	U2522	U2449	G2298	G2298	G2228	G2157	C2097	U2021	U1939	A1847	G1770
A2753	U2688	A2602	G2523	A2450	G2300	G2300	G2229	G2158	U2098	U2022	U1940	A1848	G1771
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C2755	G2690	U2604	G2525	C2455	G2302	G2302	C2231	G2161	G2101	U2028	U1946	G1857	A1772
U2756	C2691	U2605	C2527	C2456	G2303	G2303	G2232	G2162	U2102	G2027	G1947	A1773	C1773
A2757	C2692	C2606	U2528	C2457	G2304	G2304	U2233	G2163	G2103	G2029	G1948	G1858	U1774
G2761	A2693	U2609	G2529	A2459	C2305	G2305	G2234	G2164	G2104	A2030	G1948	G1859	U1775
G2762	G2694	G2610	A2530	U2462	C2306	G2306	G2235	C2165	C2105	A2031	U1951	C1860	G1776
A2764	U2697	U2611	A2531	C2463	G2307	G2307	C2236	G2166	G2106	G2032	A1952	G1861	U1779
U2765	C2698	G2612	A2534	C2464	G2308	G2308	G2237	U2172	G2112	C2040	C1958	A1877	A1780
G2766	C2699	U2613	C2535	C2465	G2309	A2310	G2238	A2173	U2113	U2041	C1962	G1878	A1789
C2767	C2700	A2614	G2536	C2466	A2311	U2312	G2239	G2174	A2114	A2043	U1963	G1879	C1790
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C2769	U2702	C2616	G2538	A2468	G2391	C2314	U2244	A2176	G2116	C2043	C1965	C1881	U1794
G2770	C2703	G2617	C2539	C2470	A2392	G2315	U2245	G2177	U2117	A2051	A1966	G1882	G1795
C2771	C2704	G2628	A2542	G2471	C2393	G2316	G2246	C2178	A2118	G2052	C1967	A1883	U1796
C2772	A2705	G2629	G2543	G2472	G2394	C2317	A2247	G2179	G2119	G2053	U1968	A1884	C1797
C2773	G2710	U2630	U2544	U2473	G2397	G2318	U2249	C2177	U2120	A2054	A1969	G1885	U1798
A2774	U2711	G2631	C2474	C2475	G2400	G2321	G2250	G2178	G2121	A1970	A1971	C1886	G1799
G2775	U2712	A2632	A2475	A2476	U2401	A2322	U2257	U2180	G2122	C2055	A1972	G1887	C1800
C2776	A2712A	G2635	A2477	A2478	C2402	G2323	C2258	G2181	U2123	G2056	G1972	G1888	A1801
G2777	G2713	G2636	U2554	A2479	G2405	A2327	C2261	G2183	G2124	A2059	G1980	A1889	A1802
A2778	G2714	U2555	C2478	G2481	U2406	A2328	U2262	C2184	G2125	A2060	U1898	G1890	A1803
U2779	G2715	G2556	G2482	C2483	A2411	G2330	C2264	G2186					
G2780	G2716	G2557	G2483										
A2781	G2717	G2558											
G2782	G2718	G2559											
G2783													



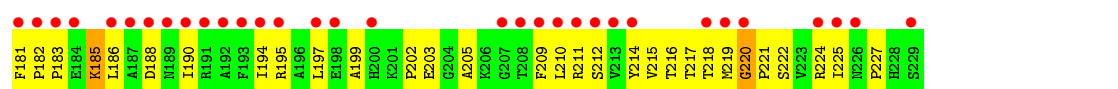
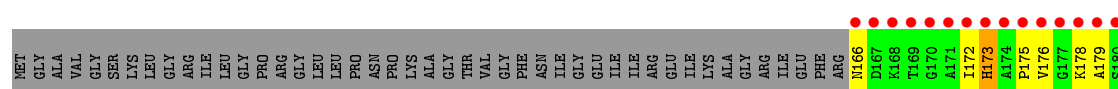
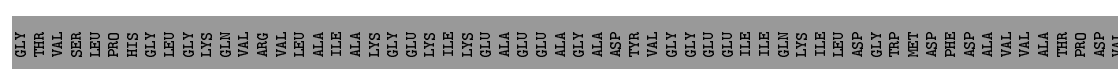
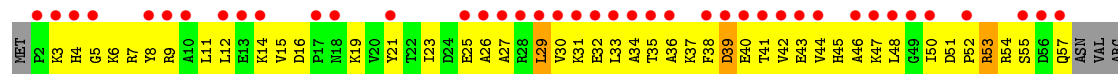
• Molecule 36: 5S RIBOSOMAL RNA



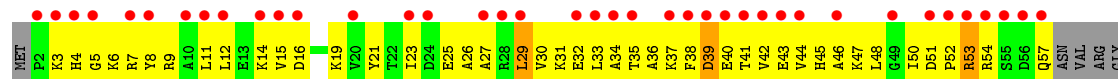
• Molecule 36: 5S RIBOSOMAL RNA



• Molecule 37: 50S RIBOSOMAL PROTEIN L1

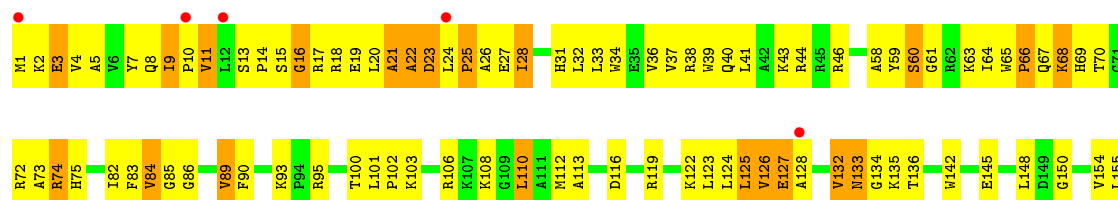


• Molecule 37: 50S RIBOSOMAL PROTEIN L1



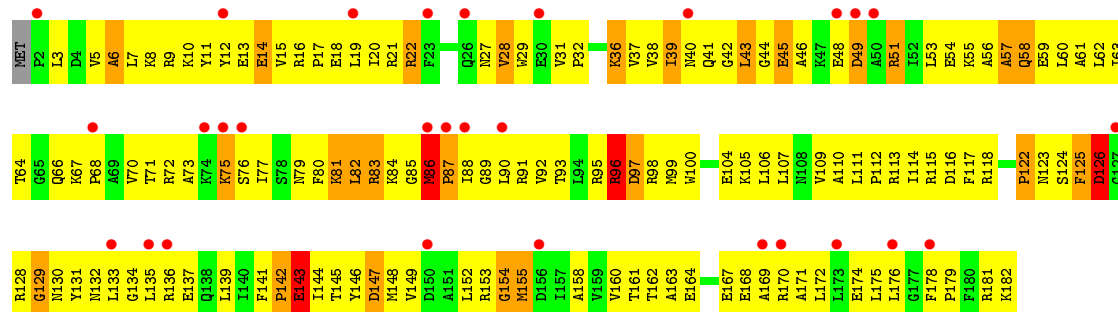




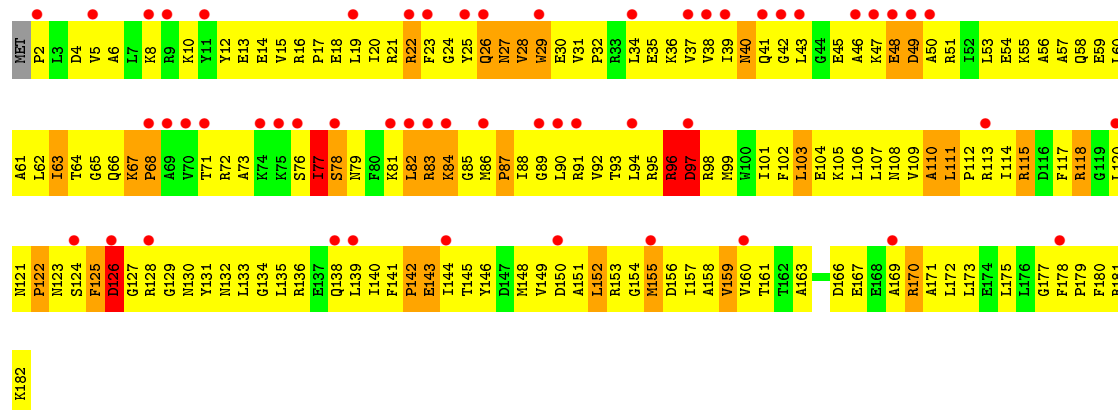




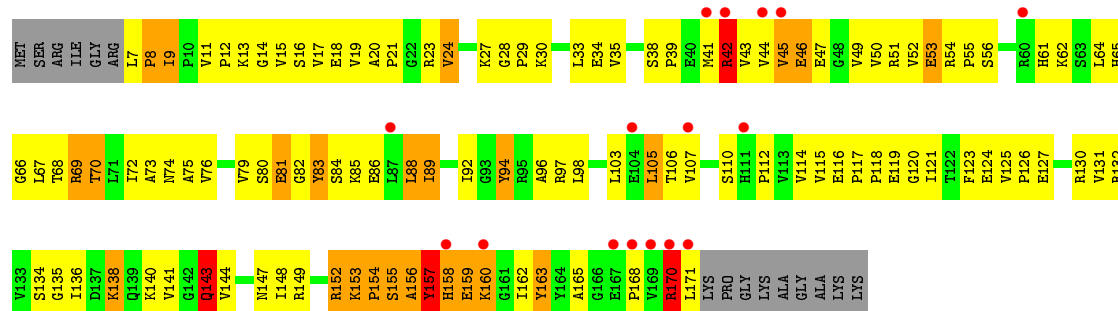
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



• Molecule 41: 50S RIBOSOMAL PROTEIN L5

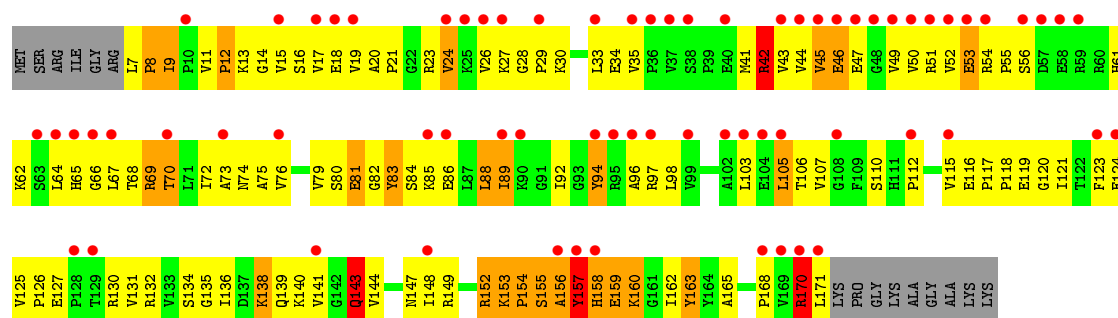


• Molecule 42: 50S RIBOSOMAL PROTEIN L6

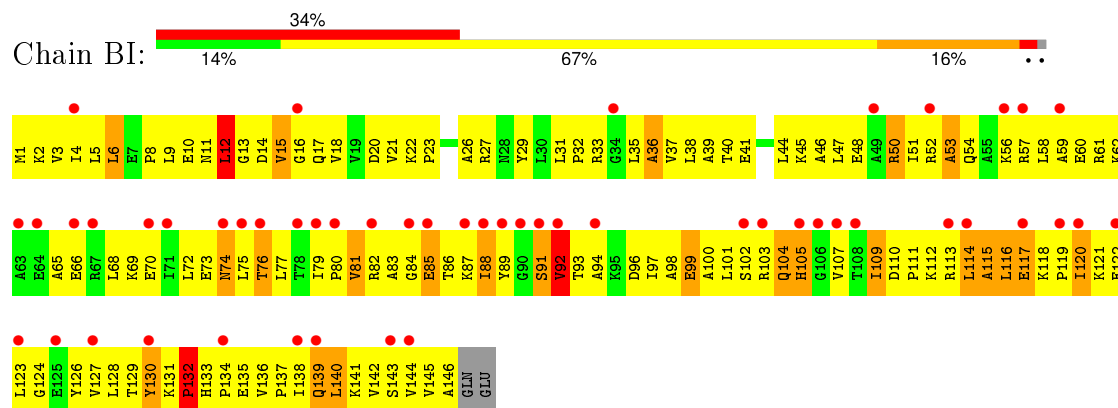


• Molecule 42: 50S RIBOSOMAL PROTEIN L6

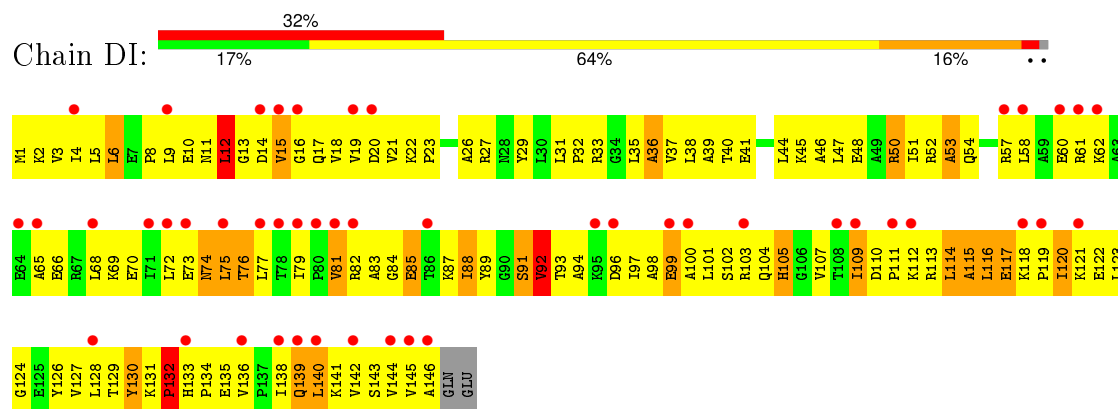




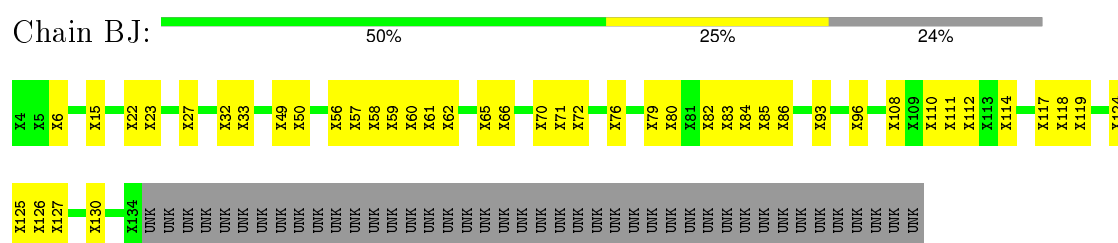
• Molecule 43: 50S RIBOSOMAL PROTEIN L9



• Molecule 43: 50S RIBOSOMAL PROTEIN L9

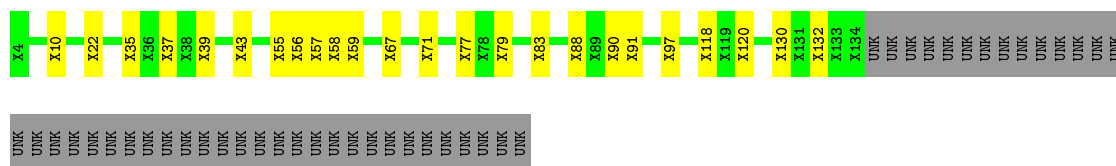


• Molecule 44: 50S RIBOSOMAL PROTEIN L10

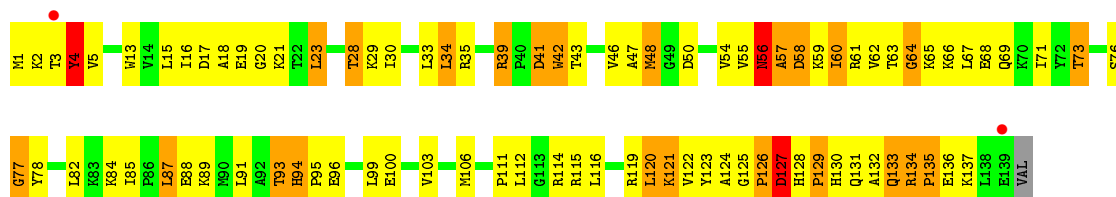


• Molecule 44: 50S RIBOSOMAL PROTEIN L10

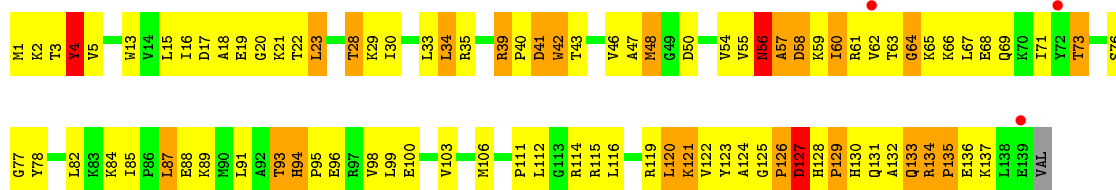




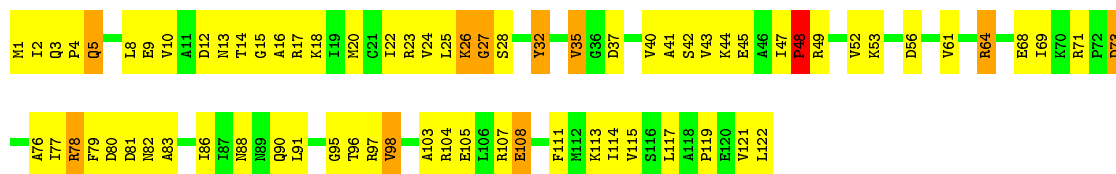
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



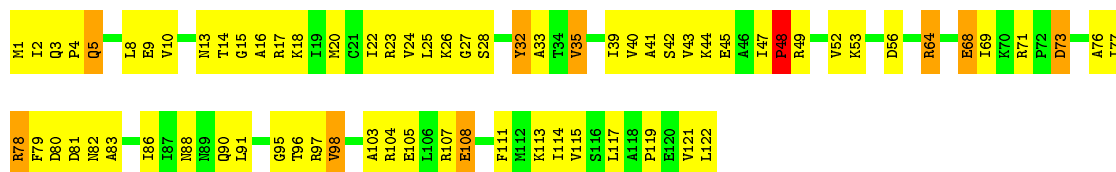
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



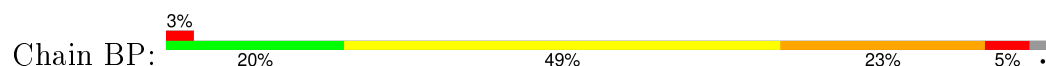
• Molecule 46: 50S RIBOSOMAL PROTEIN L14

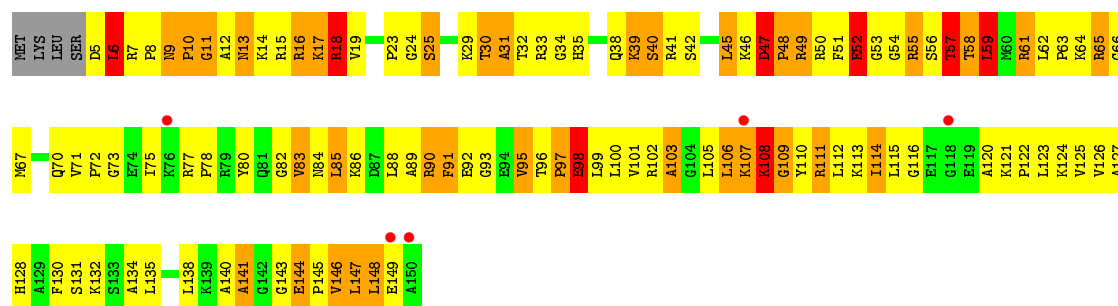


• Molecule 46: 50S RIBOSOMAL PROTEIN L14

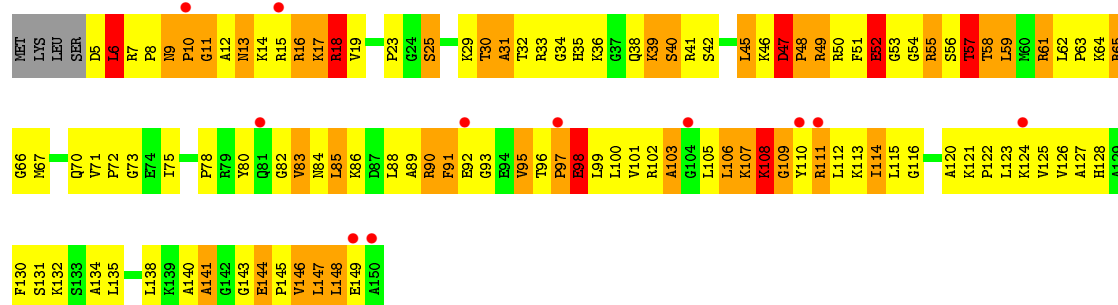
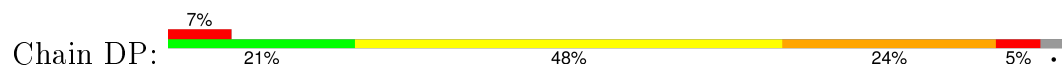


• Molecule 47: 50S RIBOSOMAL PROTEIN L15

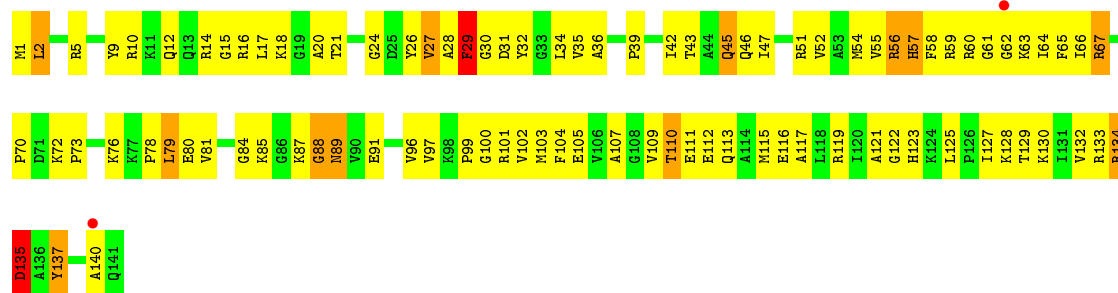




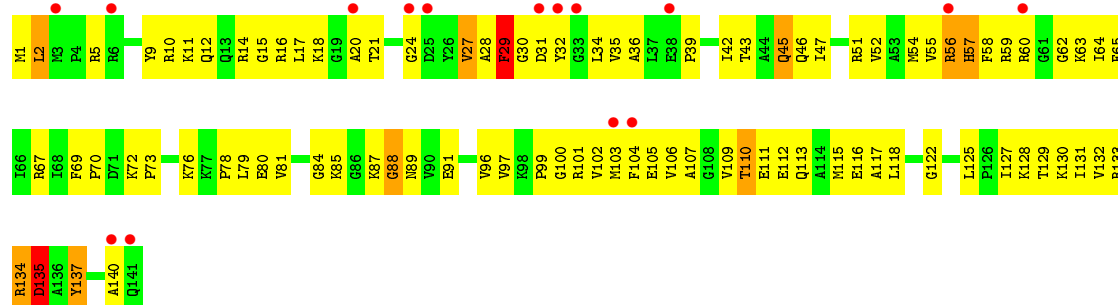
• Molecule 47: 50S RIBOSOMAL PROTEIN L15



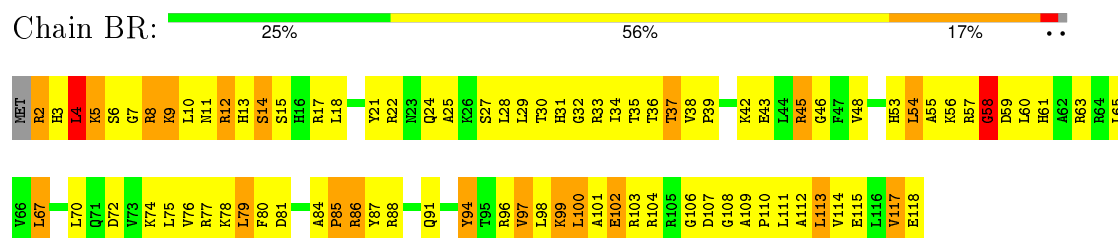
• Molecule 48: 50S RIBOSOMAL PROTEIN L16



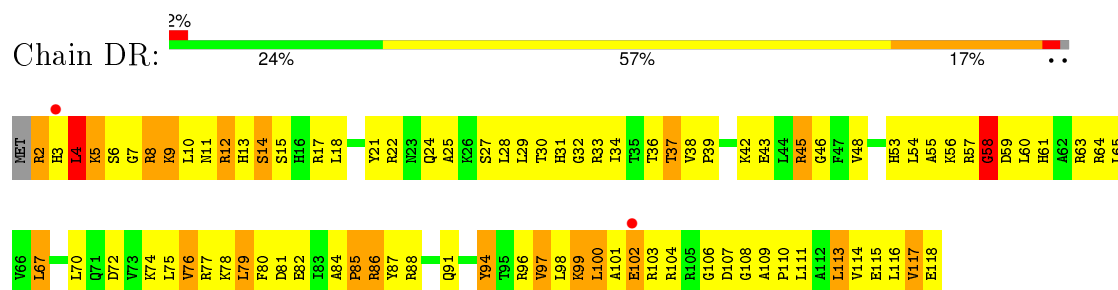
• Molecule 48: 50S RIBOSOMAL PROTEIN L16



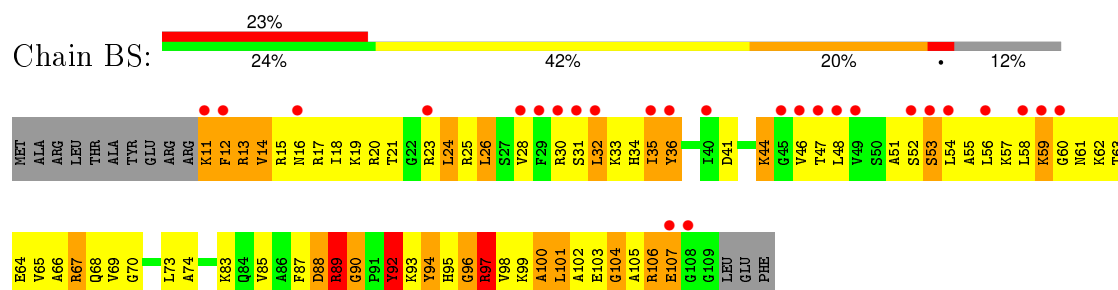
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



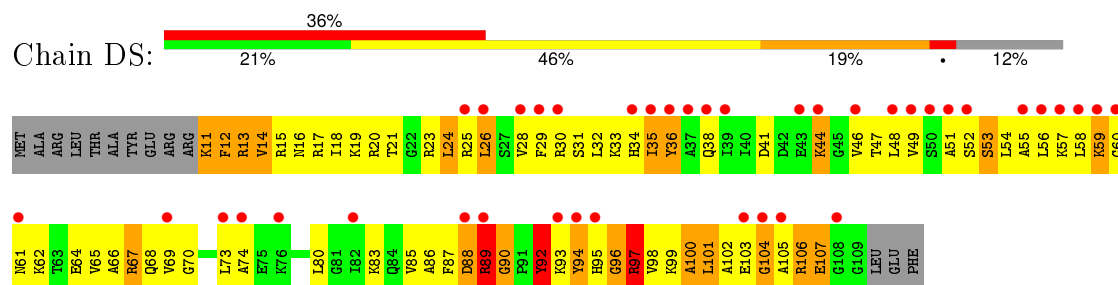
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



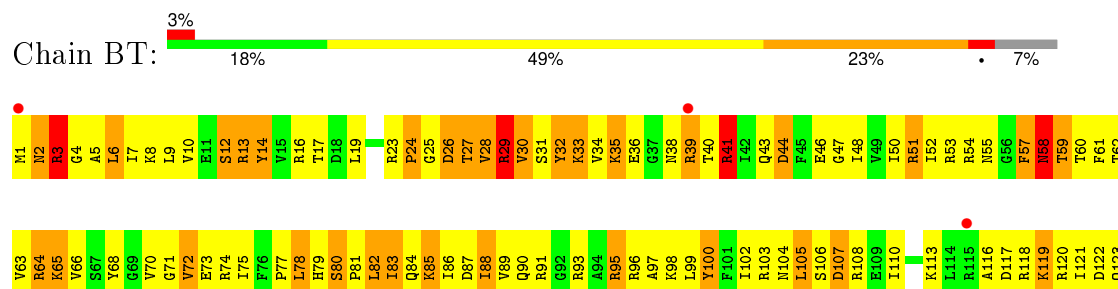
• Molecule 50: 50S RIBOSOMAL PROTEIN L18

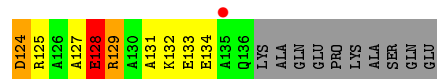


• Molecule 50: 50S RIBOSOMAL PROTEIN L18

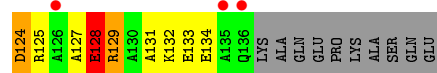
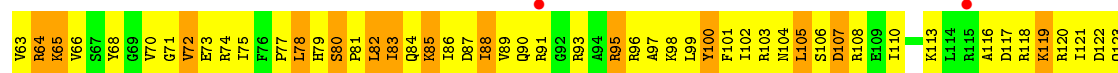
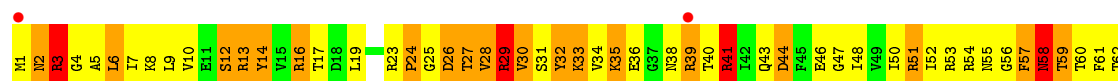
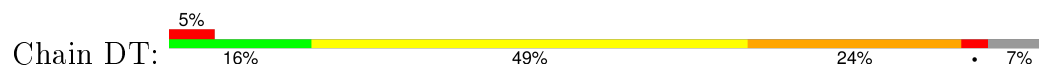


• Molecule 51: 50S RIBOSOMAL PROTEIN L19

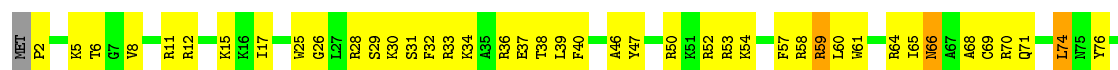
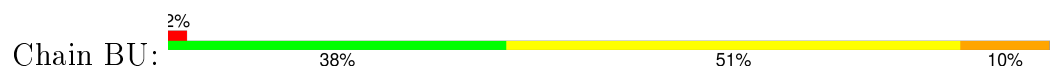




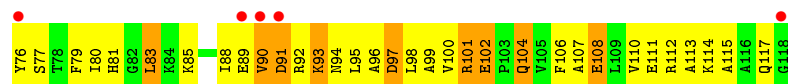
• Molecule 51: 50S RIBOSOMAL PROTEIN L19



• Molecule 52: 50S RIBOSOMAL PROTEIN L20



• Molecule 52: 50S RIBOSOMAL PROTEIN L20

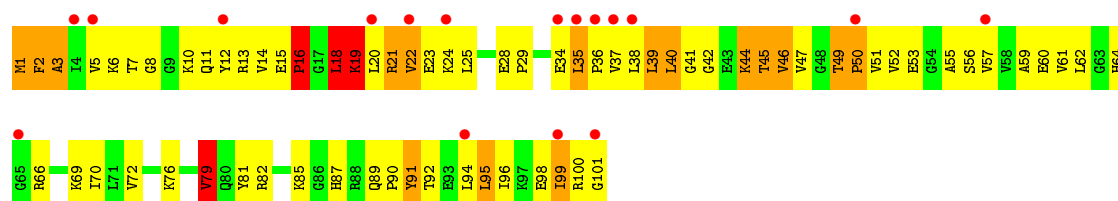


• Molecule 53: 50S RIBOSOMAL PROTEIN L21

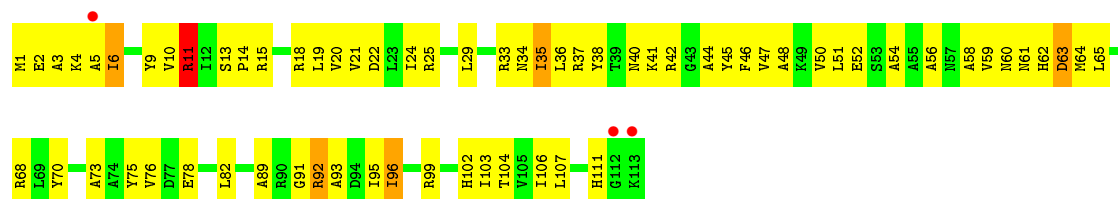
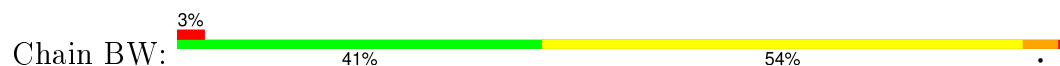


• Molecule 53: 50S RIBOSOMAL PROTEIN L21

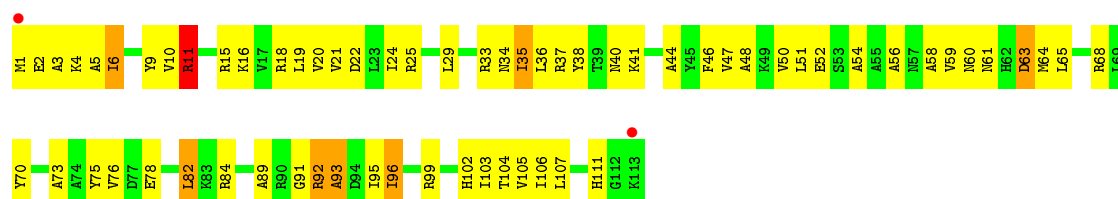
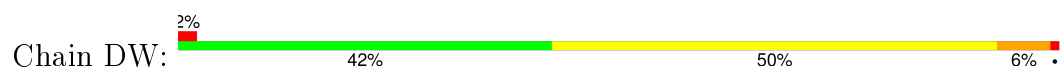




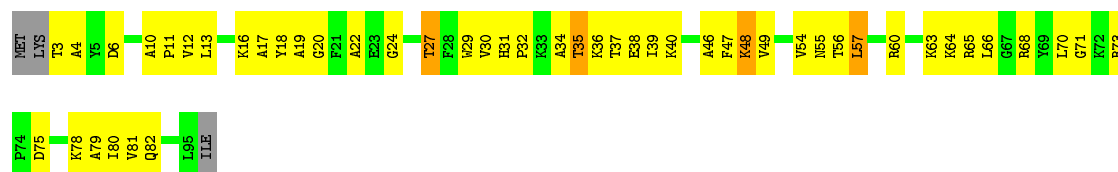
● Molecule 54: 50S RIBOSOMAL PROTEIN L22



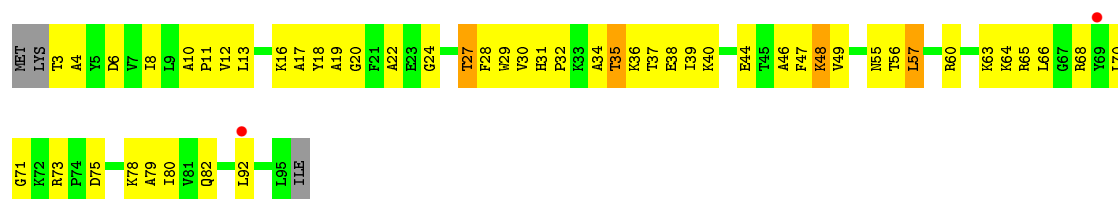
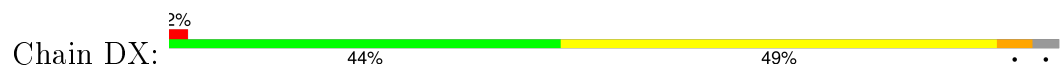
● Molecule 54: 50S RIBOSOMAL PROTEIN L22



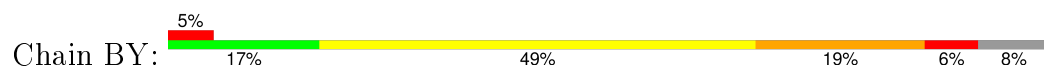
● Molecule 55: 50S RIBOSOMAL PROTEIN L23



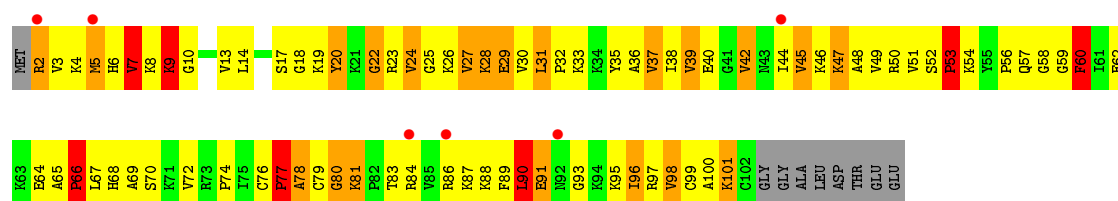
● Molecule 55: 50S RIBOSOMAL PROTEIN L23



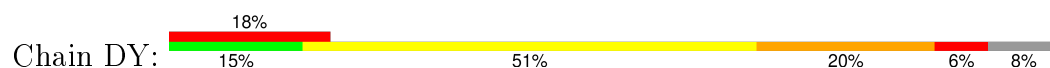
● Molecule 56: 50S RIBOSOMAL PROTEIN L24







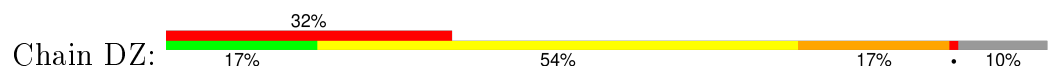
• Molecule 56: 50S RIBOSOMAL PROTEIN L24



• 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.12Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.250 , 0.280 0.274 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	71.3	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 92.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1045150 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	298096	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.44	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

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	1333	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	227	1
4	CD	1703	0	1766	223	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	47	0
14	CN	492	0	532	52	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	327	0
22	CV	1667	0	857	235	0
22	CY	1667	0	854	330	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	1764	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	DA	61341	0	30928	1844	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	2	0
58	AN	1	0	0	1	0
58	CD	1	0	0	2	0
58	CN	1	0	0	1	0
All	All	298096	0	201782	19801	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 19801 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	3
2	CB	233/256 (91%)	152 (65%)	57 (24%)	24 (10%)	1	4
3	AC	205/239 (86%)	141 (69%)	43 (21%)	21 (10%)	1	4
3	CC	205/239 (86%)	142 (69%)	40 (20%)	23 (11%)	0	3
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%)	1	4
5	CE	149/162 (92%)	110 (74%)	25 (17%)	14 (9%)	1	4
6	AF	99/101 (98%)	77 (78%)	15 (15%)	7 (7%)	1	8
6	CF	99/101 (98%)	76 (77%)	17 (17%)	6 (6%)	2	11
7	AG	153/156 (98%)	108 (71%)	41 (27%)	4 (3%)	7	32
7	CG	153/156 (98%)	110 (72%)	39 (26%)	4 (3%)	7	32
8	AH	136/138 (99%)	100 (74%)	29 (21%)	7 (5%)	2	15
8	CH	136/138 (99%)	99 (73%)	29 (21%)	8 (6%)	2	12
9	AI	121/128 (94%)	90 (74%)	22 (18%)	9 (7%)	1	7
9	CI	121/128 (94%)	91 (75%)	20 (16%)	10 (8%)	1	6
10	AJ	97/105 (92%)	76 (78%)	17 (18%)	4 (4%)	3	20
10	CJ	97/105 (92%)	76 (78%)	17 (18%)	4 (4%)	3	20
11	AK	117/129 (91%)	83 (71%)	26 (22%)	8 (7%)	1	8
11	CK	117/129 (91%)	83 (71%)	26 (22%)	8 (7%)	1	8
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%)	1	3
15	CO	86/89 (97%)	50 (58%)	27 (31%)	9 (10%)	1	3
16	AP	82/88 (93%)	48 (58%)	24 (29%)	10 (12%)	0	2
16	CP	82/88 (93%)	49 (60%)	24 (29%)	9 (11%)	0	3
17	AQ	98/105 (93%)	70 (71%)	22 (22%)	6 (6%)	2	11
17	CQ	98/105 (93%)	71 (72%)	20 (20%)	7 (7%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	68/88 (77%)	44 (65%)	18 (26%)	6 (9%)	1	5
18	CR	68/88 (77%)	44 (65%)	18 (26%)	6 (9%)	1	5
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%)	4	23
25	D0	82/85 (96%)	66 (80%)	13 (16%)	3 (4%)	4	23
26	B1	92/98 (94%)	68 (74%)	13 (14%)	11 (12%)	0	2
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	7
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	5
28	D3	58/60 (97%)	44 (76%)	9 (16%)	5 (9%)	1	5
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	1
30	D5	54/60 (90%)	43 (80%)	3 (6%)	8 (15%)	0	1
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%)	7	32
37	DC	116/229 (51%)	94 (81%)	19 (16%)	3 (3%)	7	32
38	BD	270/276 (98%)	209 (77%)	32 (12%)	29 (11%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DD	270/276 (98%)	207 (77%)	34 (13%)	29 (11%)	0	3
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	1
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	1
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	2
45	DN	137/140 (98%)	101 (74%)	20 (15%)	16 (12%)	0	2
46	BO	120/122 (98%)	99 (82%)	14 (12%)	7 (6%)	2	12
46	DO	120/122 (98%)	96 (80%)	16 (13%)	8 (7%)	1	9
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	5
48	DQ	139/141 (99%)	99 (71%)	28 (20%)	12 (9%)	1	5
49	BR	115/118 (98%)	88 (76%)	13 (11%)	14 (12%)	0	2
49	DR	115/118 (98%)	87 (76%)	14 (12%)	14 (12%)	0	2
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	15
52	DU	115/118 (98%)	88 (76%)	20 (17%)	7 (6%)	2	11
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	7
54	DW	111/113 (98%)	91 (82%)	13 (12%)	7 (6%)	2	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BX	91/96 (95%)	71 (78%)	15 (16%)	5 (6%)	2	13
55	DX	91/96 (95%)	67 (74%)	19 (21%)	5 (6%)	2	13
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	1
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	2

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 ⓘ

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%)	15	49
2	CB	202/220 (92%)	187 (93%)	15 (7%)	17	51
3	AC	160/188 (85%)	145 (91%)	15 (9%)	11	39
3	CC	160/188 (85%)	146 (91%)	14 (9%)	12	43
4	AD	180/181 (99%)	162 (90%)	18 (10%)	9	34
4	CD	180/181 (99%)	162 (90%)	18 (10%)	9	34
5	AE	115/123 (94%)	107 (93%)	8 (7%)	19	54
5	CE	115/123 (94%)	107 (93%)	8 (7%)	19	54
6	AF	90/90 (100%)	87 (97%)	3 (3%)	45	79
6	CF	90/90 (100%)	87 (97%)	3 (3%)	45	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	126/127 (99%)	121 (96%)	5 (4%)	38	75
7	CG	126/127 (99%)	121 (96%)	5 (4%)	38	75
8	AH	119/119 (100%)	109 (92%)	10 (8%)	14	46
8	CH	119/119 (100%)	109 (92%)	10 (8%)	14	46
9	AI	98/99 (99%)	90 (92%)	8 (8%)	14	47
9	CI	98/99 (99%)	90 (92%)	8 (8%)	14	47
10	AJ	88/92 (96%)	83 (94%)	5 (6%)	25	62
10	CJ	88/92 (96%)	83 (94%)	5 (6%)	25	62
11	AK	90/99 (91%)	85 (94%)	5 (6%)	26	62
11	CK	90/99 (91%)	85 (94%)	5 (6%)	26	62
12	AL	104/111 (94%)	85 (82%)	19 (18%)	2	9
12	CL	104/111 (94%)	84 (81%)	20 (19%)	2	8
13	AM	94/101 (93%)	84 (89%)	10 (11%)	8	31
13	CM	94/101 (93%)	84 (89%)	10 (11%)	8	31
14	AN	49/50 (98%)	47 (96%)	2 (4%)	37	74
14	CN	49/50 (98%)	47 (96%)	2 (4%)	37	74
15	AO	79/80 (99%)	75 (95%)	4 (5%)	29	66
15	CO	79/80 (99%)	75 (95%)	4 (5%)	29	66
16	AP	72/74 (97%)	66 (92%)	6 (8%)	14	46
16	CP	72/74 (97%)	66 (92%)	6 (8%)	14	46
17	AQ	94/97 (97%)	90 (96%)	4 (4%)	35	72
17	CQ	94/97 (97%)	90 (96%)	4 (4%)	35	72
18	AR	61/77 (79%)	59 (97%)	2 (3%)	45	79
18	CR	61/77 (79%)	59 (97%)	2 (3%)	45	79
19	AS	69/80 (86%)	62 (90%)	7 (10%)	9	33
19	CS	69/80 (86%)	61 (88%)	8 (12%)	7	27
20	AT	76/82 (93%)	71 (93%)	5 (7%)	21	56
20	CT	76/82 (93%)	71 (93%)	5 (7%)	21	56
21	AU	19/22 (86%)	17 (90%)	2 (10%)	8	31
21	CU	19/22 (86%)	18 (95%)	1 (5%)	28	64
25	B0	66/67 (98%)	59 (89%)	7 (11%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	D0	66/67 (98%)	59 (89%)	7 (11%)	8	31
26	B1	78/83 (94%)	70 (90%)	8 (10%)	9	32
26	D1	78/83 (94%)	68 (87%)	10 (13%)	5	21
27	B2	66/67 (98%)	57 (86%)	9 (14%)	5	19
27	D2	66/67 (98%)	60 (91%)	6 (9%)	12	40
28	B3	51/52 (98%)	48 (94%)	3 (6%)	24	60
28	D3	51/52 (98%)	48 (94%)	3 (6%)	24	60
29	B4	51/63 (81%)	42 (82%)	9 (18%)	2	10
29	D4	51/63 (81%)	42 (82%)	9 (18%)	2	10
30	B5	47/52 (90%)	42 (89%)	5 (11%)	8	31
30	D5	47/52 (90%)	42 (89%)	5 (11%)	8	31
31	B6	49/52 (94%)	43 (88%)	6 (12%)	6	24
31	D6	49/52 (94%)	43 (88%)	6 (12%)	6	24
32	B7	40/42 (95%)	35 (88%)	5 (12%)	6	22
32	D7	40/42 (95%)	36 (90%)	4 (10%)	9	34
33	B8	53/55 (96%)	44 (83%)	9 (17%)	2	11
33	D8	53/55 (96%)	44 (83%)	9 (17%)	2	11
34	B9	34/34 (100%)	33 (97%)	1 (3%)	50	81
34	D9	34/34 (100%)	33 (97%)	1 (3%)	50	81
37	BC	99/181 (55%)	94 (95%)	5 (5%)	29	66
37	DC	99/181 (55%)	94 (95%)	5 (5%)	29	66
38	BD	213/218 (98%)	185 (87%)	28 (13%)	5	21
38	DD	213/218 (98%)	187 (88%)	26 (12%)	6	24
39	BE	165/166 (99%)	144 (87%)	21 (13%)	5	22
39	DE	165/166 (99%)	143 (87%)	22 (13%)	5	20
40	BF	165/166 (99%)	149 (90%)	16 (10%)	10	36
40	DF	165/166 (99%)	149 (90%)	16 (10%)	10	36
41	BG	155/156 (99%)	140 (90%)	15 (10%)	10	36
41	DG	155/156 (99%)	140 (90%)	15 (10%)	10	36
42	BH	137/148 (93%)	121 (88%)	16 (12%)	7	26
42	DH	137/148 (93%)	121 (88%)	16 (12%)	7	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BI	122/124 (98%)	112 (92%)	10 (8%)	14	47
43	DI	122/124 (98%)	112 (92%)	10 (8%)	14	47
45	BN	117/119 (98%)	101 (86%)	16 (14%)	4	19
45	DN	117/119 (98%)	101 (86%)	16 (14%)	4	19
46	BO	100/100 (100%)	94 (94%)	6 (6%)	24	60
46	DO	100/100 (100%)	94 (94%)	6 (6%)	24	60
47	BP	112/116 (97%)	93 (83%)	19 (17%)	2	11
47	DP	112/116 (97%)	93 (83%)	19 (17%)	2	11
48	BQ	110/111 (99%)	100 (91%)	10 (9%)	12	40
48	DQ	110/111 (99%)	101 (92%)	9 (8%)	14	47
49	BR	100/101 (99%)	87 (87%)	13 (13%)	5	21
49	DR	100/101 (99%)	86 (86%)	14 (14%)	4	18
50	BS	77/88 (88%)	64 (83%)	13 (17%)	2	11
50	DS	77/88 (88%)	64 (83%)	13 (17%)	2	11
51	BT	118/127 (93%)	96 (81%)	22 (19%)	2	9
51	DT	118/127 (93%)	95 (80%)	23 (20%)	2	7
52	BU	92/94 (98%)	83 (90%)	9 (10%)	10	36
52	DU	92/94 (98%)	81 (88%)	11 (12%)	6	24
53	BV	82/82 (100%)	67 (82%)	15 (18%)	2	9
53	DV	82/82 (100%)	68 (83%)	14 (17%)	2	11
54	BW	91/92 (99%)	81 (89%)	10 (11%)	8	30
54	DW	91/92 (99%)	81 (89%)	10 (11%)	8	30
55	BX	74/78 (95%)	69 (93%)	5 (7%)	20	55
55	DX	74/78 (95%)	69 (93%)	5 (7%)	20	55
56	BY	84/91 (92%)	70 (83%)	14 (17%)	3	11
56	DY	84/91 (92%)	69 (82%)	15 (18%)	2	10
57	BZ	162/179 (90%)	140 (86%)	22 (14%)	5	19
57	DZ	162/179 (90%)	145 (90%)	17 (10%)	8	31
All	All	9790/10432 (94%)	8794 (90%)	996 (10%)	9	33

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

Mol	Chain	Res	Type
54	BW	11	ARG
6	CF	63	TYR
51	DT	95	ARG
55	BX	68	ARG
2	CB	87	ARG

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

Mol	Chain	Res	Type
51	BT	90	GLN
4	CD	62	GLN
48	DQ	123	HIS
52	BU	117	GLN
2	CB	37	ASN

### 5.3.3 RNA ⓘ

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
35	BA	2405	G
1	CA	429	U
35	DA	2126	A
35	BA	2439	A
1	CA	60	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	20,29,30	0.77	1 (5%)	27,39,42	1.40	3 (11%)
22	AG9	AY	36	22	20,29,30	1.38	2 (10%)	27,39,42	1.53	4 (14%)
22	AG9	CV	36	22	20,29,30	1.55	2 (10%)	27,39,42	1.40	3 (11%)
22	AG9	CY	36	22	20,29,30	1.88	4 (20%)	27,39,42	1.39	4 (14%)

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	0/14/47/48	0/2/2/2
22	AG9	AY	36	22	1/1/9/13	0/14/47/48	0/2/2/2
22	AG9	CV	36	22	1/1/9/13	0/14/47/48	0/2/2/2
22	AG9	CY	36	22	1/1/9/13	0/14/47/48	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	AV	36	AG9	C2-N3	2.44	1.35	1.30
22	CY	36	AG9	C2-N2	2.74	1.38	1.34
22	AY	36	AG9	C2-N3	2.89	1.36	1.30
22	CY	36	AG9	C1'-N1	2.90	1.56	1.47
22	CY	36	AG9	C2-N3	3.23	1.36	1.30

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AY	36	AG9	N1-C2-N3	-4.92	118.76	124.16
22	CV	36	AG9	N1-C2-N3	-4.82	118.87	124.16
22	AV	36	AG9	N1-C2-N3	-4.78	118.92	124.16
22	CY	36	AG9	N1-C2-N3	-4.52	119.20	124.16
22	AY	36	AG9	C2'-C1'-N1	2.48	120.41	113.08

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

There are no torsion outliers.

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	CV	36	AG9	12	0
22	CY	36	AG9	7	0

## 5.5 Carbohydrates

There are no carbohydrates 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	CM	5
13	AM	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1504/1522 (98%)	0.62	103 (6%) 20 7	44, 101, 184, 200	0
1	CA	1504/1522 (98%)	0.61	114 (7%) 17 6	55, 115, 186, 200	0
2	AB	235/256 (91%)	0.73	32 (13%) 4 2	75, 134, 176, 198	0
2	CB	235/256 (91%)	1.28	57 (24%) 1 0	94, 148, 183, 200	0
3	AC	207/239 (86%)	0.84	28 (13%) 4 2	82, 127, 157, 179	0
3	CC	207/239 (86%)	1.26	54 (26%) 1 0	92, 141, 170, 185	0
4	AD	208/209 (99%)	0.67	17 (8%) 14 5	64, 112, 142, 179	0
4	CD	208/209 (99%)	0.30	8 (3%) 44 21	56, 99, 135, 157	0
5	AE	151/162 (93%)	0.45	8 (5%) 30 13	65, 95, 142, 167	0
5	CE	151/162 (93%)	0.99	28 (18%) 2 1	69, 119, 151, 160	0
6	AF	101/101 (100%)	0.12	0 100 100	59, 98, 138, 173	0
6	CF	101/101 (100%)	0.12	3 (2%) 54 29	64, 110, 133, 173	0
7	AG	155/156 (99%)	1.26	36 (23%) 1 0	76, 123, 155, 198	0
7	CG	155/156 (99%)	1.19	37 (23%) 1 0	94, 131, 160, 194	0
8	AH	138/138 (100%)	0.39	7 (5%) 32 13	61, 101, 128, 144	0
8	CH	138/138 (100%)	0.77	14 (10%) 9 3	83, 121, 148, 166	0
9	AI	127/128 (99%)	1.72	44 (34%) 0 0	81, 148, 176, 191	0
9	CI	127/128 (99%)	2.13	62 (48%) 0 0	99, 153, 181, 193	0
10	AJ	99/105 (94%)	1.88	45 (45%) 0 0	71, 149, 177, 185	0
10	CJ	99/105 (94%)	2.45	55 (55%) 0 0	97, 159, 182, 189	0
11	AK	119/129 (92%)	0.56	10 (8%) 14 4	63, 94, 136, 187	0
11	CK	119/129 (92%)	0.60	14 (11%) 6 2	78, 108, 141, 176	0
12	AL	125/135 (92%)	1.10	24 (19%) 2 1	53, 93, 146, 180	0
12	CL	125/135 (92%)	1.16	28 (22%) 1 0	63, 111, 149, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	AM	119/126 (94%)	1.37	35 (29%)	1	0	75, 129, 161, 178	0
13	CM	119/126 (94%)	2.06	50 (42%)	0	0	96, 150, 169, 186	0
14	AN	60/61 (98%)	1.43	16 (26%)	1	0	71, 118, 145, 157	0
14	CN	60/61 (98%)	1.59	23 (38%)	0	0	108, 143, 166, 187	0
15	AO	88/89 (98%)	0.44	4 (4%)	37	17	60, 97, 130, 148	0
15	CO	88/89 (98%)	0.70	9 (10%)	9	3	67, 110, 138, 146	0
16	AP	84/88 (95%)	1.11	15 (17%)	2	1	67, 112, 156, 178	0
16	CP	84/88 (95%)	0.52	4 (4%)	34	15	60, 87, 137, 157	0
17	AQ	100/105 (95%)	0.67	10 (10%)	9	3	74, 109, 138, 151	0
17	CQ	100/105 (95%)	0.81	12 (12%)	6	2	70, 109, 139, 165	0
18	AR	70/88 (79%)	0.63	5 (7%)	19	7	69, 98, 139, 157	0
18	CR	70/88 (79%)	0.82	7 (10%)	9	3	77, 111, 148, 156	0
19	AS	79/93 (84%)	1.97	29 (36%)	0	0	89, 137, 171, 185	0
19	CS	79/93 (84%)	2.49	39 (49%)	0	0	112, 154, 178, 200	0
20	AT	99/106 (93%)	1.16	17 (17%)	2	1	65, 117, 160, 167	0
20	CT	99/106 (93%)	0.93	12 (12%)	6	2	66, 107, 151, 163	0
21	AU	25/27 (92%)	2.19	14 (56%)	0	0	84, 120, 146, 156	0
21	CU	25/27 (92%)	4.05	19 (76%)	0	0	91, 135, 171, 188	0
22	AV	77/78 (98%)	1.51	23 (29%)	1	0	65, 141, 179, 199	0
22	AY	77/78 (98%)	1.64	26 (33%)	0	0	90, 140, 185, 189	0
22	CV	77/78 (98%)	2.26	37 (48%)	0	0	94, 175, 196, 200	0
22	CY	77/78 (98%)	2.93	47 (61%)	0	0	138, 176, 197, 200	0
23	AW	78/78 (100%)	2.28	39 (50%)	0	0	70, 173, 191, 199	0
23	CW	78/78 (100%)	3.41	56 (71%)	0	0	99, 188, 200, 200	0
24	AX	12/24 (50%)	1.12	1 (8%)	14	5	59, 88, 157, 160	0
24	CX	12/24 (50%)	1.99	5 (41%)	0	0	92, 163, 185, 185	0
25	B0	84/85 (98%)	0.79	8 (9%)	10	4	39, 66, 124, 167	0
25	D0	84/85 (98%)	1.31	21 (25%)	1	0	71, 105, 146, 165	0
26	B1	94/98 (95%)	0.09	0	100	100	33, 61, 114, 141	0
26	D1	94/98 (95%)	0.25	3 (3%)	51	27	43, 74, 127, 149	0
27	B2	71/72 (98%)	-0.06	1 (1%)	78	60	41, 70, 122, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
27	D2	71/72 (98%)	0.26	4 (5%)	28 11	57, 97, 139, 178	0
28	B3	60/60 (100%)	0.42	2 (3%)	50 26	42, 63, 108, 167	0
28	D3	60/60 (100%)	1.36	15 (25%)	1 0	65, 109, 149, 175	0
29	B4	58/71 (81%)	1.37	12 (20%)	1 0	96, 144, 171, 187	0
29	D4	58/71 (81%)	1.37	15 (25%)	1 0	86, 165, 194, 200	0
30	B5	56/60 (93%)	-0.09	0	100 100	25, 63, 126, 148	0
30	D5	56/60 (93%)	0.20	1 (1%)	71 50	48, 80, 128, 146	0
31	B6	50/54 (92%)	3.64	39 (78%)	0 0	99, 140, 171, 180	0
31	D6	50/54 (92%)	4.81	41 (82%)	0 0	113, 150, 174, 191	0
32	B7	48/49 (97%)	0.17	1 (2%)	67 44	23, 42, 83, 129	0
32	D7	48/49 (97%)	0.34	1 (2%)	67 44	35, 54, 98, 131	0
33	B8	64/65 (98%)	0.42	2 (3%)	52 28	30, 61, 107, 123	0
33	D8	64/65 (98%)	0.74	7 (10%)	7 2	46, 89, 134, 177	0
34	B9	37/37 (100%)	5.44	35 (94%)	0 0	91, 136, 157, 159	0
34	D9	37/37 (100%)	6.17	36 (97%)	0 0	126, 149, 172, 183	0
35	BA	2848/2915 (97%)	0.37	129 (4%)	37 17	20, 56, 184, 200	0
35	DA	2848/2915 (97%)	0.43	158 (5%)	29 12	39, 82, 186, 200	0
36	BB	119/122 (97%)	0.67	1 (0%)	87 75	52, 81, 149, 178	0
36	DB	119/122 (97%)	0.92	10 (8%)	14 4	102, 151, 183, 195	0
37	BC	120/229 (52%)	3.80	88 (73%)	0 0	119, 168, 189, 200	0
37	DC	120/229 (52%)	3.55	82 (68%)	0 0	132, 170, 187, 199	0
38	BD	272/276 (98%)	0.01	5 (1%)	71 50	24, 55, 93, 150	0
38	DD	272/276 (98%)	0.13	4 (1%)	76 58	37, 73, 110, 144	0
39	BE	205/206 (99%)	0.20	8 (3%)	43 21	20, 62, 129, 165	0
39	DE	205/206 (99%)	0.34	6 (2%)	55 31	41, 82, 136, 159	0
40	BF	208/210 (99%)	0.31	13 (6%)	23 9	22, 63, 144, 195	0
40	DF	208/210 (99%)	0.26	7 (3%)	49 24	38, 90, 145, 184	0
41	BG	181/182 (99%)	1.05	29 (16%)	3 1	51, 103, 155, 182	0
41	DG	181/182 (99%)	1.36	54 (29%)	1 0	102, 141, 167, 183	0
42	BH	165/180 (91%)	0.64	16 (9%)	10 3	49, 86, 136, 174	0
42	DH	165/180 (91%)	2.06	69 (41%)	0 0	102, 139, 167, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BI	146/148 (98%)	1.82	51 (34%) 0 0	55, 147, 187, 200	0
43	DI	146/148 (98%)	1.71	48 (32%) 0 0	59, 139, 183, 200	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BN	139/140 (99%)	0.05	2 (1%) 78 60	36, 64, 118, 147	0
45	DN	139/140 (99%)	0.43	3 (2%) 65 42	69, 104, 136, 155	0
46	BO	122/122 (100%)	-0.10	0 100 100	33, 60, 94, 116	0
46	DO	122/122 (100%)	0.09	0 100 100	54, 83, 110, 141	0
47	BP	146/150 (97%)	0.55	5 (3%) 49 24	29, 74, 128, 189	0
47	DP	146/150 (97%)	0.72	11 (7%) 17 6	41, 98, 144, 173	0
48	BQ	141/141 (100%)	0.32	2 (1%) 78 60	38, 67, 109, 143	0
48	DQ	141/141 (100%)	0.86	15 (10%) 8 3	63, 113, 153, 178	0
49	BR	117/118 (99%)	0.12	0 100 100	36, 62, 103, 136	0
49	DR	117/118 (99%)	0.20	2 (1%) 73 52	42, 76, 118, 151	0
50	BS	99/112 (88%)	1.26	26 (26%) 1 0	52, 95, 141, 160	0
50	DS	99/112 (88%)	2.00	40 (40%) 0 0	101, 137, 163, 186	0
51	BT	136/146 (93%)	0.09	4 (2%) 55 31	47, 78, 140, 181	0
51	DT	136/146 (93%)	0.35	7 (5%) 32 13	58, 92, 151, 176	0
52	BU	117/118 (99%)	0.05	2 (1%) 73 52	27, 53, 102, 144	0
52	DU	117/118 (99%)	0.48	7 (5%) 25 10	46, 97, 137, 163	0
53	BV	101/101 (100%)	0.06	2 (1%) 68 46	24, 72, 124, 168	0
53	DV	101/101 (100%)	1.03	17 (16%) 2 1	53, 116, 146, 171	0
54	BW	113/113 (100%)	0.08	3 (2%) 58 34	28, 52, 105, 180	0
54	DW	113/113 (100%)	0.10	2 (1%) 71 50	49, 71, 119, 165	0
55	BX	93/96 (96%)	-0.13	0 100 100	29, 63, 100, 141	0
55	DX	93/96 (96%)	0.19	2 (2%) 65 42	55, 83, 115, 138	0
56	BY	101/110 (91%)	0.38	6 (5%) 26 11	47, 89, 131, 157	0
56	DY	101/110 (91%)	1.08	20 (19%) 1 0	60, 106, 149, 164	0
57	BZ	185/206 (89%)	1.64	56 (30%) 1 0	51, 113, 163, 188	0
57	DZ	185/206 (89%)	1.81	65 (35%) 0 0	99, 144, 171, 189	0
All	All	21266/22572 (94%)	0.77	2703 (12%) 5 2	20, 98, 177, 200	0

The worst 5 of 2703 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	BI	88	ILE	22.7
37	BC	171	ALA	19.8
35	BA	277	C	19.1
34	D9	34	GLN	17.7
48	DQ	141	GLN	16.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
22	AG9	AY	36	28/29	0.88	0.34	1.83	43,59,79,79	0
22	AG9	CY	36	28/29	0.75	0.51	1.44	33,49,70,70	0
22	AG9	CV	36	28/29	0.81	0.42	0.75	33,49,70,70	0
22	AG9	AV	36	28/29	0.90	0.26	-0.17	43,59,79,79	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
58	ZN	CD	1000	1/1	0.95	0.29	-0.26	200,200,200,200	0
58	ZN	AD	1000	1/1	0.84	0.25	-0.95	165,165,165,165	0
58	ZN	AN	1000	1/1	0.95	0.08	-1.47	88,88,88,88	0
58	ZN	CN	1000	1/1	0.84	0.07	-1.60	178,178,178,178	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.