



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2019 – 04:11 PM EDT

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

<https://www.wwpdb.org/validation/2017/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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

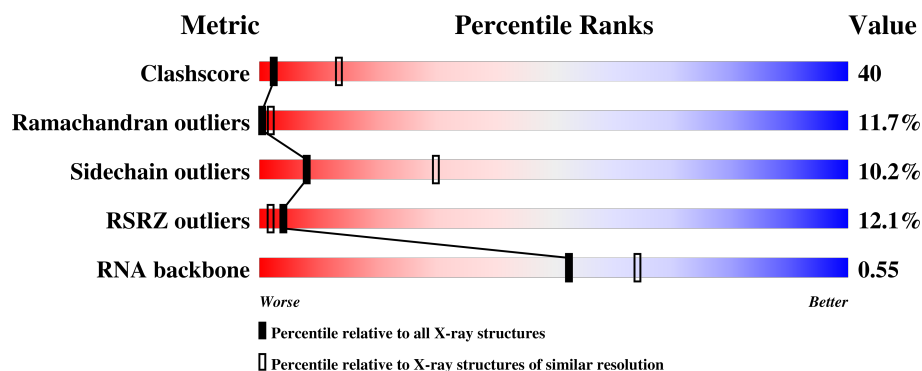
# 1 Overall quality at a glance ⓘ

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	122126	1042 (3.10-3.10)
Ramachandran outliers	120053	1010 (3.10-3.10)
Sidechain outliers	120020	1010 (3.10-3.10)
RSRZ outliers	108989	1089 (3.12-3.08)
RNA backbone	2636	1015 (3.44-2.76)

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>6%</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>12%</div> <div>21%</div> <div>59%</div> <div>12%</div> <div>8%</div> </div>
2	CB	256	<div> <div>21%</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	

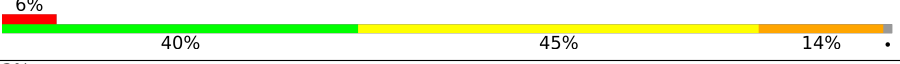

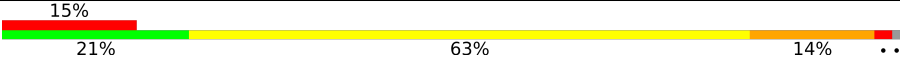
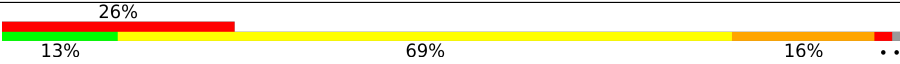
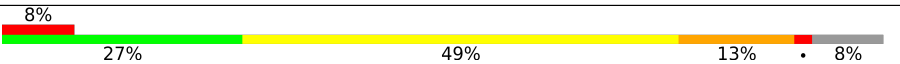
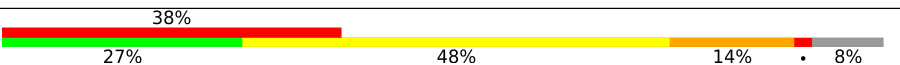
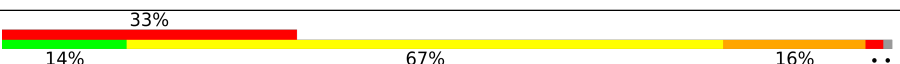
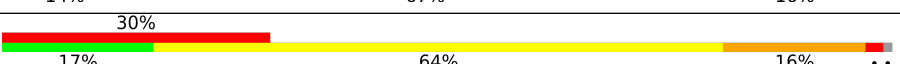
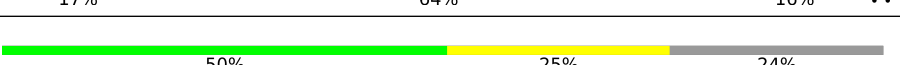
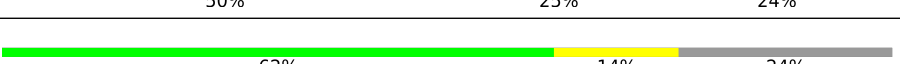
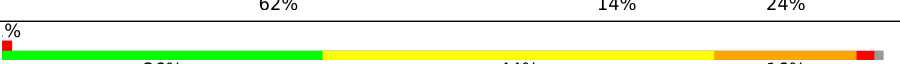
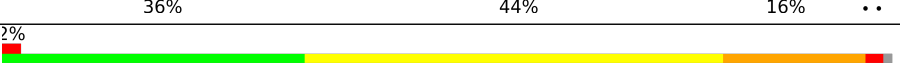
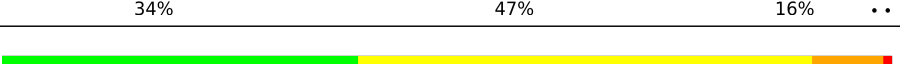
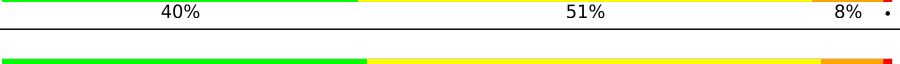


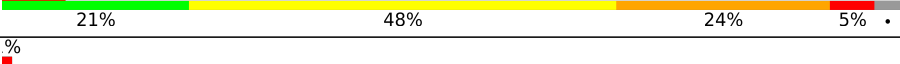
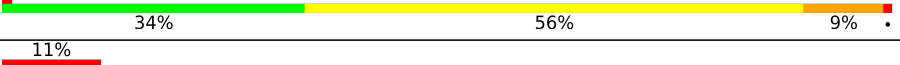

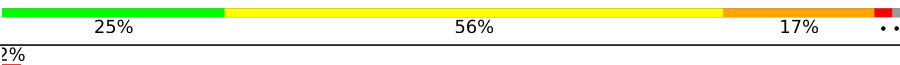
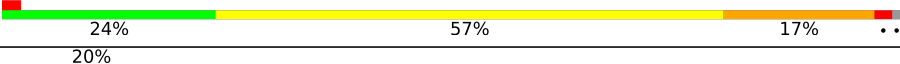
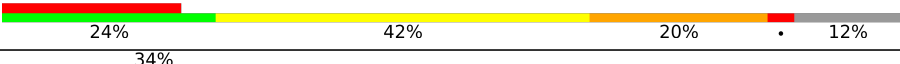


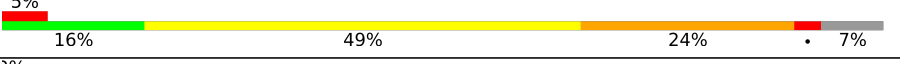
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Mol	Chain	Length	Quality of chain
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2915	
35	DA	2915	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
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	-
22	AG9	CY	36	X	-	-	X
58	ZN	AD	1000	-	-	X	-
58	ZN	AN	1000	-	-	X	-
58	ZN	CD	1000	-	-	X	-
58	ZN	CN	1000	-	-	X	-

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 298096 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE.

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

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

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

- Molecule 24 is a RNA chain called MRNA.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			734	460	148	125	1			
26	D1	94	Total	C	N	O	S	0	0	1
			734	460	148	125	1			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	56	Total	C	N	O	S	0	0	1
			428	267	87	69	5			
30	D5	56	Total	C	N	O	S	0	0	1
			428	267	87	69	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
31	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	48	Total	C	N	O	S	0	0	1
			410	251	103	54	2			
32	D7	48	Total	C	N	O	S	0	0	1
			410	251	103	54	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			
35	DA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			
37	DC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

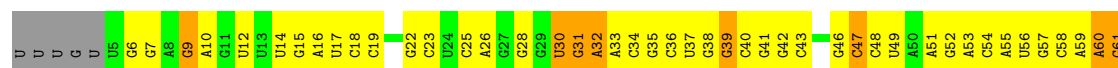
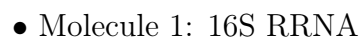
- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

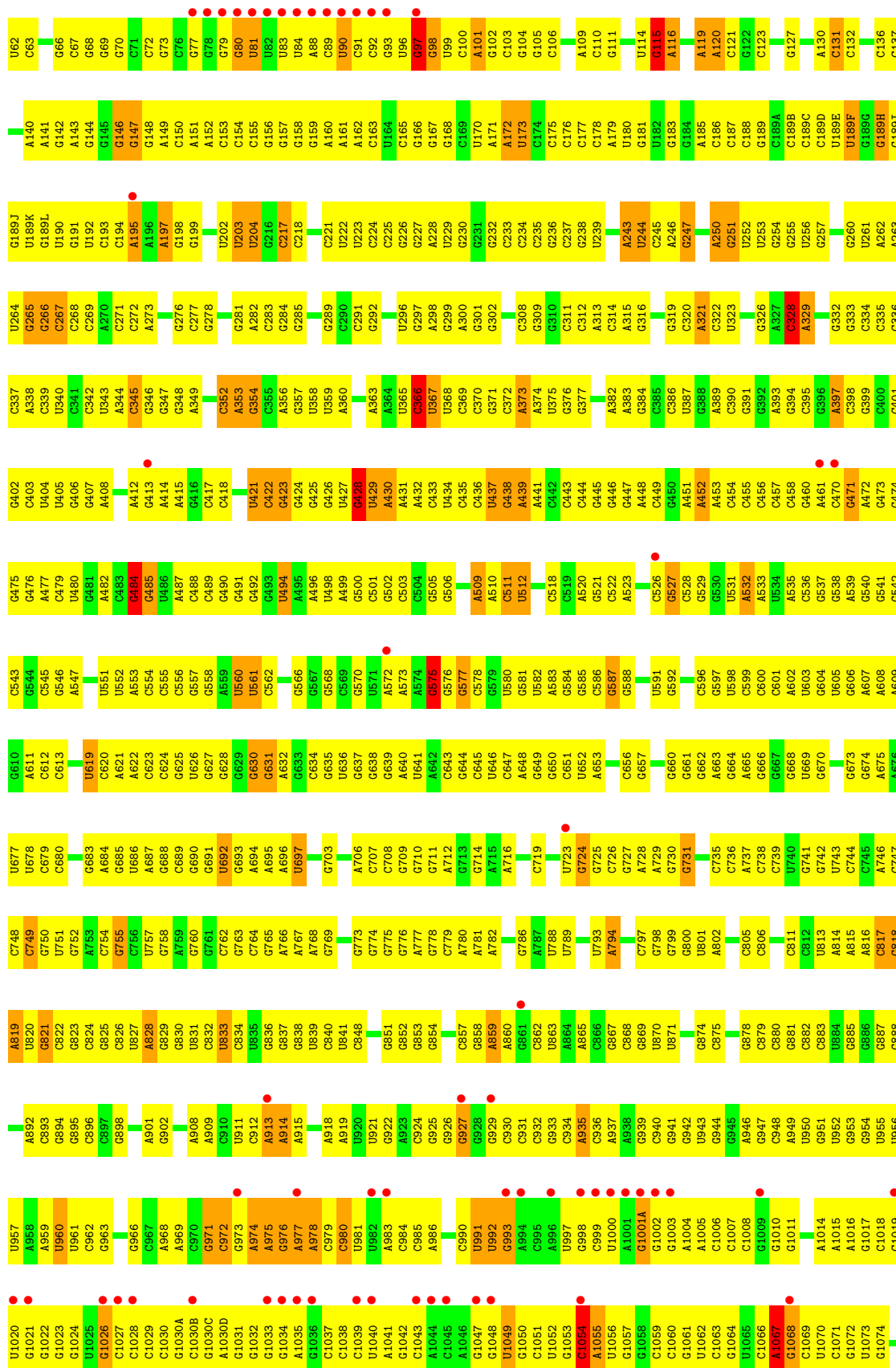
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			
57	DZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			

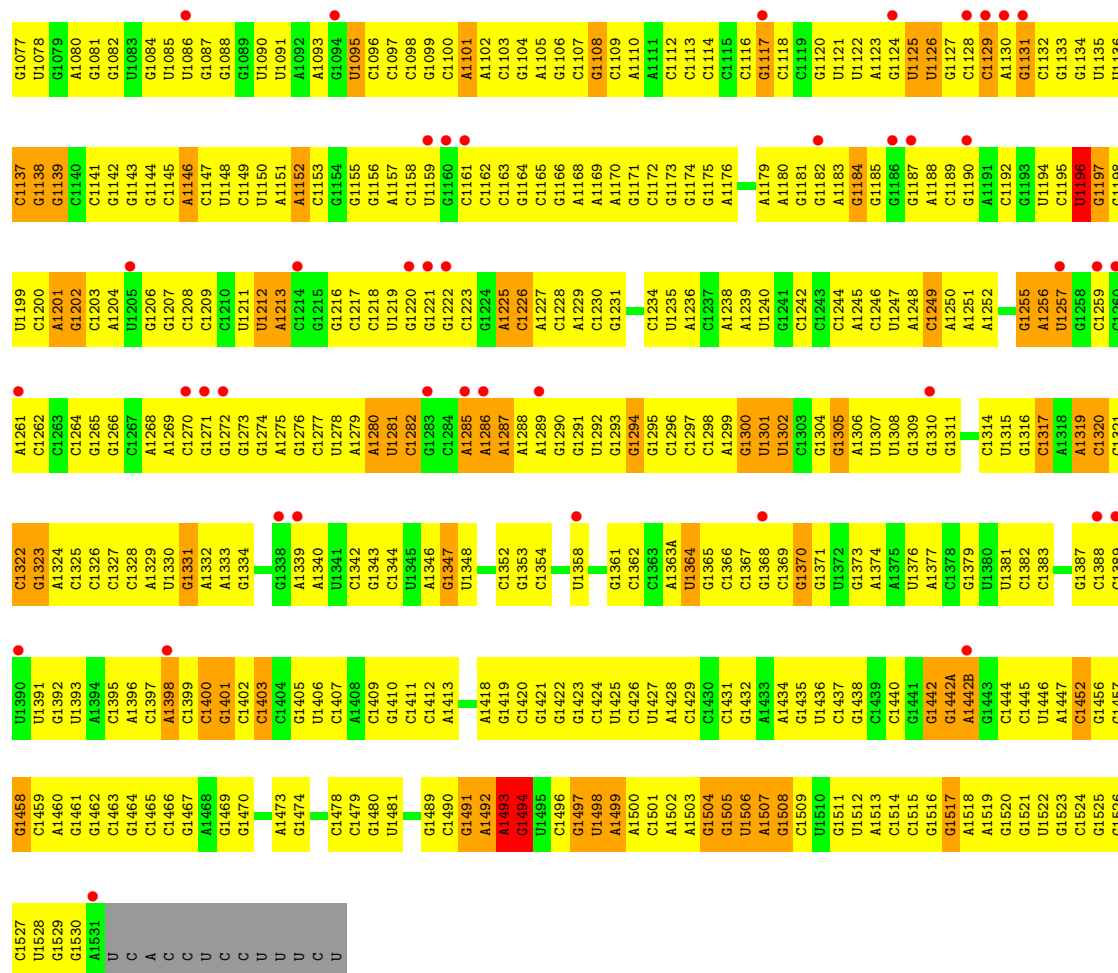
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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		



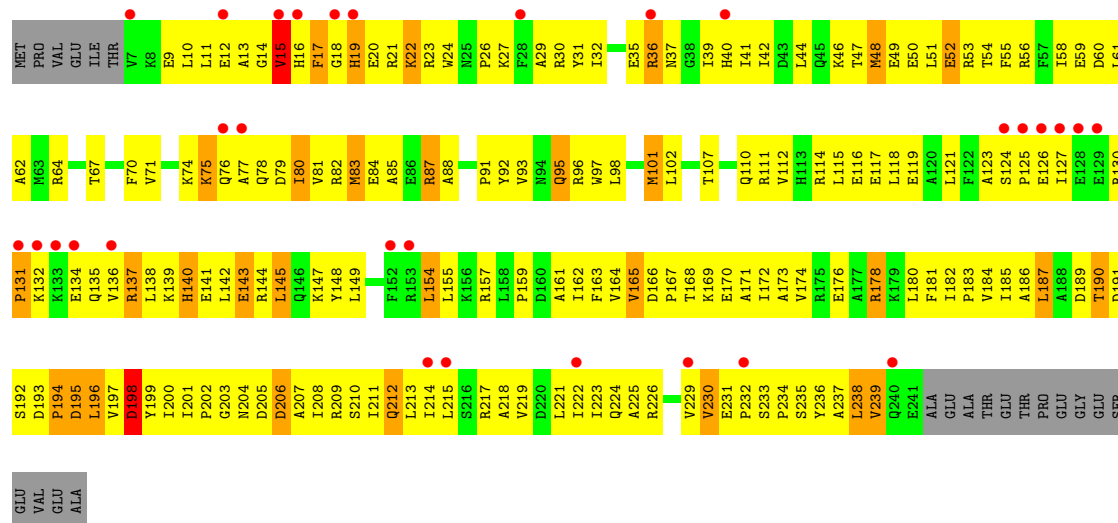




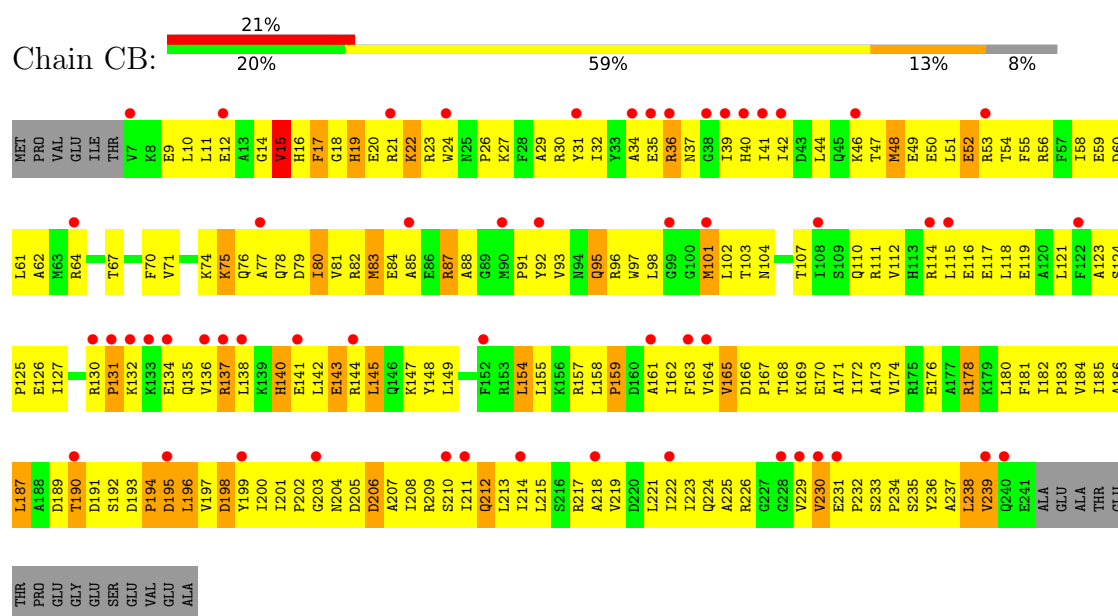


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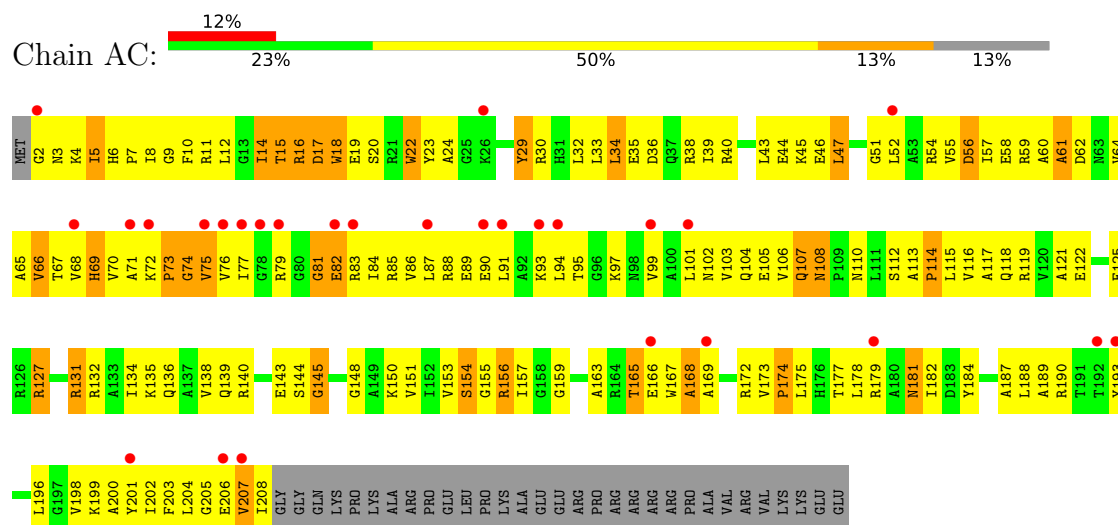
Chain AB: 12% 21% 59% 12% 8%



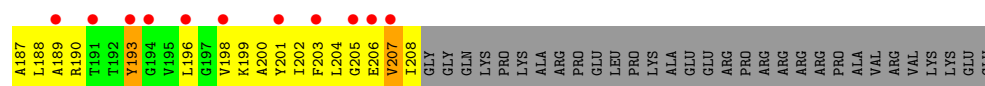
### • Molecule 2: 30S RIBOSOMAL PROTEIN S2



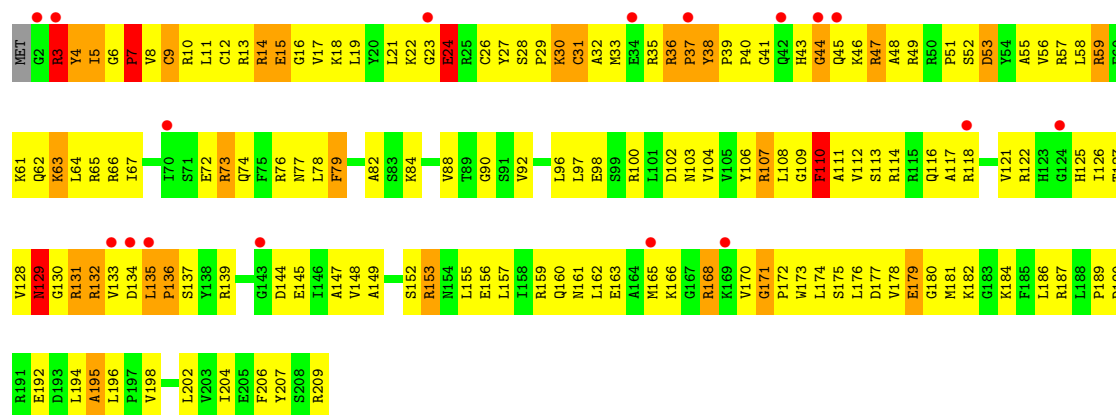
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



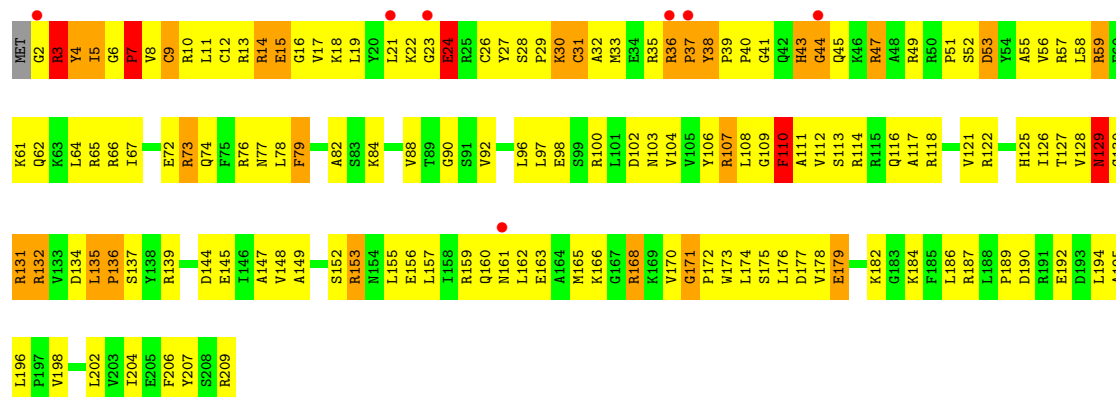




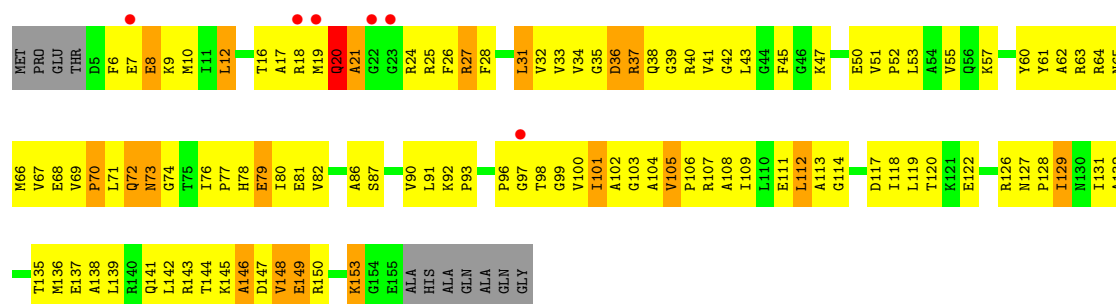
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



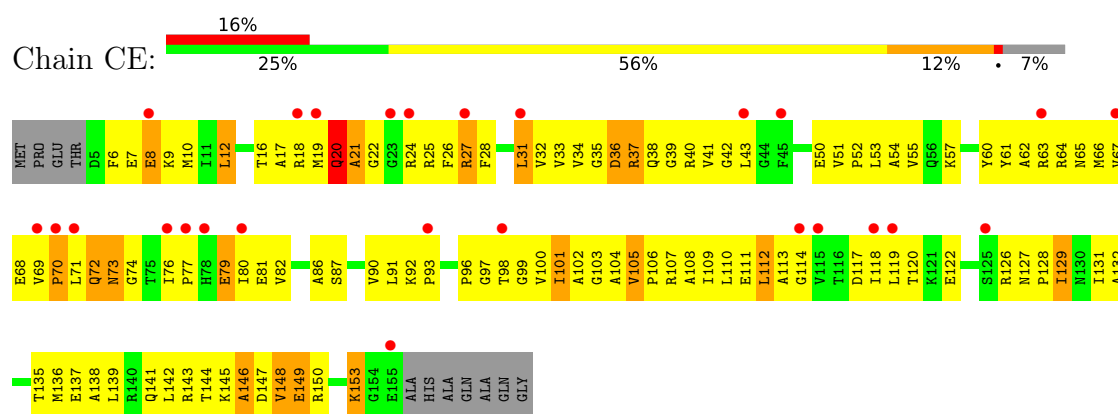
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

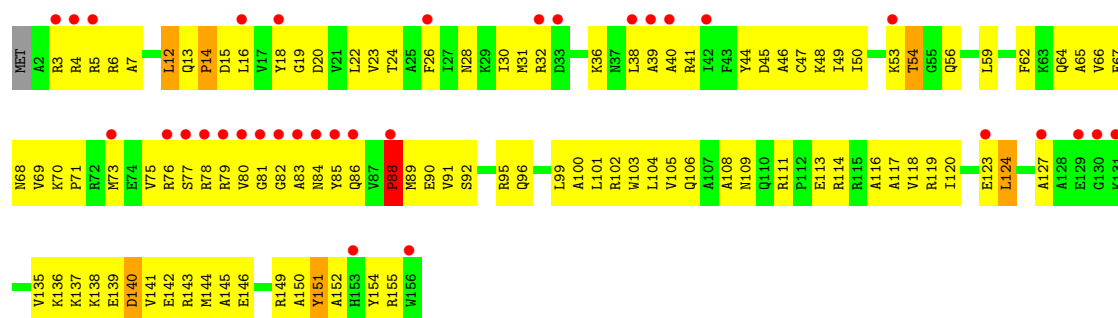


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

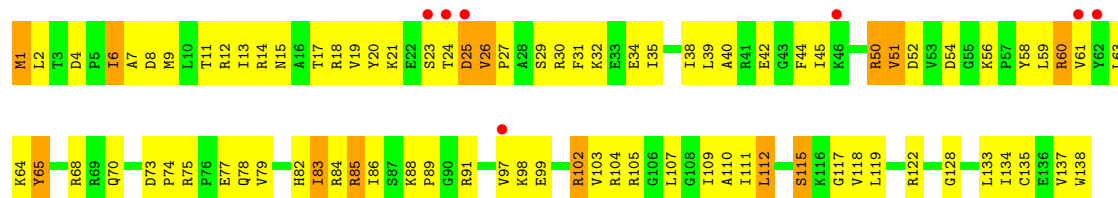


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

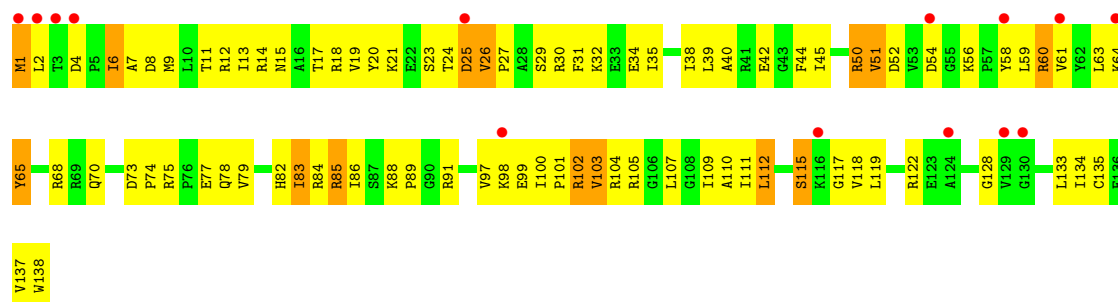




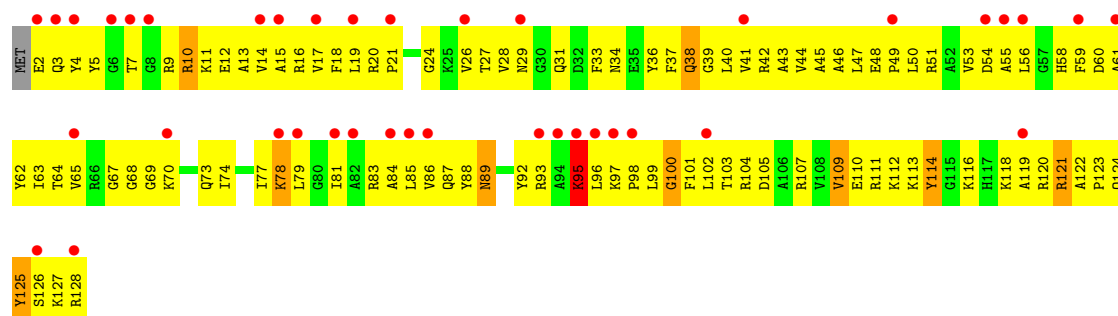
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

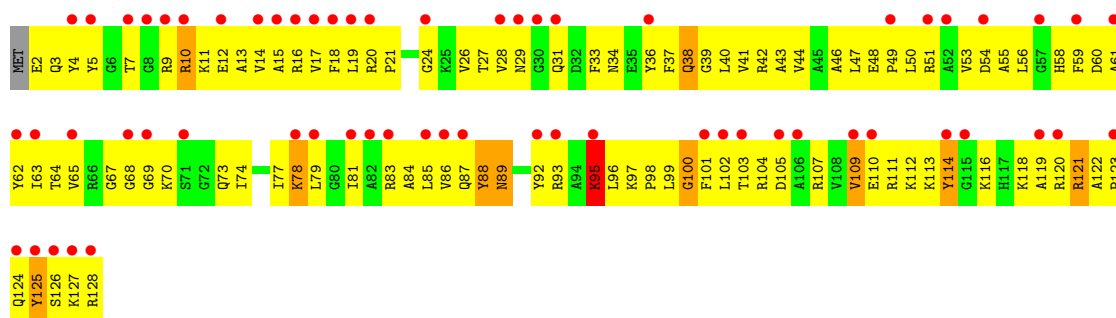


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

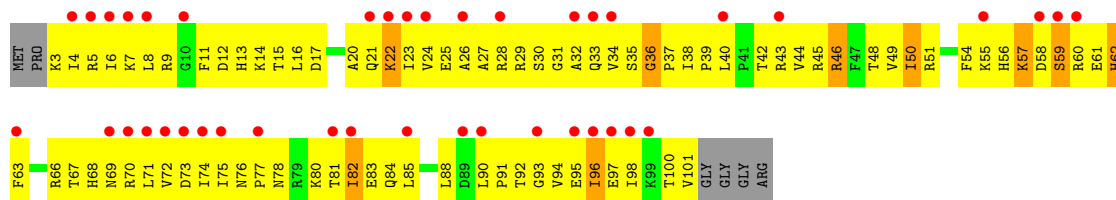


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

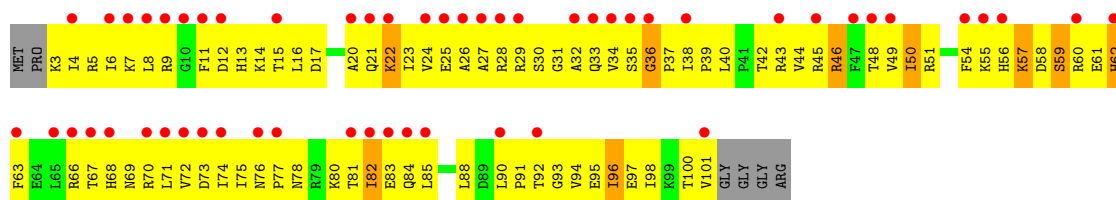




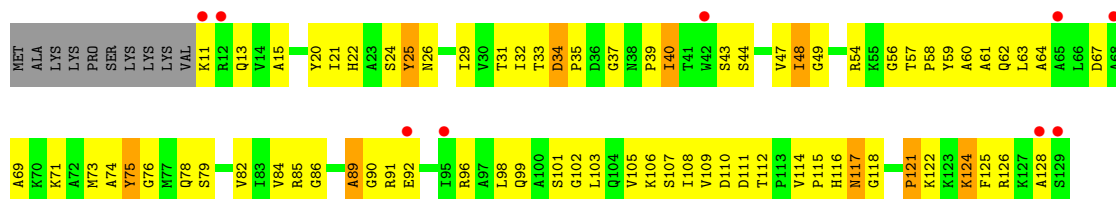
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



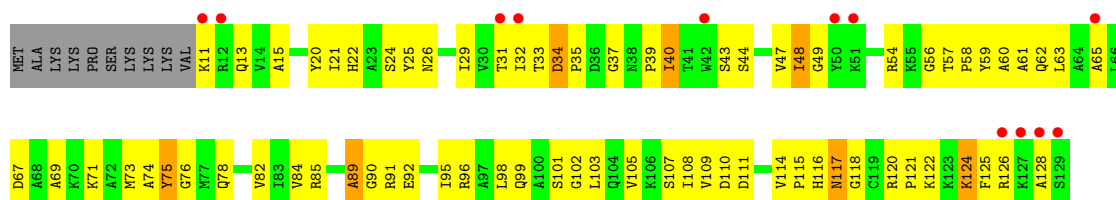
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



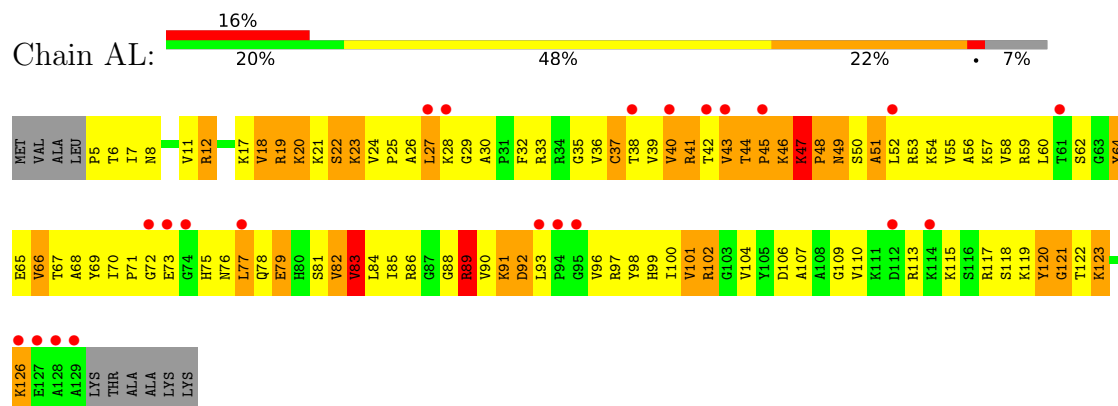
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



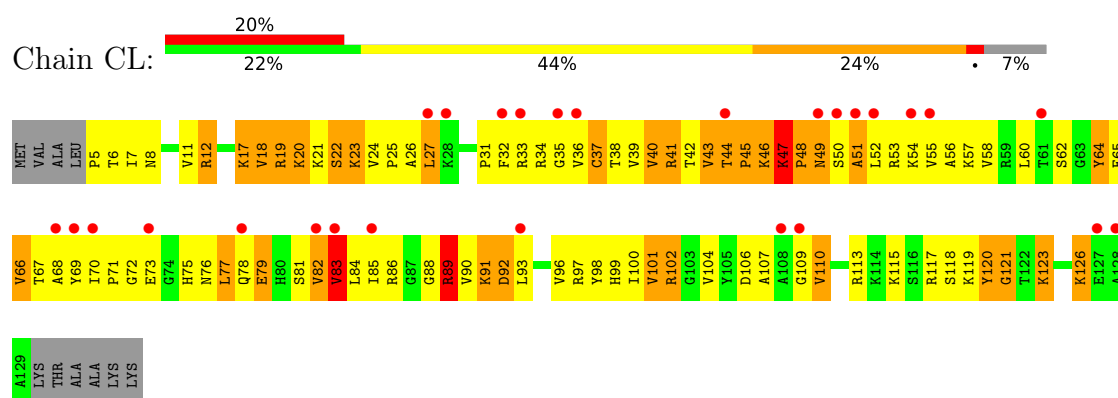
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



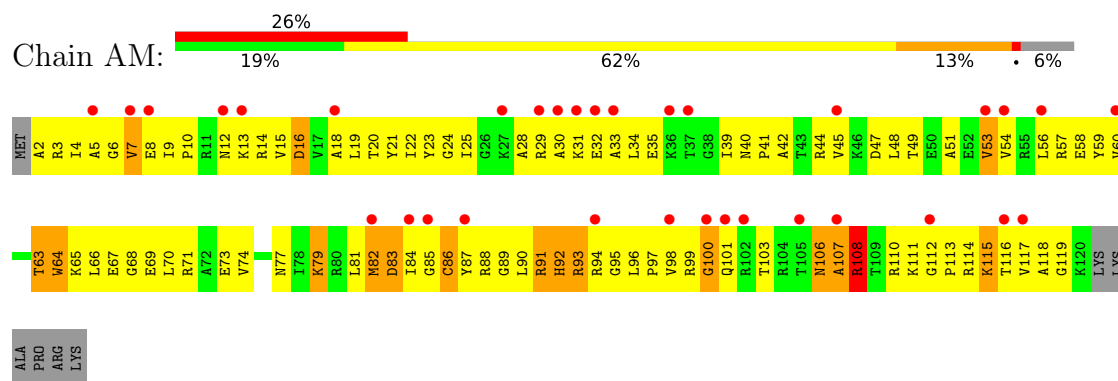
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



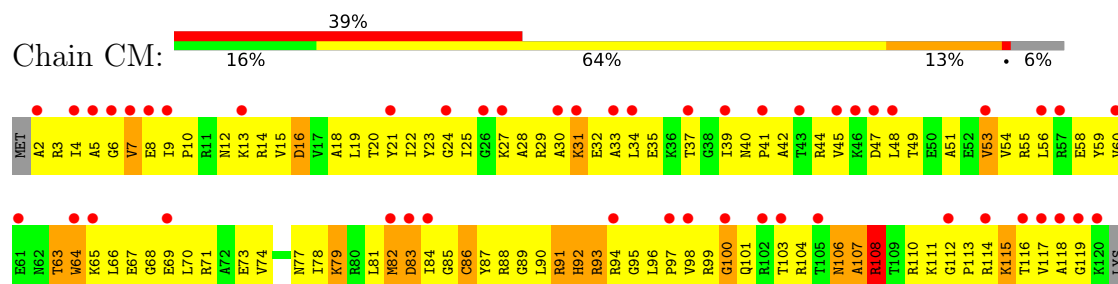
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

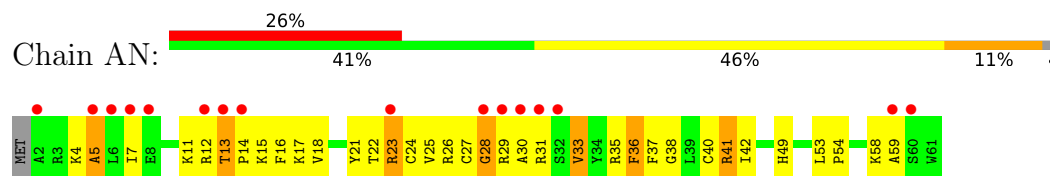


- Molecule 13: 30S RIBOSOMAL PROTEIN S13

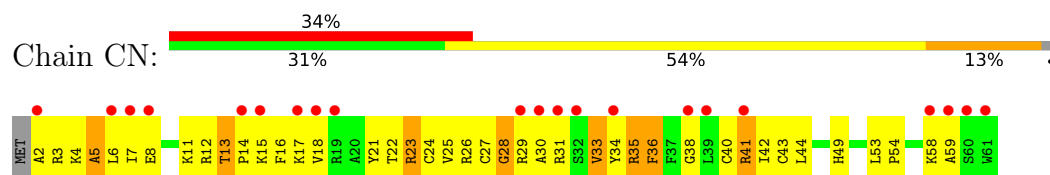


LYS  
ALA  
PRO  
ARG  
LYS

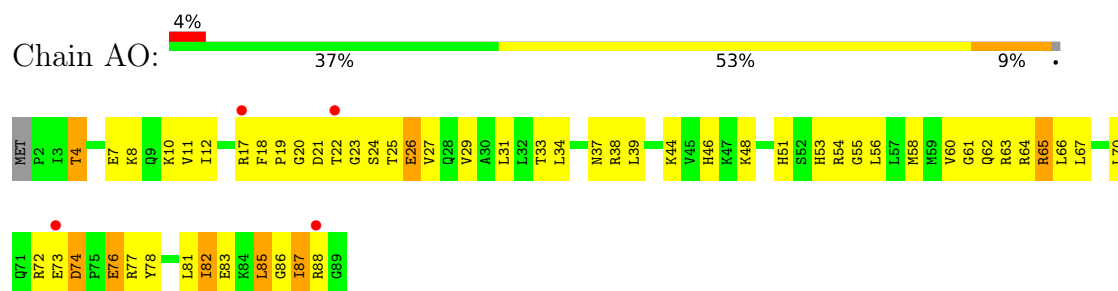
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



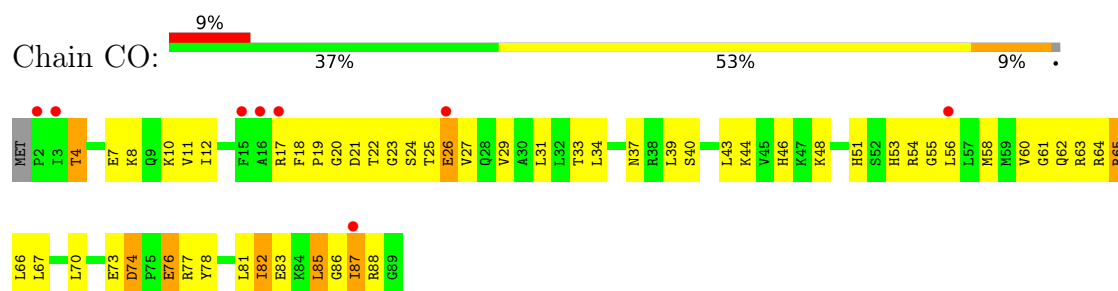
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



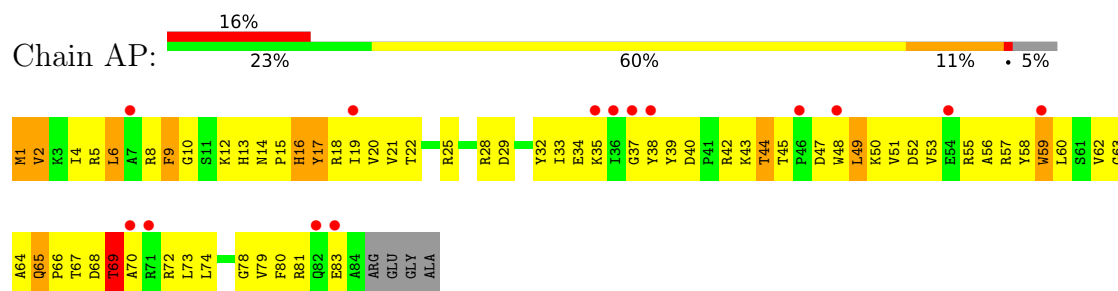
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

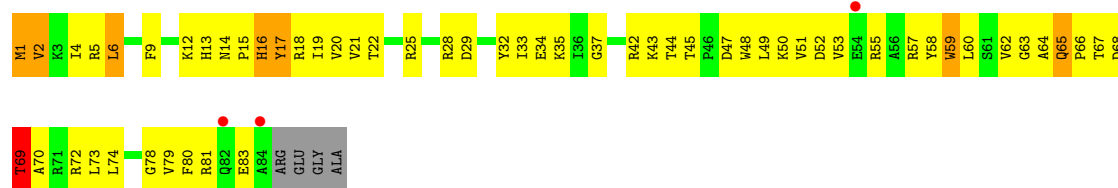


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

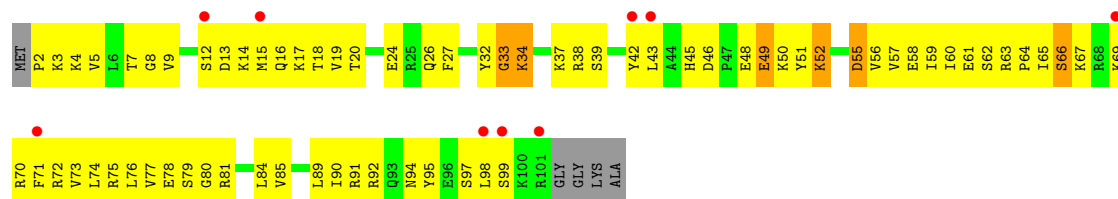


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

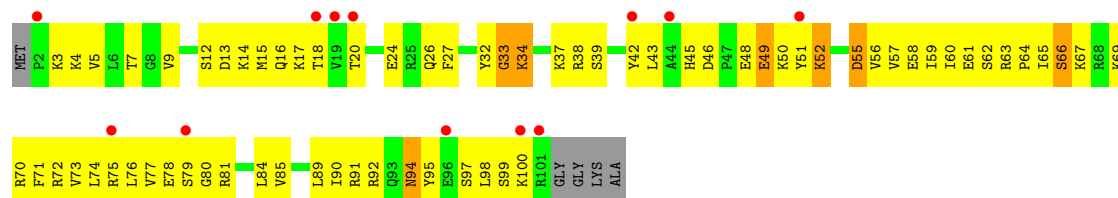




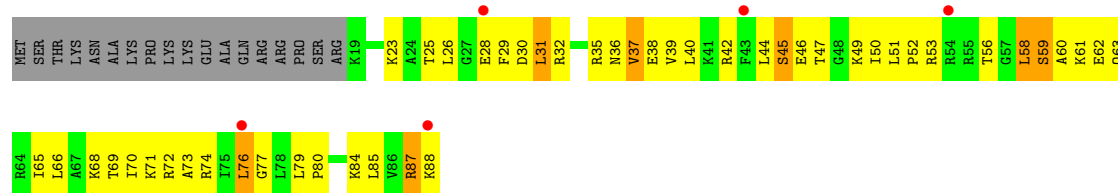
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



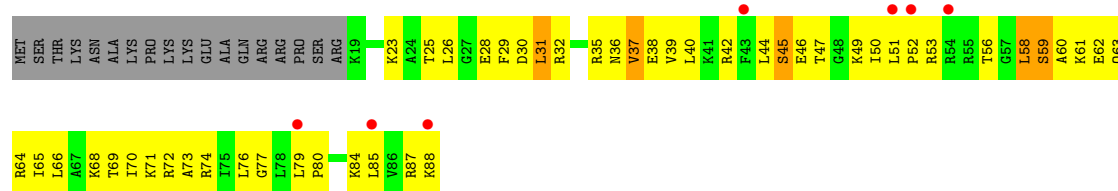
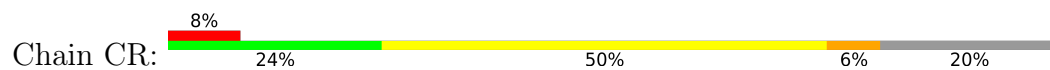
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



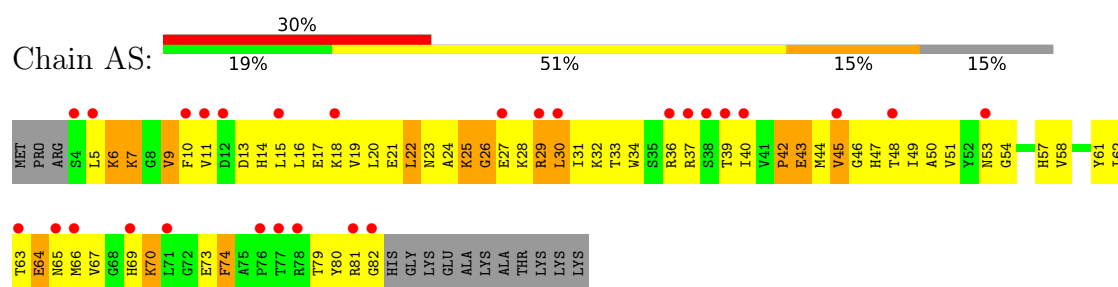
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



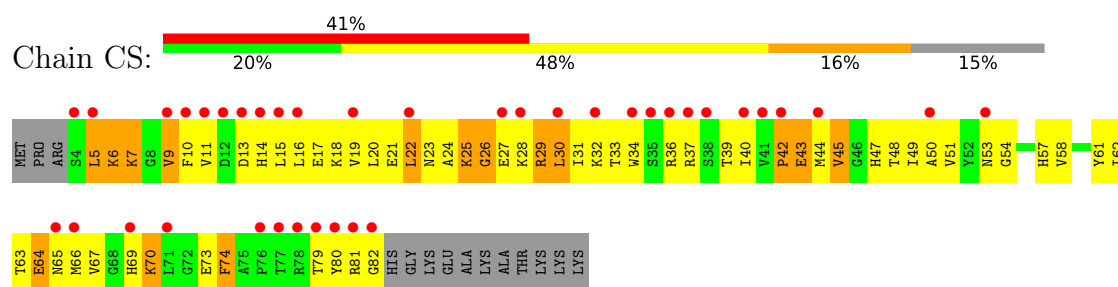
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



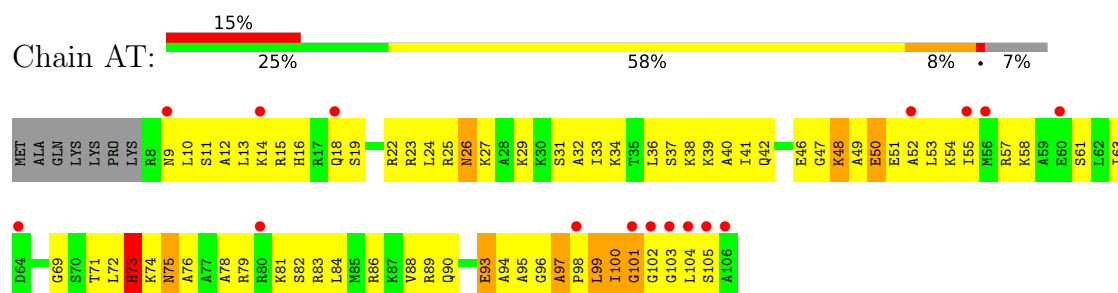
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



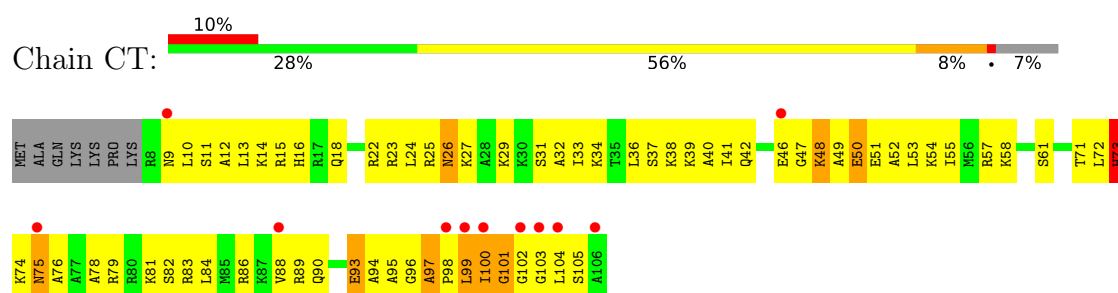
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



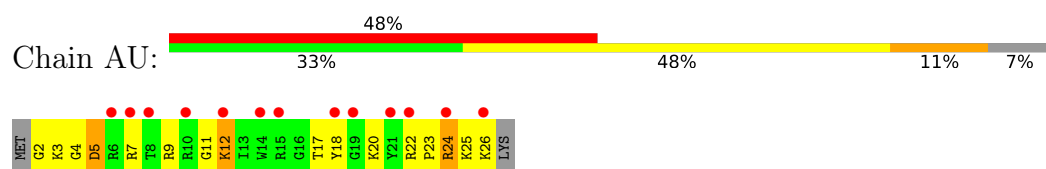
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



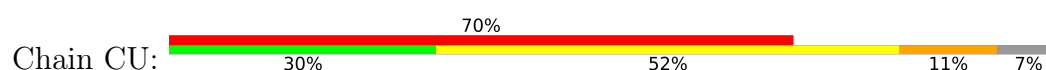
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



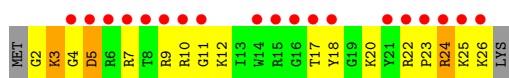
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



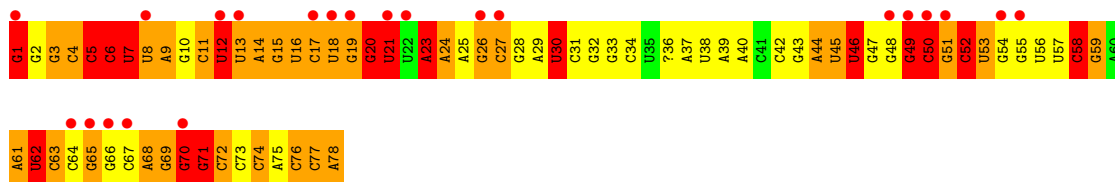
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



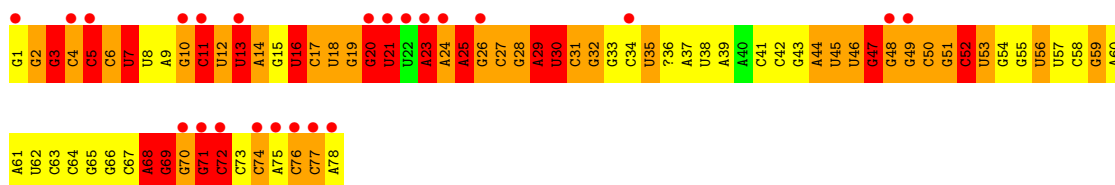




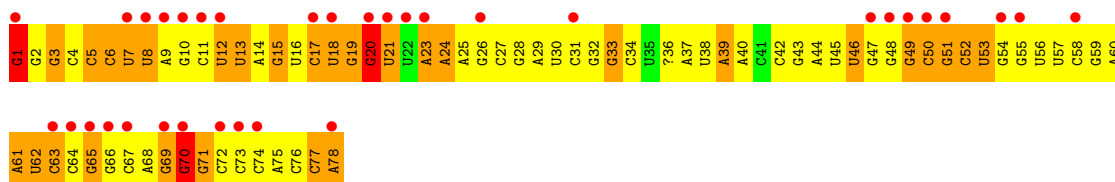
- Molecule 22: E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE



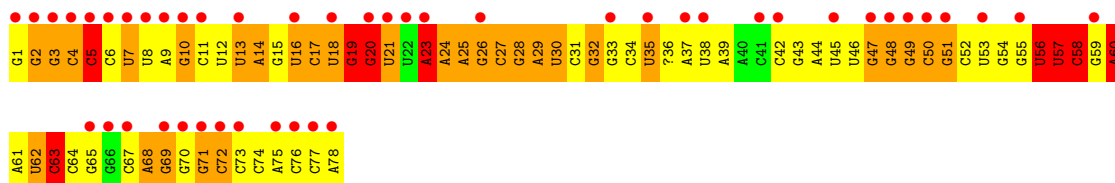
- Molecule 22: E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE



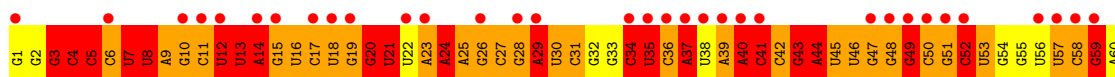
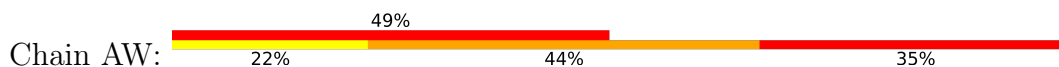
- Molecule 22: E-SITE TRNA ILE2 AGMATIDINE OR P-SITE TRNA ILE2 AGMATIDINE



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

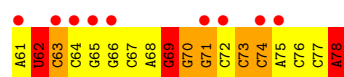
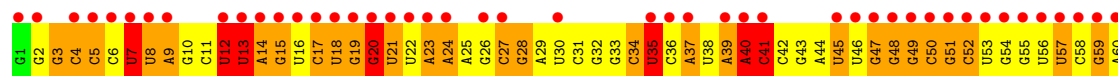
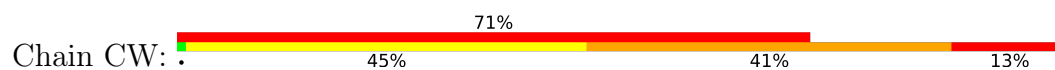


- Molecule 23: A-SITE TRNA ILE2 AGMATIDINE

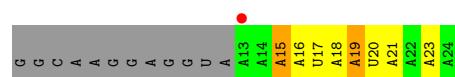




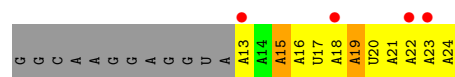
● Molecule 23: A-SITE TRNA ILE2 AGMATIDINE



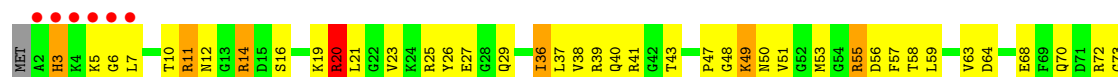
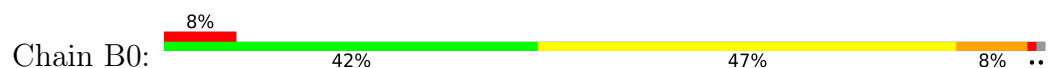
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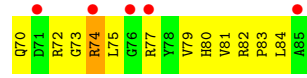
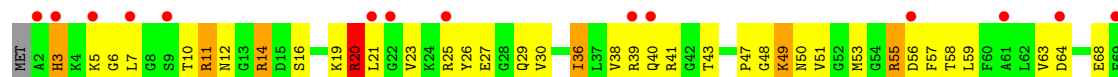
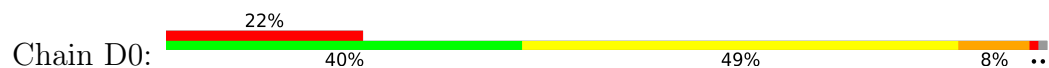
● Molecule 24: MRNA



● Molecule 25: 50S RIBOSOMAL PROTEIN L27

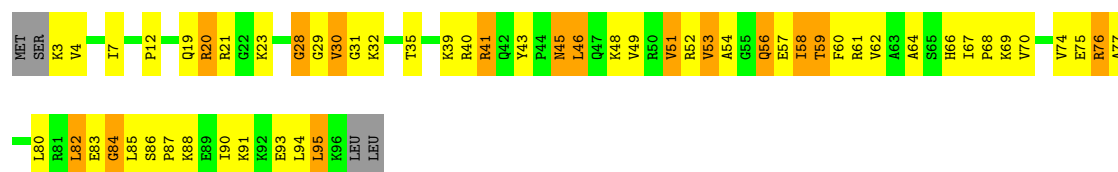


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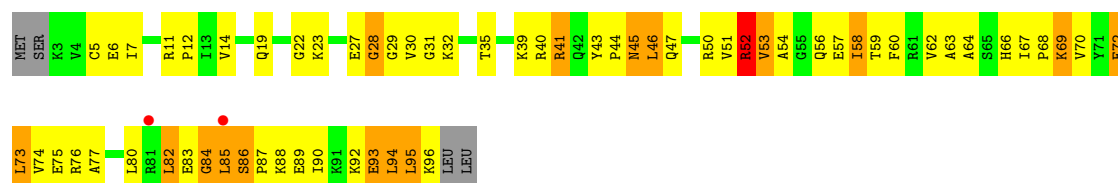


● Molecule 26: 50S RIBOSOMAL PROTEIN L28

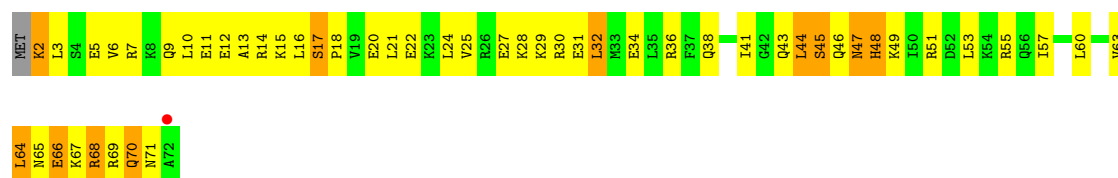




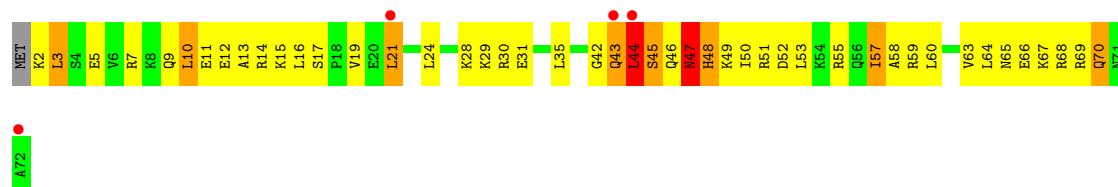
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



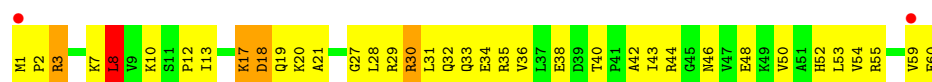
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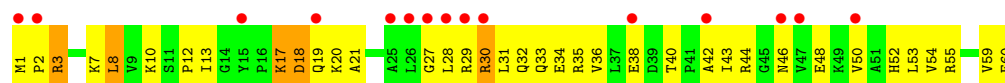
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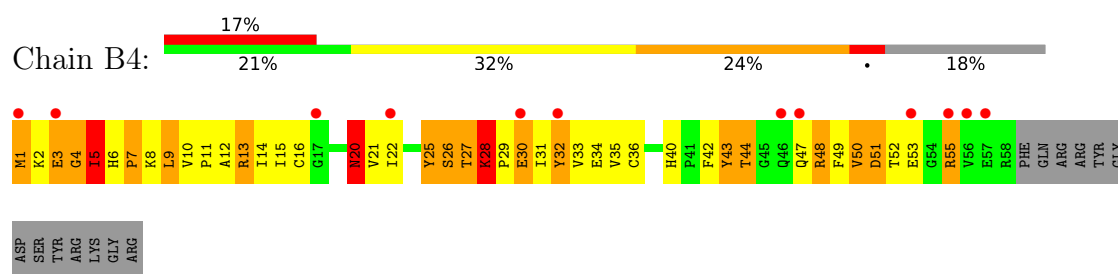
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



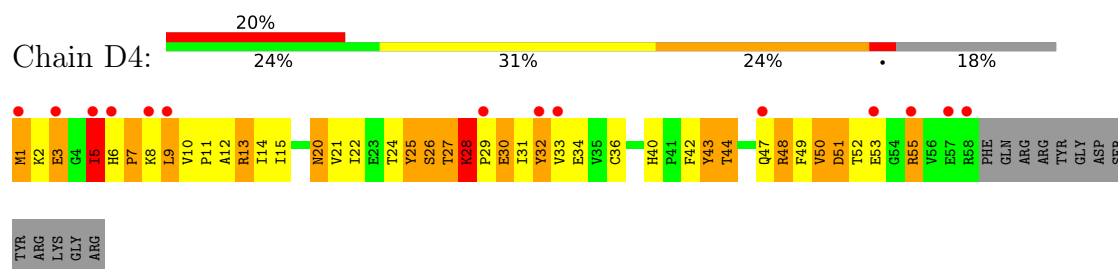
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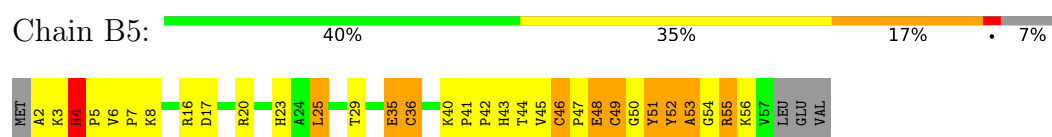
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



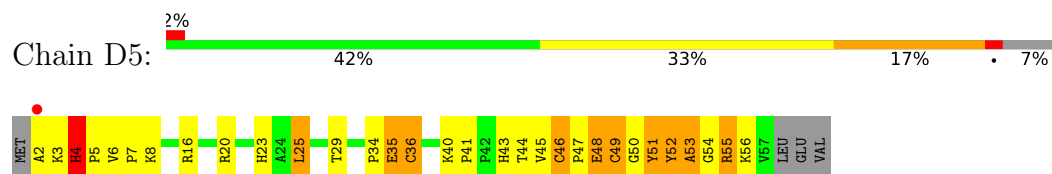
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



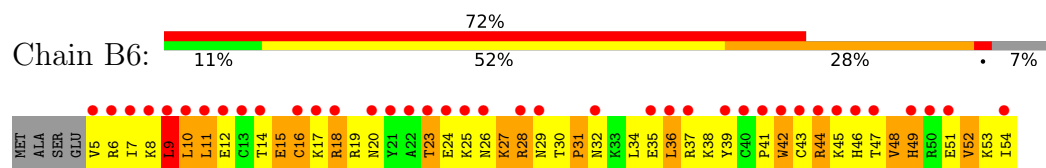
- Molecule 30: 50S RIBOSOMAL PROTEIN L32



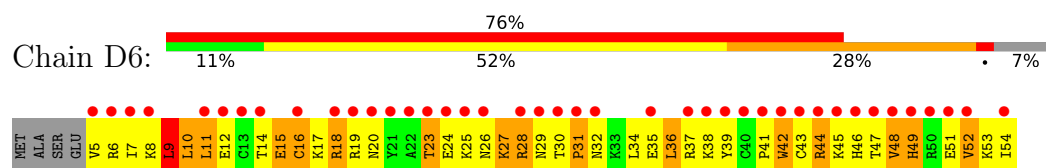
- Molecule 30: 50S RIBOSOMAL PROTEIN L32



- Molecule 31: 50S RIBOSOMAL PROTEIN L33



- Molecule 31: 50S RIBOSOMAL PROTEIN L33

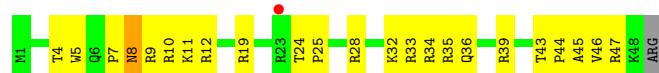


- Molecule 32: 50S RIBOSOMAL PROTEIN L34

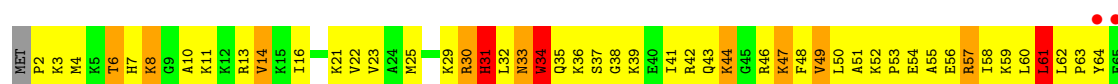




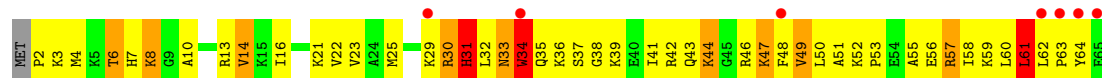
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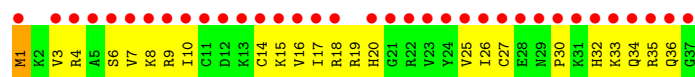
• Molecule 33: 50S RIBOSOMAL PROTEIN L35



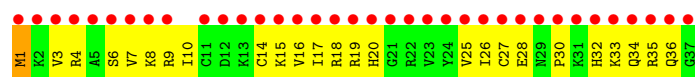
• Molecule 33: 50S RIBOSOMAL PROTEIN L35



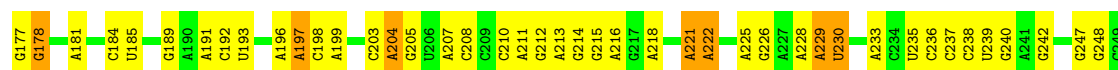
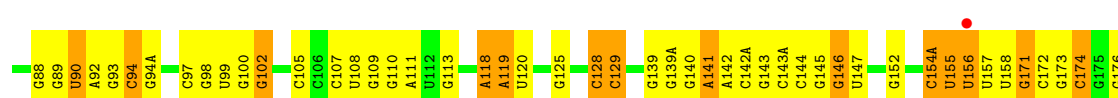
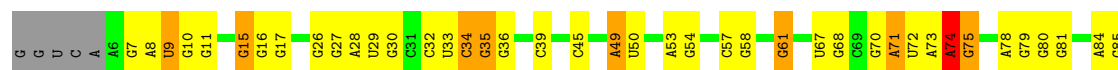
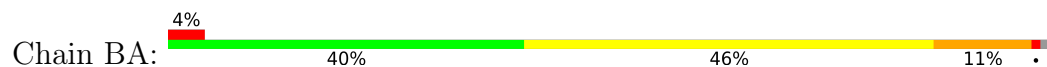
• Molecule 34: 50S RIBOSOMAL PROTEIN L36

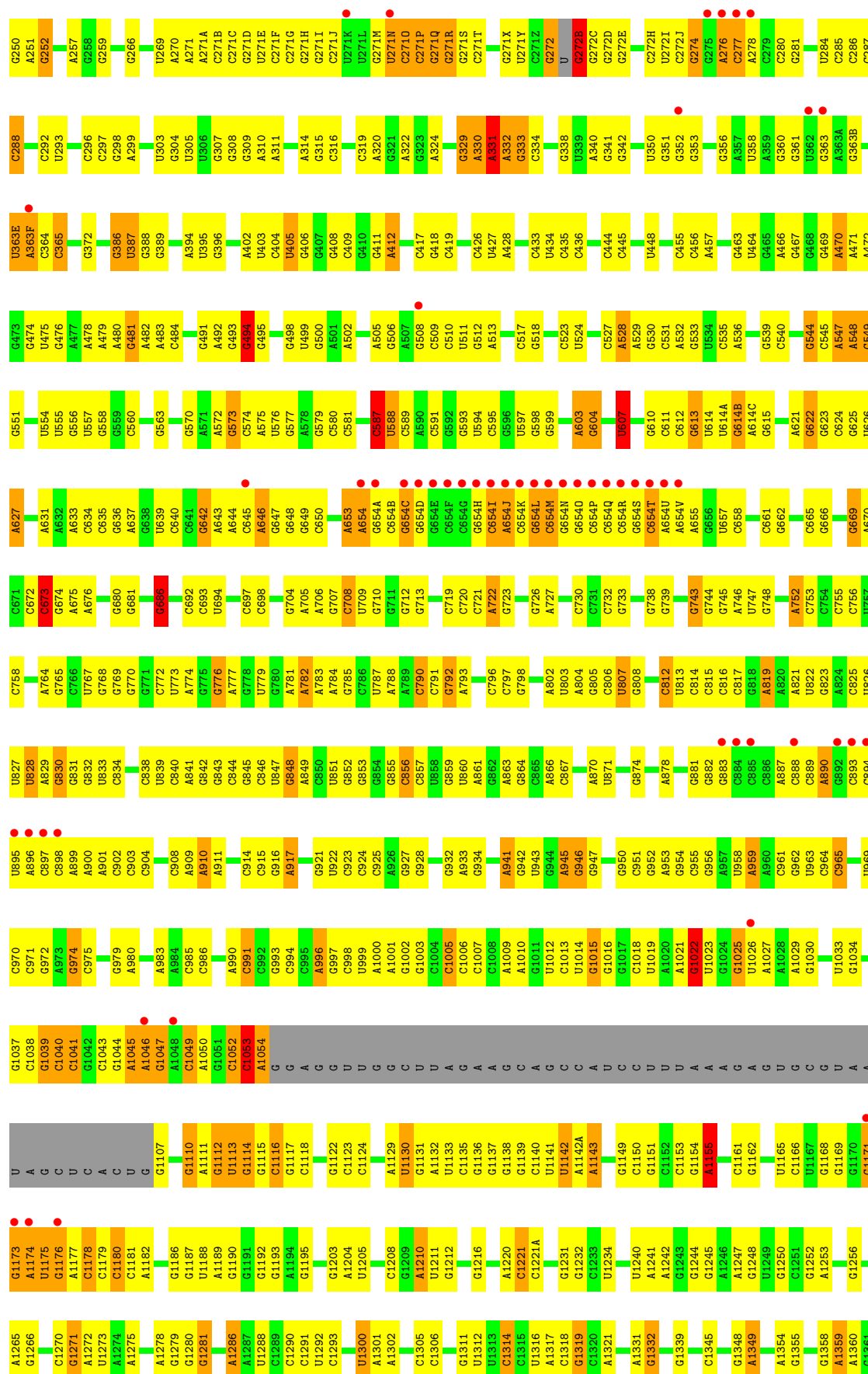


• Molecule 34: 50S RIBOSOMAL PROTEIN L36

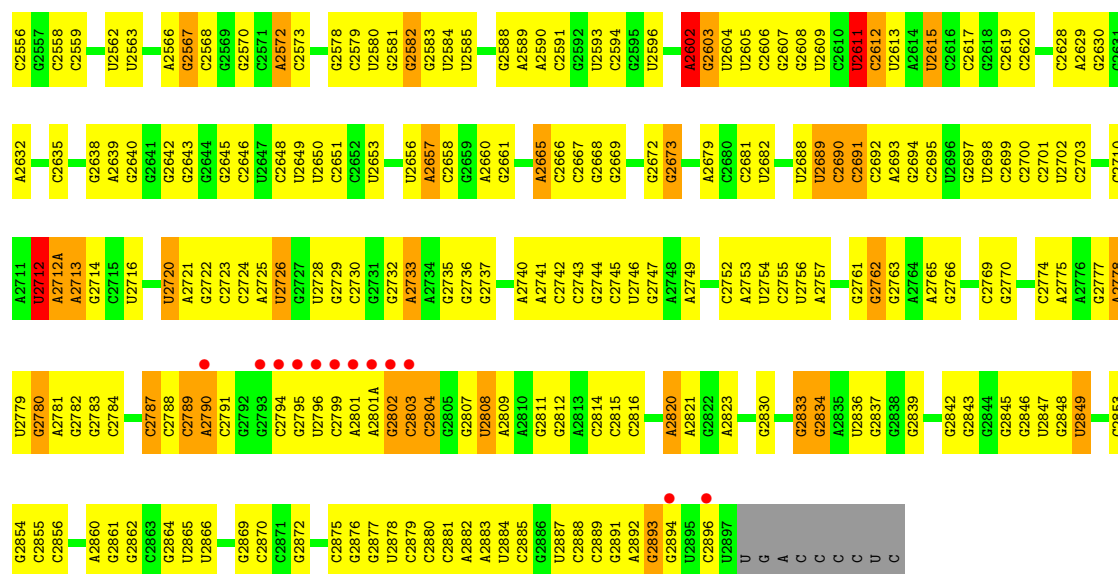


• Molecule 35: 23S RIBOSOMAL RNA

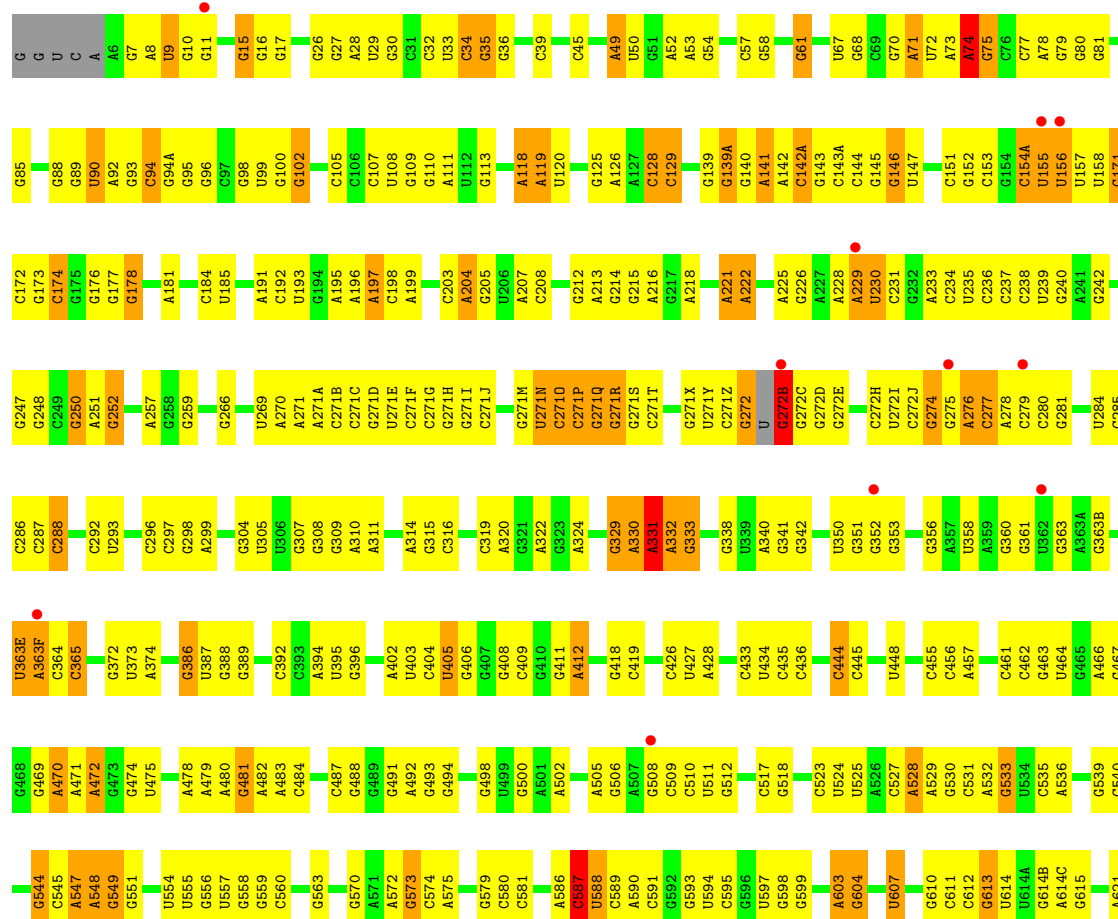








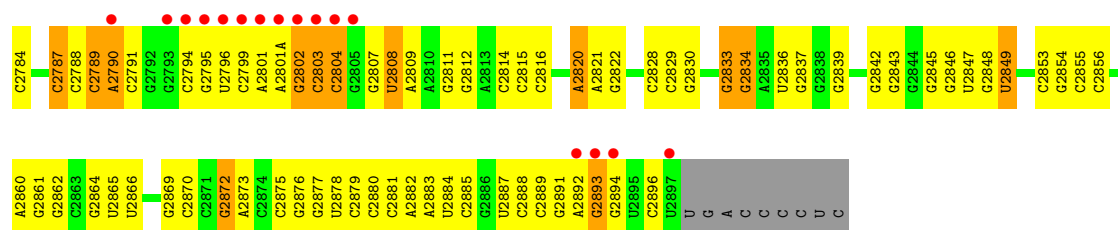
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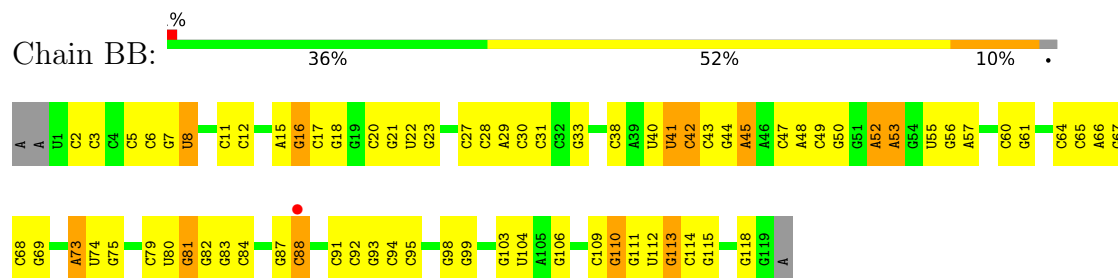


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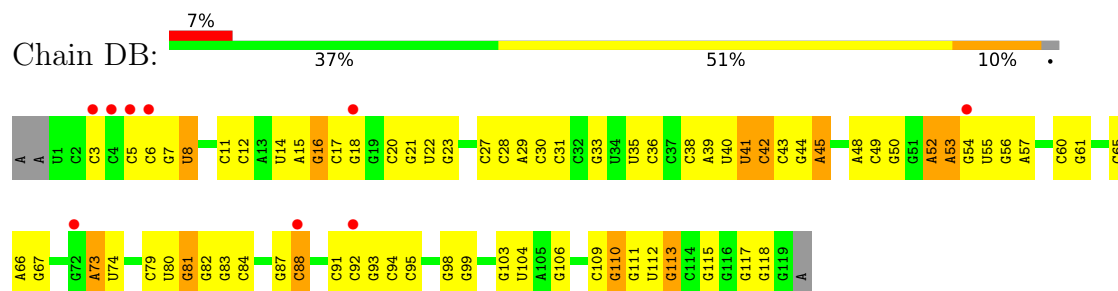
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C2689	U2604	G2526	G2455	A2377	U2232	C2161	G2107	U2028	G1947	A1773	
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C2692	C2606	U2528	G2459	G2381	G2234	C2163	G2103	G2029	G1948	U1859	U1775
A2693		G2529	A2459	C2382	G2235	C2164	G2104	A2030	G1948	G1860	G1776
G2694	U2609	A2530	U2462	G2383	C2236	G2165	C2105	A2031	U1951	G1861	
G2697	C2610	A2531	C2463	G2384	G2237	G2166	G2106	G2032	A1952	G1862	U1779
A2765	U2611	A2534	C2464	A2385	U2238	U2167	C2107	A2033	A1953	G1863	A1780
G2766	U2613	G2535	C2465	C2386	G2239	G2168	C2108	U2034	G1954	U1864	
C2767	A2614	G2536	C2466	G2389	A2311	A2169	U2109	G2035	U1955	G1865	A1784
C2701	U2615	U2537	C2467	U2390	G2312	A2170	C2110	C2036		C1866	A1785
U2702	C2616	C2538	G2468	G2391	U2243	A2171	C2111		G1958	A1876	A1786
C2703	C2617	U2539	A2469	G2392	U2244	U2172	G2112	U2041	C1962	A1877	
C2704		G2539	G2470	A2393	U2245	A2173	U2113	A2114	U1963	G1878	A1789
A2705	C2628	A2542	C2471	C2394	G2246	C2174	G2114	C2042	G1964	C1879	C1790
C2772	G2629	G2543	G2472	C2397	U2248	C2175	G2115	C2043	C1965	C1880	A1791
C2773	U2630	G2544	U2473	G2397	U2249	A2176	G2116		C1966	C1881	
A2775	A2631	G2544	U2474	G2397	U2250	C2177	U2117	C2050	A1966	G1882	U1794
U2776	U2552	G2544	C2475	G2400	G2251	C2178	A2118	A2051	G1967	G1883	C1795
G2777	A2632	G2553	A2476	U2401	U2257	C2179	G2119	G2052	G1968	A1884	U1796
A2778	C2635	U2554	C2477	C2402	C2258	U2180	G2120	G2053	A1969	A1885	C1797
U2779	U2555	A2478	A2478	G2405	G2261	G2181	G2121	A2054	G1970	C1886	U1798
G2780	G2638	C2556	G2481	U2406	C2262	G2182	U2122	C2055	A1971	C1887	G1899
A2781	U2639	G2557	G2482	G2483	U2263	C2183	G2123	G2056	A1972	G1888	C1800
G2782	C2640	G2558	G2483	A2411	C2185	G2184	G2124	A2059	G1980	A1889	A1802
G2783		C2559	C2483		G2186		A2126	A2060	A1981	U1998	A1803



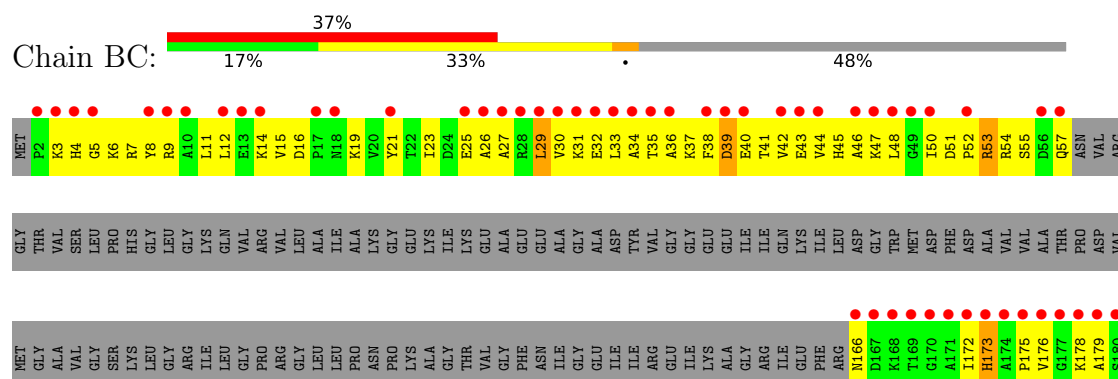
• Molecule 36: 5S RIBOSOMAL RNA



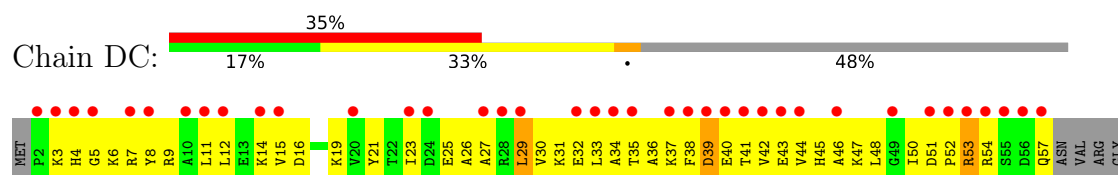
• Molecule 36: 5S RIBOSOMAL RNA

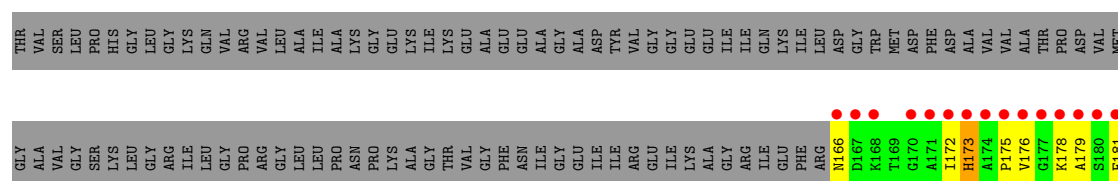


• Molecule 37: 50S RIBOSOMAL PROTEIN L1

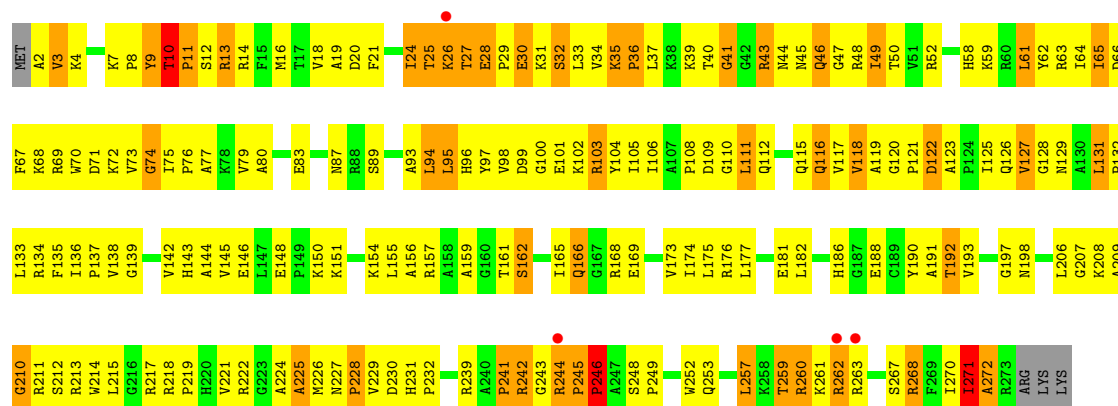


• Molecule 37: 50S RIBOSOMAL PROTEIN L1

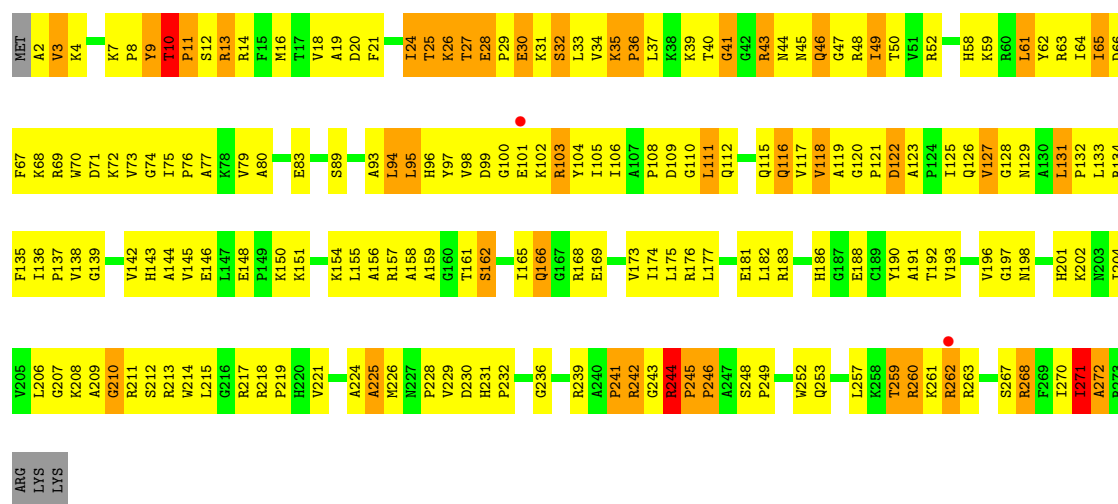




### • Molecule 38: 50S RIBOSOMAL PROTEIN L2

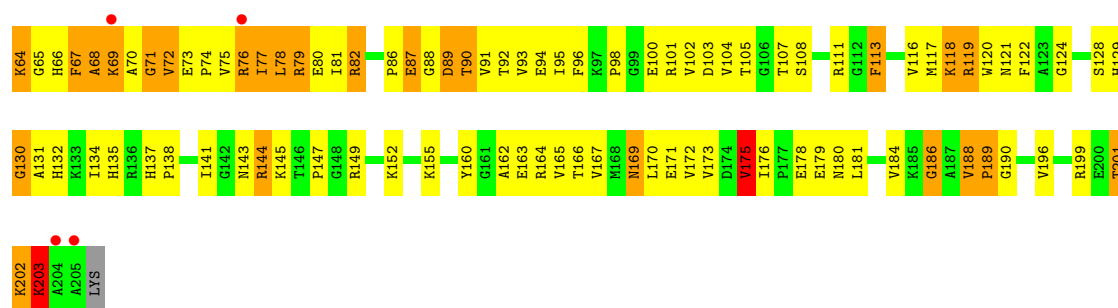


### • Molecule 38: 50S RIBOSOMAL PROTEIN L2

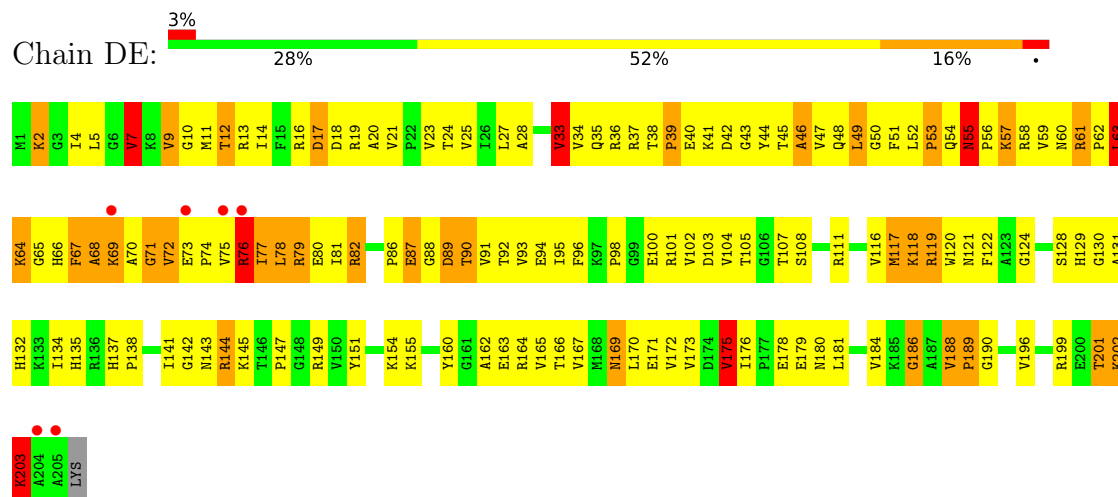


### • Molecule 39: 50S RIBOSOMAL PROTEIN L3

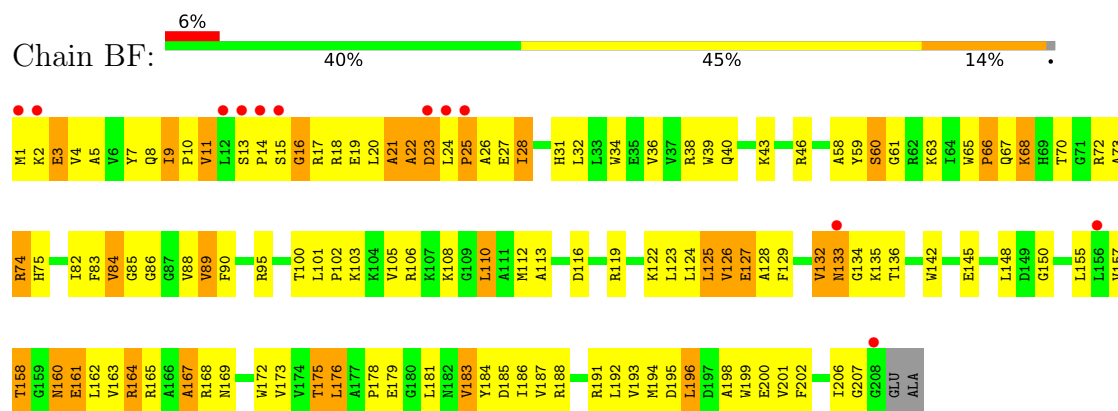




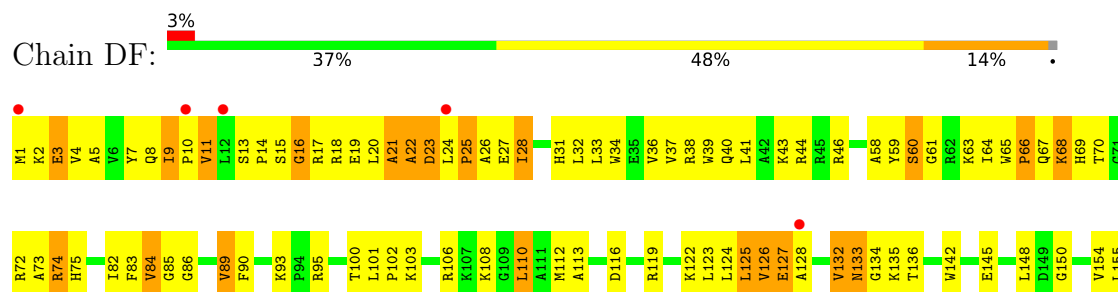
• Molecule 39: 50S RIBOSOMAL PROTEIN L3



• Molecule 40: 50S RIBOSOMAL PROTEIN L4

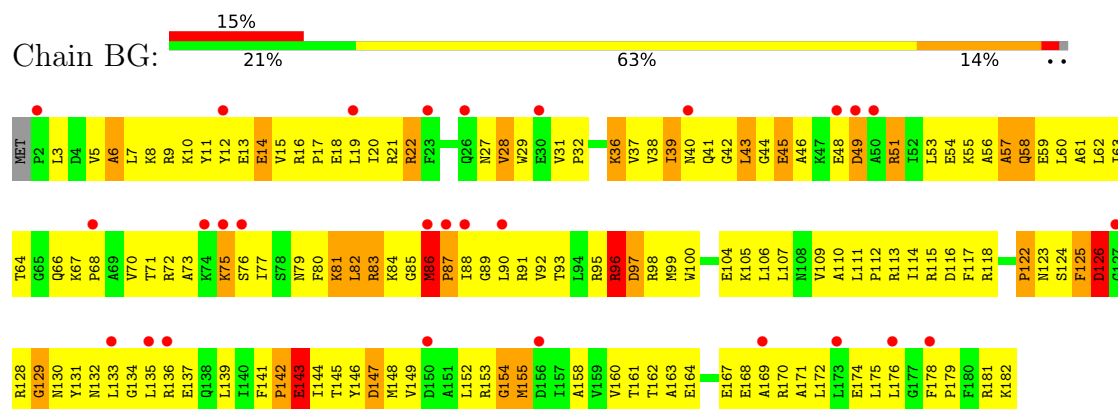


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

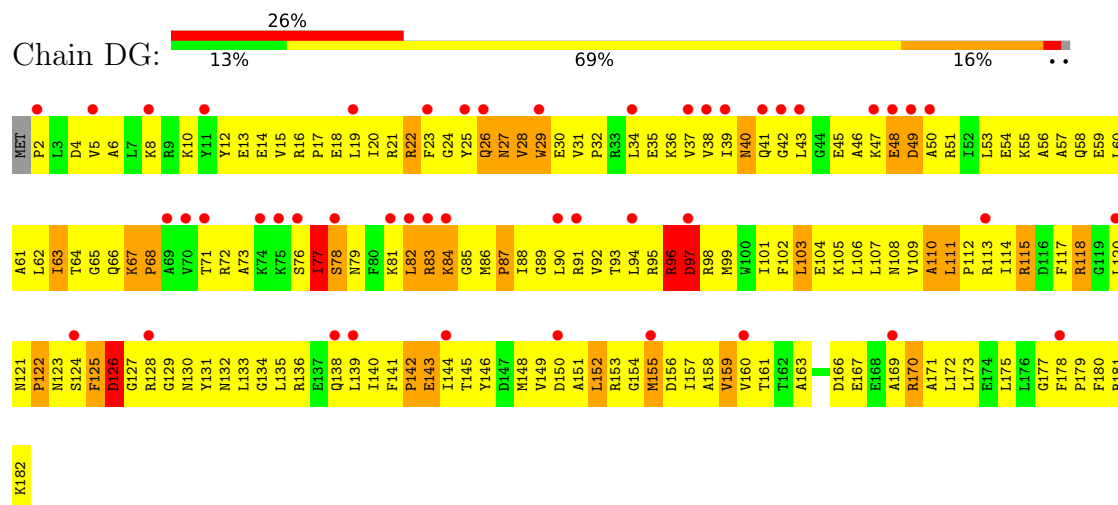




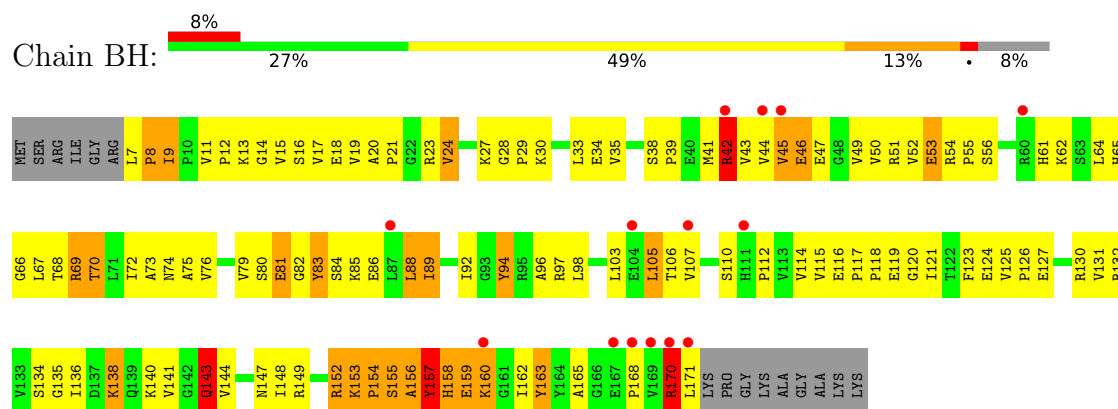
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



• Molecule 41: 50S RIBOSOMAL PROTEIN L5

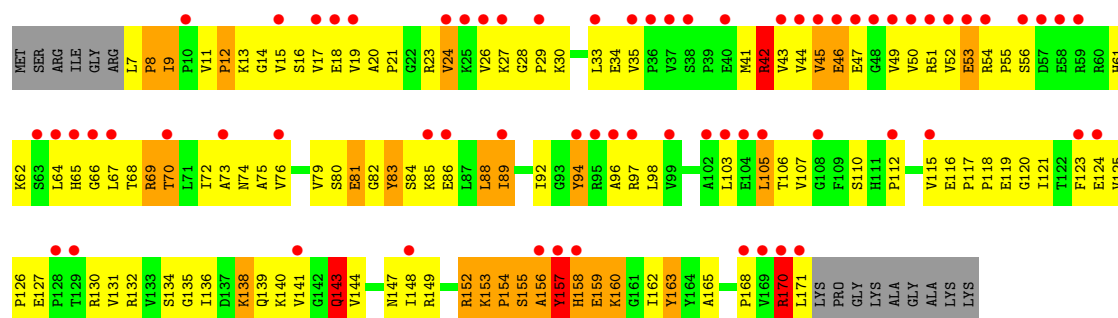


• Molecule 42: 50S RIBOSOMAL PROTEIN L6

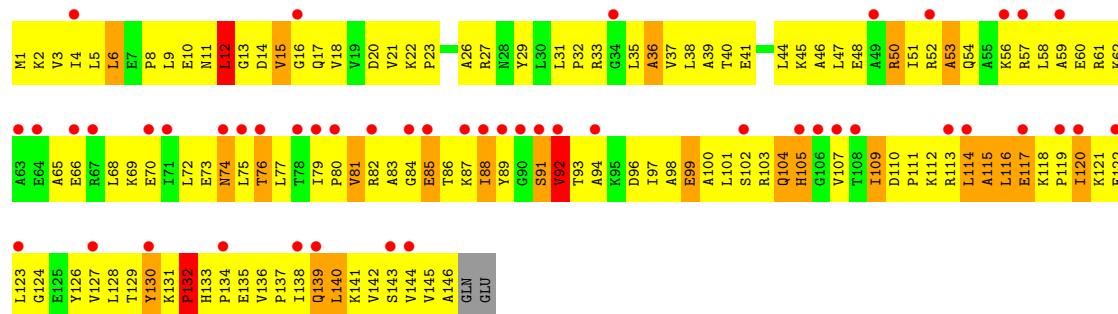


• Molecule 42: 50S RIBOSOMAL PROTEIN L6

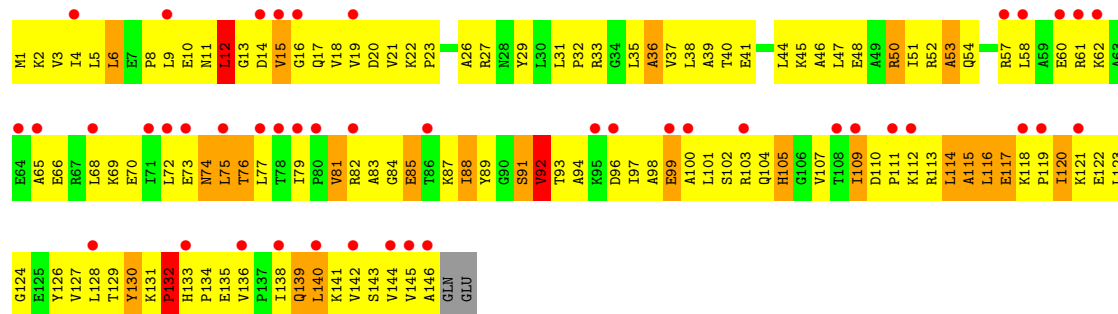




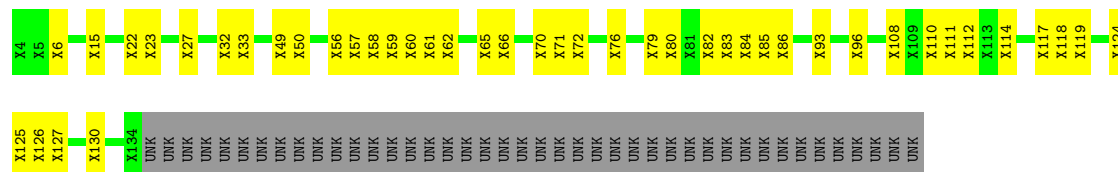
• Molecule 43: 50S RIBOSOMAL PROTEIN L9



• Molecule 43: 50S RIBOSOMAL PROTEIN L9

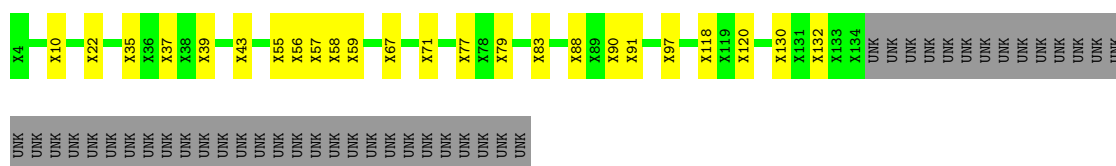


• Molecule 44: 50S RIBOSOMAL PROTEIN L10

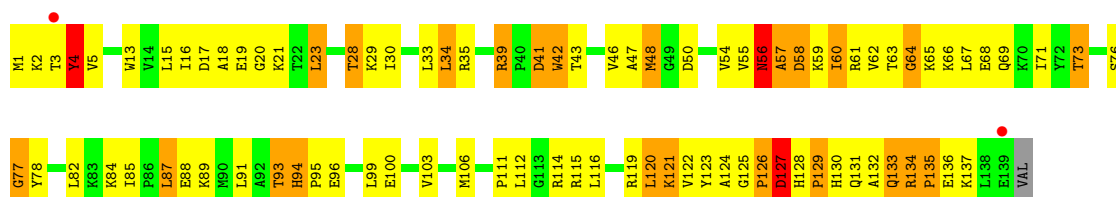


• Molecule 44: 50S RIBOSOMAL PROTEIN L10

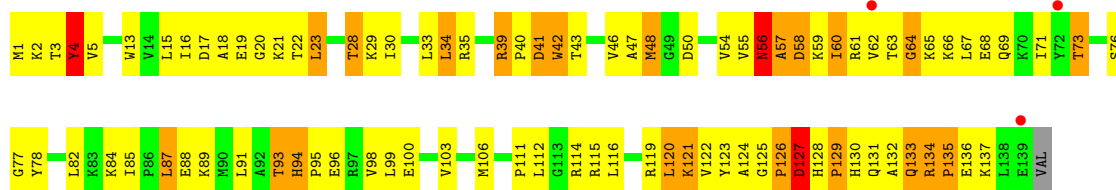




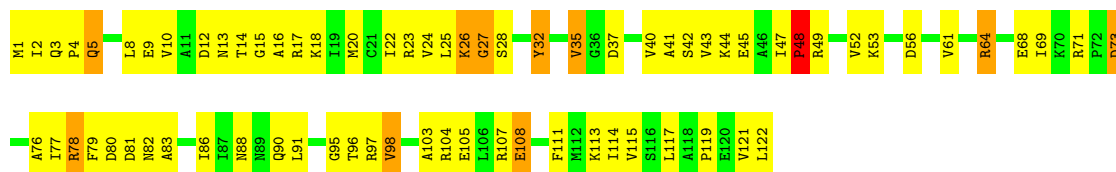
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



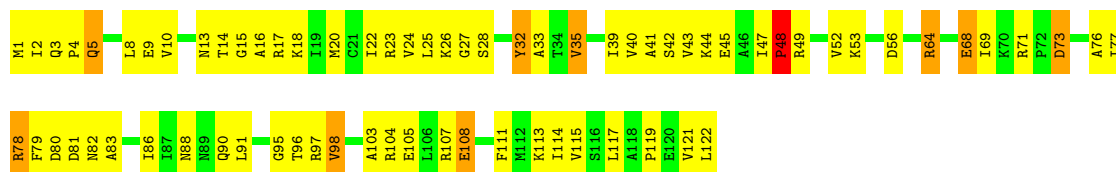
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



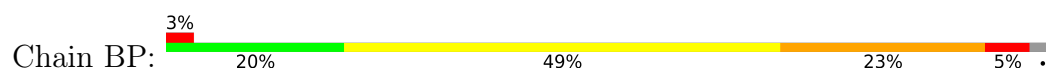
• Molecule 46: 50S RIBOSOMAL PROTEIN L14



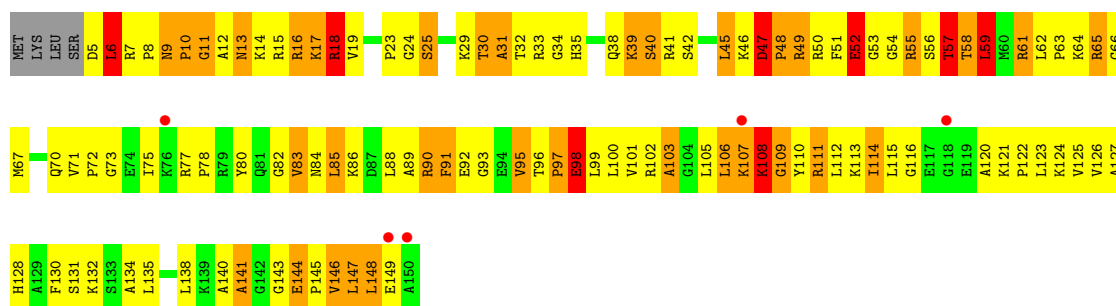
• Molecule 46: 50S RIBOSOMAL PROTEIN L14



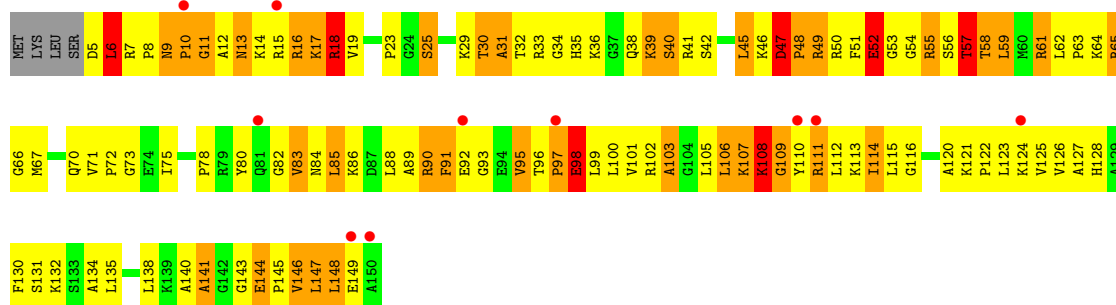
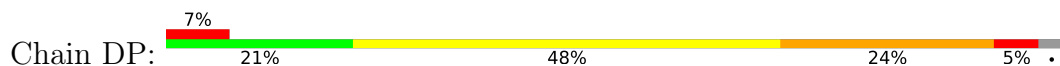
• Molecule 47: 50S RIBOSOMAL PROTEIN L15



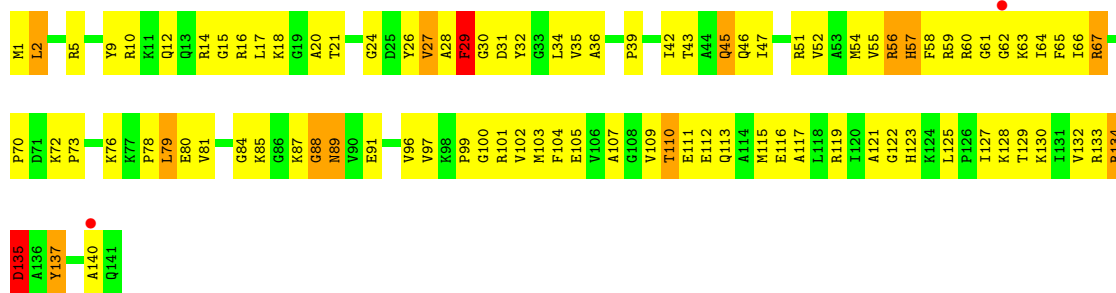
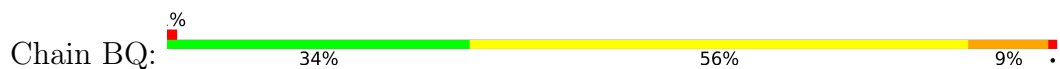




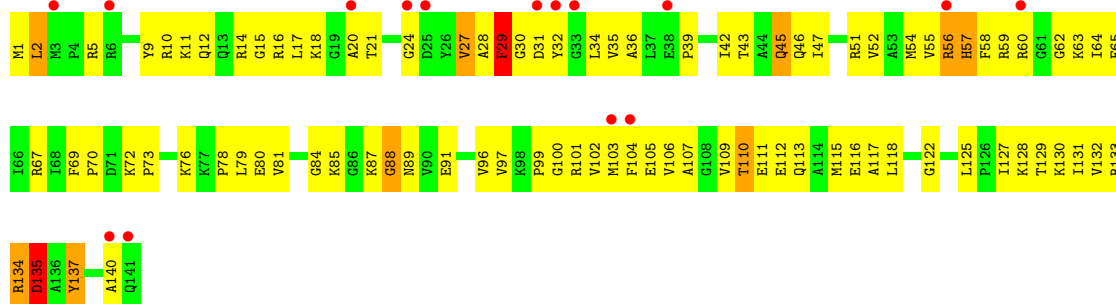
• Molecule 47: 50S RIBOSOMAL PROTEIN L15



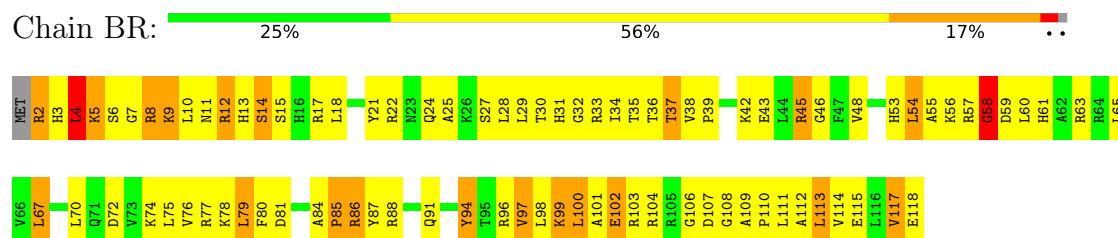
• Molecule 48: 50S RIBOSOMAL PROTEIN L16



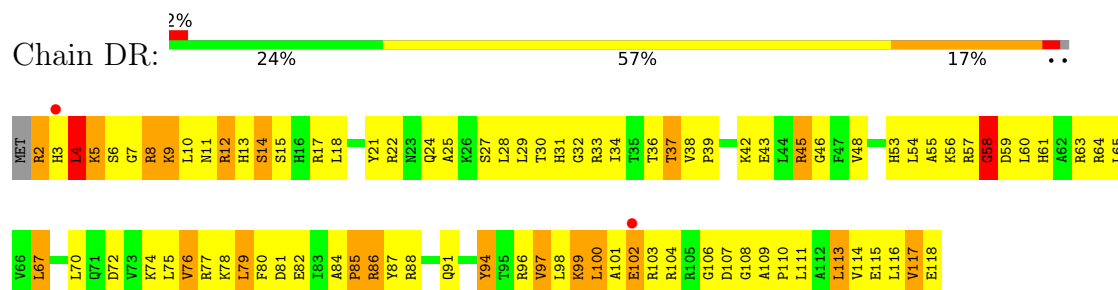
• Molecule 48: 50S RIBOSOMAL PROTEIN L16



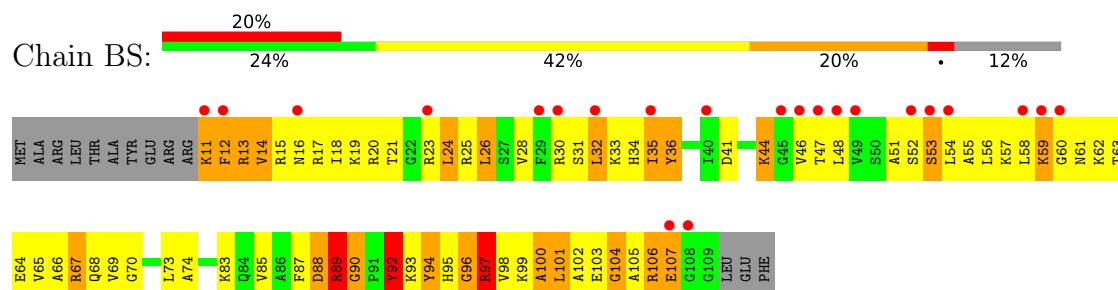
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



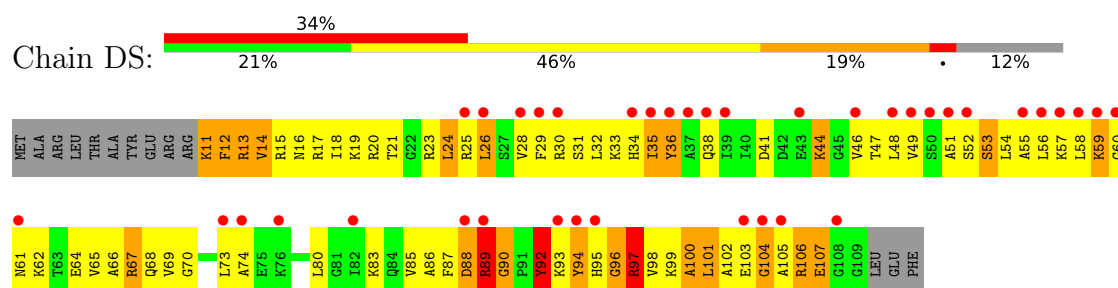
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



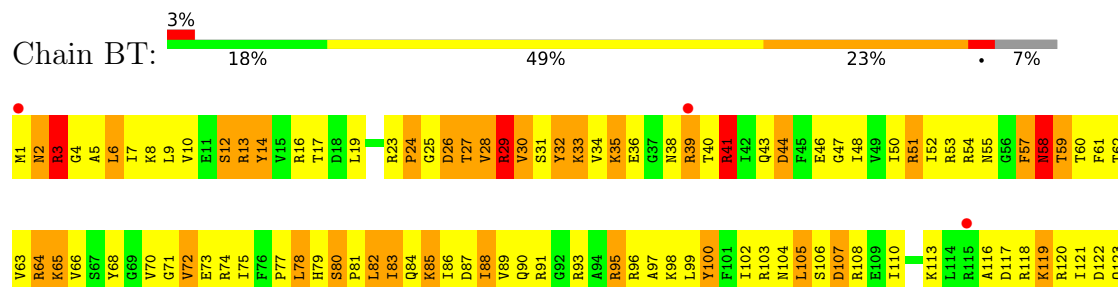
• Molecule 50: 50S RIBOSOMAL PROTEIN L18

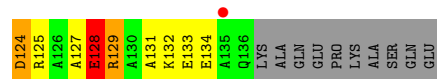


• Molecule 50: 50S RIBOSOMAL PROTEIN L18

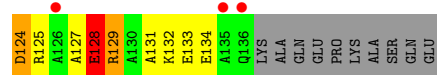
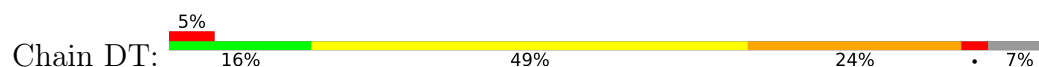


• Molecule 51: 50S RIBOSOMAL PROTEIN L19

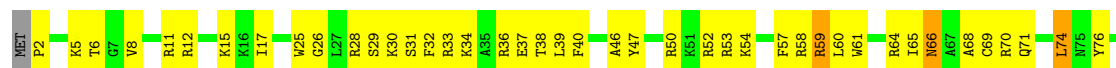




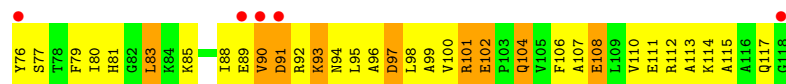
● Molecule 51: 50S RIBOSOMAL PROTEIN L19



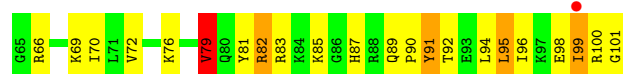
• Molecule 52: 50S RIBOSOMAL PROTEIN L20



● Molecule 52: 50S RIBOSOMAL PROTEIN L20

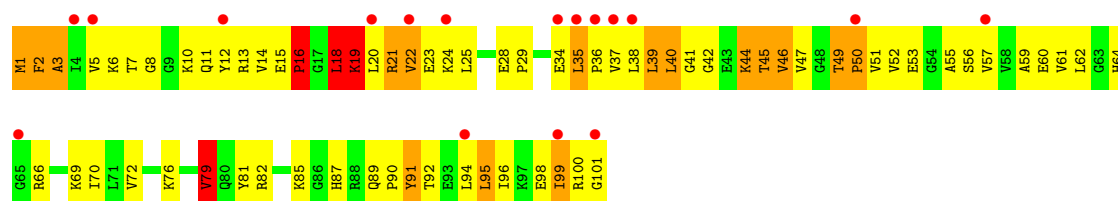


● Molecule 53: 50S RIBOSOMAL PROTEIN L21

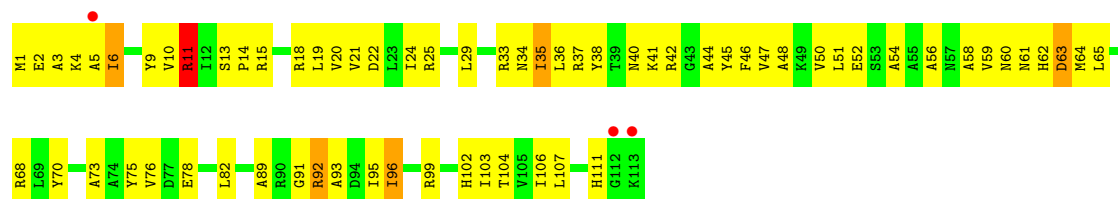
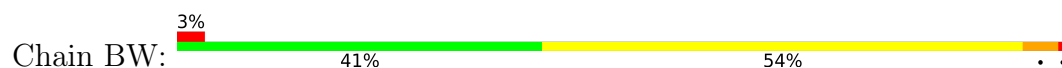


● Molecule 53: 50S RIBOSOMAL PROTEIN L21

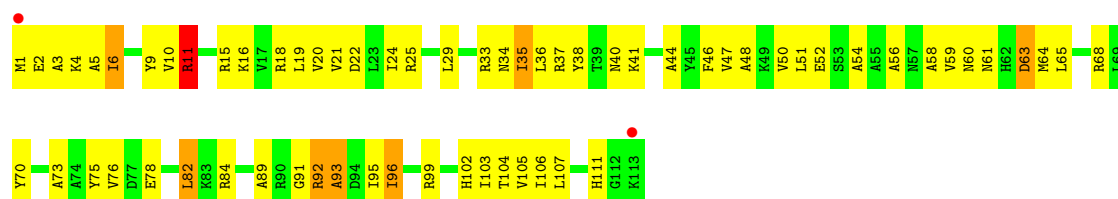
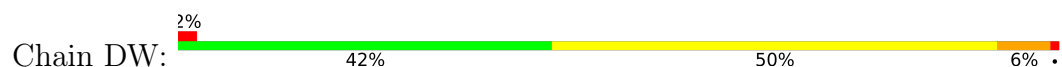




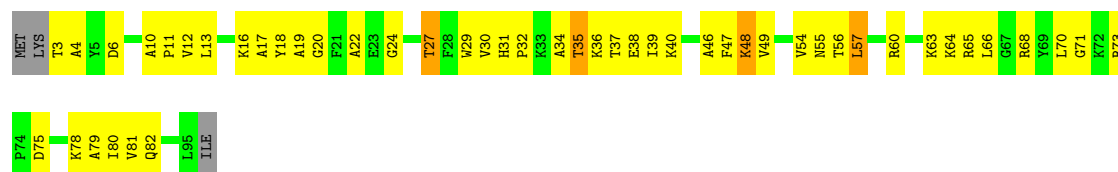
● Molecule 54: 50S RIBOSOMAL PROTEIN L22



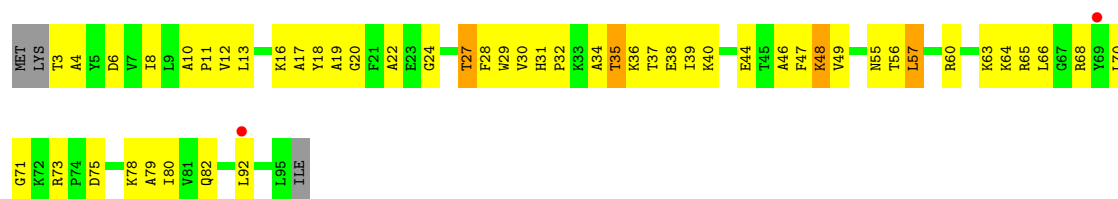
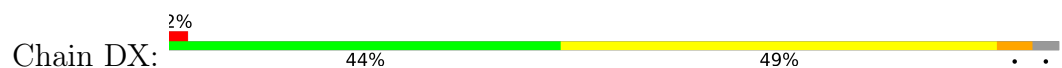
● Molecule 54: 50S RIBOSOMAL PROTEIN L22



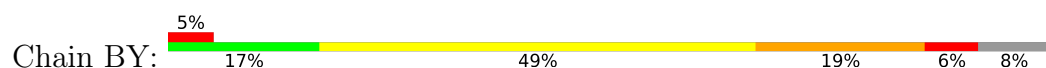
● Molecule 55: 50S RIBOSOMAL PROTEIN L23

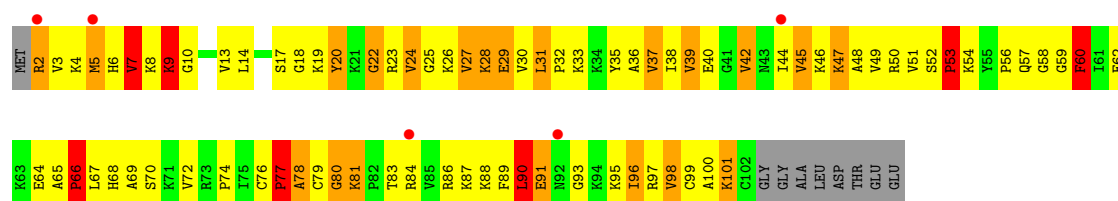


● Molecule 55: 50S RIBOSOMAL PROTEIN L23

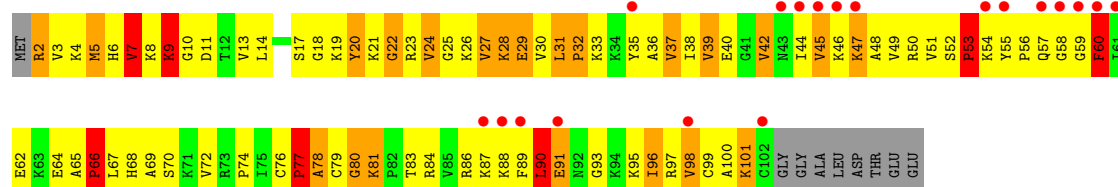
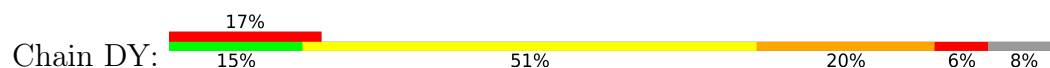


● Molecule 56: 50S RIBOSOMAL PROTEIN L24

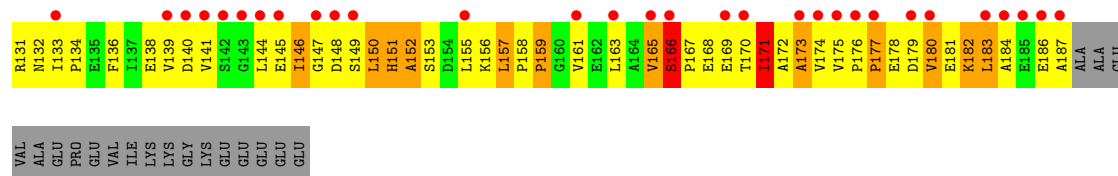
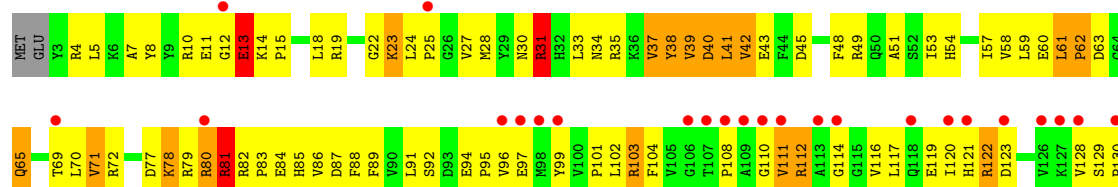




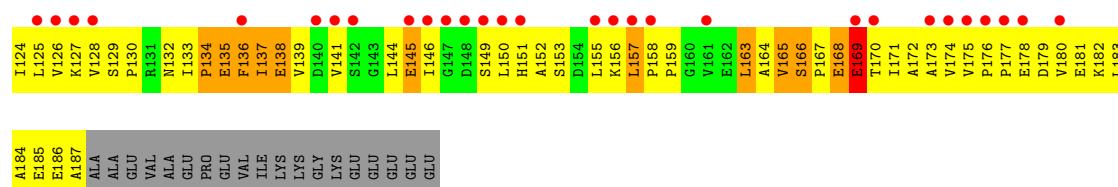
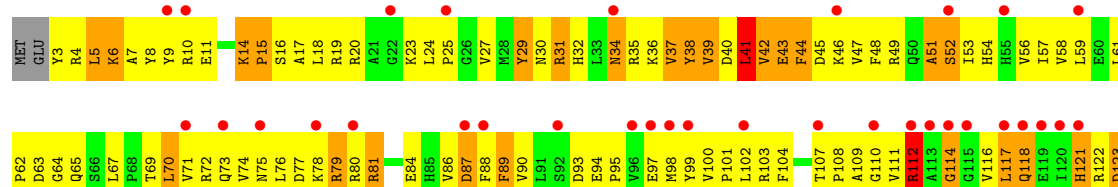
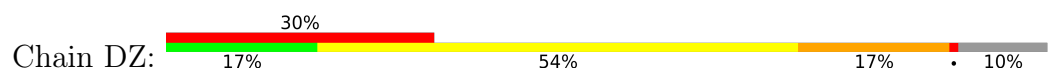
• Molecule 56: 50S RIBOSOMAL PROTEIN L24



• Molecule 57: 50S RIBOSOMAL PROTEIN L25



• Molecule 57: 50S RIBOSOMAL PROTEIN L25



## 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 0.273 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
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 , 91.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	298096	wwPDB-VP
Average B, all atoms (Å <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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.44	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	1334	0
1	CA	32329	0	16318	1413	0
2	AB	1901	0	1951	265	0
2	CB	1901	0	1951	274	0
3	AC	1613	0	1677	225	0
3	CC	1613	0	1677	239	0
4	AD	1703	0	1765	229	1
4	CD	1703	0	1766	226	0
5	AE	1147	0	1207	149	0
5	CE	1147	0	1207	155	0
6	AF	843	0	857	81	0
6	CF	843	0	857	81	1
7	AG	1257	0	1296	124	0
7	CG	1257	0	1296	123	0
8	AH	1116	0	1177	123	0
8	CH	1116	0	1177	126	0
9	AI	1010	0	1035	154	0
9	CI	1010	0	1035	159	0
10	AJ	795	0	840	181	0
10	CJ	795	0	840	178	0
11	AK	885	0	904	85	0
11	CK	885	0	904	85	0
12	AL	971	0	1057	215	0
12	CL	971	0	1057	213	0
13	AM	938	0	991	131	0
13	CM	938	0	991	131	0
14	AN	492	0	531	49	0
14	CN	492	0	532	54	0
15	AO	734	0	771	57	0

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

The worst 5 of 19809 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CY:57:U:C6	57:DZ:182:LYS:HA	1.08	1.58
1:CA:1196:U:C4	24:CX:23:A:C5	1.96	1.53
22:CY:57:U:H6	57:DZ:182:LYS:CA	1.20	1.50
1:CA:1196:U:O4	24:CX:23:A:C4	1.70	1.45
22:CY:62:U:O2'	57:DZ:186:GLU:CB	1.68	1.39

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:27:TYR:OH	6:CF:15:ASP:OD2[4_455]	2.05	0.15

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	153 (66%)	55 (24%)	25 (11%)	0	3
2	CB	233/256 (91%)	152 (65%)	57 (24%)	24 (10%)	0	3
3	AC	205/239 (86%)	141 (69%)	43 (21%)	21 (10%)	0	4
3	CC	205/239 (86%)	142 (69%)	40 (20%)	23 (11%)	0	2
4	AD	206/209 (99%)	133 (65%)	46 (22%)	27 (13%)	0	1
4	CD	206/209 (99%)	135 (66%)	44 (21%)	27 (13%)	0	1
5	AE	149/162 (92%)	111 (74%)	24 (16%)	14 (9%)	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	7
6	CF	99/101 (98%)	76 (77%)	17 (17%)	6 (6%)	1	10
7	AG	153/156 (98%)	108 (71%)	41 (27%)	4 (3%)	6	29
7	CG	153/156 (98%)	110 (72%)	39 (26%)	4 (3%)	6	29
8	AH	136/138 (99%)	100 (74%)	29 (21%)	7 (5%)	2	14
8	CH	136/138 (99%)	99 (73%)	29 (21%)	8 (6%)	2	11
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	5
10	AJ	97/105 (92%)	76 (78%)	17 (18%)	4 (4%)	3	18
10	CJ	97/105 (92%)	76 (78%)	17 (18%)	4 (4%)	3	18
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%)	0	3
15	CO	86/89 (97%)	50 (58%)	27 (31%)	9 (10%)	0	3
16	AP	82/88 (93%)	48 (58%)	24 (29%)	10 (12%)	0	1
16	CP	82/88 (93%)	49 (60%)	24 (29%)	9 (11%)	0	3
17	AQ	98/105 (93%)	70 (71%)	22 (22%)	6 (6%)	1	10
17	CQ	98/105 (93%)	71 (72%)	20 (20%)	7 (7%)	1	7

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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	21
25	D0	82/85 (96%)	66 (80%)	13 (16%)	3 (4%)	4	21
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	0
30	D5	54/60 (90%)	43 (80%)	3 (6%)	8 (15%)	0	0
31	B6	48/54 (89%)	22 (46%)	12 (25%)	14 (29%)	0	0
31	D6	48/54 (89%)	22 (46%)	12 (25%)	14 (29%)	0	0
32	B7	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
32	D7	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
33	B8	62/65 (95%)	41 (66%)	13 (21%)	8 (13%)	0	1
33	D8	62/65 (95%)	41 (66%)	13 (21%)	8 (13%)	0	1
34	B9	35/37 (95%)	28 (80%)	7 (20%)	0	100	100
34	D9	35/37 (95%)	28 (80%)	7 (20%)	0	100	100
37	BC	116/229 (51%)	94 (81%)	19 (16%)	3 (3%)	6	29
37	DC	116/229 (51%)	94 (81%)	19 (16%)	3 (3%)	6	29
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	11
46	DO	120/122 (98%)	96 (80%)	16 (13%)	8 (7%)	1	8
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	1
49	DR	115/118 (98%)	87 (76%)	14 (12%)	14 (12%)	0	1
50	BS	97/112 (87%)	54 (56%)	24 (25%)	19 (20%)	0	0
50	DS	97/112 (87%)	52 (54%)	26 (27%)	19 (20%)	0	0
51	BT	134/146 (92%)	85 (63%)	19 (14%)	30 (22%)	0	0
51	DT	134/146 (92%)	86 (64%)	18 (13%)	30 (22%)	0	0
52	BU	115/118 (98%)	90 (78%)	19 (16%)	6 (5%)	2	14
52	DU	115/118 (98%)	88 (76%)	20 (17%)	7 (6%)	1	10
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%)	1	9

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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	0
57	DZ	183/206 (89%)	111 (61%)	42 (23%)	30 (16%)	0	0
All	All	11600/12592 (92%)	7946 (68%)	2292 (20%)	1362 (12%)	0	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%)	13	44
2	CB	202/220 (92%)	187 (93%)	15 (7%)	15	47
3	AC	160/188 (85%)	145 (91%)	15 (9%)	9	35
3	CC	160/188 (85%)	146 (91%)	14 (9%)	11	39
4	AD	180/181 (99%)	162 (90%)	18 (10%)	8	31
4	CD	180/181 (99%)	162 (90%)	18 (10%)	8	31
5	AE	115/123 (94%)	107 (93%)	8 (7%)	16	49
5	CE	115/123 (94%)	107 (93%)	8 (7%)	16	49
6	AF	90/90 (100%)	87 (97%)	3 (3%)	41	74
6	CF	90/90 (100%)	87 (97%)	3 (3%)	41	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	126/127 (99%)	121 (96%)	5 (4%)	34	69
7	CG	126/127 (99%)	121 (96%)	5 (4%)	34	69
8	AH	119/119 (100%)	109 (92%)	10 (8%)	12	41
8	CH	119/119 (100%)	109 (92%)	10 (8%)	12	41
9	AI	98/99 (99%)	90 (92%)	8 (8%)	12	42
9	CI	98/99 (99%)	90 (92%)	8 (8%)	12	42
10	AJ	88/92 (96%)	83 (94%)	5 (6%)	23	56
10	CJ	88/92 (96%)	83 (94%)	5 (6%)	23	56
11	AK	90/99 (91%)	85 (94%)	5 (6%)	23	57
11	CK	90/99 (91%)	85 (94%)	5 (6%)	23	57
12	AL	104/111 (94%)	85 (82%)	19 (18%)	2	8
12	CL	104/111 (94%)	84 (81%)	20 (19%)	1	7
13	AM	94/101 (93%)	84 (89%)	10 (11%)	7	28
13	CM	94/101 (93%)	84 (89%)	10 (11%)	7	28
14	AN	49/50 (98%)	47 (96%)	2 (4%)	33	68
14	CN	49/50 (98%)	47 (96%)	2 (4%)	33	68
15	AO	79/80 (99%)	75 (95%)	4 (5%)	26	60
15	CO	79/80 (99%)	75 (95%)	4 (5%)	26	60
16	AP	72/74 (97%)	66 (92%)	6 (8%)	12	42
16	CP	72/74 (97%)	66 (92%)	6 (8%)	12	42
17	AQ	94/97 (97%)	90 (96%)	4 (4%)	32	66
17	CQ	94/97 (97%)	90 (96%)	4 (4%)	32	66
18	AR	61/77 (79%)	59 (97%)	2 (3%)	41	74
18	CR	61/77 (79%)	59 (97%)	2 (3%)	41	74
19	AS	69/80 (86%)	62 (90%)	7 (10%)	8	31
19	CS	69/80 (86%)	61 (88%)	8 (12%)	6	24
20	AT	76/82 (93%)	71 (93%)	5 (7%)	18	51
20	CT	76/82 (93%)	71 (93%)	5 (7%)	18	51
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	29
21	CU	19/22 (86%)	18 (95%)	1 (5%)	25	59
25	B0	66/67 (98%)	59 (89%)	7 (11%)	7	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	D0	66/67 (98%)	59 (89%)	7 (11%)	7	28
26	B1	78/83 (94%)	70 (90%)	8 (10%)	8	30
26	D1	78/83 (94%)	68 (87%)	10 (13%)	5	20
27	B2	66/67 (98%)	57 (86%)	9 (14%)	4	17
27	D2	66/67 (98%)	60 (91%)	6 (9%)	10	37
28	B3	51/52 (98%)	48 (94%)	3 (6%)	21	55
28	D3	51/52 (98%)	48 (94%)	3 (6%)	21	55
29	B4	51/63 (81%)	42 (82%)	9 (18%)	2	9
29	D4	51/63 (81%)	42 (82%)	9 (18%)	2	9
30	B5	47/52 (90%)	42 (89%)	5 (11%)	7	28
30	D5	47/52 (90%)	42 (89%)	5 (11%)	7	28
31	B6	49/52 (94%)	43 (88%)	6 (12%)	5	21
31	D6	49/52 (94%)	43 (88%)	6 (12%)	5	21
32	B7	40/42 (95%)	35 (88%)	5 (12%)	5	20
32	D7	40/42 (95%)	36 (90%)	4 (10%)	8	31
33	B8	53/55 (96%)	44 (83%)	9 (17%)	2	10
33	D8	53/55 (96%)	44 (83%)	9 (17%)	2	10
34	B9	34/34 (100%)	33 (97%)	1 (3%)	45	76
34	D9	34/34 (100%)	33 (97%)	1 (3%)	45	76
37	BC	99/181 (55%)	94 (95%)	5 (5%)	26	60
37	DC	99/181 (55%)	94 (95%)	5 (5%)	26	60
38	BD	213/218 (98%)	185 (87%)	28 (13%)	4	19
38	DD	213/218 (98%)	187 (88%)	26 (12%)	5	21
39	BE	165/166 (99%)	144 (87%)	21 (13%)	5	20
39	DE	165/166 (99%)	143 (87%)	22 (13%)	4	18
40	BF	165/166 (99%)	149 (90%)	16 (10%)	9	33
40	DF	165/166 (99%)	149 (90%)	16 (10%)	9	33
41	BG	155/156 (99%)	140 (90%)	15 (10%)	9	33
41	DG	155/156 (99%)	140 (90%)	15 (10%)	9	33
42	BH	137/148 (93%)	121 (88%)	16 (12%)	6	24
42	DH	137/148 (93%)	121 (88%)	16 (12%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BI	122/124 (98%)	112 (92%)	10 (8%)	12	42
43	DI	122/124 (98%)	112 (92%)	10 (8%)	12	42
45	BN	117/119 (98%)	101 (86%)	16 (14%)	4	17
45	DN	117/119 (98%)	101 (86%)	16 (14%)	4	17
46	BO	100/100 (100%)	94 (94%)	6 (6%)	21	54
46	DO	100/100 (100%)	94 (94%)	6 (6%)	21	54
47	BP	112/116 (97%)	93 (83%)	19 (17%)	2	10
47	DP	112/116 (97%)	93 (83%)	19 (17%)	2	10
48	BQ	110/111 (99%)	100 (91%)	10 (9%)	10	37
48	DQ	110/111 (99%)	101 (92%)	9 (8%)	12	42
49	BR	100/101 (99%)	87 (87%)	13 (13%)	4	19
49	DR	100/101 (99%)	86 (86%)	14 (14%)	4	17
50	BS	77/88 (88%)	64 (83%)	13 (17%)	2	10
50	DS	77/88 (88%)	64 (83%)	13 (17%)	2	10
51	BT	118/127 (93%)	96 (81%)	22 (19%)	2	8
51	DT	118/127 (93%)	95 (80%)	23 (20%)	1	6
52	BU	92/94 (98%)	83 (90%)	9 (10%)	9	32
52	DU	92/94 (98%)	81 (88%)	11 (12%)	5	22
53	BV	82/82 (100%)	67 (82%)	15 (18%)	2	8
53	DV	82/82 (100%)	68 (83%)	14 (17%)	2	10
54	BW	91/92 (99%)	81 (89%)	10 (11%)	7	27
54	DW	91/92 (99%)	81 (89%)	10 (11%)	7	27
55	BX	74/78 (95%)	69 (93%)	5 (7%)	17	50
55	DX	74/78 (95%)	69 (93%)	5 (7%)	17	50
56	BY	84/91 (92%)	70 (83%)	14 (17%)	2	10
56	DY	84/91 (92%)	69 (82%)	15 (18%)	2	9
57	BZ	162/179 (90%)	140 (86%)	22 (14%)	4	17
57	DZ	162/179 (90%)	145 (90%)	17 (10%)	7	29
All	All	9790/10432 (94%)	8794 (90%)	996 (10%)	8	30

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 [i](#)

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

5 of 1644 RNA backbone outliers are listed below:

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

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Mol	Chain	Res	Type
1	AA	47	C

5 of 171 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
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	22,29,30	0.77	1 (4%)	25,39,42	1.05	2 (8%)
22	AG9	AY	36	22	22,29,30	1.36	2 (9%)	25,39,42	1.21	3 (12%)
22	AG9	CV	36	22	22,29,30	1.55	2 (9%)	25,39,42	1.04	2 (8%)
22	AG9	CY	36	22	22,29,30	1.86	4 (18%)	25,39,42	1.09	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	AG9	AV	36	22	1/1/9/13	3/14/47/48	0/2/2/2
22	AG9	AY	36	22	1/1/9/13	7/14/47/48	0/2/2/2
22	AG9	CV	36	22	1/1/9/13	3/14/47/48	0/2/2/2
22	AG9	CY	36	22	1/1/9/13	7/14/47/48	0/2/2/2

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

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

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

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

All (4) chirality outliers are listed below:

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

5 of 20 torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 36 short contacts:

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



## 5.5 Carbohydrates [i](#)

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%)	0.58	95 (6%) 20 8	44, 101, 184, 200	0
1	CA	1504/1522 (98%)	0.57	103 (6%) 17 7	55, 115, 186, 200	0
2	AB	235/256 (91%)	0.69	30 (12%) 3 1	75, 134, 176, 198	0
2	CB	235/256 (91%)	1.22	55 (23%) 0 0	94, 148, 183, 200	0
3	AC	207/239 (86%)	0.80	28 (13%) 3 1	82, 127, 157, 179	0
3	CC	207/239 (86%)	1.21	51 (24%) 0 0	92, 141, 170, 185	0
4	AD	208/209 (99%)	0.63	17 (8%) 11 4	64, 112, 142, 179	0
4	CD	208/209 (99%)	0.27	7 (3%) 45 23	56, 99, 135, 157	0
5	AE	151/162 (93%)	0.42	6 (3%) 38 18	65, 95, 142, 167	0
5	CE	151/162 (93%)	0.95	26 (17%) 1 1	69, 119, 151, 160	0
6	AF	101/101 (100%)	0.10	0 100 100	59, 98, 138, 173	0
6	CF	101/101 (100%)	0.10	3 (2%) 50 26	64, 110, 133, 173	0
7	AG	155/156 (99%)	1.21	35 (22%) 0 0	76, 123, 155, 198	0
7	CG	155/156 (99%)	1.14	33 (21%) 1 0	94, 131, 160, 194	0
8	AH	138/138 (100%)	0.35	7 (5%) 28 12	61, 101, 128, 144	0
8	CH	138/138 (100%)	0.73	14 (10%) 7 2	83, 121, 148, 166	0
9	AI	127/128 (99%)	1.66	39 (30%) 0 0	81, 148, 176, 191	0
9	CI	127/128 (99%)	2.05	61 (48%) 0 0	99, 153, 181, 193	0
10	AJ	99/105 (94%)	1.82	41 (41%) 0 0	71, 149, 177, 185	0
10	CJ	99/105 (94%)	2.37	54 (54%) 0 0	97, 159, 182, 189	0
11	AK	119/129 (92%)	0.52	9 (7%) 14 5	63, 94, 136, 187	0
11	CK	119/129 (92%)	0.57	12 (10%) 7 2	78, 108, 141, 176	0
12	AL	125/135 (92%)	1.05	22 (17%) 1 1	53, 93, 146, 180	0
12	CL	125/135 (92%)	1.11	27 (21%) 0 0	63, 111, 149, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
13	AM	119/126 (94%)	1.32	33 (27%)	0	0	75, 129, 161, 178	0
13	CM	119/126 (94%)	1.99	49 (41%)	0	0	96, 150, 169, 186	0
14	AN	60/61 (98%)	1.37	16 (26%)	0	0	71, 118, 145, 157	0
14	CN	60/61 (98%)	1.53	21 (35%)	0	0	108, 143, 166, 187	0
15	AO	88/89 (98%)	0.41	4 (4%)	33	16	60, 97, 130, 148	0
15	CO	88/89 (98%)	0.65	8 (9%)	9	3	67, 110, 138, 146	0
16	AP	84/88 (95%)	1.07	14 (16%)	1	1	67, 112, 156, 178	0
16	CP	84/88 (95%)	0.48	3 (3%)	42	21	60, 87, 137, 157	0
17	AQ	100/105 (95%)	0.63	9 (9%)	9	3	74, 109, 138, 151	0
17	CQ	100/105 (95%)	0.77	12 (12%)	4	2	70, 109, 139, 165	0
18	AR	70/88 (79%)	0.58	5 (7%)	16	6	69, 98, 139, 157	0
18	CR	70/88 (79%)	0.78	7 (10%)	7	2	77, 111, 148, 156	0
19	AS	79/93 (84%)	1.90	28 (35%)	0	0	89, 137, 171, 185	0
19	CS	79/93 (84%)	2.41	38 (48%)	0	0	112, 154, 178, 200	0
20	AT	99/106 (93%)	1.11	16 (16%)	1	1	65, 117, 160, 167	0
20	CT	99/106 (93%)	0.89	11 (11%)	5	2	66, 107, 151, 163	0
21	AU	25/27 (92%)	2.10	13 (52%)	0	0	84, 120, 146, 156	0
21	CU	25/27 (92%)	3.92	19 (76%)	0	0	91, 135, 171, 188	0
22	AV	77/78 (98%)	1.44	22 (28%)	0	0	65, 141, 179, 199	0
22	AY	77/78 (98%)	1.56	23 (29%)	0	0	90, 140, 185, 189	0
22	CV	77/78 (98%)	2.17	34 (44%)	0	0	94, 175, 196, 200	0
22	CY	77/78 (98%)	2.82	46 (59%)	0	0	138, 176, 197, 200	0
23	AW	78/78 (100%)	2.19	38 (48%)	0	0	70, 173, 191, 199	0
23	CW	78/78 (100%)	3.28	55 (70%)	0	0	99, 188, 200, 200	0
24	AX	12/24 (50%)	1.04	1 (8%)	11	4	59, 88, 157, 160	0
24	CX	12/24 (50%)	1.89	4 (33%)	0	0	92, 163, 185, 185	0
25	B0	84/85 (98%)	0.75	7 (8%)	11	4	39, 66, 124, 167	0
25	D0	84/85 (98%)	1.26	19 (22%)	0	0	71, 105, 146, 165	0
26	B1	94/98 (95%)	0.07	0	100	100	33, 61, 114, 141	0
26	D1	94/98 (95%)	0.22	2 (2%)	63	42	43, 74, 127, 149	0
27	B2	71/72 (98%)	-0.09	1 (1%)	75	56	41, 70, 122, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
27	D2	71/72 (98%)	0.24	4 (5%)	24 10	57, 97, 139, 178	0
28	B3	60/60 (100%)	0.39	2 (3%)	46 24	42, 63, 108, 167	0
28	D3	60/60 (100%)	1.31	15 (25%)	0 0	65, 109, 149, 175	0
29	B4	58/71 (81%)	1.32	12 (20%)	1 0	96, 144, 171, 187	0
29	D4	58/71 (81%)	1.32	14 (24%)	0 0	86, 165, 194, 200	0
30	B5	56/60 (93%)	-0.11	0	100 100	25, 63, 126, 148	0
30	D5	56/60 (93%)	0.17	1 (1%)	68 46	48, 80, 128, 146	0
31	B6	50/54 (92%)	3.53	39 (78%)	0 0	99, 140, 171, 180	0
31	D6	50/54 (92%)	4.67	41 (82%)	0 0	113, 150, 174, 191	0
32	B7	48/49 (97%)	0.14	1 (2%)	63 42	23, 42, 83, 129	0
32	D7	48/49 (97%)	0.31	1 (2%)	63 42	35, 54, 98, 131	0
33	B8	64/65 (98%)	0.39	2 (3%)	49 26	30, 61, 107, 123	0
33	D8	64/65 (98%)	0.70	7 (10%)	5 2	46, 89, 134, 177	0
34	B9	37/37 (100%)	5.29	35 (94%)	0 0	91, 136, 157, 159	0
34	D9	37/37 (100%)	6.00	36 (97%)	0 0	126, 149, 172, 183	0
35	BA	2848/2915 (97%)	0.34	124 (4%)	34 16	20, 56, 184, 200	0
35	DA	2848/2915 (97%)	0.40	150 (5%)	26 11	39, 82, 186, 200	0
36	BB	119/122 (97%)	0.63	1 (0%)	86 72	52, 81, 149, 178	0
36	DB	119/122 (97%)	0.87	9 (7%)	14 5	102, 151, 183, 195	0
37	BC	120/229 (52%)	3.70	85 (70%)	0 0	119, 168, 189, 200	0
37	DC	120/229 (52%)	3.45	81 (67%)	0 0	132, 170, 187, 199	0
38	BD	272/276 (98%)	-0.02	4 (1%)	73 54	24, 55, 93, 150	0
38	DD	272/276 (98%)	0.11	2 (0%)	87 75	37, 73, 110, 144	0
39	BE	205/206 (99%)	0.17	7 (3%)	45 23	20, 62, 129, 165	0
39	DE	205/206 (99%)	0.31	6 (2%)	51 28	41, 82, 136, 159	0
40	BF	208/210 (99%)	0.28	12 (5%)	23 10	22, 63, 144, 195	0
40	DF	208/210 (99%)	0.23	7 (3%)	45 23	38, 90, 145, 184	0
41	BG	181/182 (99%)	1.00	28 (15%)	2 1	51, 103, 155, 182	0
41	DG	181/182 (99%)	1.30	47 (25%)	0 0	102, 141, 167, 183	0
42	BH	165/180 (91%)	0.61	14 (8%)	11 4	49, 86, 136, 174	0
42	DH	165/180 (91%)	1.99	68 (41%)	0 0	102, 139, 167, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BI	146/148 (98%)	1.76	49 (33%) 0 0	55, 147, 187, 200	0
43	DI	146/148 (98%)	1.65	45 (30%) 0 0	59, 139, 183, 200	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BN	139/140 (99%)	0.02	2 (1%) 75 56	36, 64, 118, 147	0
45	DN	139/140 (99%)	0.39	3 (2%) 62 40	69, 104, 136, 155	0
46	BO	122/122 (100%)	-0.11	0 100 100	33, 60, 94, 116	0
46	DO	122/122 (100%)	0.07	0 100 100	54, 83, 110, 141	0
47	BP	146/150 (97%)	0.51	5 (3%) 45 23	29, 74, 128, 189	0
47	DP	146/150 (97%)	0.68	10 (6%) 17 7	41, 98, 144, 173	0
48	BQ	141/141 (100%)	0.29	2 (1%) 75 56	38, 67, 109, 143	0
48	DQ	141/141 (100%)	0.81	15 (10%) 6 2	63, 113, 153, 178	0
49	BR	117/118 (99%)	0.09	0 100 100	36, 62, 103, 136	0
49	DR	117/118 (99%)	0.17	2 (1%) 70 48	42, 76, 118, 151	0
50	BS	99/112 (88%)	1.21	22 (22%) 0 0	52, 95, 141, 160	0
50	DS	99/112 (88%)	1.93	38 (38%) 0 0	101, 137, 163, 186	0
51	BT	136/146 (93%)	0.06	4 (2%) 51 28	47, 78, 140, 181	0
51	DT	136/146 (93%)	0.31	7 (5%) 28 12	58, 92, 151, 176	0
52	BU	117/118 (99%)	0.03	2 (1%) 70 48	27, 53, 102, 144	0
52	DU	117/118 (99%)	0.45	7 (5%) 22 9	46, 97, 137, 163	0
53	BV	101/101 (100%)	0.03	1 (0%) 82 67	24, 72, 124, 168	0
53	DV	101/101 (100%)	0.98	17 (16%) 1 1	53, 116, 146, 171	0
54	BW	113/113 (100%)	0.05	3 (2%) 54 30	28, 52, 105, 180	0
54	DW	113/113 (100%)	0.07	2 (1%) 68 46	49, 71, 119, 165	0
55	BX	93/96 (96%)	-0.15	0 100 100	29, 63, 100, 141	0
55	DX	93/96 (96%)	0.16	2 (2%) 62 40	55, 83, 115, 138	0
56	BY	101/110 (91%)	0.35	5 (4%) 29 13	47, 89, 131, 157	0
56	DY	101/110 (91%)	1.03	19 (18%) 1 0	60, 106, 149, 164	0
57	BZ	185/206 (89%)	1.59	54 (29%) 0 0	51, 113, 163, 188	0
57	DZ	185/206 (89%)	1.74	62 (33%) 0 0	99, 144, 171, 189	0
All	All	21266/22572 (94%)	0.72	2566 (12%) 4 2	20, 98, 177, 200	0

The worst 5 of 2566 RSRZ outliers are listed below:

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

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
22	AG9	CY	36	28/29	0.75	0.51	33,49,70,70	0
22	AG9	CV	36	28/29	0.81	0.42	33,49,70,70	0
22	AG9	AY	36	28/29	0.88	0.34	43,59,79,79	0
22	AG9	AV	36	28/29	0.90	0.26	43,59,79,79	0

## 6.3 Carbohydrates [i](#)

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

## 6.5 Other polymers [i](#)

There are no such residues in this entry.