wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 2, 2024 – 11:24 am GMT

PDB ID	:	4V5G
Title	:	The crystal structure of the 70S ribosome bound to EF-Tu and tRNA
Authors	:	Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.
Deposited on	:	2009-09-01
Resolution	:	3.60 Å(reported)

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

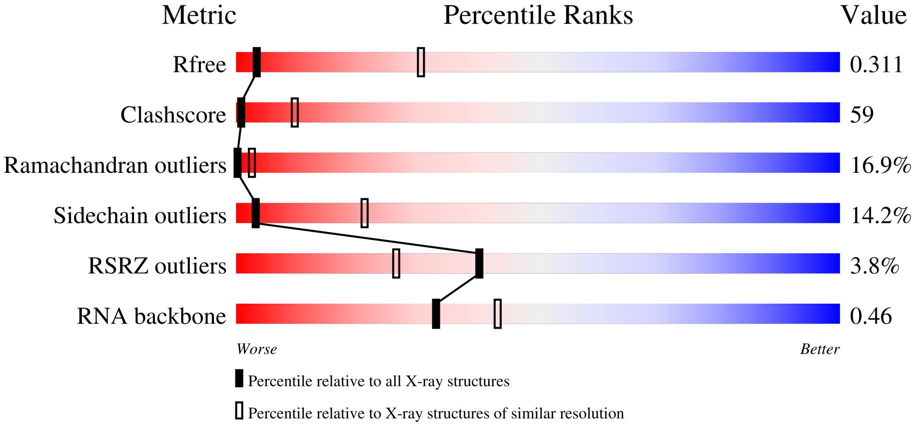
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

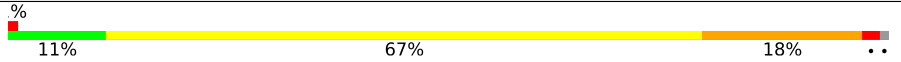
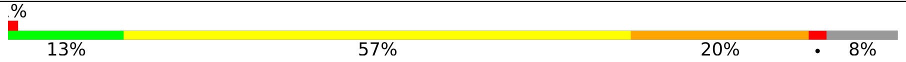
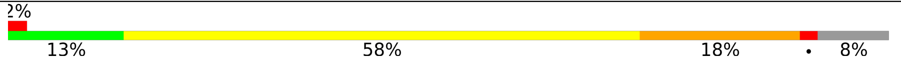
The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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

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

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Mol	Chain	Length	Quality of chain
3	AC	239	14% 57% 15% 13%
3	CC	239	% 16% 56% 14% 13%
4	AD	209	14% 59% 24% •
4	CD	209	14% 57% 26% •
5	AE	162	20% 60% 12% • 7%
5	CE	162	% 22% 59% 12% • 7%
6	AF	101	29% 56% 14% •
6	CF	101	% 24% 60% 15% •
7	AG	156	2% 22% 52% 25% ••
7	CG	156	4% 21% 54% 24% ••
8	AH	138	% 22% 57% 21% •
8	CH	138	18% 62% 20% •
9	AI	128	4% 14% 69% 16% ••
9	CI	128	2% 13% 70% 16% ••
10	AJ	105	9% 15% 52% 24% • 6%
10	CJ	105	10% 14% 53% 24% • 6%
11	AK	129	3% 19% 64% 9% 8%
11	CK	129	3% 20% 63% 9% 8%
12	AL	135	% 17% 52% 23% • 7%
12	CL	135	% 19% 50% 24% • 7%
13	AM	126	5% 10% 65% 22% • •
13	CM	126	4% 10% 66% 21% • •
14	AN	61	2% 10% 54% 33% • •
14	CN	61	2% 13% 54% 28% • •
15	AO	89	% 25% 53% 15% 7% •

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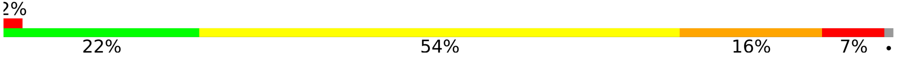
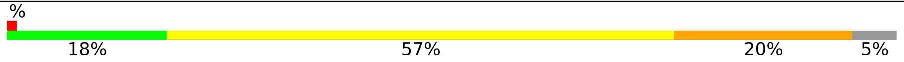
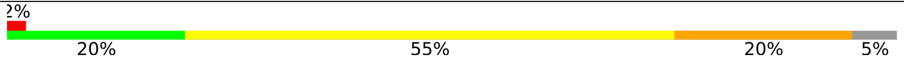
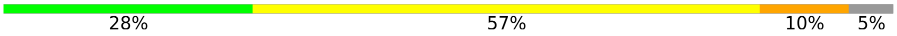
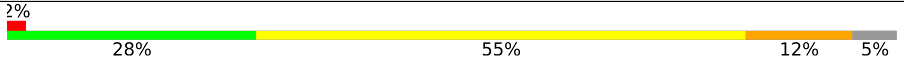
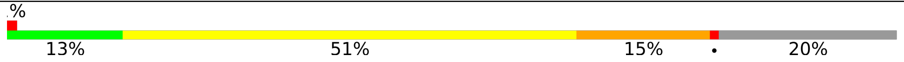
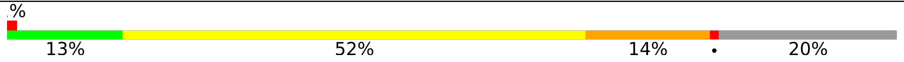
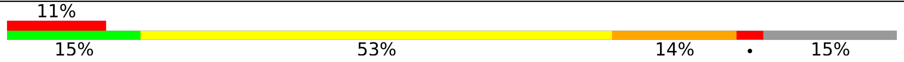
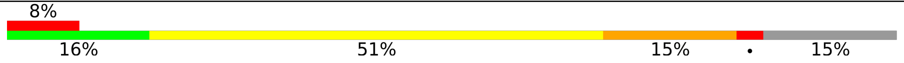
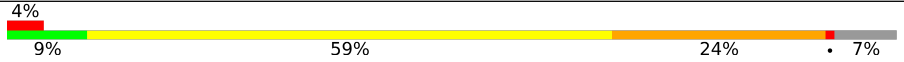
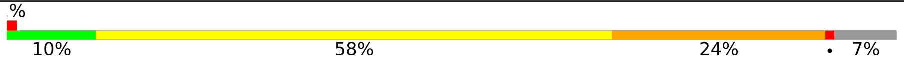
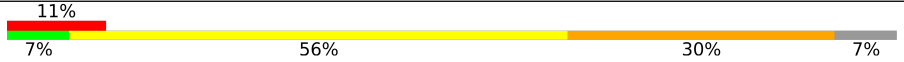
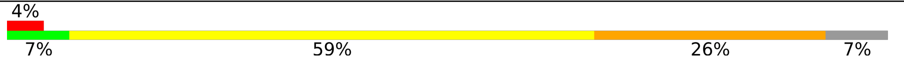
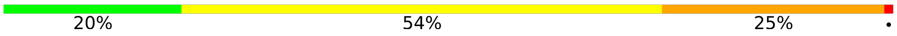
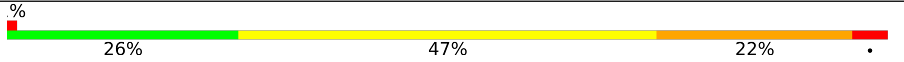
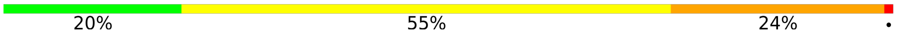
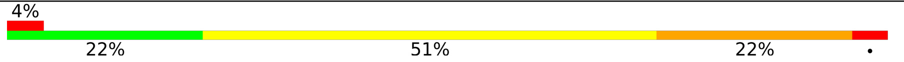
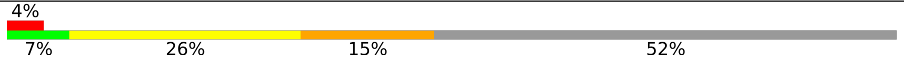
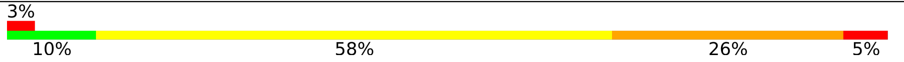
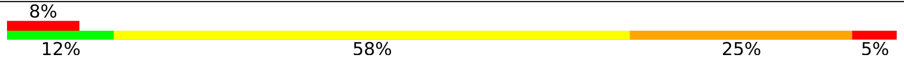
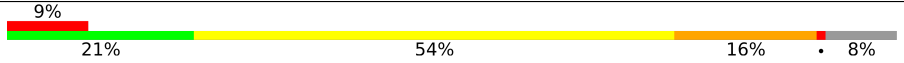
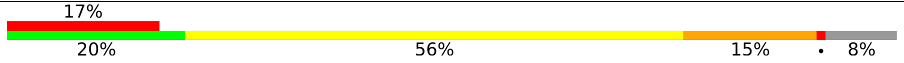
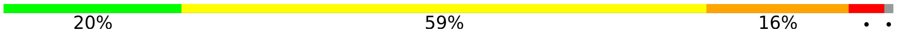
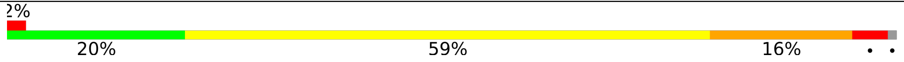
Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	AW	76	
22	CV	76	
22	CW	76	
23	AX	27	
23	CX	27	
24	AY	77	
24	CY	77	
25	AZ	406	
25	CZ	406	
26	B0	85	
26	D0	85	

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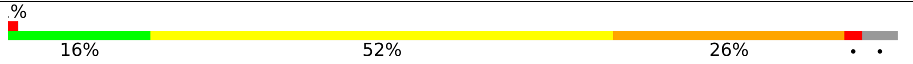
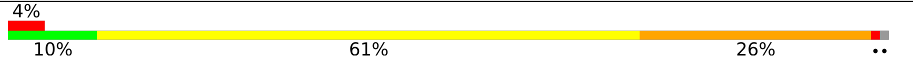
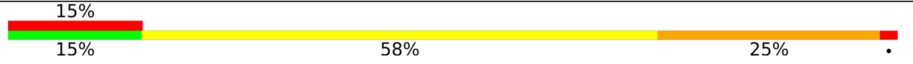
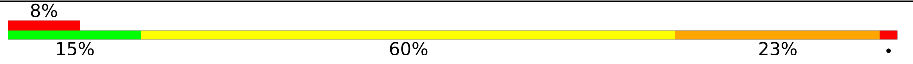
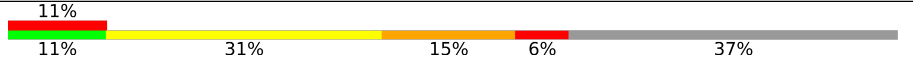
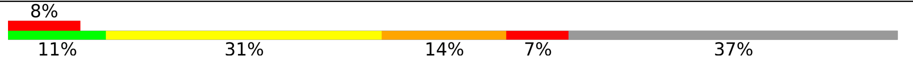
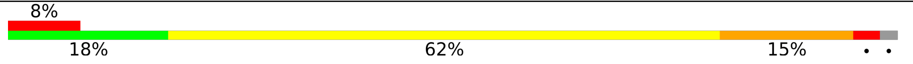
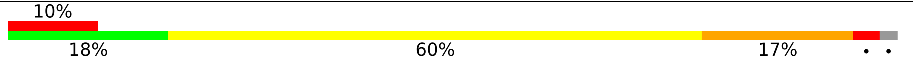
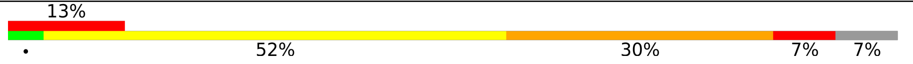
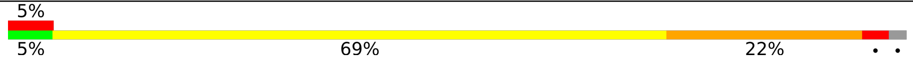
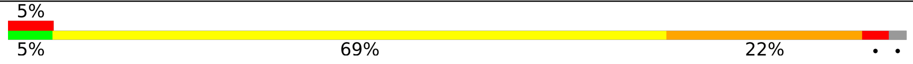
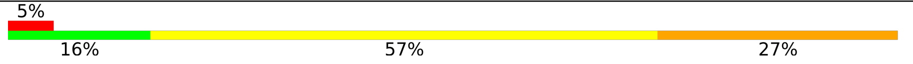
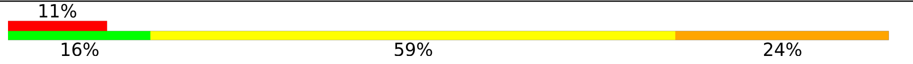
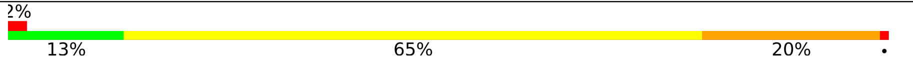
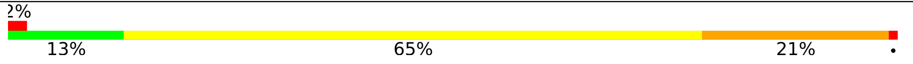
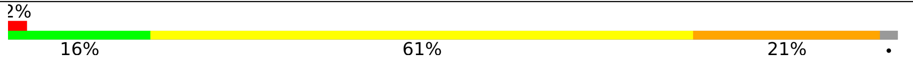
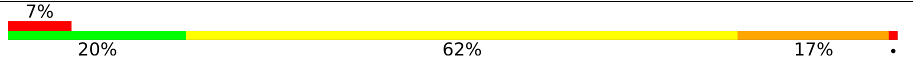
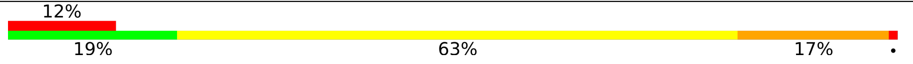
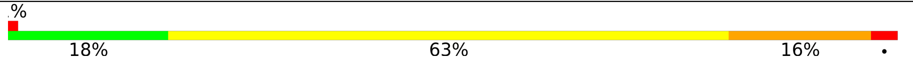
Mol	Chain	Length	Quality of chain
27	B1	98	
27	D1	98	
28	B2	72	
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229	
39	BD	276	

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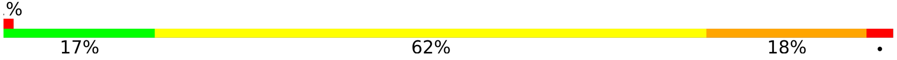
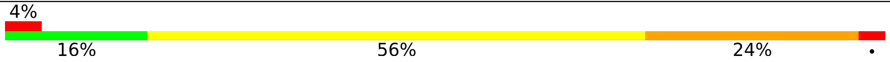
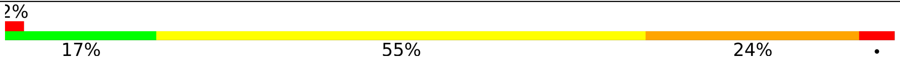
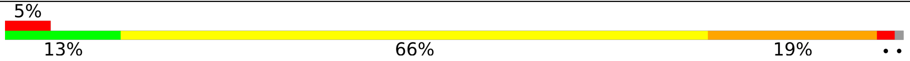
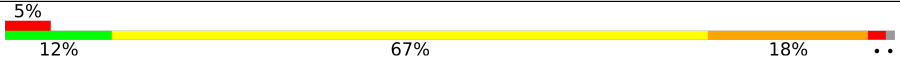
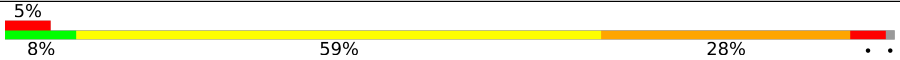
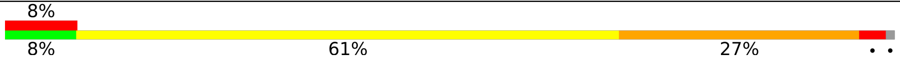
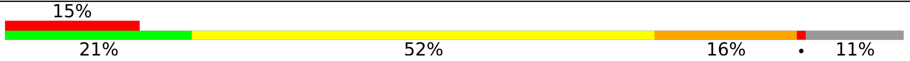
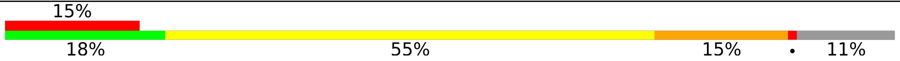
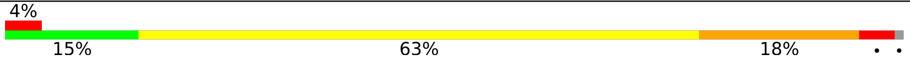
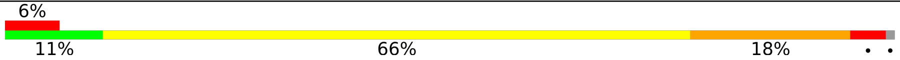
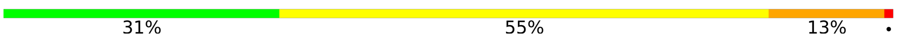
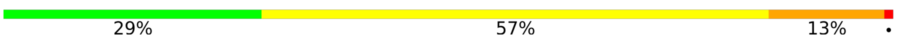
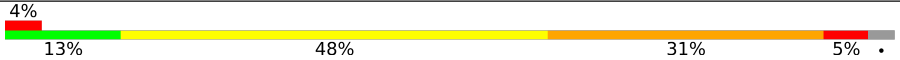
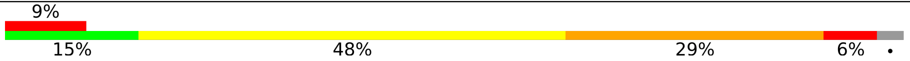
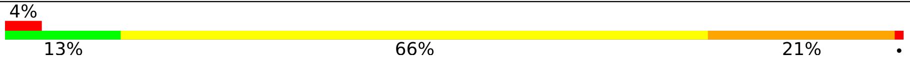
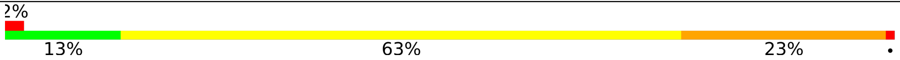
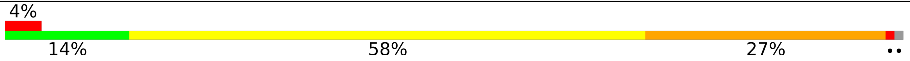
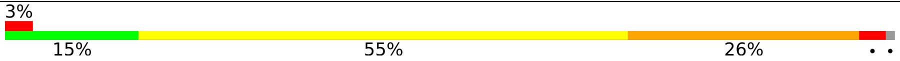
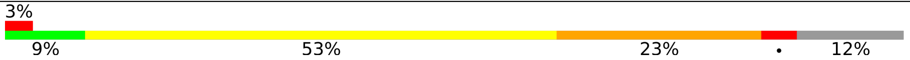
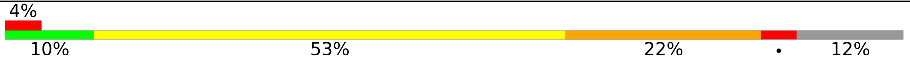
Mol	Chain	Length	Quality of chain
39	DD	276	 % 17% 62% 18% •
40	BE	206	 4% 16% 56% 24% •
40	DE	206	 2% 17% 55% 24% •
41	BF	210	 5% 13% 66% 19% • •
41	DF	210	 5% 12% 67% 18% • •
42	BG	182	 5% 8% 59% 28% • •
42	DG	182	 8% 8% 61% 27% • •
43	BH	180	 15% 21% 52% 16% • 11%
43	DH	180	 15% 18% 55% 15% • 11%
44	BJ	173	 64% 12% 24%
44	DJ	173	 66% 10% 24%
45	BK	147	 67% 29% •
45	DK	147	 69% 27% •
46	BN	140	 4% 15% 63% 18% • •
46	DN	140	 6% 11% 66% 18% • •
47	BO	122	 31% 55% 13% •
47	DO	122	 29% 57% 13% •
48	BP	150	 4% 13% 48% 31% 5% •
48	DP	150	 9% 15% 48% 29% 6% •
49	BQ	141	 4% 13% 66% 21% •
49	DQ	141	 2% 13% 63% 23% •
50	BR	118	 4% 14% 58% 27% ••
50	DR	118	 3% 15% 55% 26% • •
51	BS	112	 3% 9% 53% 23% • 12%
51	DS	112	 4% 10% 53% 22% • 12%

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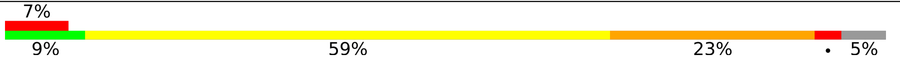
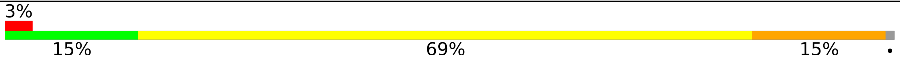
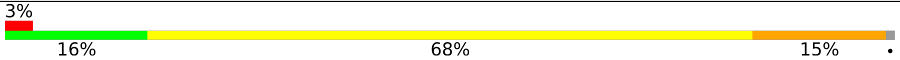
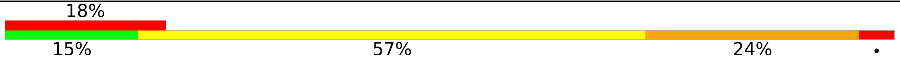
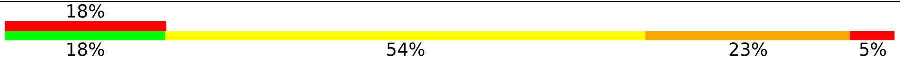
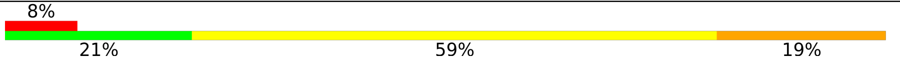
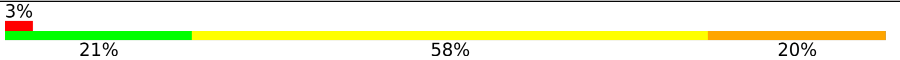
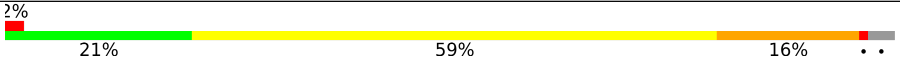
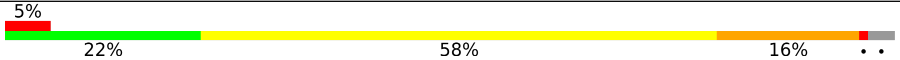
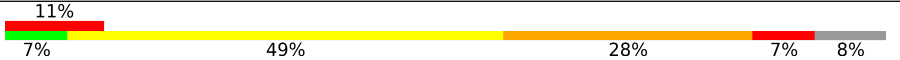
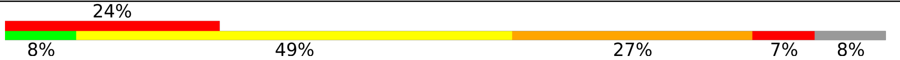
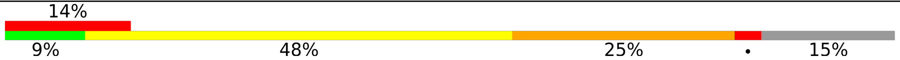
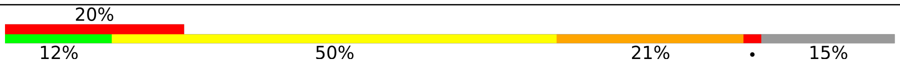
Mol	Chain	Length	Quality of chain
52	BT	146	
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	H2U	AY	16	-	-	-	X
24	H2U	CY	16	-	-	-	X
24	H2U	CY	17	-	-	-	X
24	PSU	CY	55	-	-	X	-
60	ZN	D9	101	-	-	X	-
61	MG	CY	101	-	-	-	X
62	GDP	AZ	501	-	-	X	-
62	GDP	CZ	501	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 306876 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 RIBOSOMAL RNA.

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

- 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 1901 1213 342 341 5	0	0	1
2	CB	235	Total C N O S 1901 1213 342 341 5	0	0	1

- 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 1613 1016 315 281 1	0	0	1
3	CC	207	Total C N O S 1613 1016 315 281 1	0	0	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 1703 1066 339 291 7	0	0	0
4	CD	208	Total C N O S 1703 1066 339 291 7	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	AV	76	1619	723	290	531	75	0	0	0
22	AW	76	1619	723	290	531	75	0	0	0
22	CV	76	1619	723	290	531	75	0	0	0
22	CW	76	1619	723	290	531	75	0	0	0

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	AX	13	272	124	50	86	12	0	0	0
23	CX	13	272	124	50	86	12	0	0	0

- Molecule 24 is a RNA chain called A-SITE TRNA THR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	AY	77	1650	741	292	541	76	0	0	0
24	CY	77	1650	741	292	541	76	0	0	0

- Molecule 25 is a protein called ELONGATION FACTOR TU-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	AZ	374	2900	1832	508	548	12	0	0	0
25	CZ	374	2900	1832	508	548	12	0	0	0

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	B1	94	732	460	146	125	1	0	0	1
27	D1	94	732	460	146	125	1	0	0	1

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	B4	45	341	218	58	61	4	0	0	1
30	D4	45	341	218	58	61	4	0	0	1

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	B5	59	459	288	90	76	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
33	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 36 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			
36	DA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			

- Molecule 37 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			
38	DC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
39	DD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	160	Total 1223	C 773	N 229	O 220	S 1	0	0	1
43	DH	160	Total 1223	C 773	N 229	O 220	S 1	0	0	1

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

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BK	141	Total 701	C 420	N 141	O 140	0	0	1
45	DK	141	Total 701	C 420	N 141	O 140	0	0	1

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
49	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
52	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

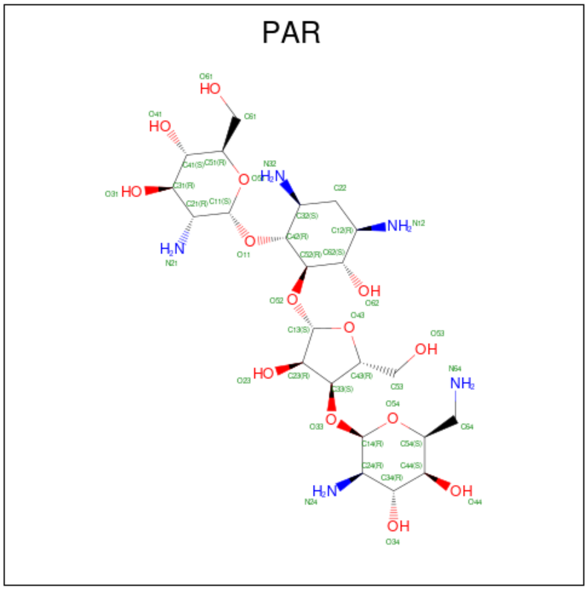
- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	176	Total 1403	C 897	N 252	O 252	S 2	0	0	0
58	DZ	176	Total 1403	C 897	N 252	O 252	S 2	0	0	0

- Molecule 59 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	AA	1	Total 42	C 23	N 5	O 14	0	0
59	CA	1	Total 42	C 23	N 5	O 14	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AD	1	Total 1	Zn 1	0	0
60	AN	1	Total 1	Zn 1	0	0
60	B4	1	Total 1	Zn 1	0	0
60	B9	1	Total 1	Zn 1	0	0
60	CD	1	Total 1	Zn 1	0	0
60	CN	1	Total 1	Zn 1	0	0

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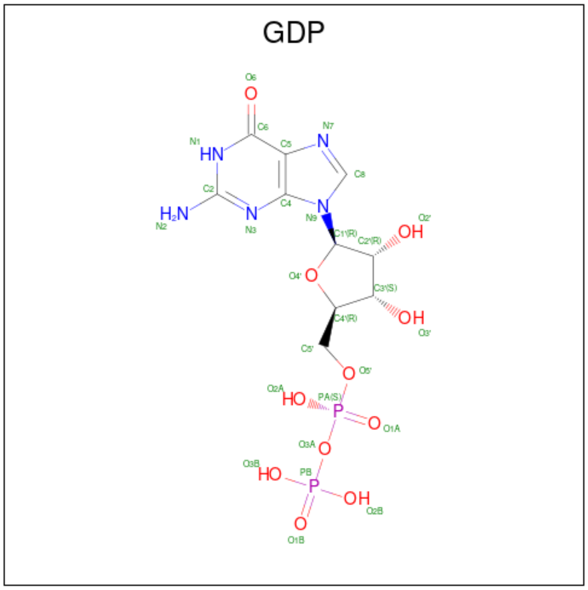
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	D4	1	Total Zn 1 1	0	0
60	D9	1	Total Zn 1 1	0	0

- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

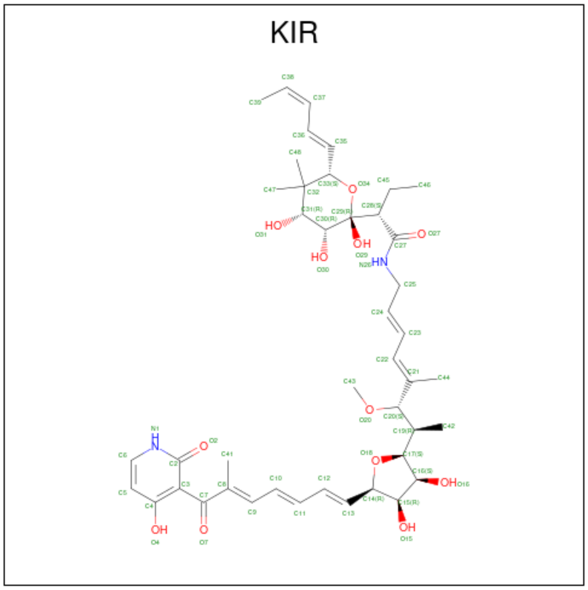
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AY	1	Total Mg 1 1	0	0
61	CY	1	Total Mg 1 1	0	0

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



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

- Molecule 63 is KIRROMYCIN (three-letter code: KIR) (formula: $C_{43}H_{60}N_2O_{12}$).

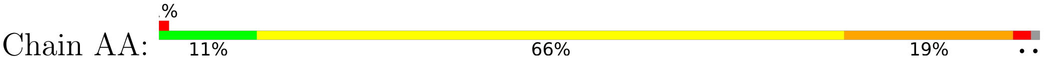


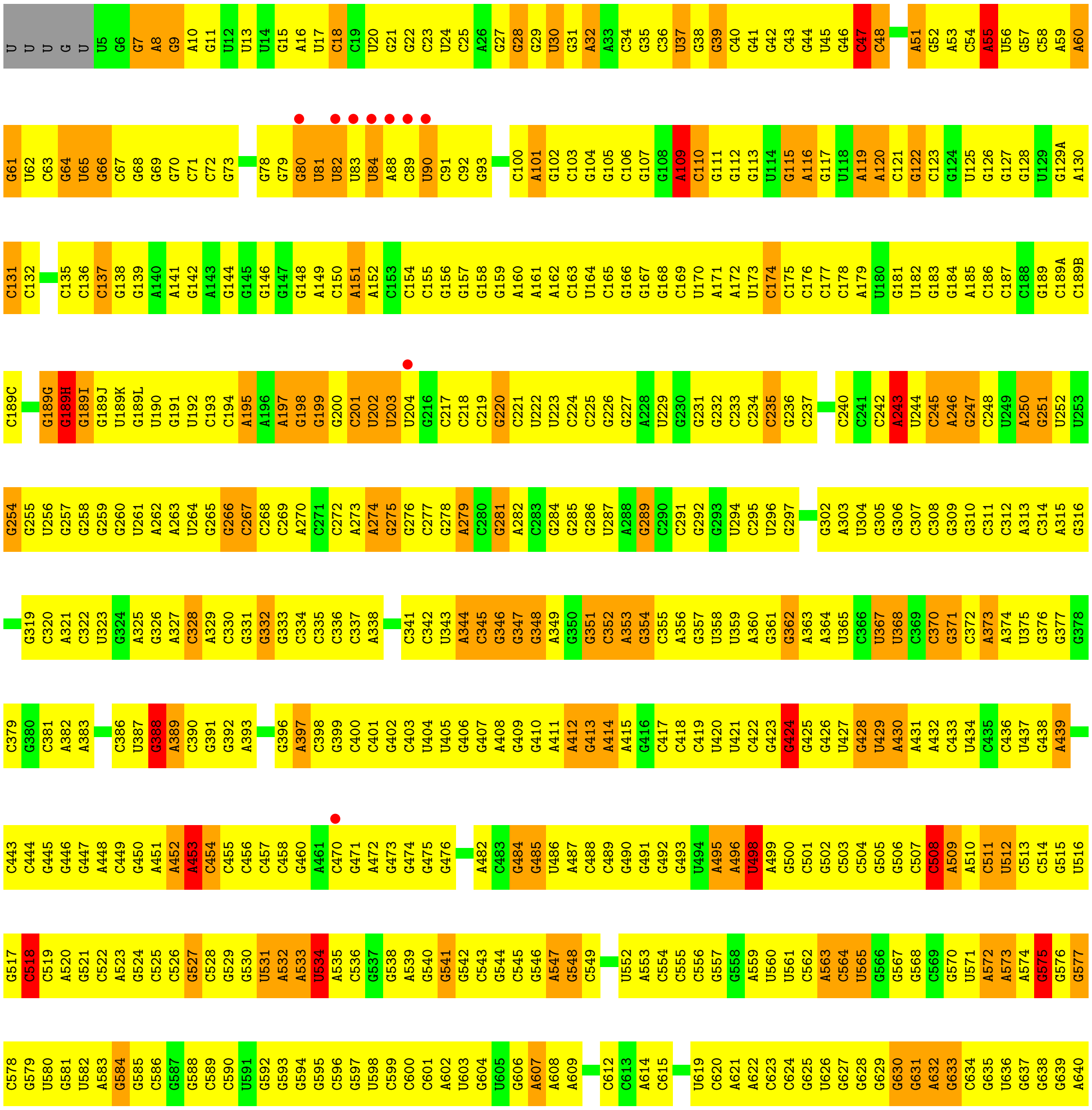
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
63	AZ	1	57	43	2	12	0	0
			Total	C	N	O		
63	CZ	1	57	43	2	12	0	0

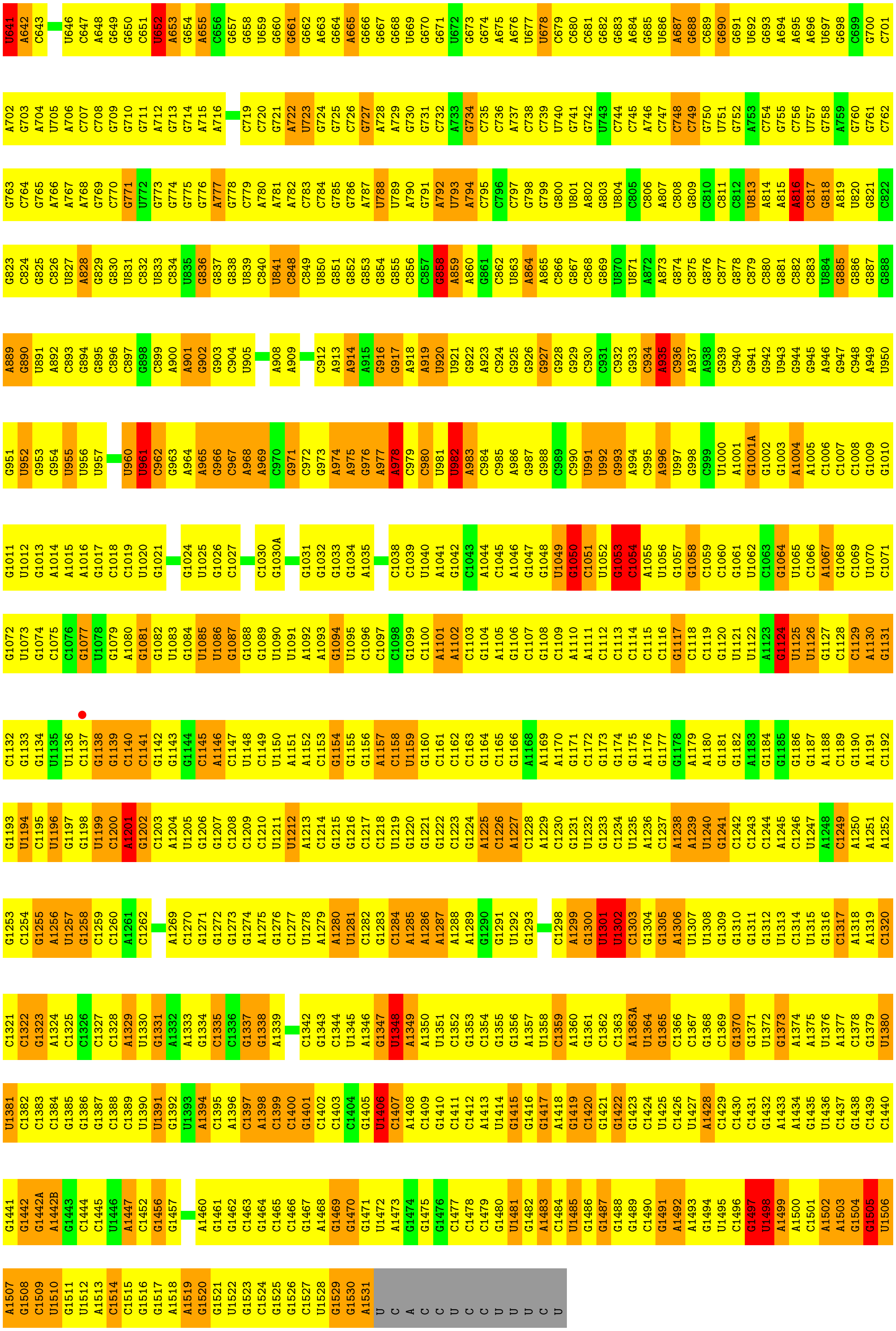
3 Residue-property plots ⓘ

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

- Molecule 1: 16S RIBOSOMAL RNA

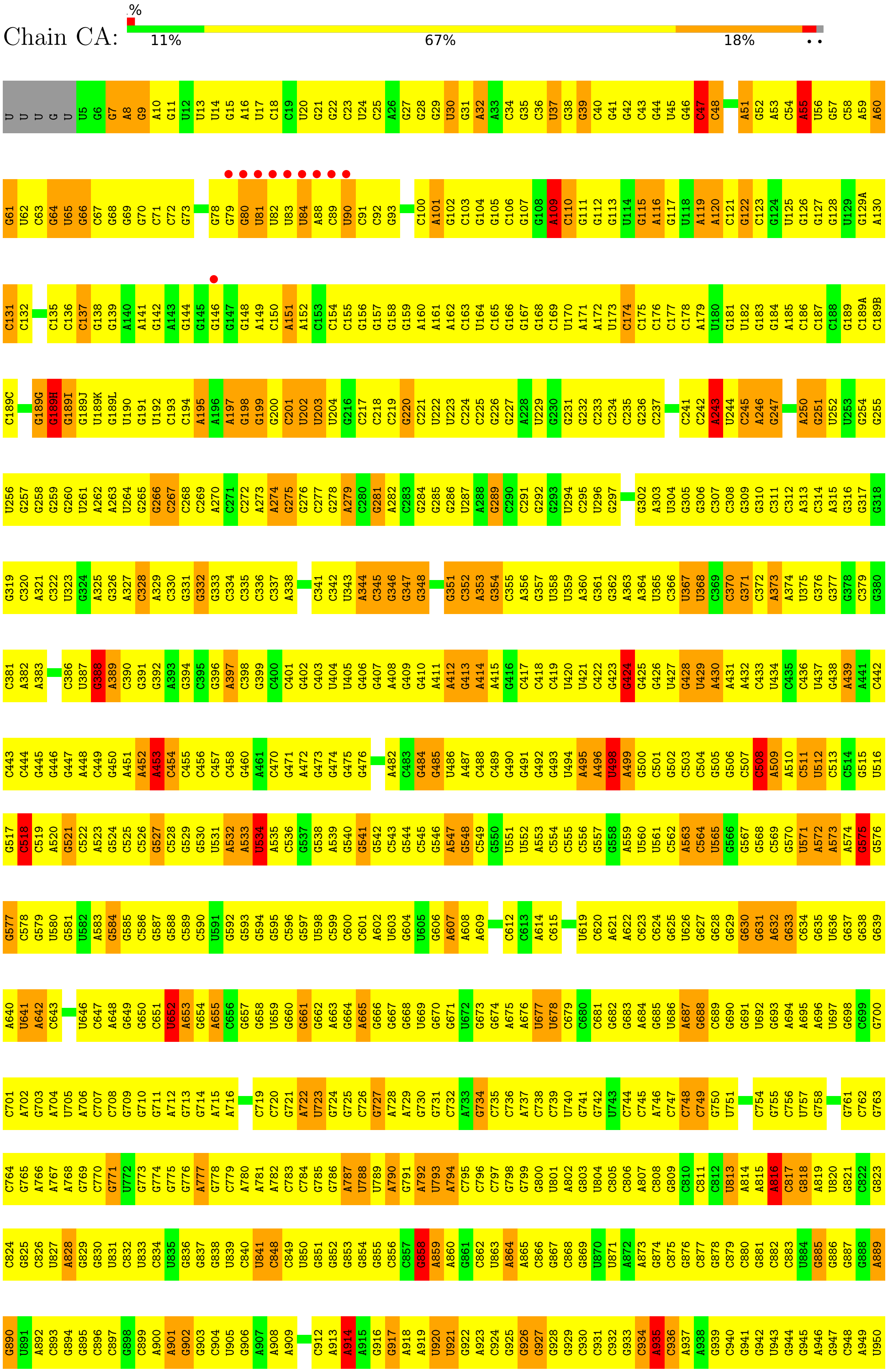


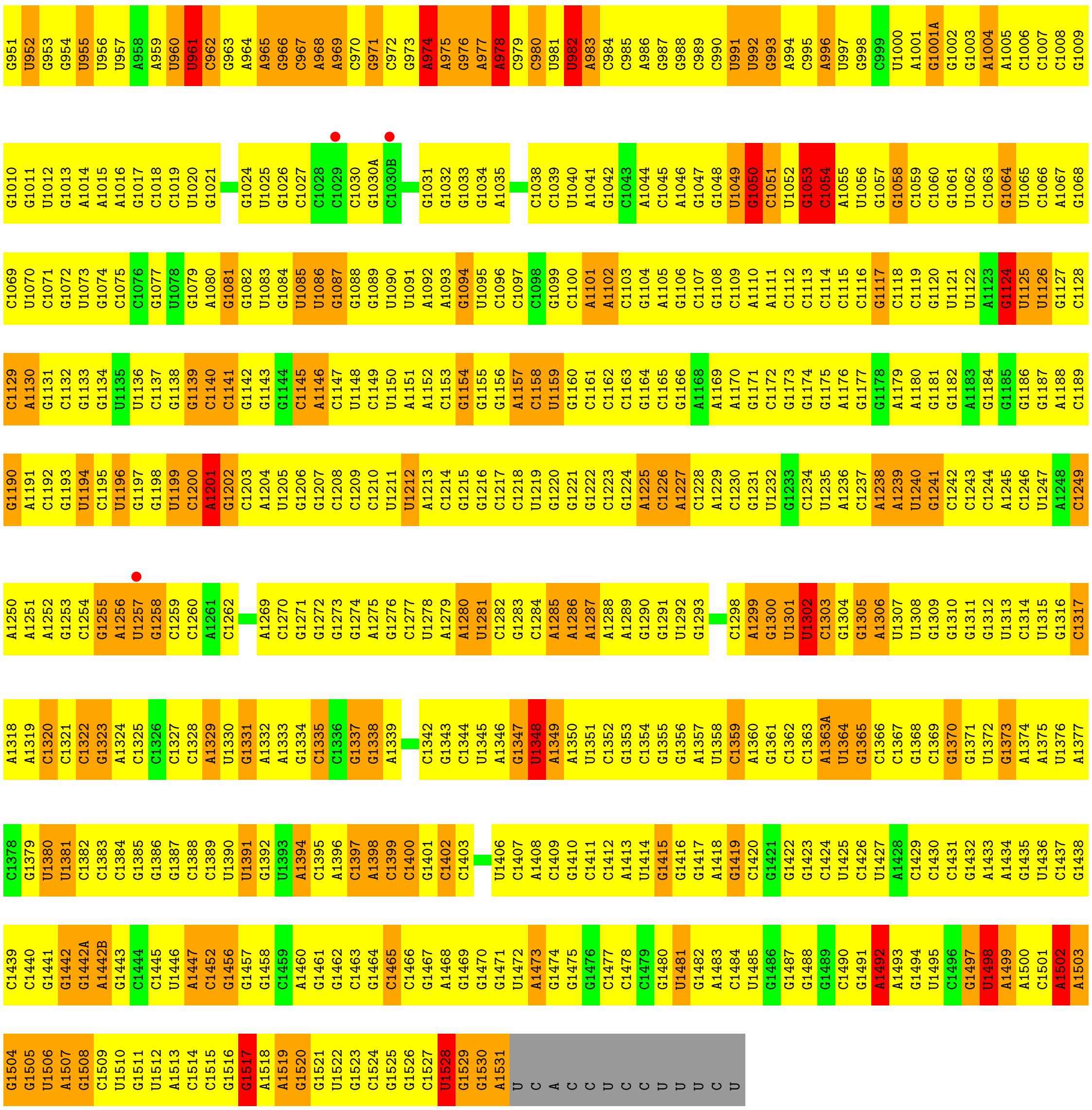




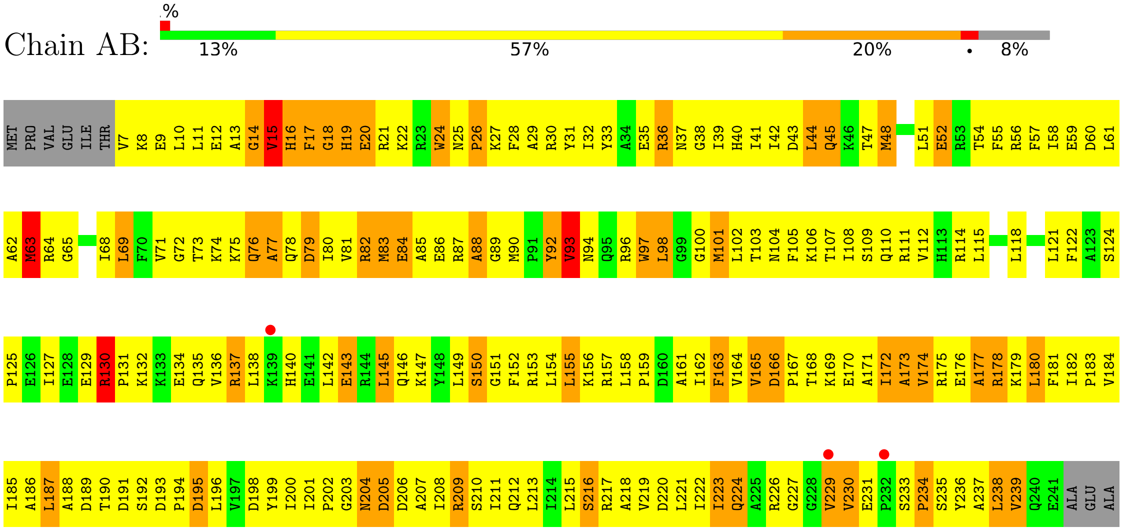
- Molecule 1: 16S RIBOSOMAL RNA

Chain CA:

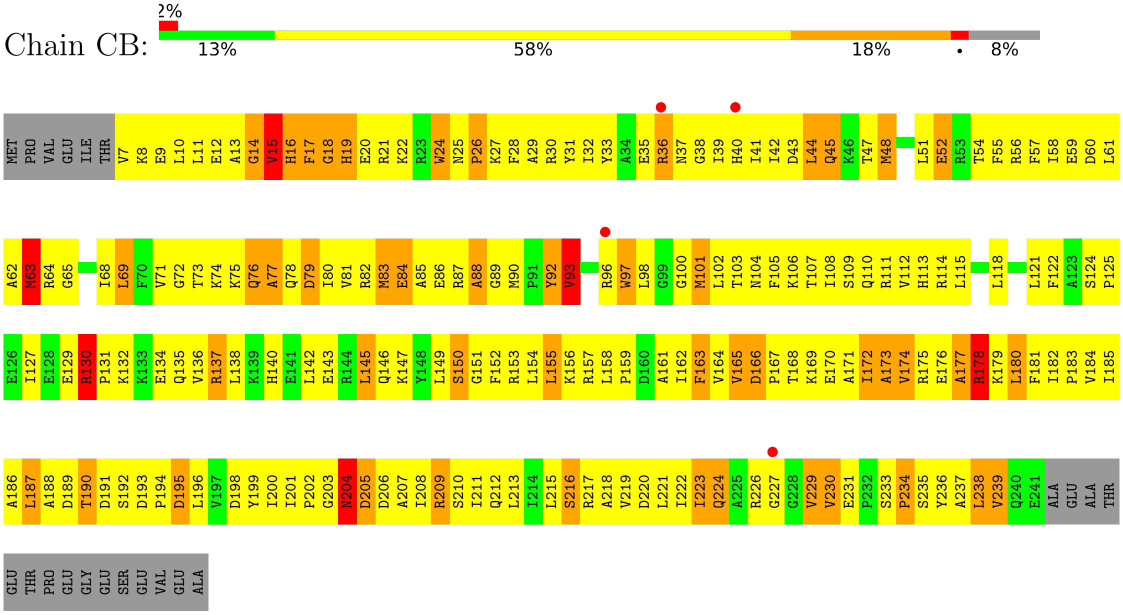

.%
11%
67%
18%
• •
U U U G U U5 G6 G7 A8 G9 A10 G11 U12 U13 U14 G15 A16 U17 C18 C19 U20 G21 G22 C23 U24 C25 A26 G27 G28 G29 U30 G31 A32 A33 C34 G35 C36 U37 G38 G39 C40 G41 G42 C43 G44 U45 G46 C47 C48 A51 G52 A53 C54 A55 U56 G57 C58 A59 A60
G61 U62 C63 G64 U65 G66 C67 G68 G69 G70 C71 C72 G73 C78 G79 G80 U81 U82 U83 U84 A88 C89 U90 C91 C92 G93 C100 A101 G102 C103 G104 G105 C106 G107 G108 A109 C110 G111 G112 G113 U114 G115 A116 G117 U118 A119 A120 C121 G122 C123 G124 U125 G126 G127 G128 U129 G129A A130
C131 C132 C135 C136 C137 G138 G139 A140 A141 G142 A143 G144 G145 G146 G147 G148 A149 C150 A151 A152 C153 C154 C155 G156 G157 G158 G159 A160 A161 A162 C163 U164 C165 G166 G167 G168 C169 U170 A171 A172 U173 C174 C175 C176 C177 C178 A179 U180 G181 U182 G183 G184 A185 C186 C187 C188 G189 C189A C189B
C189C G189G G189H G189I G189J U189K G189L U190 G191 U192 C193 C194 A195 A196 A197 G198 G199 G200 C201 U202 U203 U204 G216 C217 C218 C219 G220 C221 U222 U223 C224 C225 G226 G227 A228 U229 G230 G231 G232 C233 C234 C235 G236 G237 C241 C242 A243 U244 C245 A246 G247 A250 G251 U252 U253 G254 G255
U256 G257 G258 G259 G260 U261 A262 A263 U264 G265 G266 C267 C268 C269 A270 C271 C272 A273 A274 G275 G276 C277 G278 A279 C280 G281 A282 C283 G284 G285 G286 U287 A288 G289 C290 C291 G292 G293 U294 C295 U296 G297 G302 A303 U304 G305 G306 C307 C308 G309 G310 C311 C312 A313 C314 A315 G316 G317 G318
G319 C320 A321 C322 U323 G324 A325 G326 A327 C328 A329 C330 G331 G332 G333 C334 C335 C336 C337 A338 C341 C342 U343 A344 C345 G346 G347 G348 G351 C352 A353 G354 C355 A356 G357 U358 U359 A360 G361 G362 A363 A364 U365 C366 U367 U368 C369 C370 G371 C372 A373 A374 U375 G376 G377 G378 C379 G380
C381 A382 A383 C386 U387 G388 A389 C390 G391 G392 A393 G394 C395 G396 A397 C398 G399 C400 C401 G402 C403 U404 U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 A415 G416 C417 C418 C419 U420 U421 C422 G423 G424 G425 G426 U427 G428 U429 A430 A431 A432 C433 U434 C435 C436 U437 G438 A439 A441 C442
C443 C444 G445 G446 G447 A448 C449 G450 A451 A452 A453 C454 C455 C456 C457 C458 G460 A461 C470 C471 A472 G473 G474 G475 G476 A482 C483 G484 G485 U486 A487 C488 C489 G490 G491 G492 G493 U494 A495 A496 U498 A499 G500 C501 G502 C503 C504 G505 G506 C507 C508 A509 A510 C511 U512 C513 C514 G515 U516
G517 C518 C519 A520 G521 C522 A523 G524 C525 C526 G527 C528 G529 G530 U531 A532 A533 U534 A535 C536 G537 G538 A539 G540 G541 C542 C543 G544 C545 G546 A547 G548 C549 G550 U551 U552 A553 C554 C555 C556 G557 G558 A559 U560 U561 C562 A563 C564 U565 G566 G567 G568 C569 G570 U571 A572 A573 A574 G575 G576
G577 C578 G579 U580 G581 U582 A583 G584 G585 C586 G587 G588 C589 C590 U591 G592 G593 G594 G595 C596 G597 U598 C599 C600 C601 A602 U603 G604 U605 G606 A607 A608 A609 C612 C613 A614 C615 U619 C620 A621 A622 C623 C624 G625 U626 G627 G628 G629 G630 G631 A632 G633 C634 G635 U636 G637 G638 G639
A640 U641 A642 C643 U646 C647 A648 G649 G650 C651 U652 A653 G654 A655 C656 G657 G658 U659 G660 G661 G662 A663 G664 A665 G666 G667 G668 U669 G670 C671 U672 G673 G674 A675 A676 U677 U678 C679 C680 C681 G682 G683 A684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 U697 G698 C699 G700
C701 A702 G703 A704 U705 A706 C707 C708 G709 G710 G711 A712 G713 G714 A715 A716 C719 C720 G721 A722 U723 G724 G725 C726 G727 A728 A729 G730 G731 C732 A733 G734 C735 C736 A737 C738 C739 U740 G741 G742 U743 C744 C745 A746 C747 C748 C749 G750 U751 C754 G755 C756 U757 G758 G761 C762 G763
C764 G765 A766 A767 A768 G769 C770 G771 U772 G773 G774 C775 G776 A777 G778 C779 A780 A781 A782 C783 C784 G785 C786 A787 U788 U789 A790 G791 A792 U793 A794 C795 C796 C797 G798 G799 G800 U801 A802 G803 U804 C805 C806 A807 C808 G809 C810 C811 C812 U813 A814 A815 A816 C817 G818 A819 U820 G821 C822 G823
C824 G825 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 G837 G838 U839 C840 U841 C848 C849 U850 G851 G852 G853 G854 G855 C856 C857 G858 A859 A860 G861 C862 U863 A864 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 C875 G876 C877 G878 C879 C880 G881 C882 C883 U884 G885 G886 G887 G888 A889
G890 U891 A892 C893 G894 G895 C896 C897 G898 C899 A900 A901 G902 G903 C904 U905 G906 A907 A908 A909 C912 A913 A914 A915 G916 G917 A918 A919 U920 U921 G922 A923 C924 G925 G926 G927 G928 G929 C930 C931 G932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 U943 G944 G945 A946 C947 C948 A949 U950



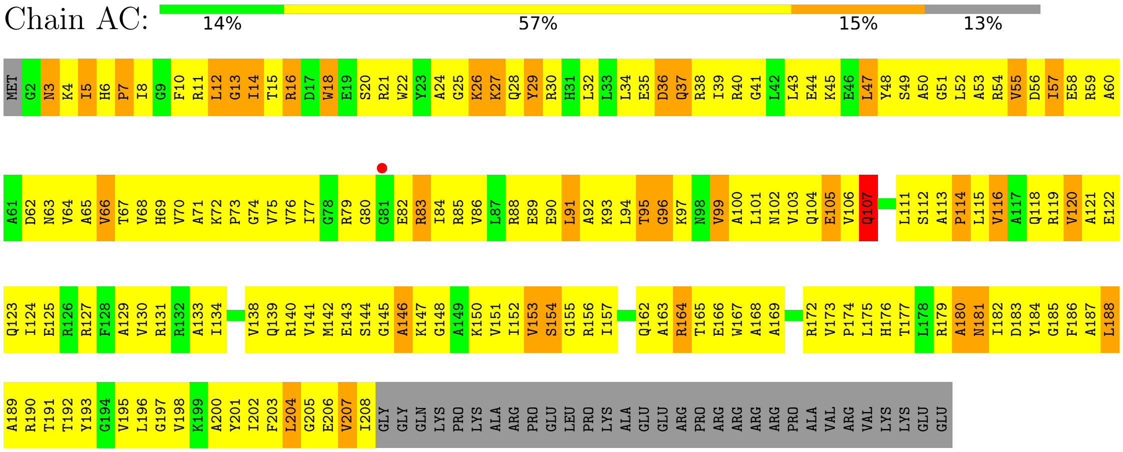
- Molecule 2: 30S RIBOSOMAL PROTEIN S2



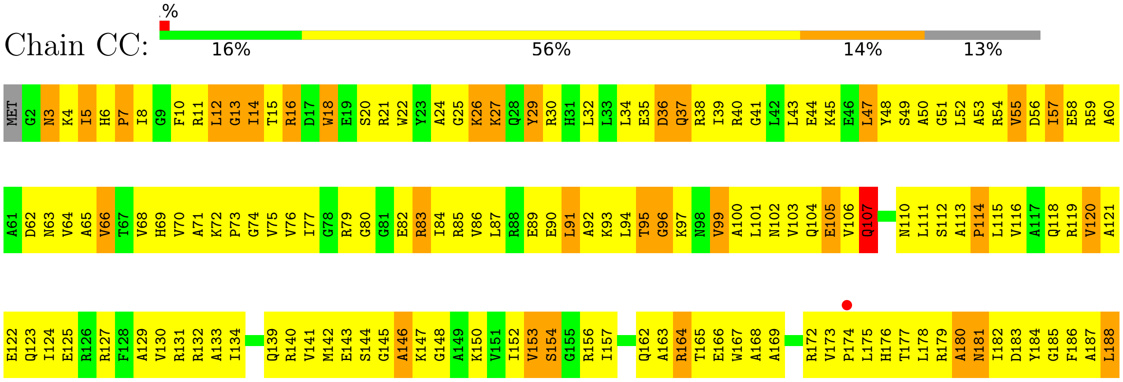
- Molecule 2: 30S RIBOSOMAL PROTEIN S2



- Molecule 3: 30S RIBOSOMAL PROTEIN S3



- Molecule 3: 30S RIBOSOMAL PROTEIN S3



A189 R190 T191 T192 Y193 G194 V195 L196 G197 V198 K199 A200 Y201 I202 F203 L204 G205 E206 V207 I208 GLY GLY GLN LYS PRO LYS ALA ARG PRO GLU LEU PRO LYS ALA GLU GLU ARG PRO ARG ARG ARG ARG ARG PRO ALA VAL ARG VAL LYS LYS GLU GLU

- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD: 14% 59% 24% •

MET G2 R3 Y4 I5 G6 P7 V8 C9 R10 L11 C12 R13 R14 E15 G16 V17 K18 L19 Y20 L21 K22 G23 E24 R25 C26 Y27 S28 P29 K30 C31 A32 M33 E34 R35 R36 P37 Y38 P39 P40 G41 Q42 H43 G44 Q45 K46 R47 A48 R49 R50 P51 S52 D53 Y54 A55 V56 R57 L58 R59 E60

K61 Q62 K63 L64 R65 R66 I67 Y68 G69 I70 S71 E72 R73 Q74 F75 R76 N77 L78 F79 E80 E81 A82 K85 K86 G87 V88 T89 G90 S91 V92 F93 L94 G95 L96 L97 E98 S99 R100 L101 D102 N103 V104 V105 Y106 R107 L108 G109 F110 A111 V112 S113 R114 R115 Q116 A117 R118 Q119 L120 V121

R122 H123 G124 H125 I126 T127 V128 N129 G130 R131 R132 V133 D134 L135 P136 S137 Y138 R139 V140 E145 A149 E150 K151 S152 R153 N154 L155 E156 L157 I158 R159 Q160 N161 L162 E163 A164 M165 K166 V170 G171 P172 W173 L174 S175 L176 D177 V178 E179 G180 M181 K182 G183 K184 F185 L186 R187 L188

P189 D190 R191 E192 D193 L194 A195 L196 P197 V198 N199 E200 Q201 L202 V203 I204 E205 F206 Y207 S208 R209

- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD: 14% 57% 26% •

MET G2 R3 Y4 I5 G6 P7 V8 C9 R10 L11 C12 R13 R14 E15 G16 V17 K18 L19 Y20 L21 K22 G23 E24 R25 C26 Y27 S28 P29 K30 C31 A32 M33 E34 R35 R36 P37 Y38 P39 P40 G41 Q42 H43 G44 Q45 K46 R47 A48 R49 R50 P51 S52 D53 Y54 A55 V56 R57 L58 R59 E60

K61 Q62 K63 L64 R65 R66 I67 Y68 G69 I70 S71 E72 R73 Q74 F75 R76 N77 L78 F79 E80 E81 K85 K86 G87 V88 T89 G90 S91 V92 F93 L94 G95 L96 L97 E98 S99 R100 L101 D102 N103 V104 V105 Y106 R107 L108 G109 F110 A111 V112 S113 R114 R115 Q116 A117 R118 Q119 L120 V121 R122

H123 G124 H125 I126 T127 V128 N129 G130 R131 R132 V133 D134 L135 P136 S137 Y138 R139 V140 E145 A149 E150 K151 S152 R153 N154 L155 E156 L157 I158 R159 Q160 N161 L162 E163 A164 M165 K166 V170 G171 P172 W173 L174 S175 L176 D177 V178 E179 G180 M181 K182 G183 K184 F185 L186 R187 L188 P189

D190 R191 E192 D193 L194 A195 L196 P197 V198 N199 E200 Q201 L202 V203 I204 E205 F206 Y207 S208 R209

- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE: 20% 60% 12% • 7%

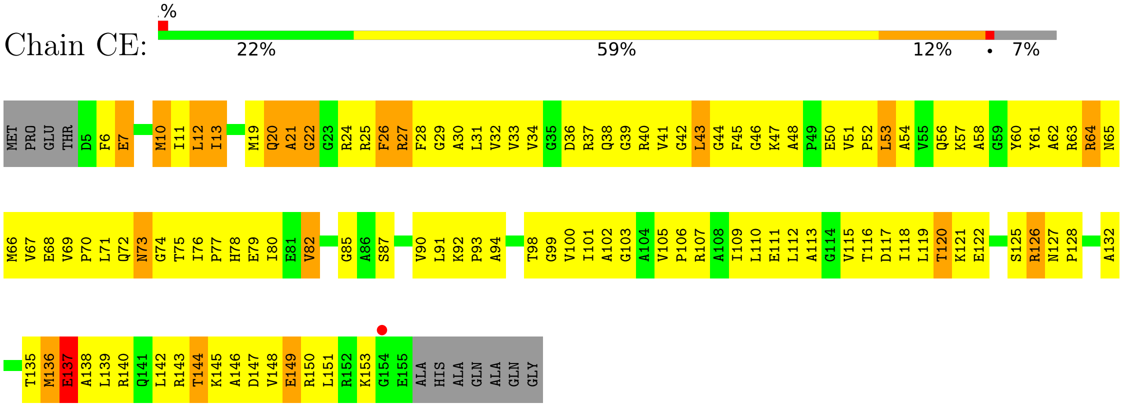
MET PRO GLU THR D5 F6 E7 M10 I11 L12 I13 M19 Q20 A21 G22 G23 R24 R25 F26 R27 F28 G29 A30 L31 V32 V33 V34 G35 D36 R37 Q38 G39 R40 V41 G42 L43 G44 F45 G46 K47 A48 P49 E50 V51 P52 L53 A54 V55 Q56 K57 A58 G59 Y60 Y61 A62 R63 R64 N65

M66 V67 E68 V69 P70 L71 Q72 N73 G74 T75 I76 P77 H78 E79 I80 E81 V82 E83 F84 G85 A86 S87 V90 L91 K92 P93 A94 T98 G99 V100 I101 A102 G103 A104 V105 P106 R107 A108 I109 L110 E111 L112 A113 G114 V115 T116 D117 I118 L119 T120 K121 E122 S125 R126 N127 P128

I131 A132 Y133 A134 T135 M136 E137 A138 L139 R140 Q141 L142 R143 T144 K145 A146 D147 V148 E149 R150 L151 R152 K153 G154 E155 ALA HIS ALA GLN ALA GLN GLY

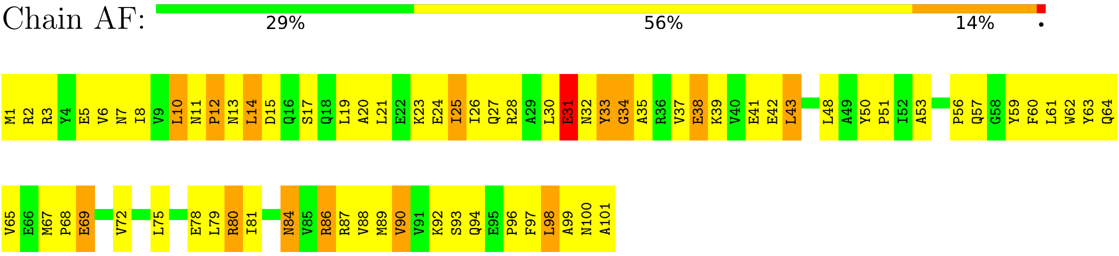
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:



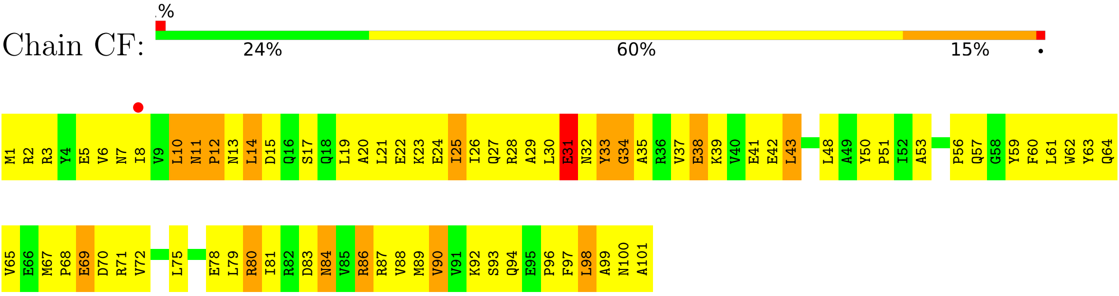
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



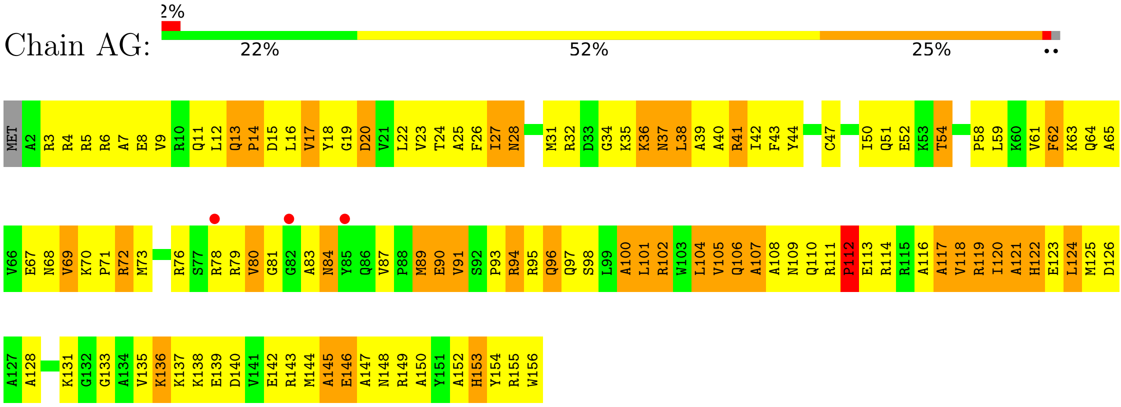
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF:



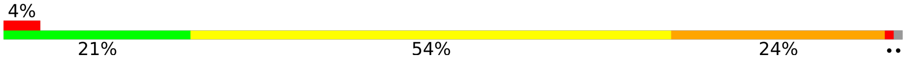
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

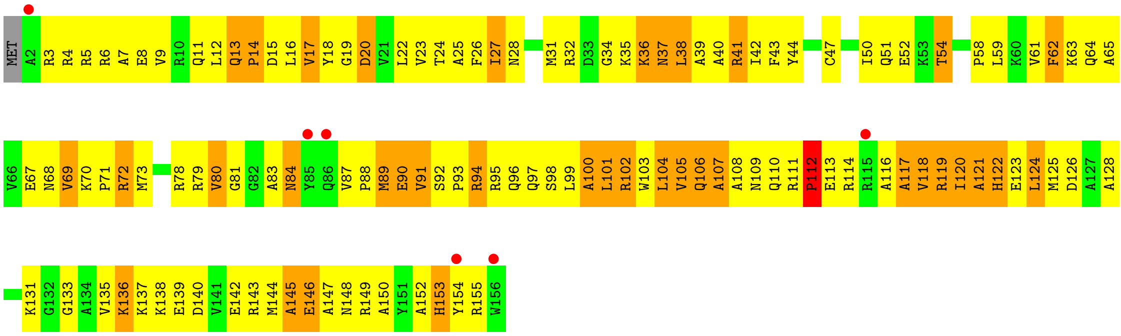
Chain AG:



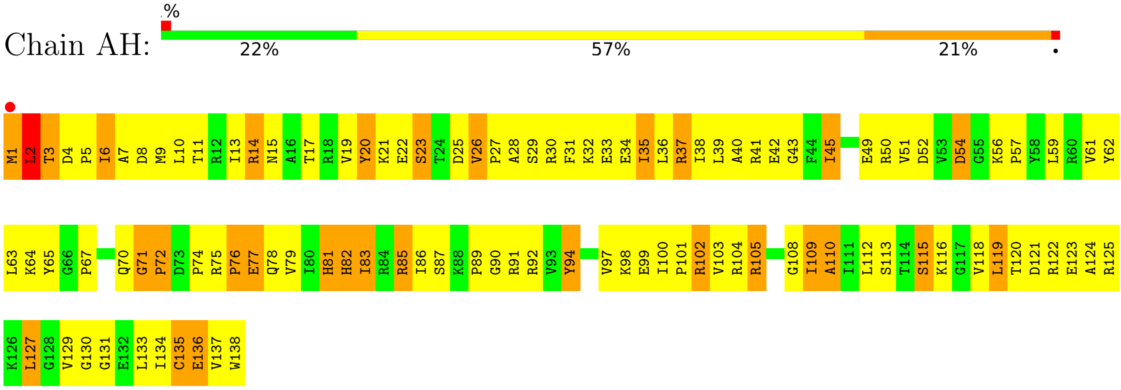
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG:

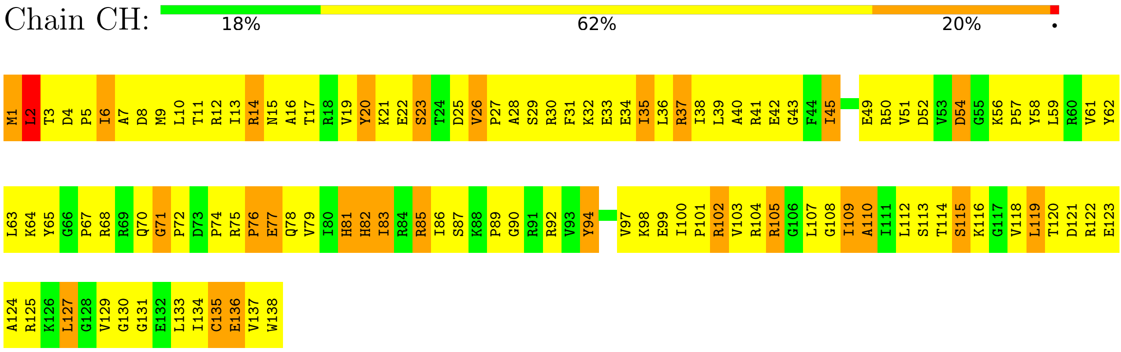




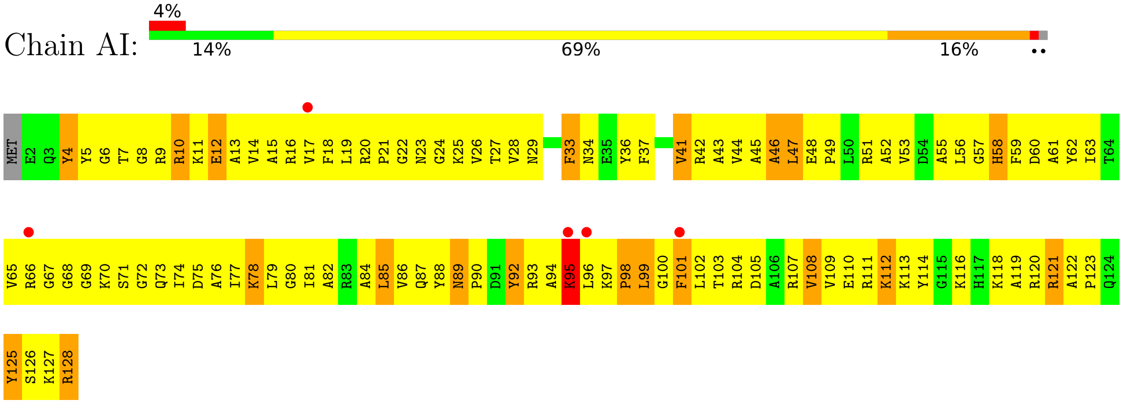
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



- Molecule 8: 30S RIBOSOMAL PROTEIN S8

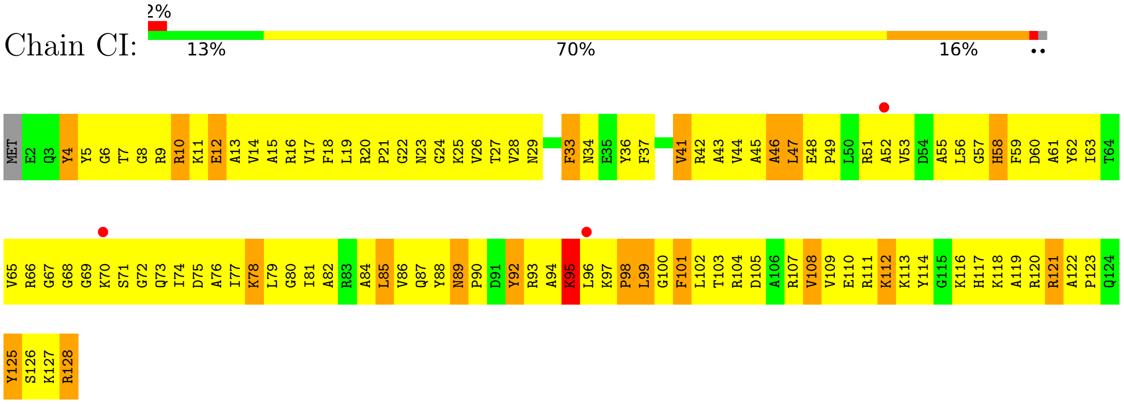


- Molecule 9: 30S RIBOSOMAL PROTEIN S9



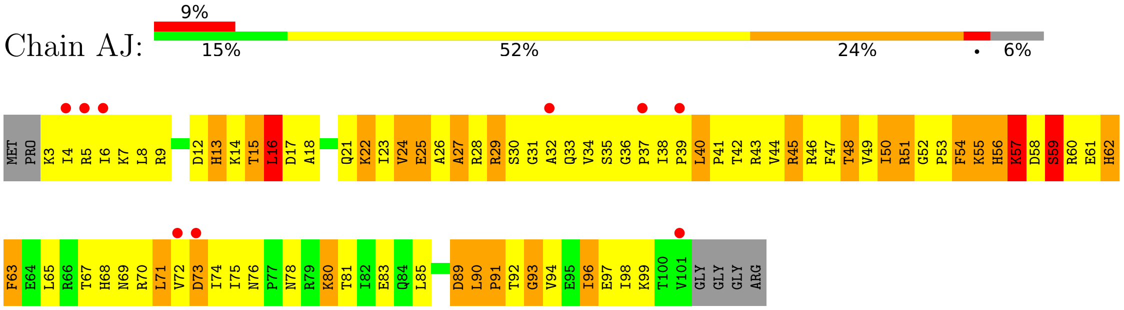
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



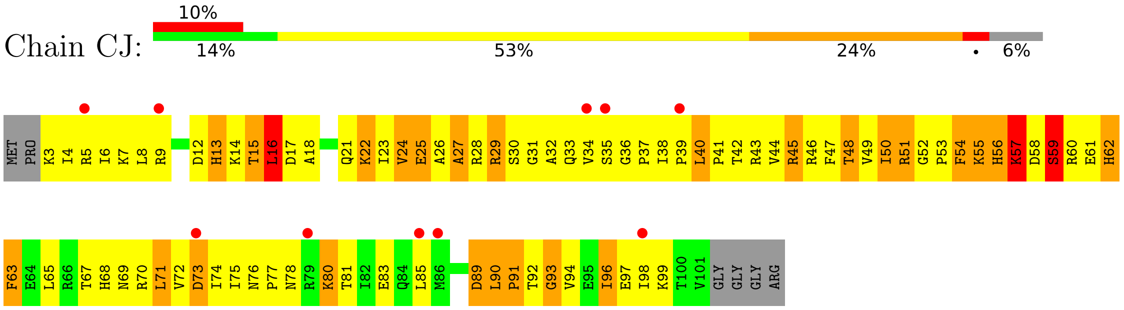
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



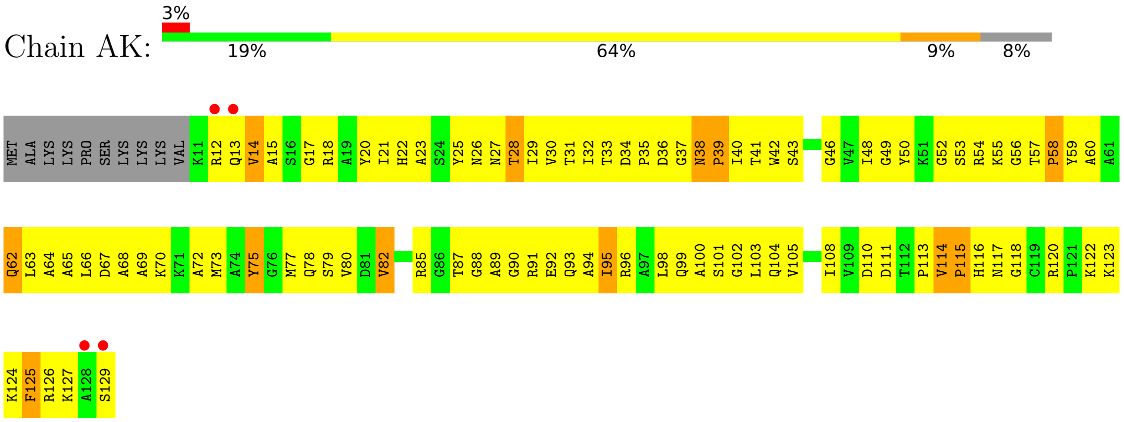
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:

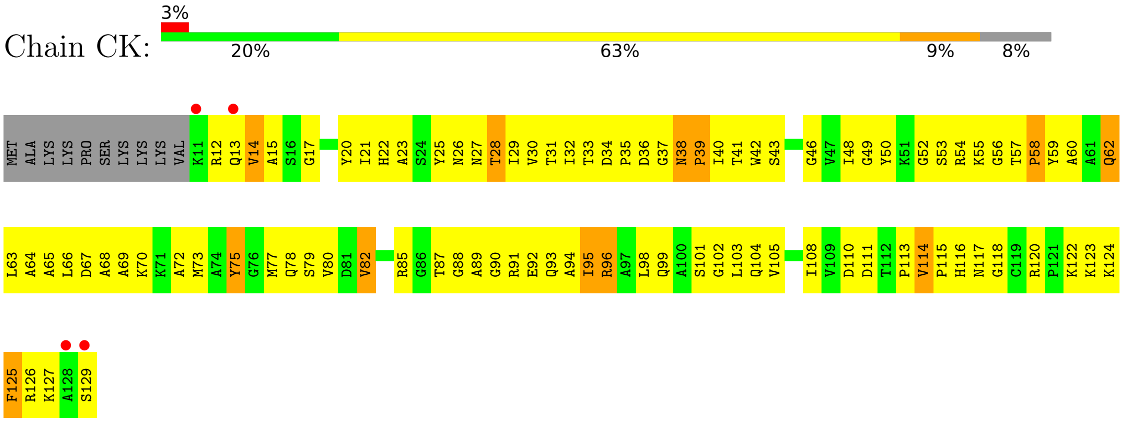


- Molecule 11: 30S RIBOSOMAL PROTEIN S11

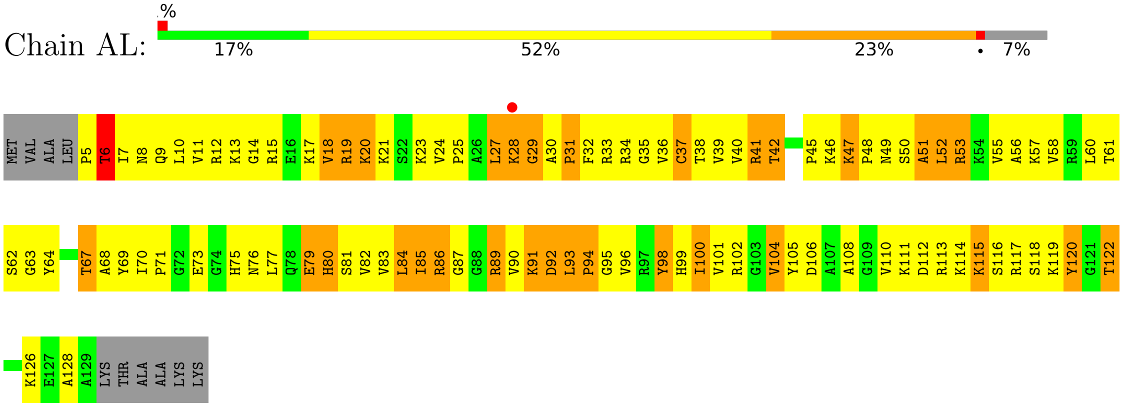
Chain AK:



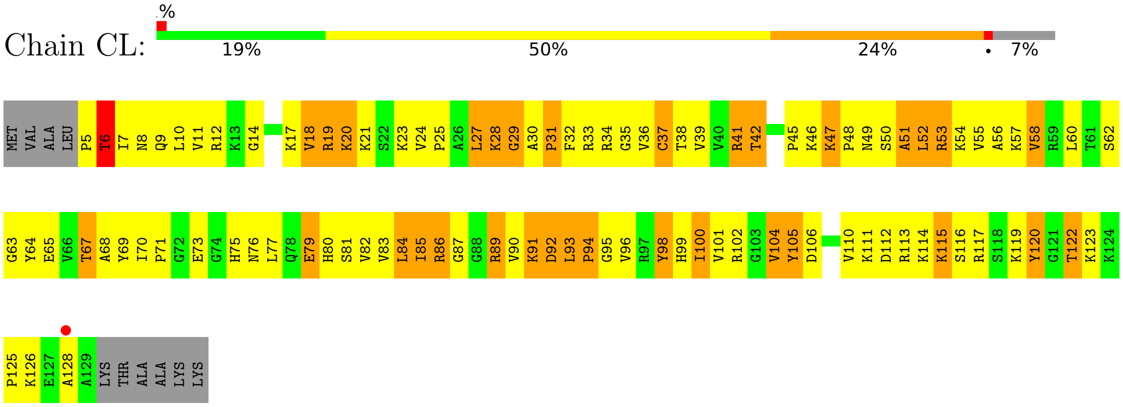
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



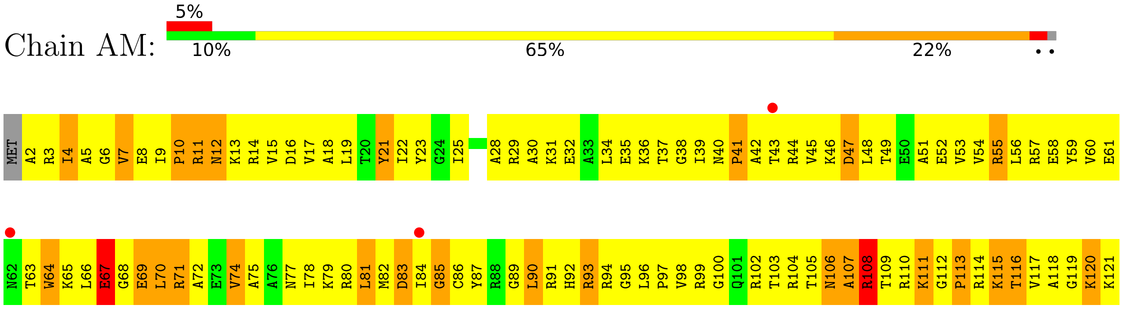
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

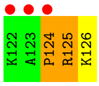


- Molecule 12: 30S RIBOSOMAL PROTEIN S12

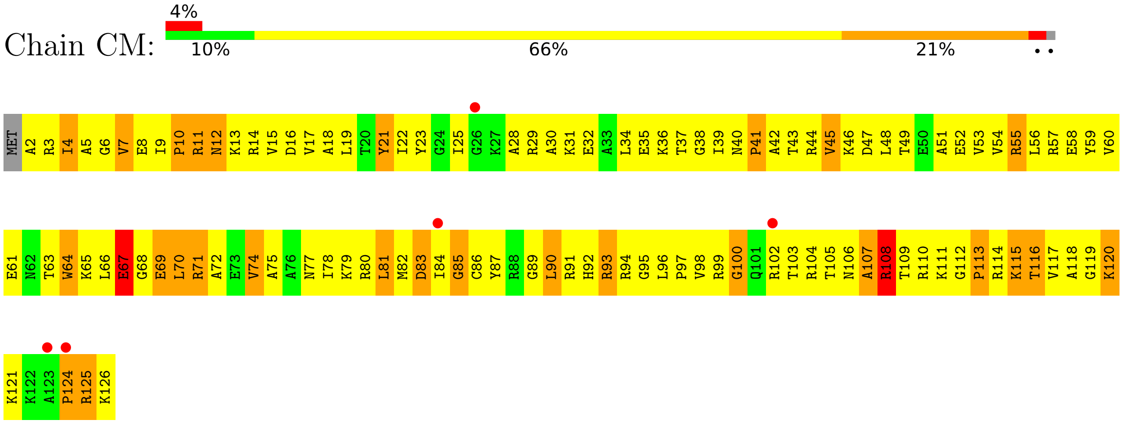


- Molecule 13: 30S RIBOSOMAL PROTEIN S13

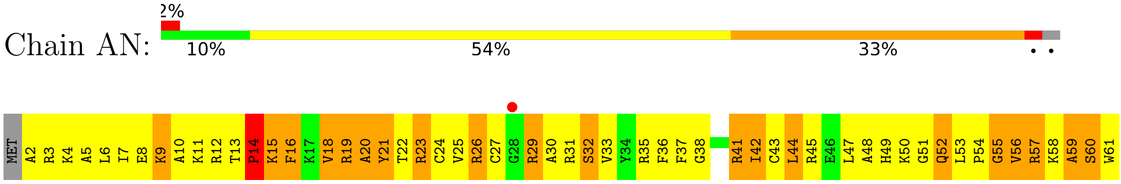




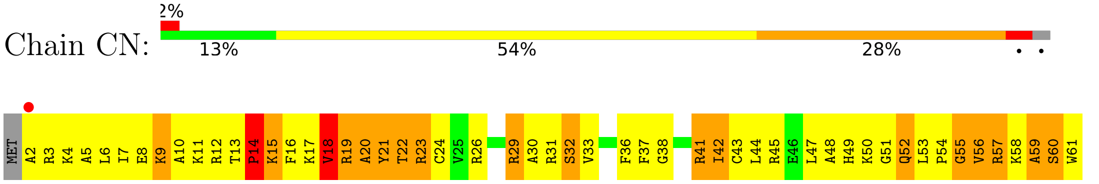
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



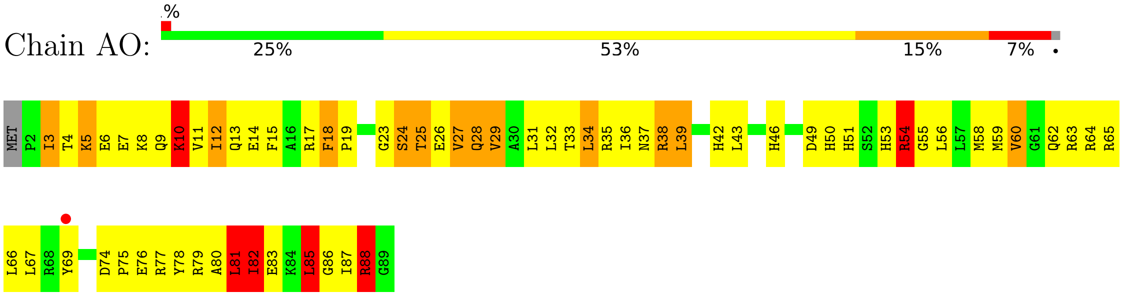
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



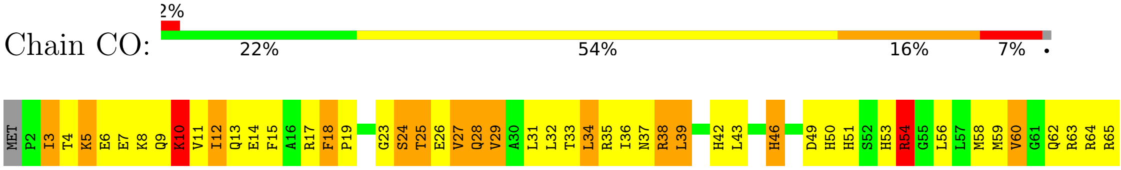
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

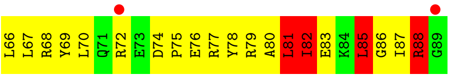


- Molecule 15: 30S RIBOSOMAL PROTEIN S15



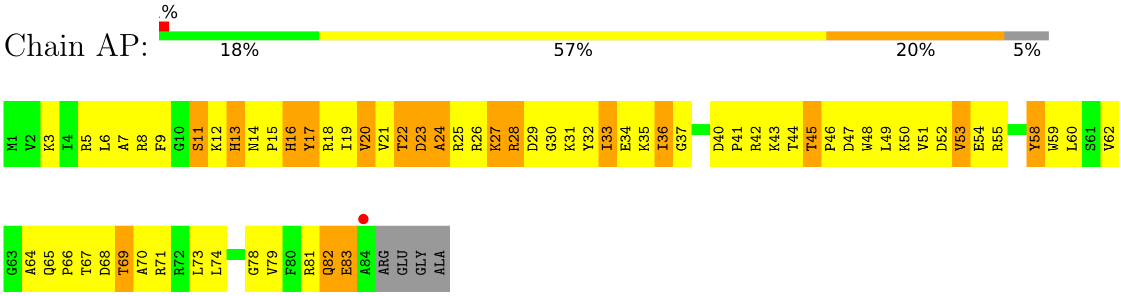
- Molecule 15: 30S RIBOSOMAL PROTEIN S15





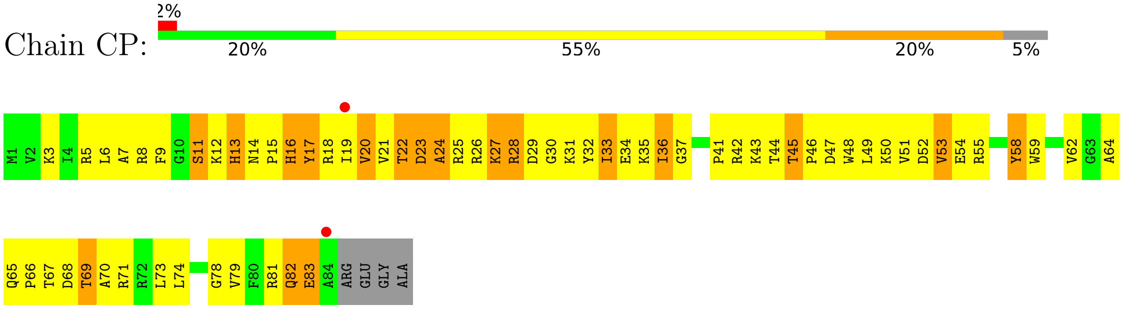
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



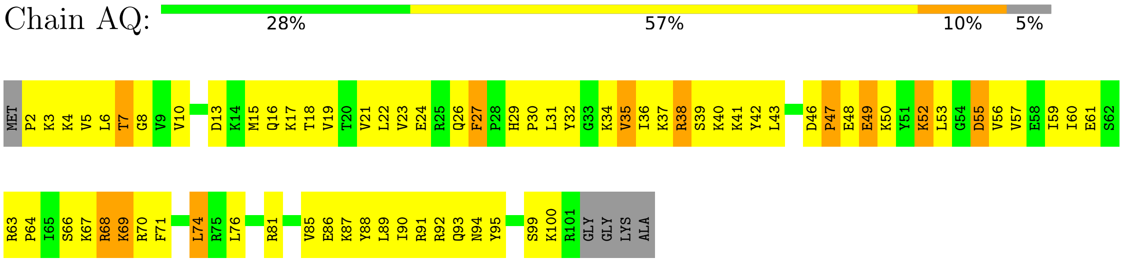
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



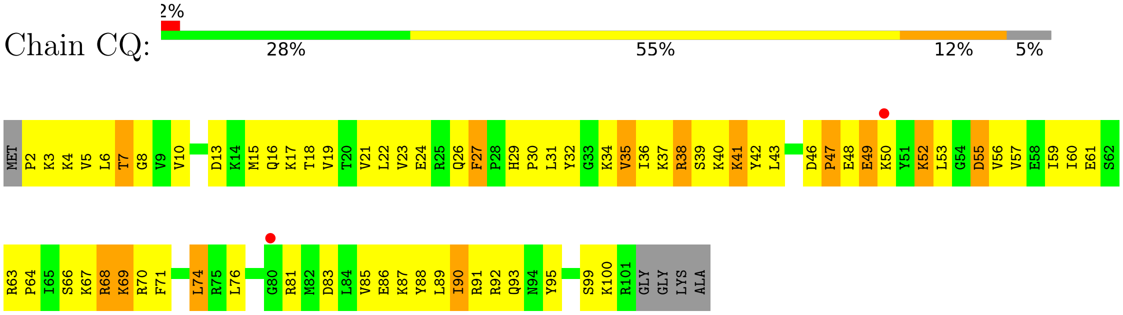
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



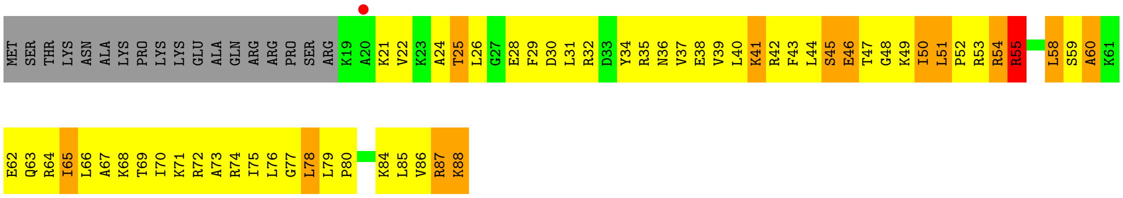
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



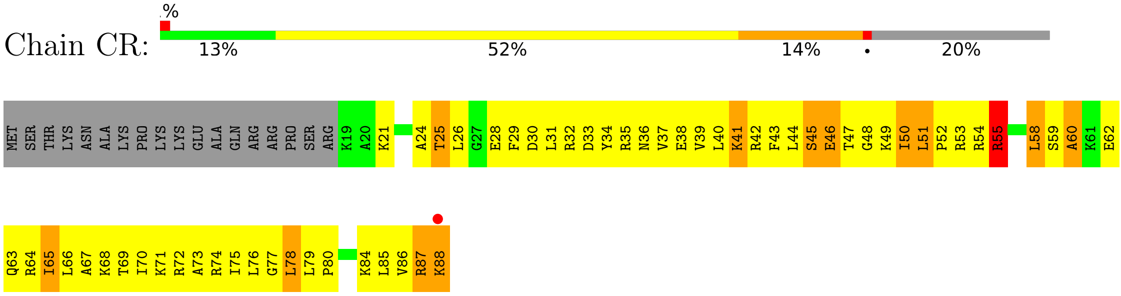
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



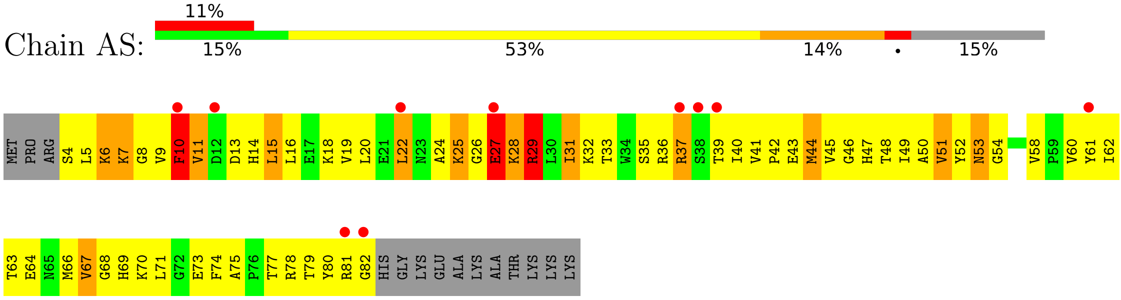
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:



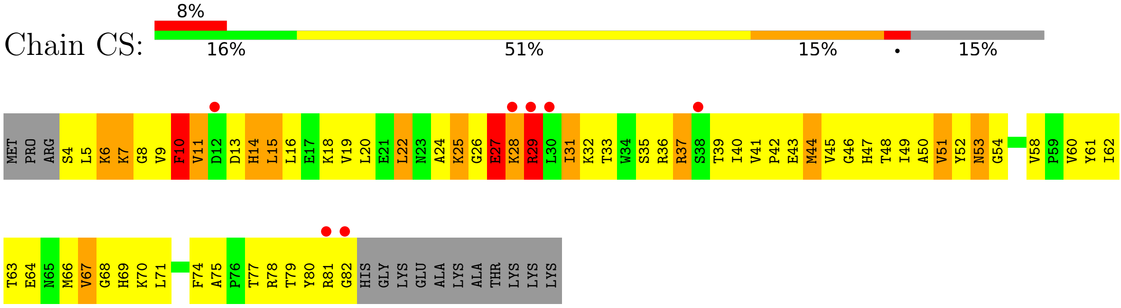
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



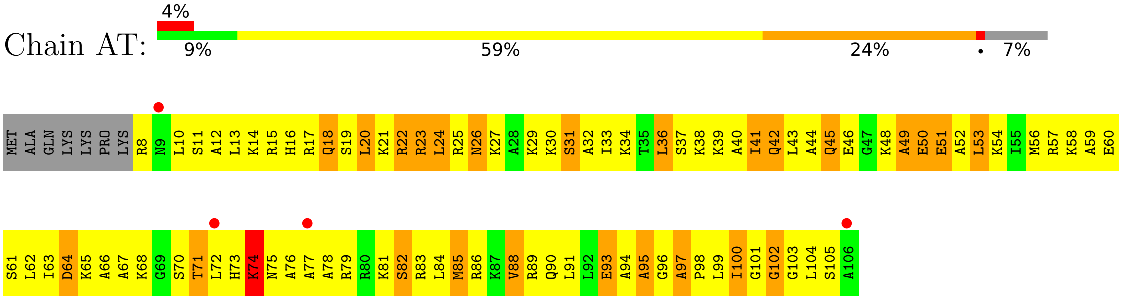
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:

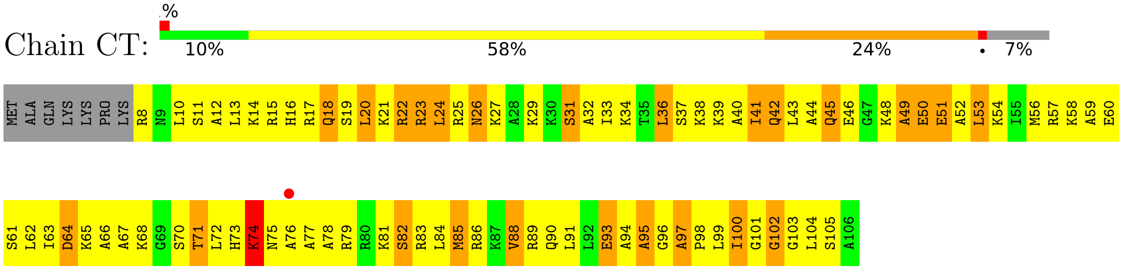


- Molecule 20: 30S RIBOSOMAL PROTEIN S20

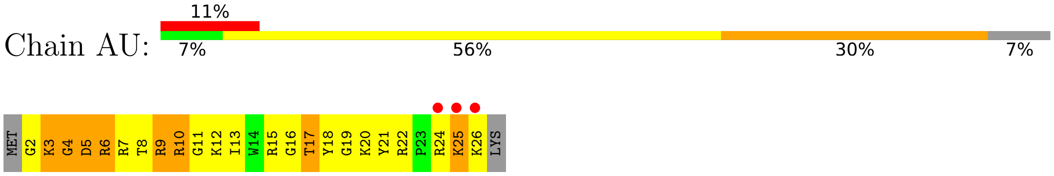
Chain AT:



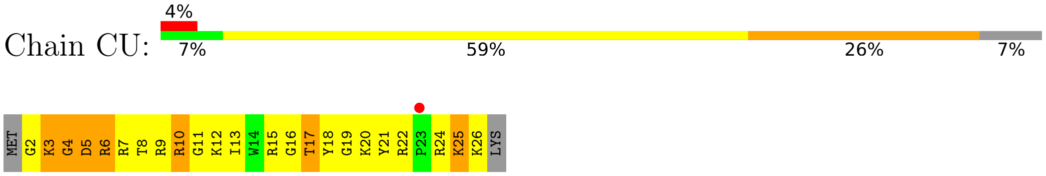
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



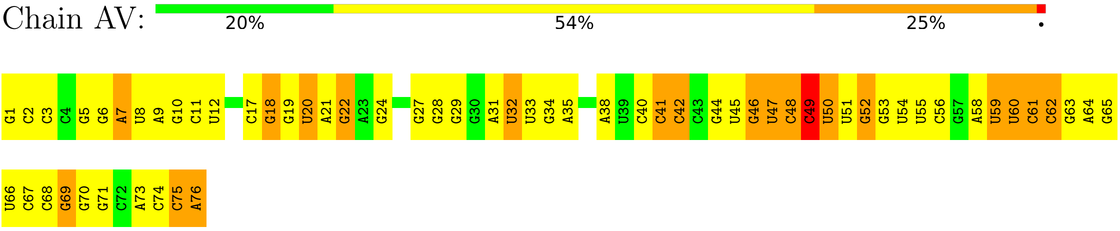
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



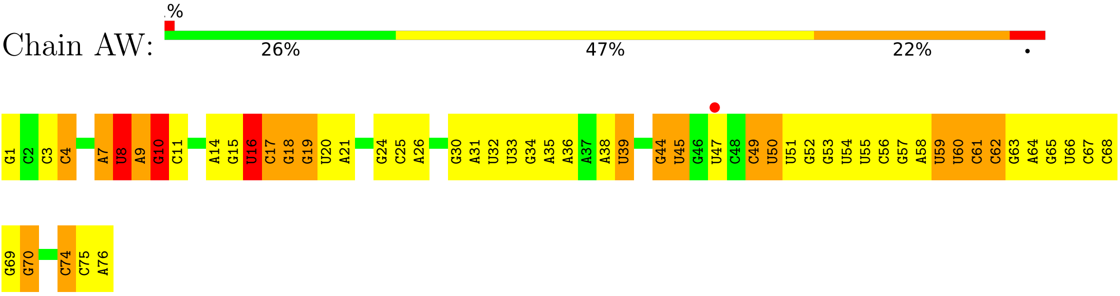
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



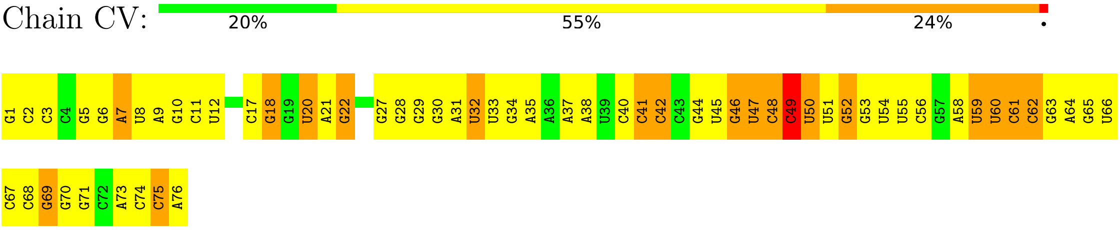
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

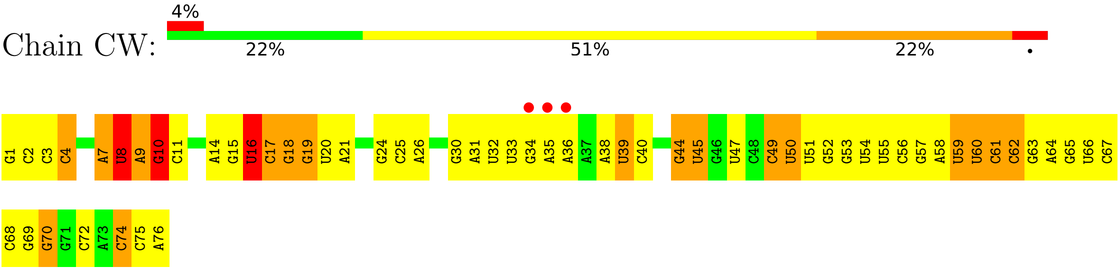


- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



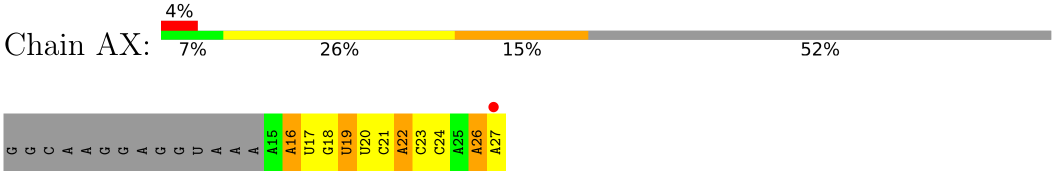
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain CW:



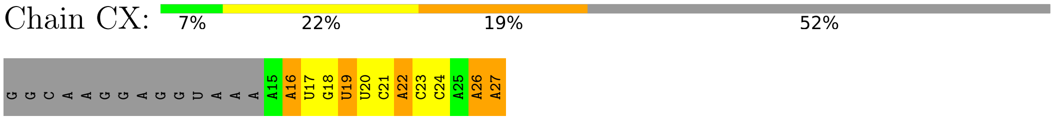
- Molecule 23: MRNA

Chain AX:



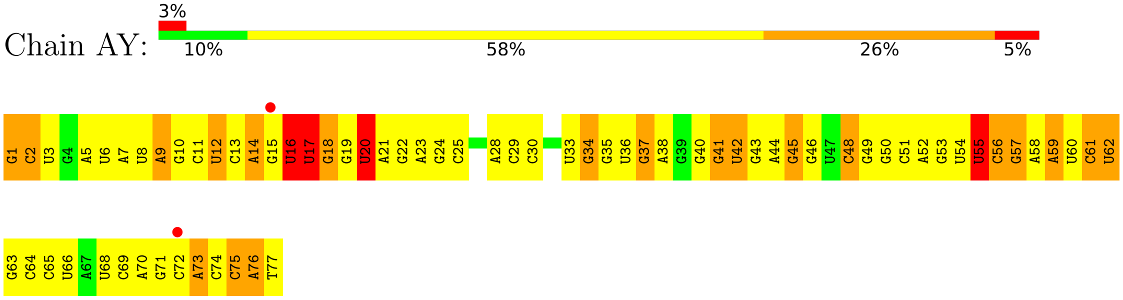
- Molecule 23: MRNA

Chain CX:



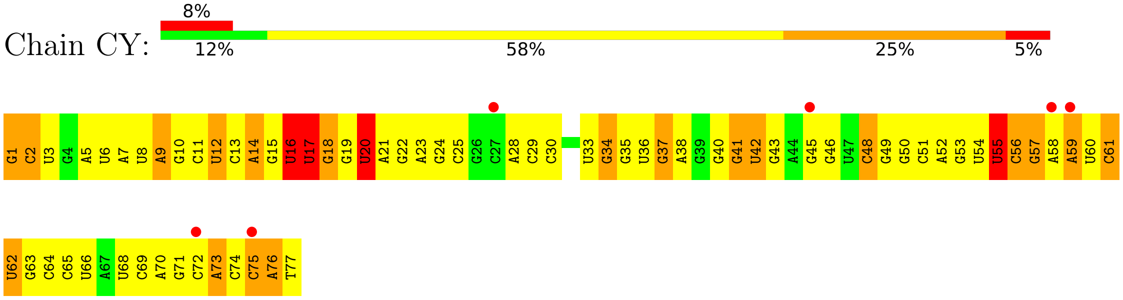
- Molecule 24: A-SITE TRNA THR

Chain AY:



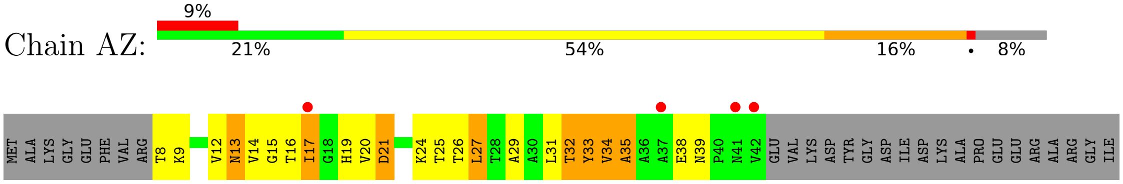
- Molecule 24: A-SITE TRNA THR

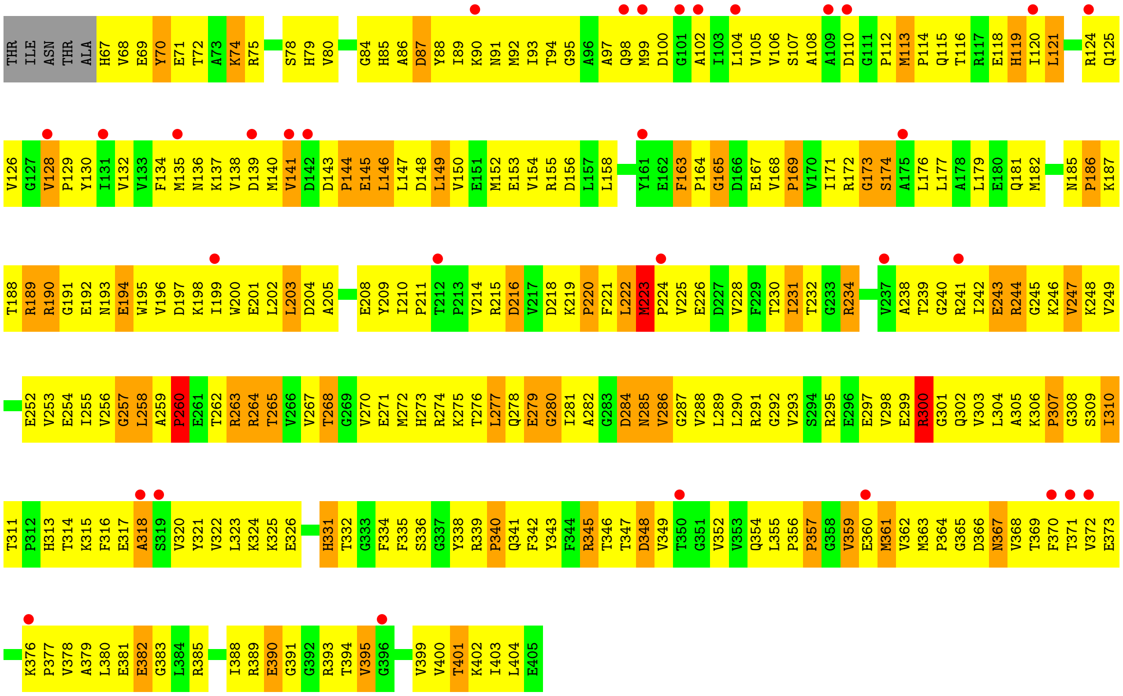
Chain CY:



- Molecule 25: ELONGATION FACTOR TU-A

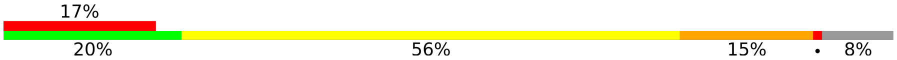
Chain AZ:

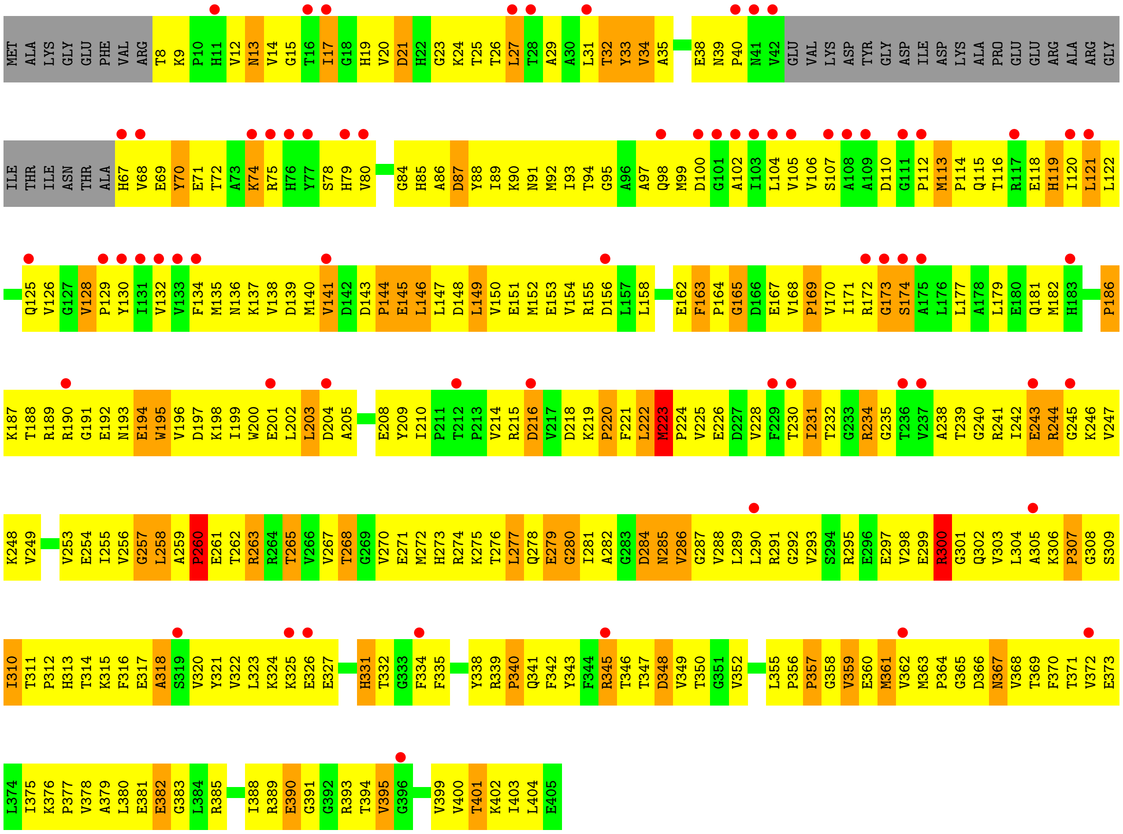




- Molecule 25: ELONGATION FACTOR TU-A

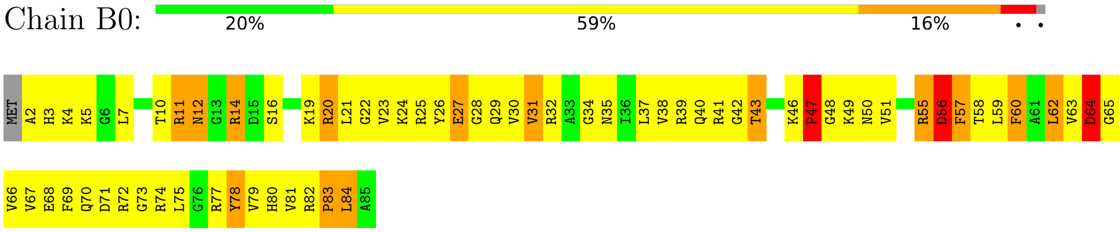
Chain CZ:





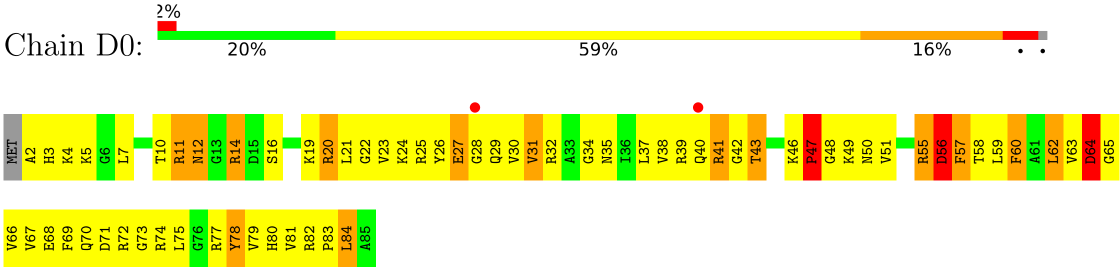
- Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain B0:



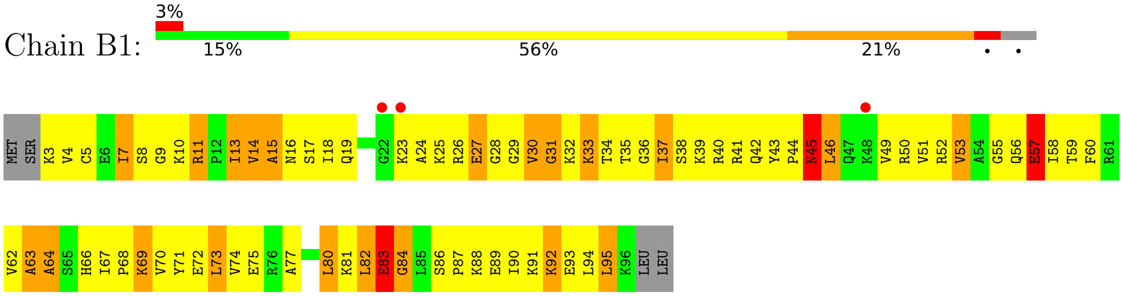
- Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain D0:



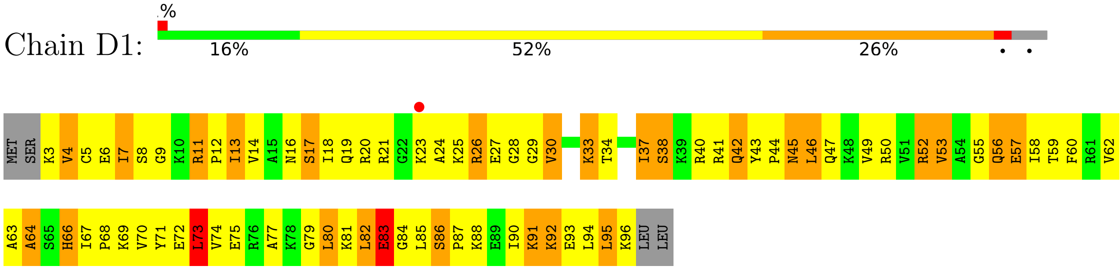
- Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain B1:



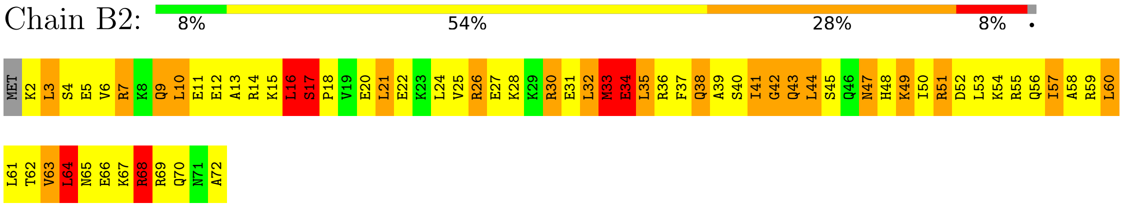
- Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain D1:



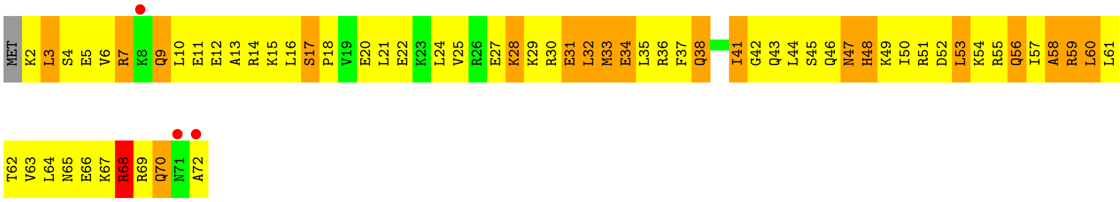
- Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain B2:



- Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain D2:

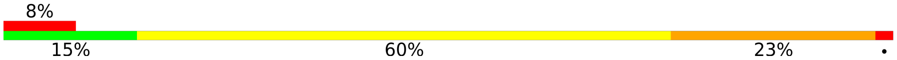


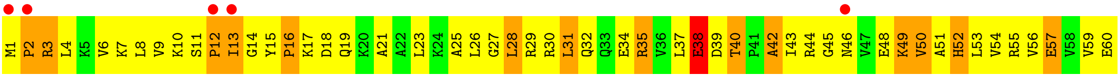
- Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain B3:

- Molecule 29: 50S RIBOSOMAL PROTEIN L30

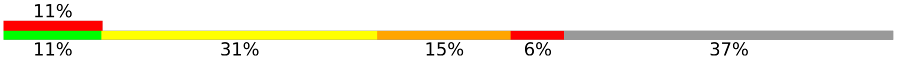
Chain D3:

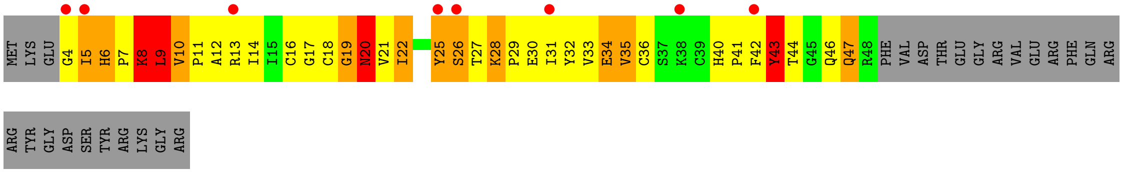




- Molecule 30: 50S RIBOSOMAL PROTEIN L31

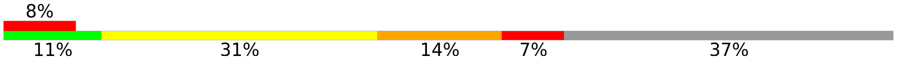
Chain B4:

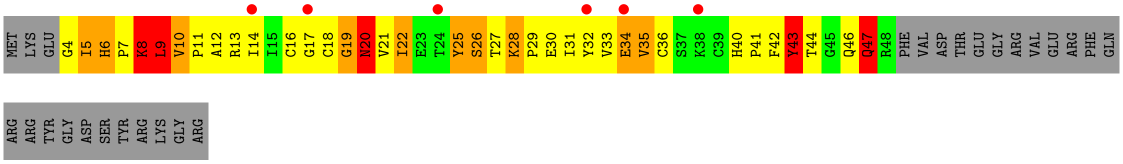




- Molecule 30: 50S RIBOSOMAL PROTEIN L31

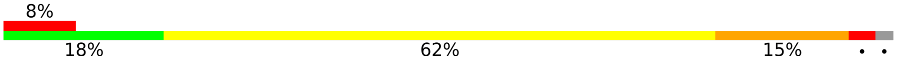
Chain D4:

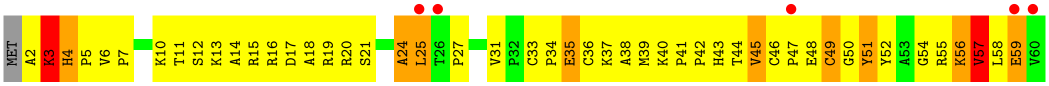




- Molecule 31: 50S RIBOSOMAL PROTEIN L32

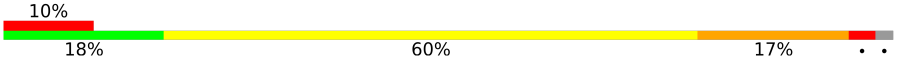
Chain B5:

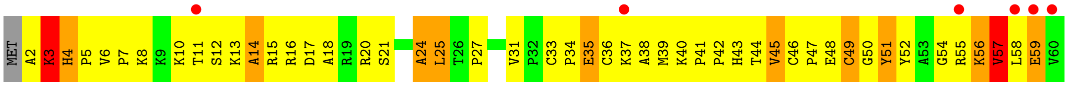




- Molecule 31: 50S RIBOSOMAL PROTEIN L32

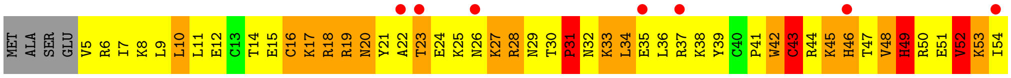
Chain D5:





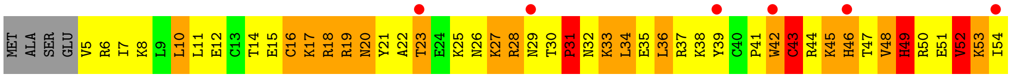
- Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain B6:



- Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain D6:



- Molecule 33: 50S RIBOSOMAL PROTEIN L34

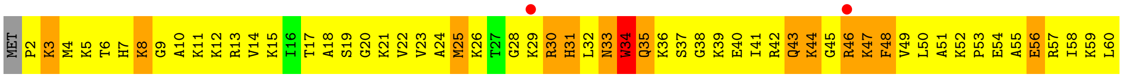
Chain B7:

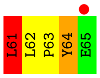
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain D7:

- Molecule 34: 50S RIBOSOMAL PROTEIN L35

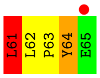
Chain B8:





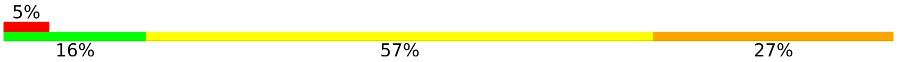
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

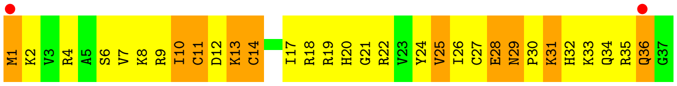
Chain D8:



• Molecule 35: 50S RIBOSOMAL PROTEIN L36

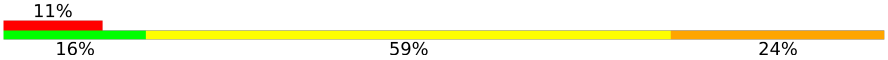
Chain B9:

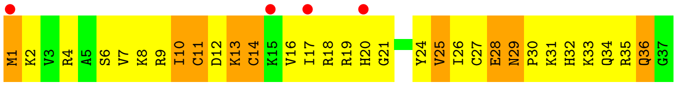




• Molecule 35: 50S RIBOSOMAL PROTEIN L36

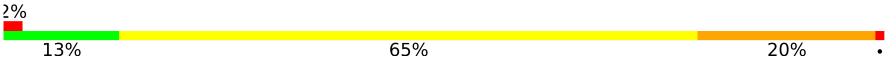
Chain D9:

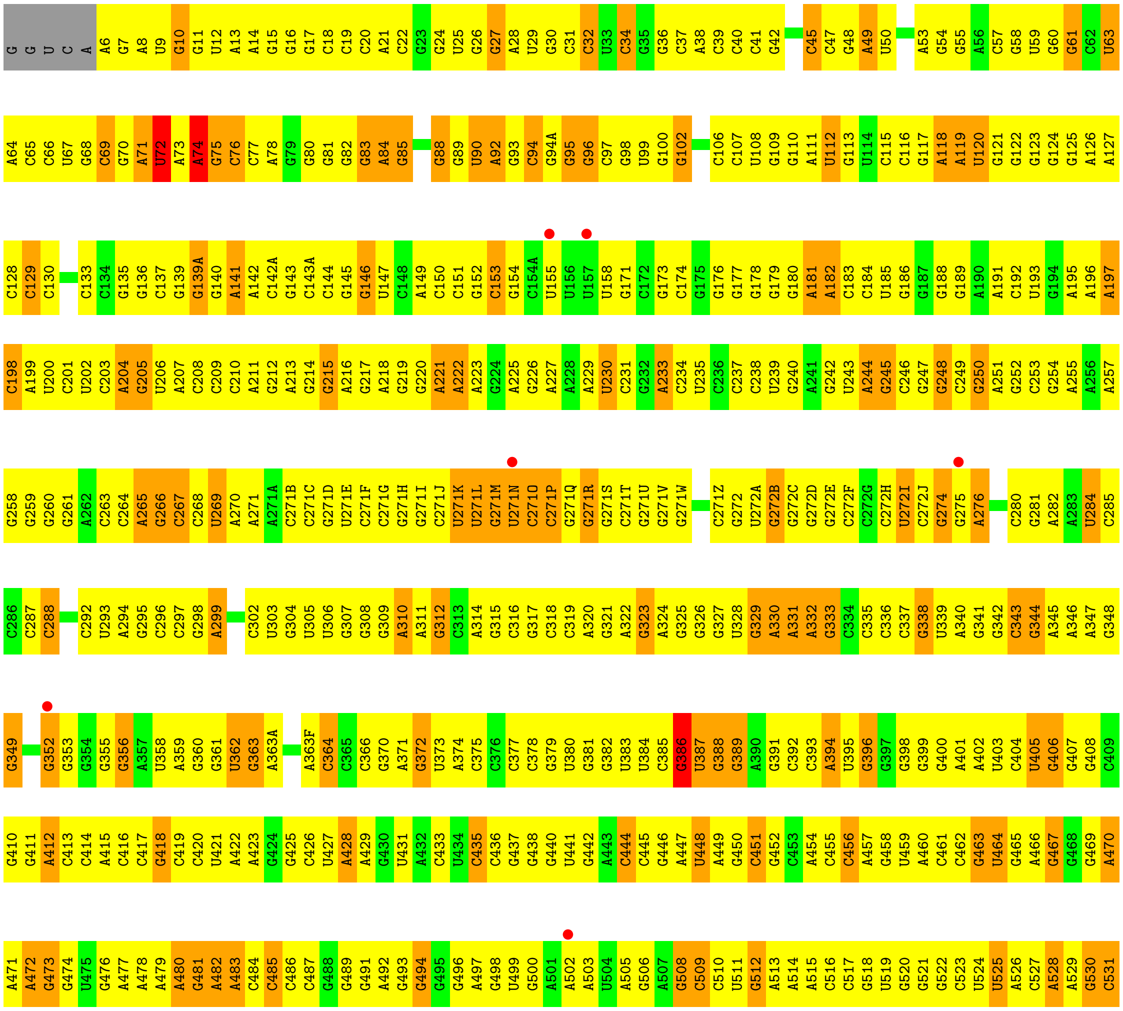


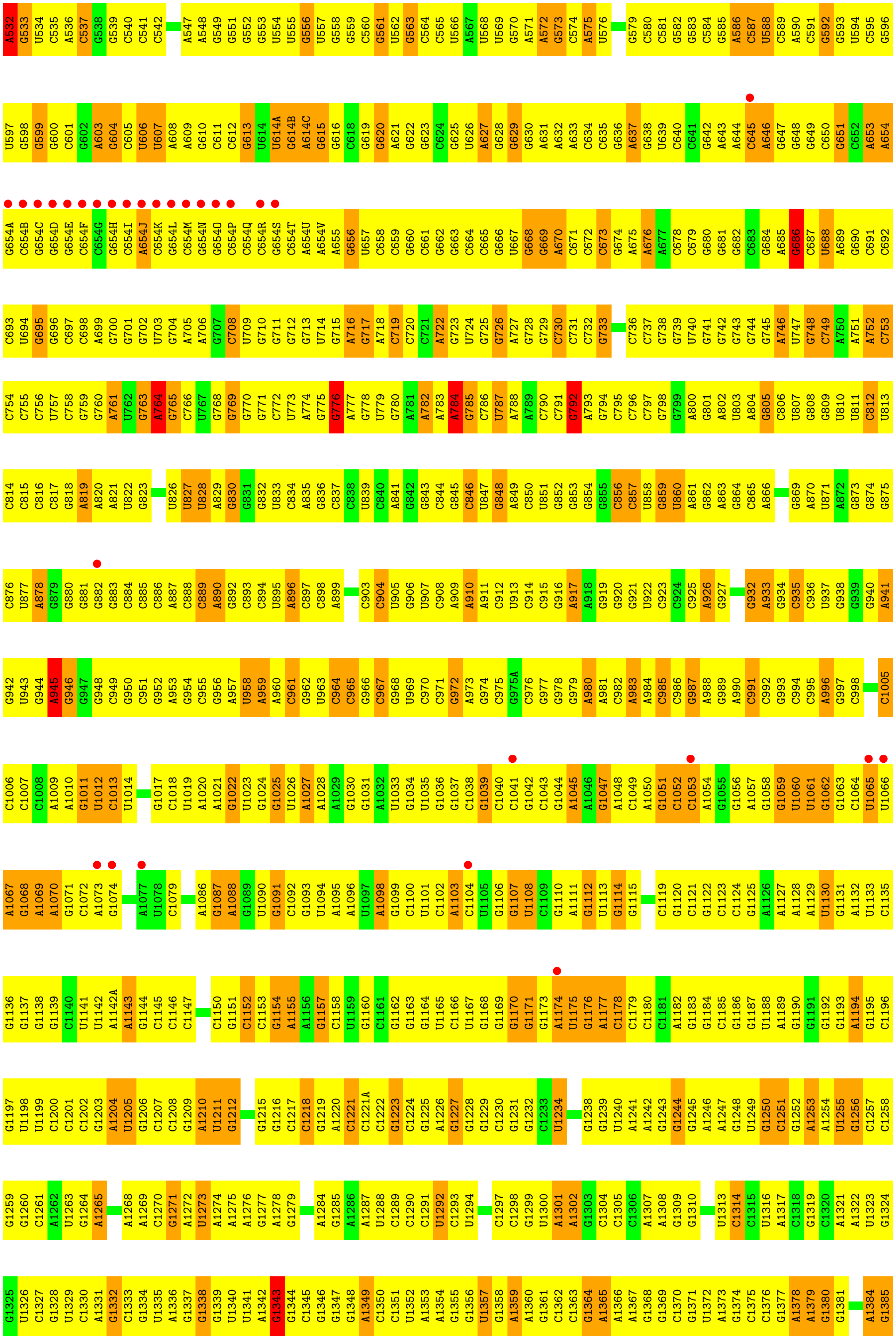


• Molecule 36: 23S RIBOSOMAL RNA

Chain BA:



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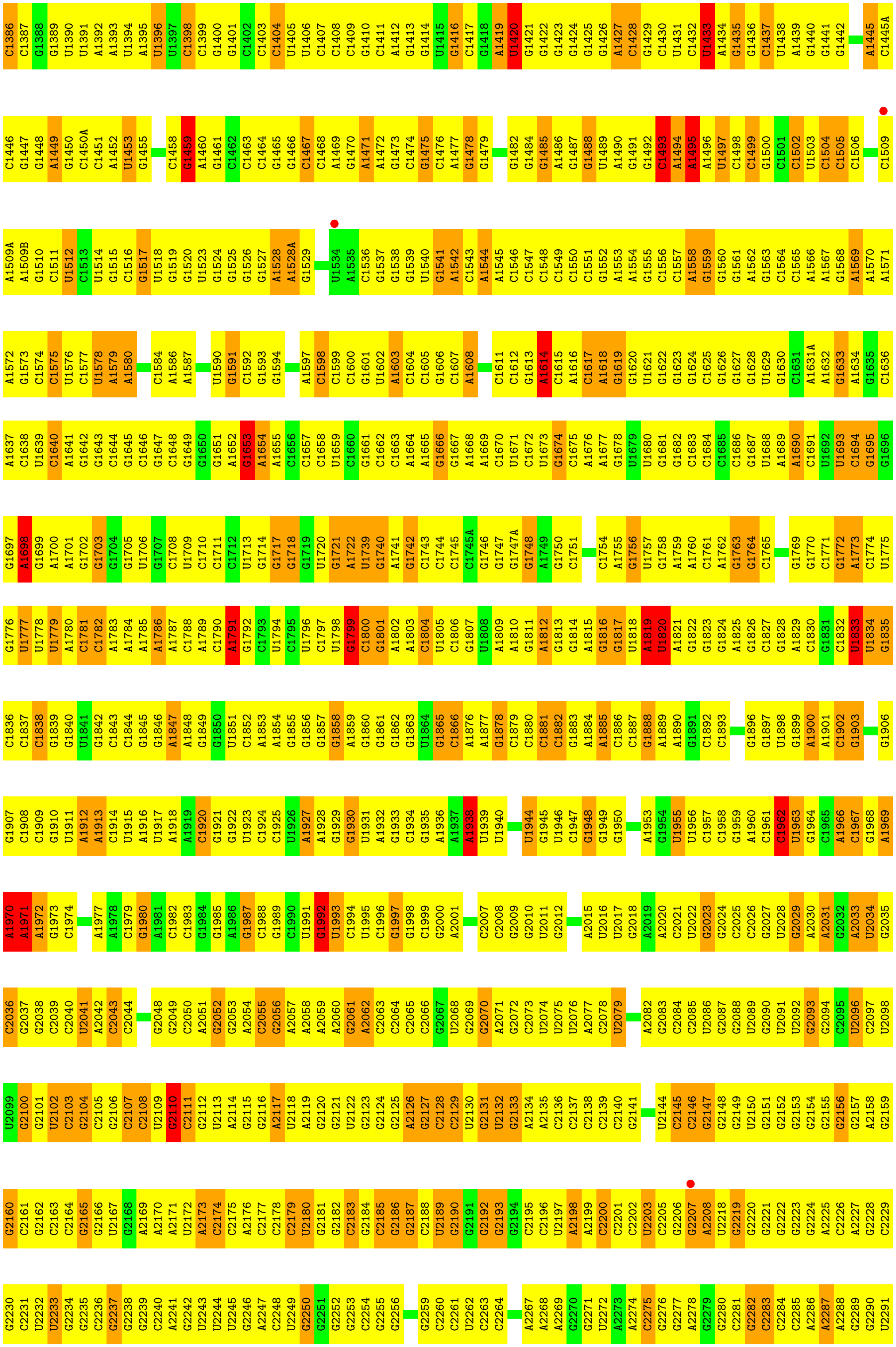
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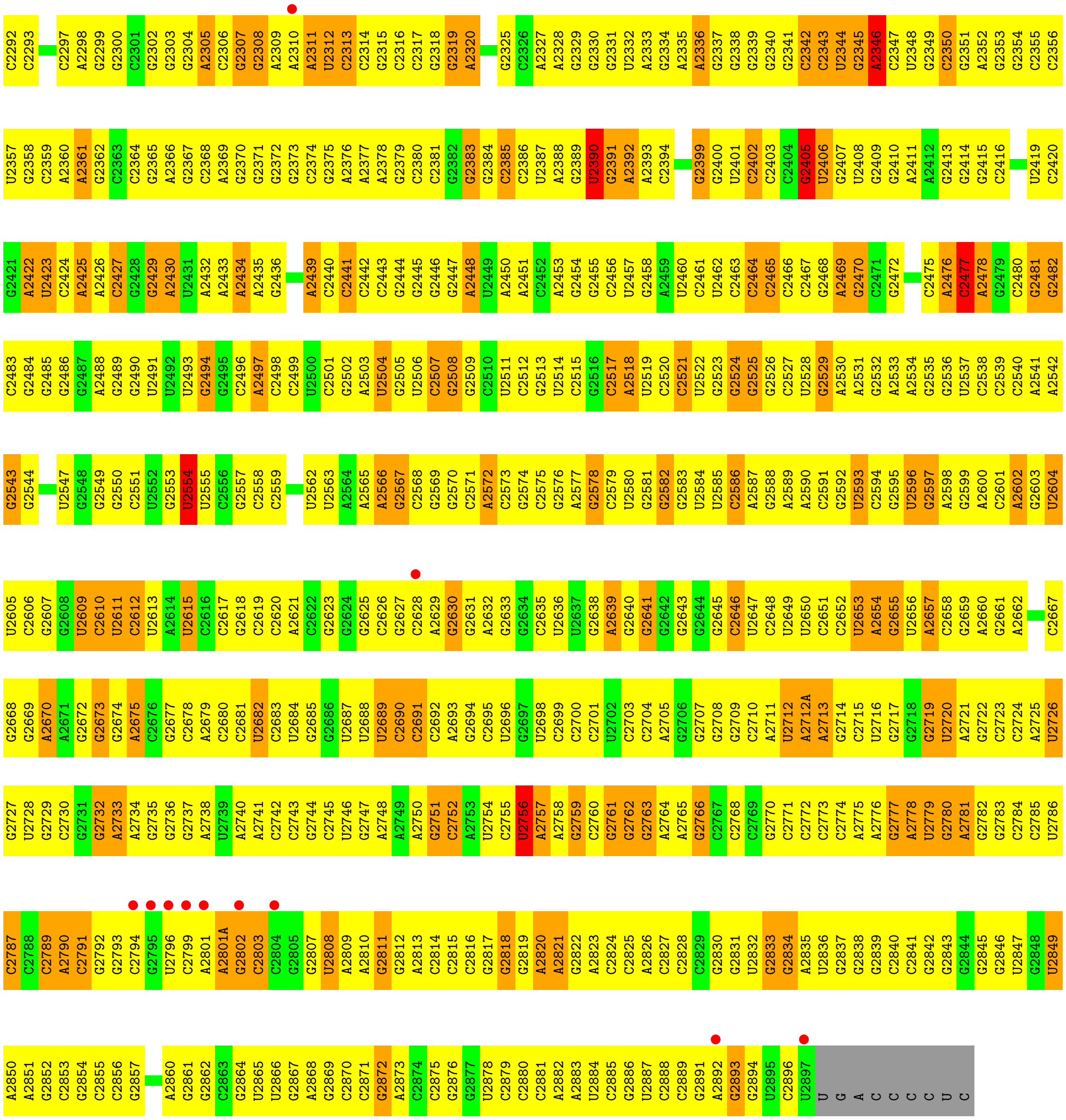
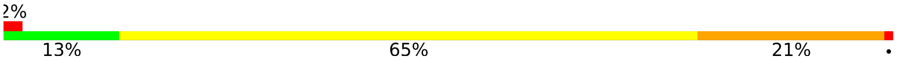
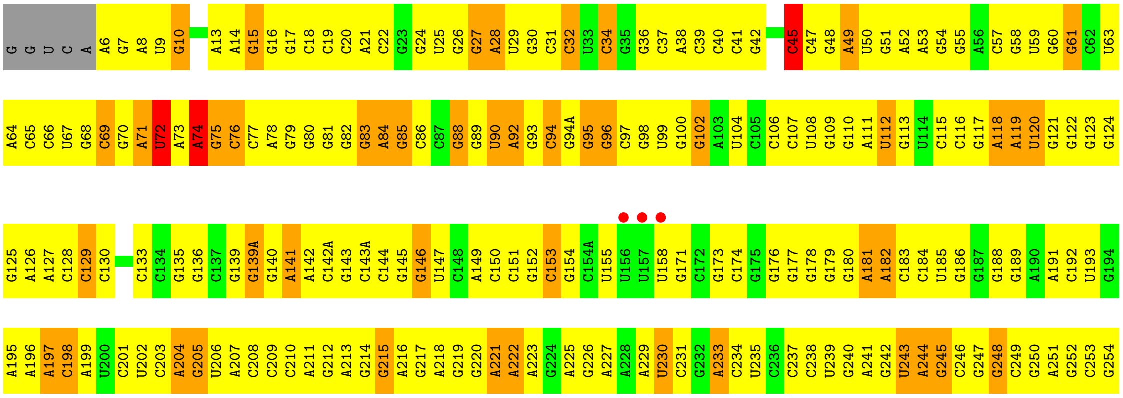
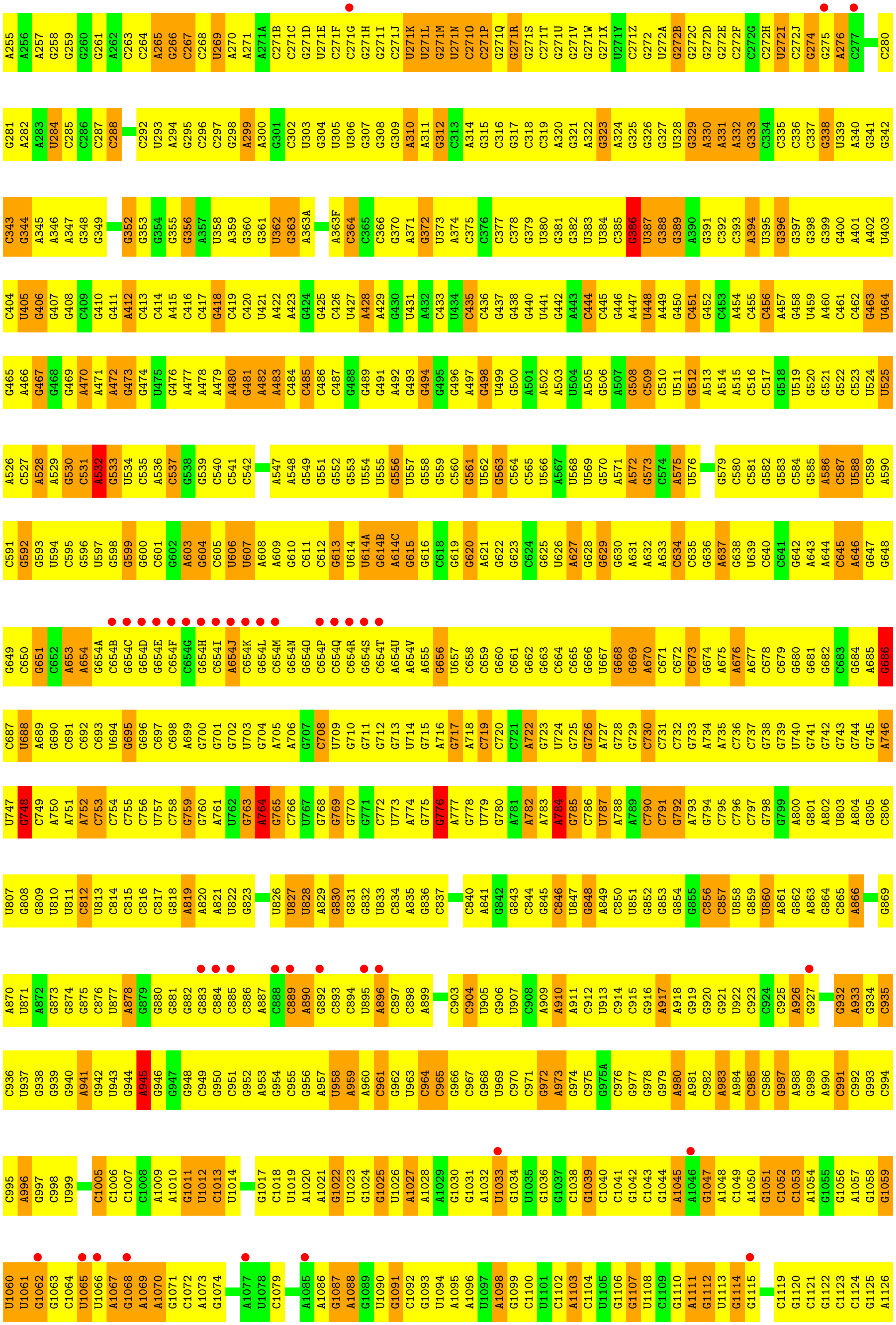


- Molecule 36: 23S RIBOSOMAL RNA

Chain DA:



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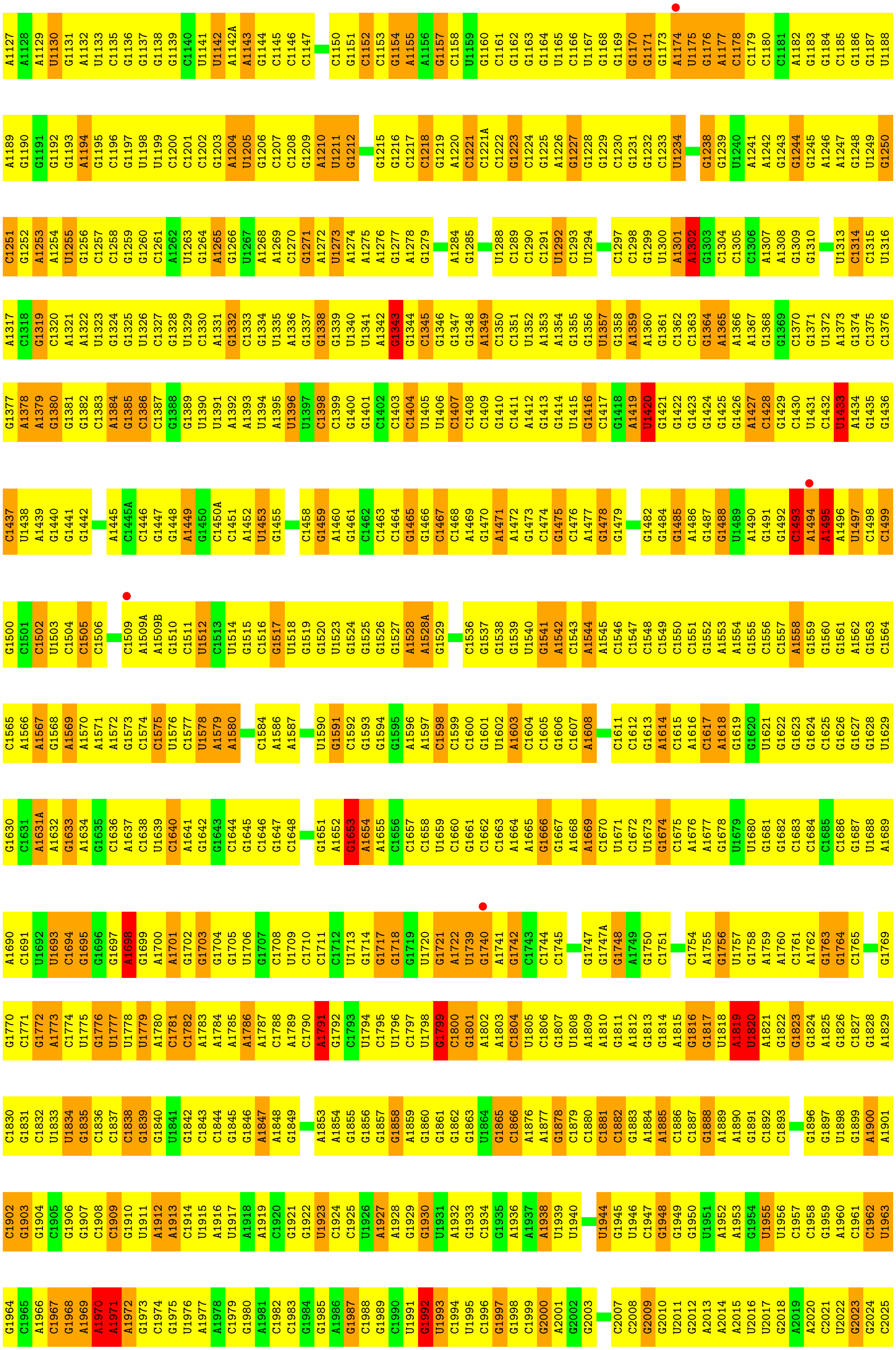
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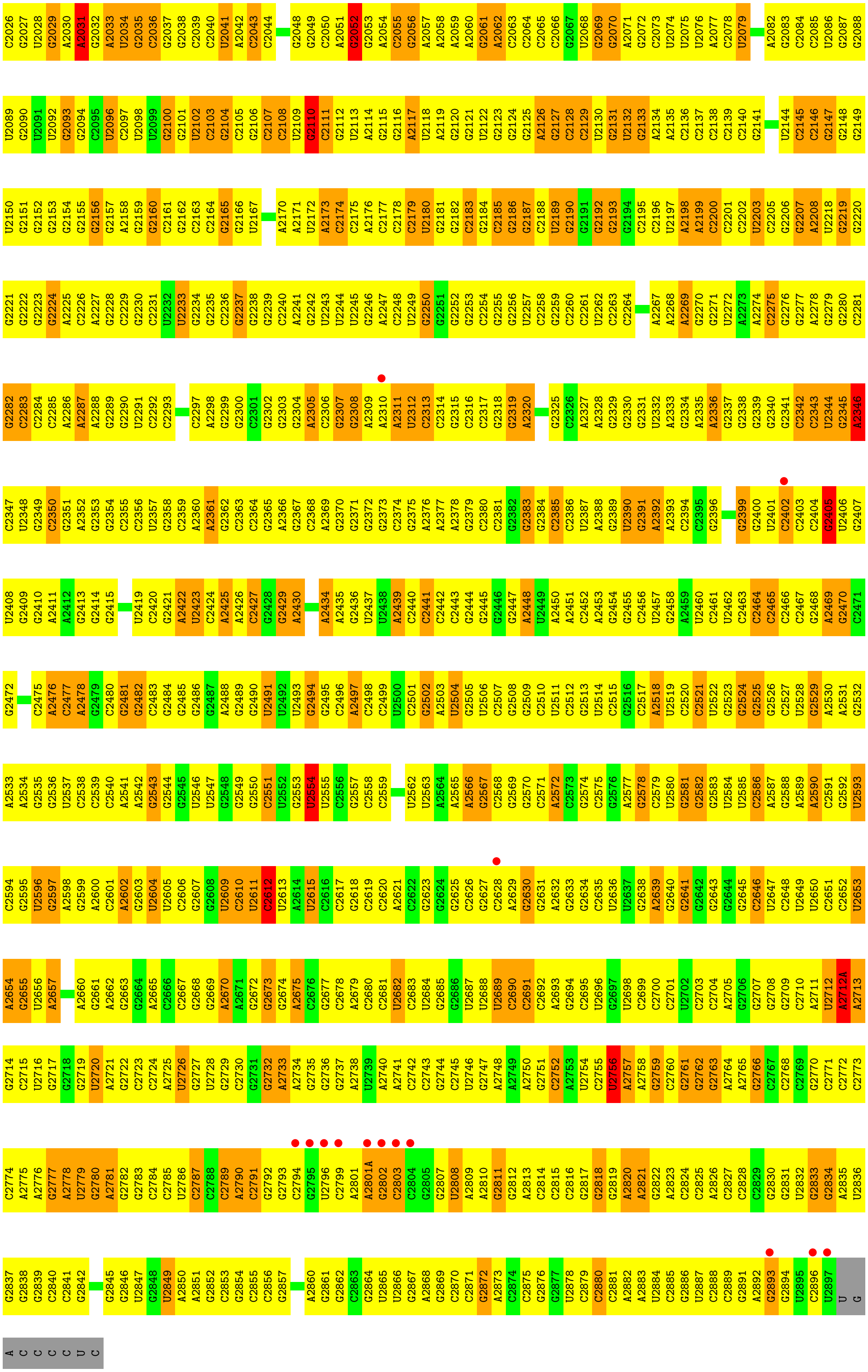
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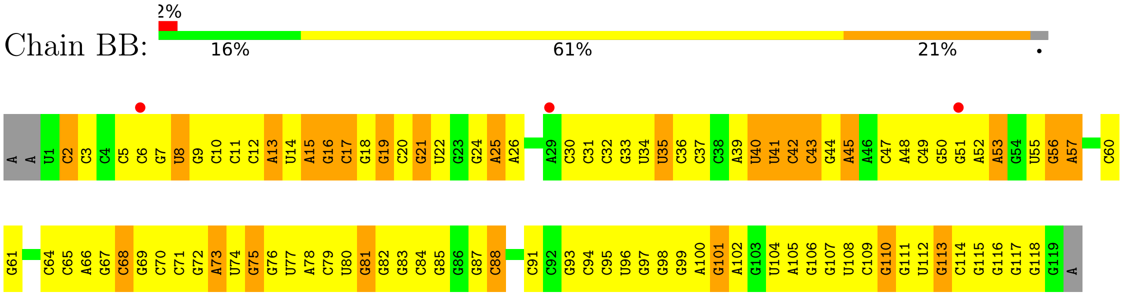
- Molecule 37: 5S RIBOSOMAL RNA



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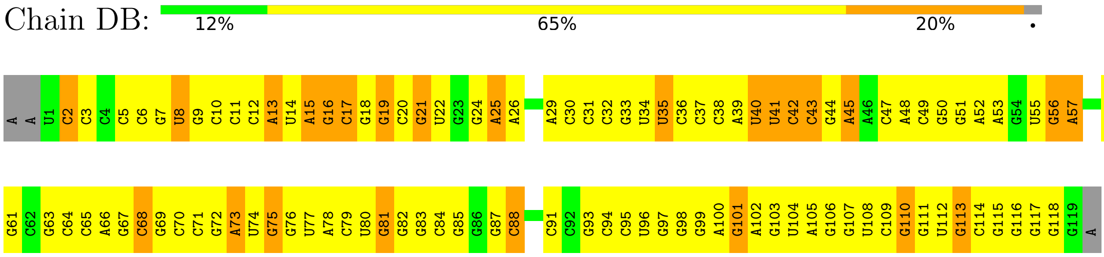

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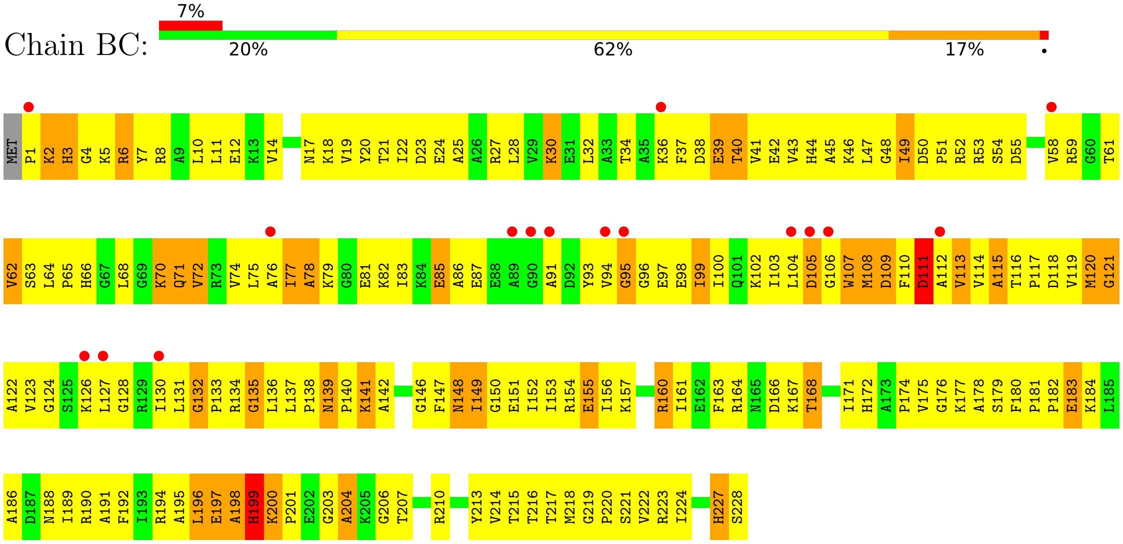

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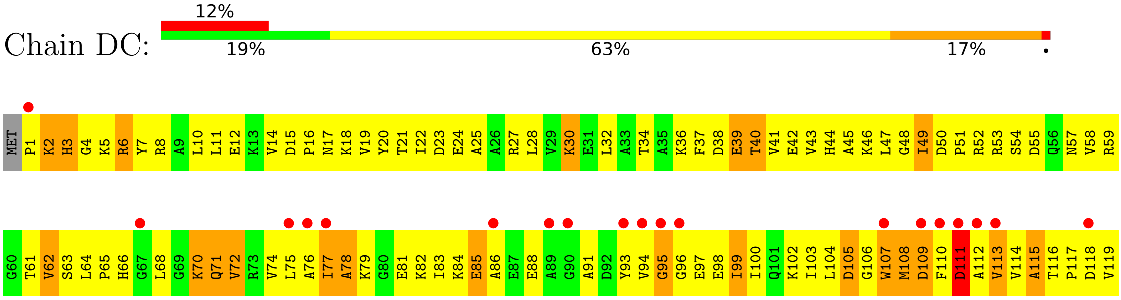

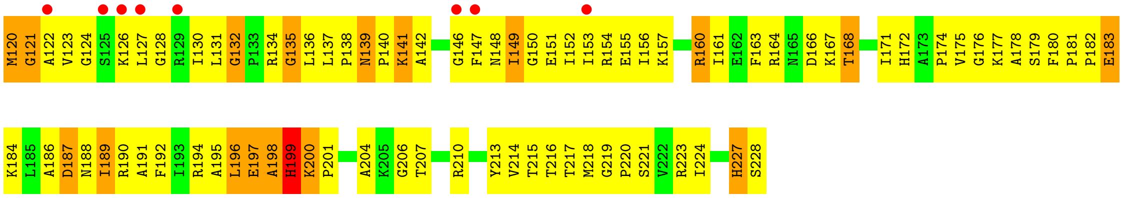

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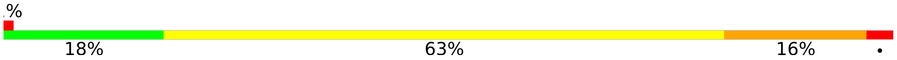

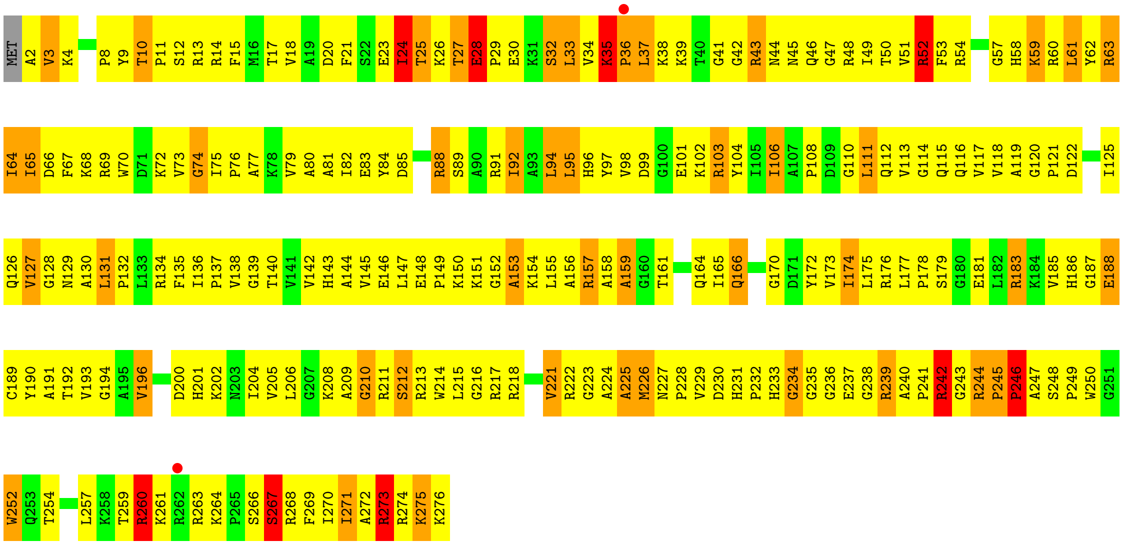

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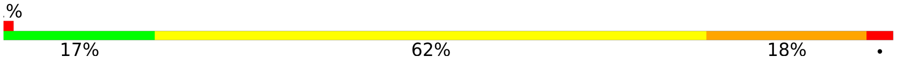

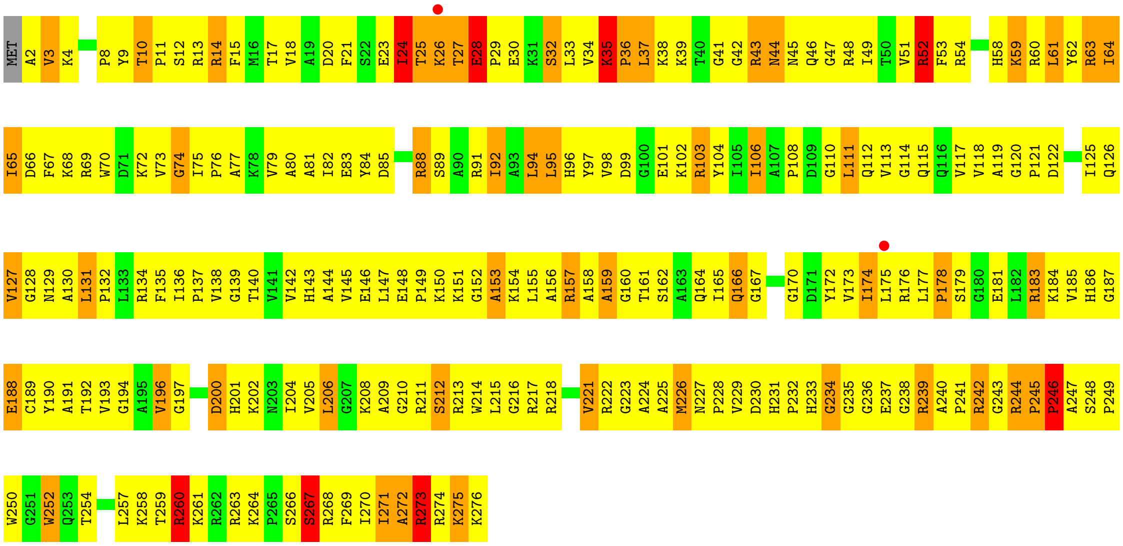

- Molecule 40: 50S RIBOSOMAL PROTEIN L3

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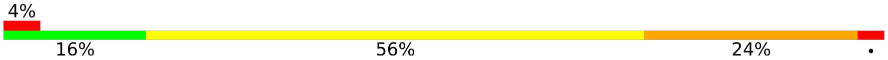

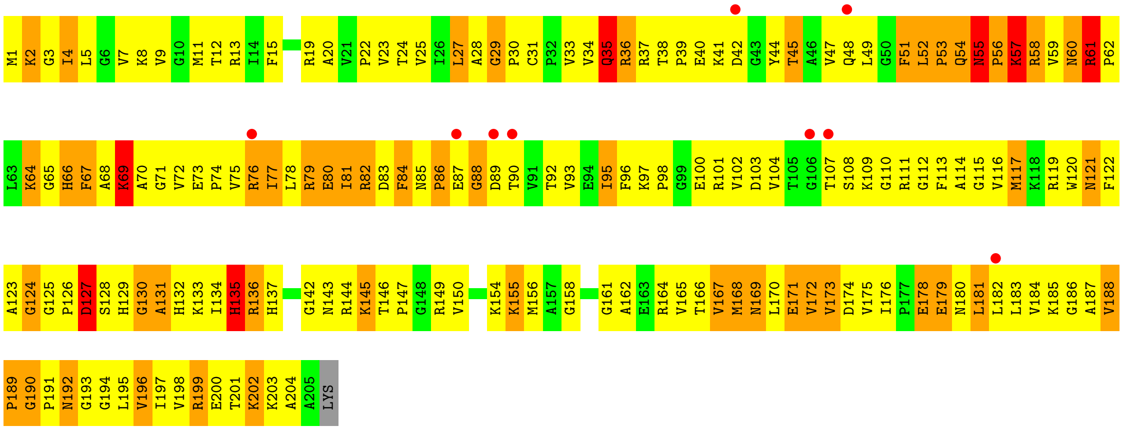

- Molecule 40: 50S RIBOSOMAL PROTEIN L3

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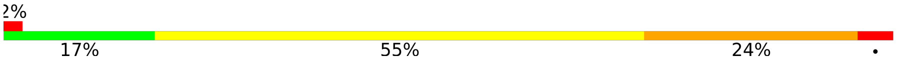
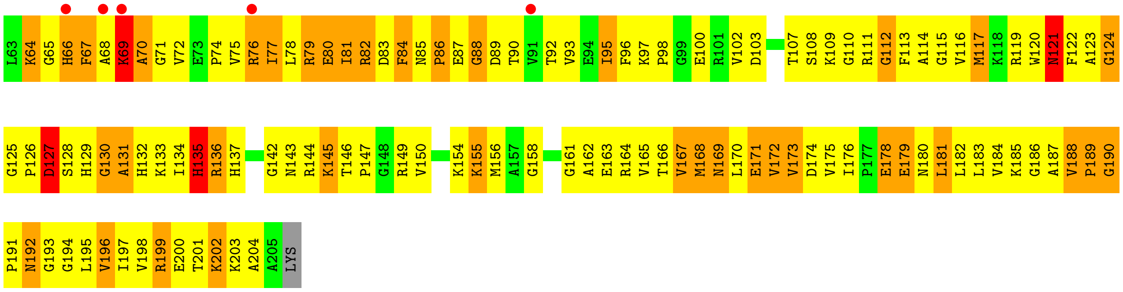
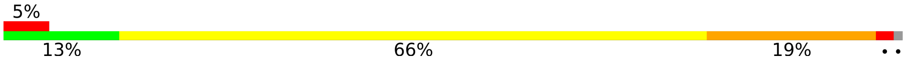
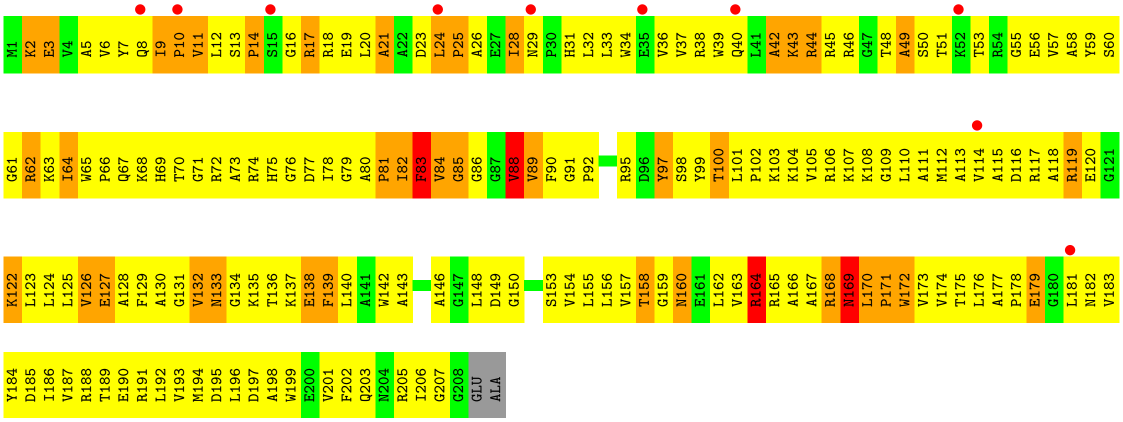




- Molecule 41: 50S RIBOSOMAL PROTEIN L4

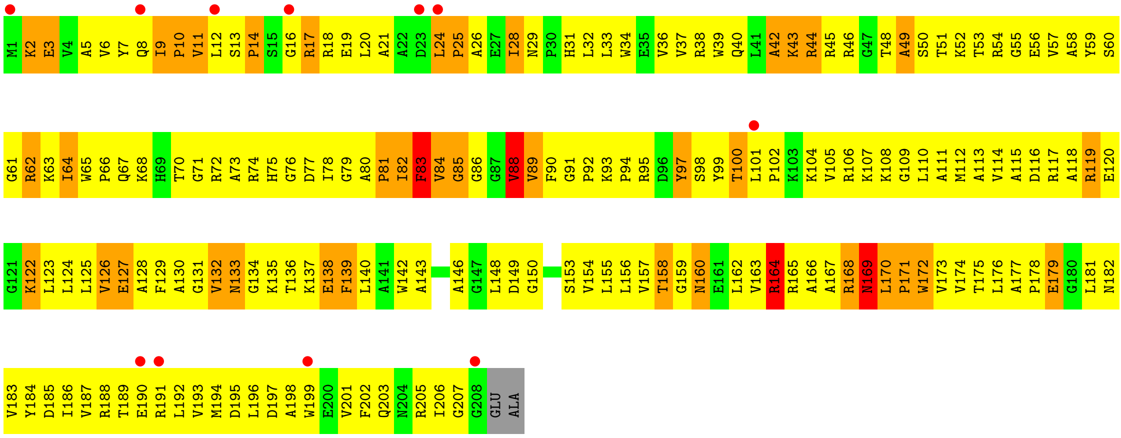
Chain BF:





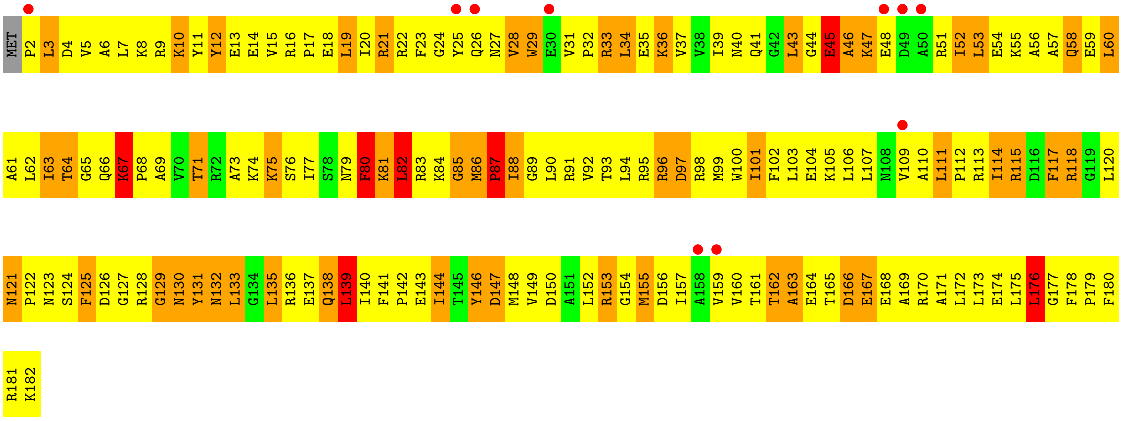
- Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain DF:



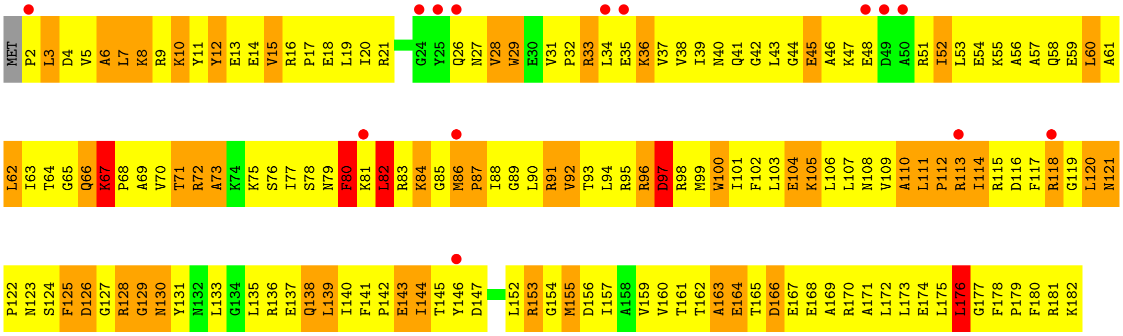
- Molecule 42: 50S RIBOSOMAL PROTEIN L5

Chain BG:



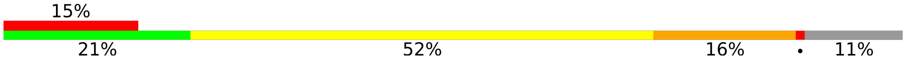
- Molecule 42: 50S RIBOSOMAL PROTEIN L5

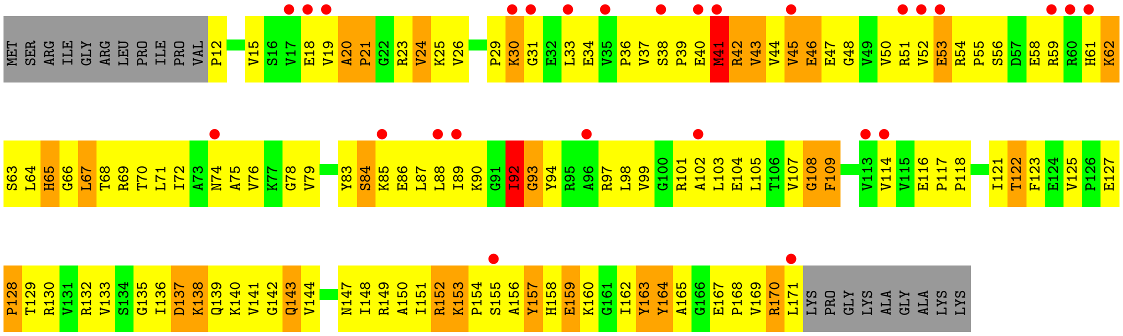
Chain DG:



- Molecule 43: 50S RIBOSOMAL PROTEIN L6

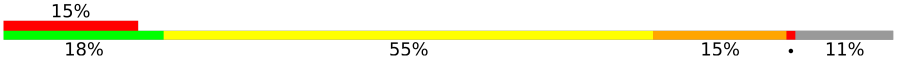
Chain BH:

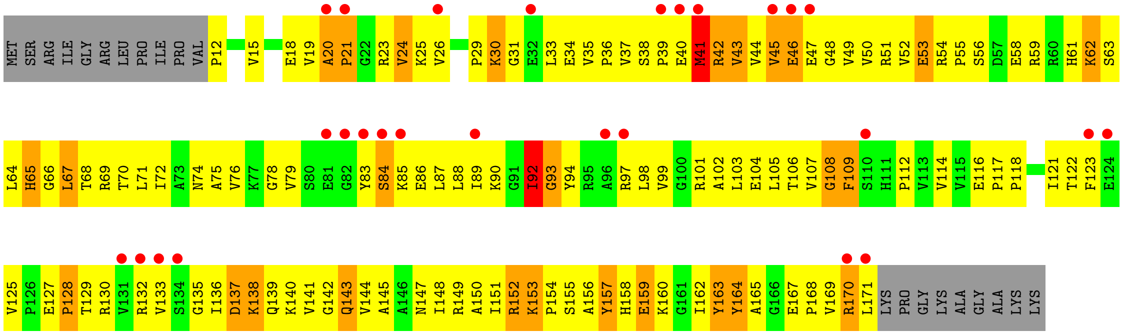




- Molecule 43: 50S RIBOSOMAL PROTEIN L6

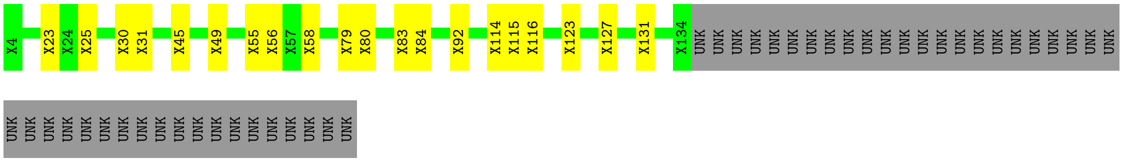
Chain DH:





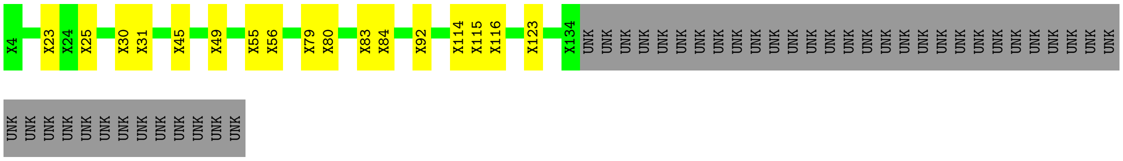
- Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



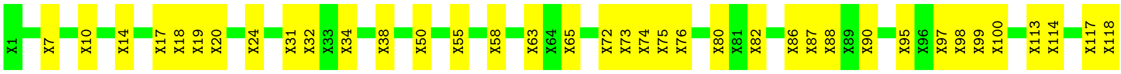
- Molecule 44: 50S RIBOSOMAL PROTEIN L10

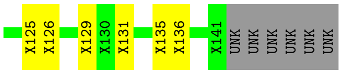
Chain DJ:



- Molecule 45: 50S RIBOSOMAL PROTEIN L11

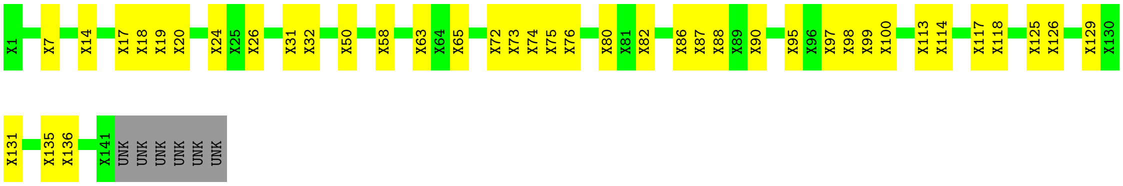
Chain BK:





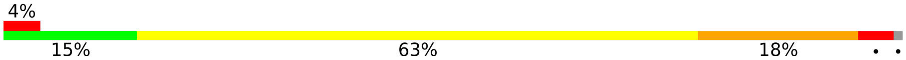
- Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain DK:



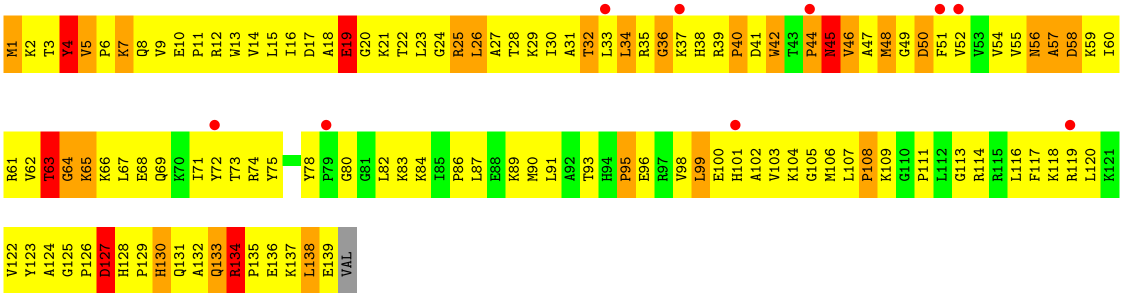
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:



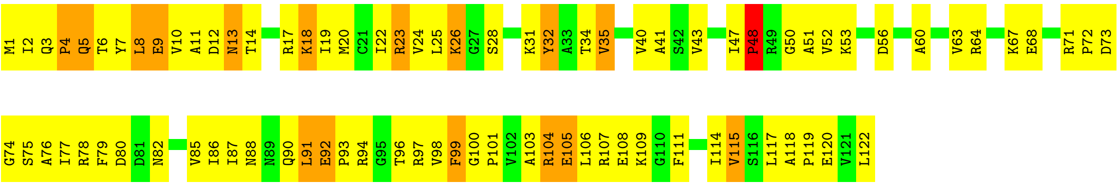
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN:

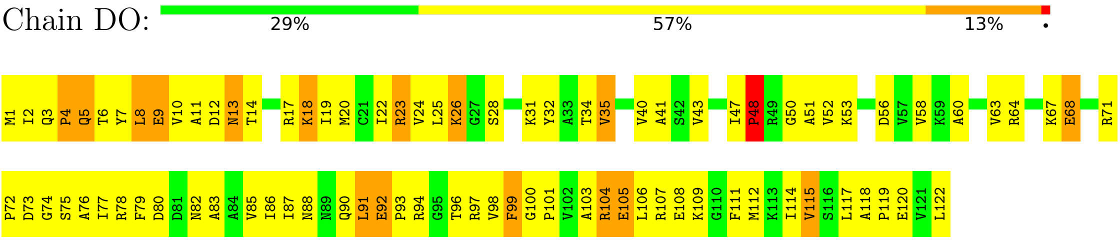


- Molecule 47: 50S RIBOSOMAL PROTEIN L14

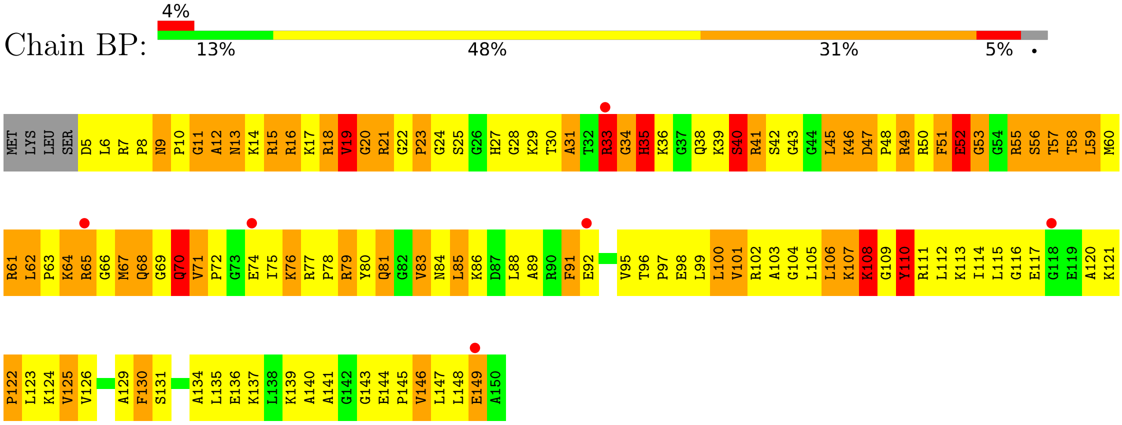
Chain BO:



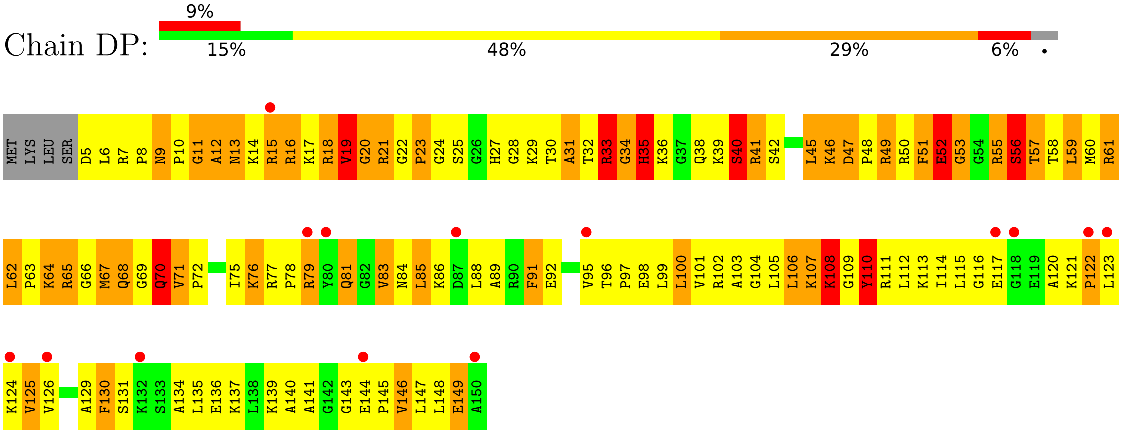
- Molecule 47: 50S RIBOSOMAL PROTEIN L14



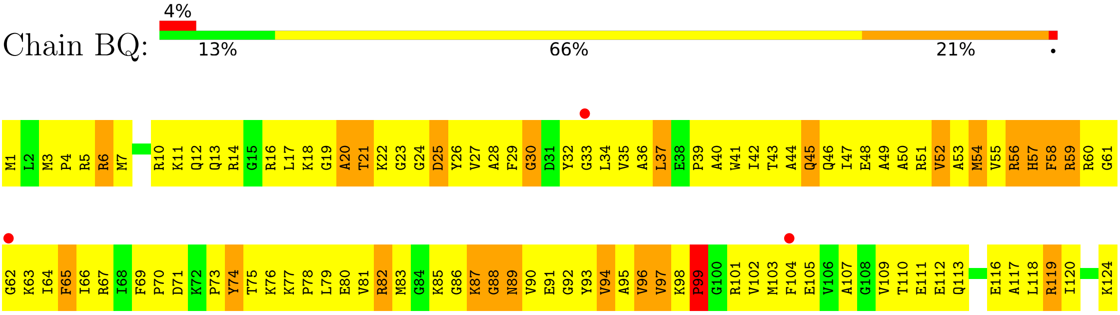
- Molecule 48: 50S RIBOSOMAL PROTEIN L15



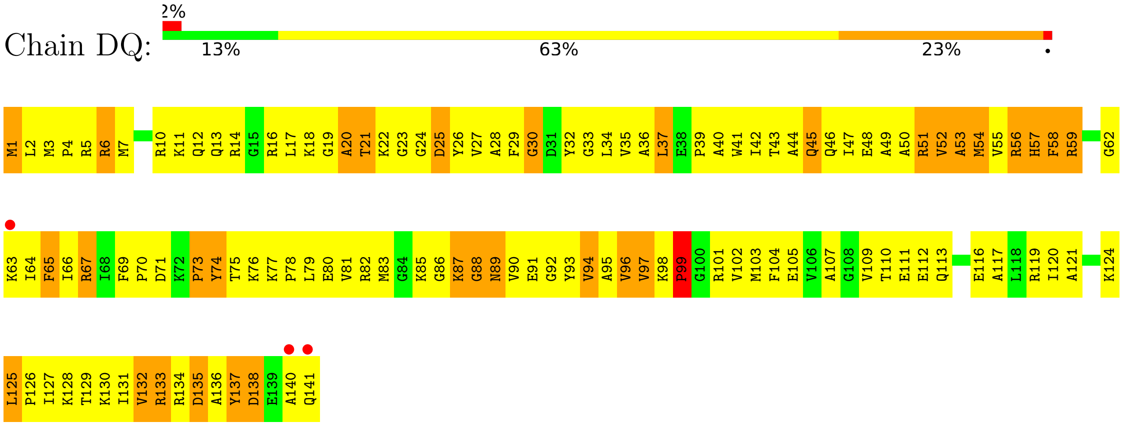
- Molecule 48: 50S RIBOSOMAL PROTEIN L15



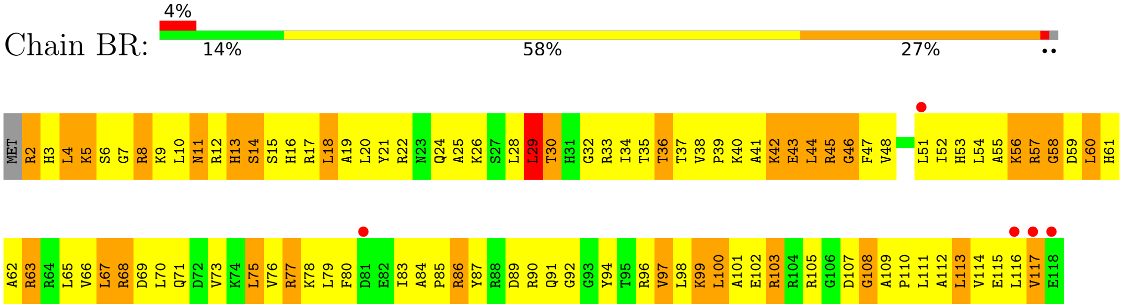
- Molecule 49: 50S RIBOSOMAL PROTEIN L16



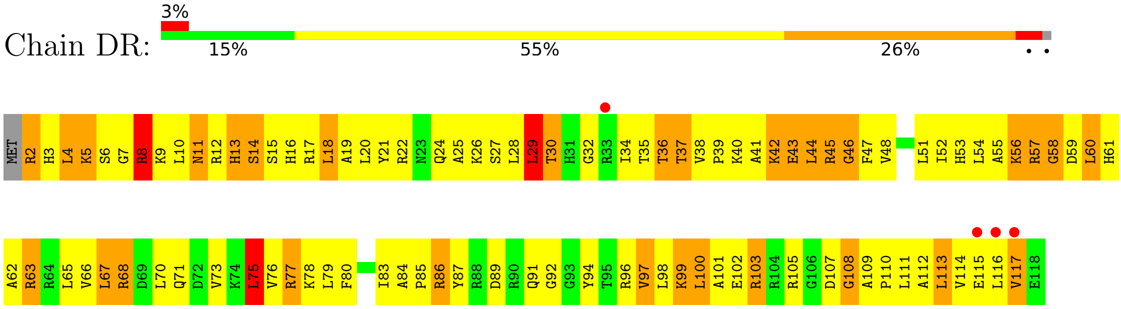
- Molecule 49: 50S RIBOSOMAL PROTEIN L16



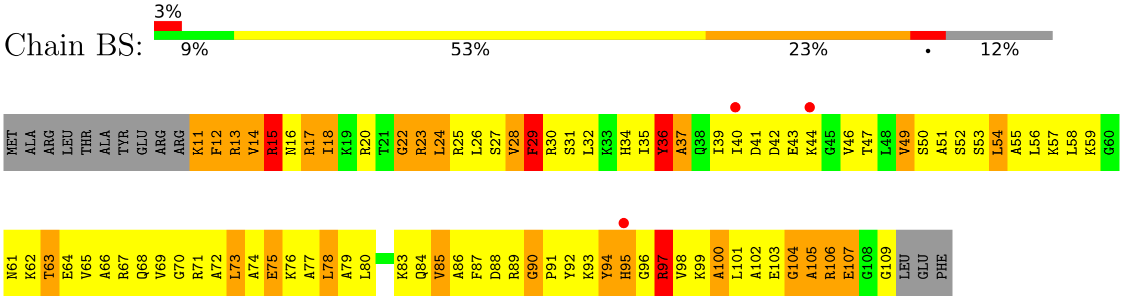
- Molecule 50: 50S RIBOSOMAL PROTEIN L17



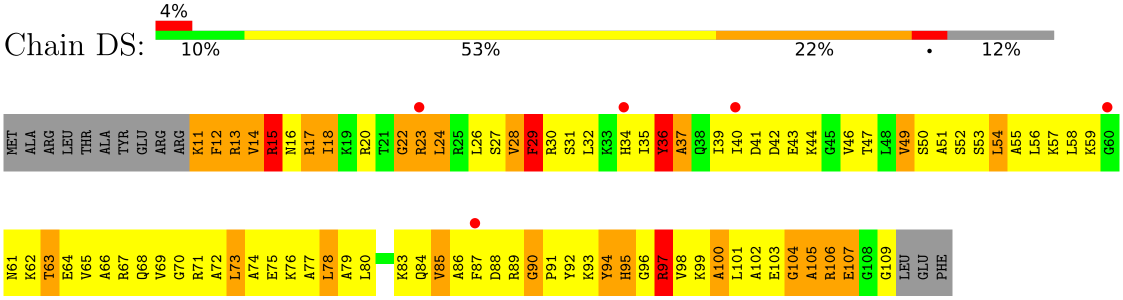
- Molecule 50: 50S RIBOSOMAL PROTEIN L17



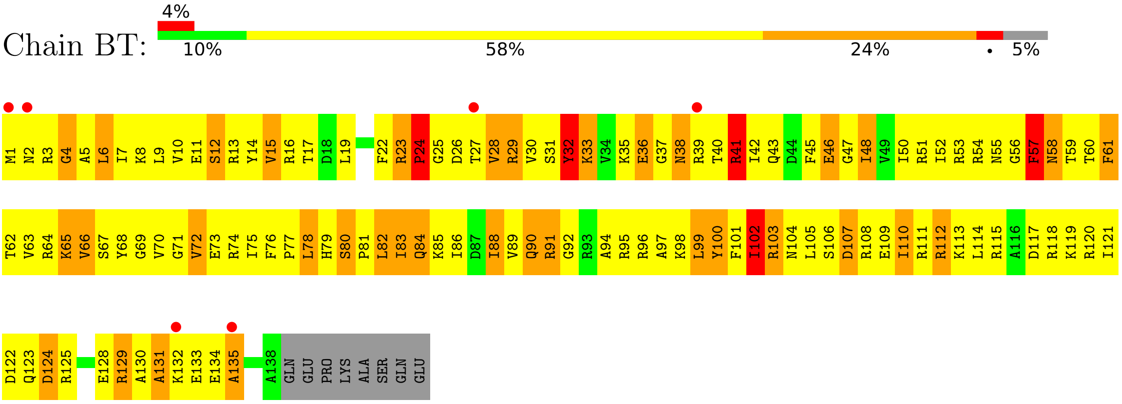
- Molecule 51: 50S RIBOSOMAL PROTEIN L18



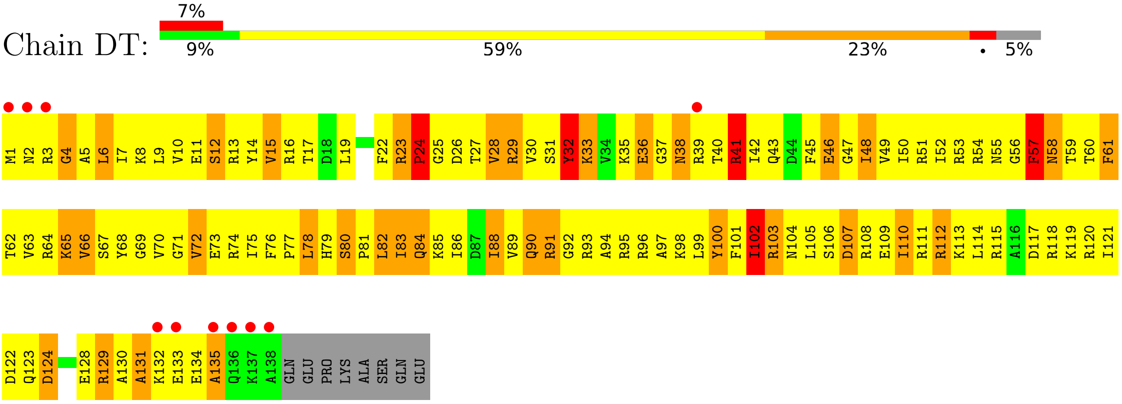
- Molecule 51: 50S RIBOSOMAL PROTEIN L18



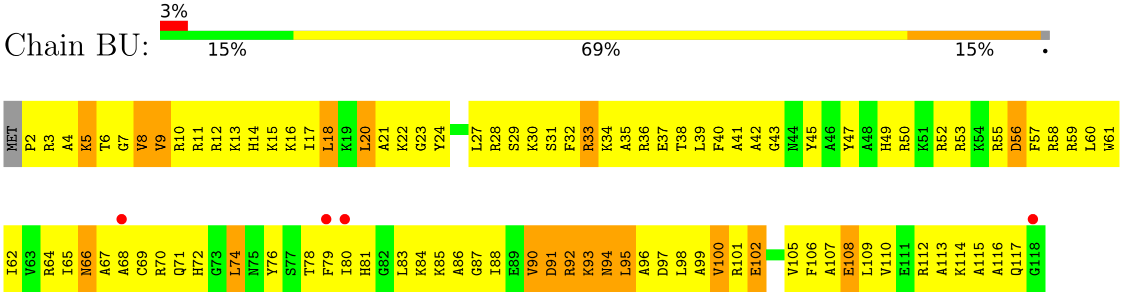
- Molecule 52: 50S RIBOSOMAL PROTEIN L19



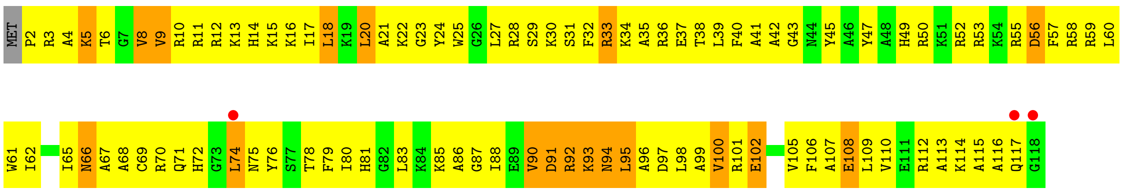
- Molecule 52: 50S RIBOSOMAL PROTEIN L19



- Molecule 53: 50S RIBOSOMAL PROTEIN L20

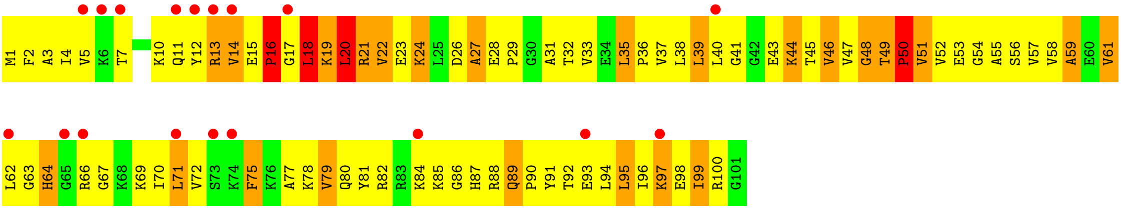


- Molecule 53: 50S RIBOSOMAL PROTEIN L20



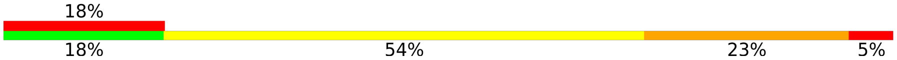
- Molecule 54: 50S RIBOSOMAL PROTEIN L21

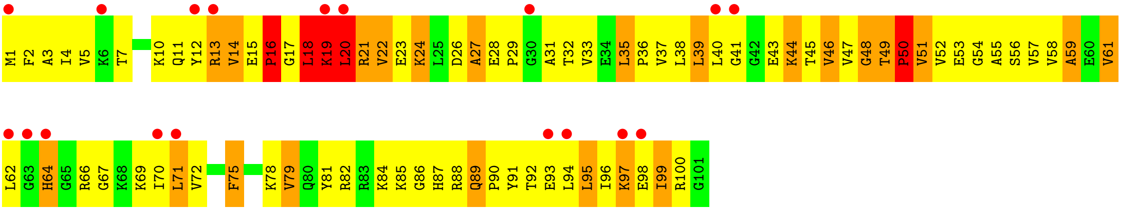
Chain BV:



- Molecule 54: 50S RIBOSOMAL PROTEIN L21

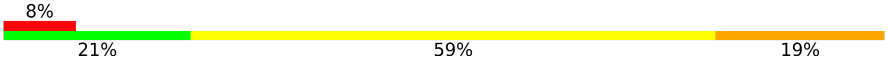
Chain DV:

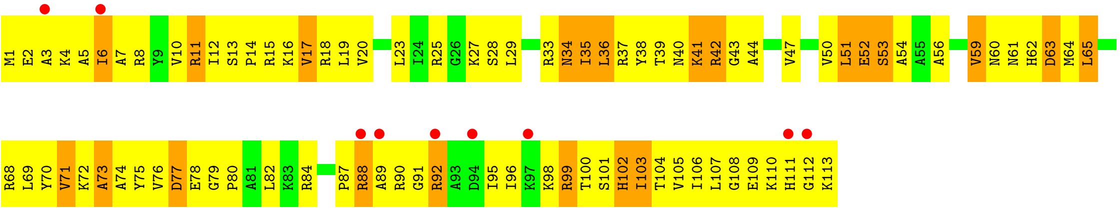




- Molecule 55: 50S RIBOSOMAL PROTEIN L22

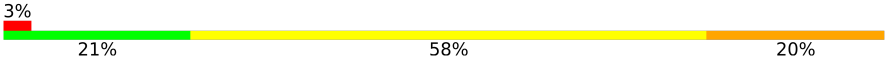
Chain BW:

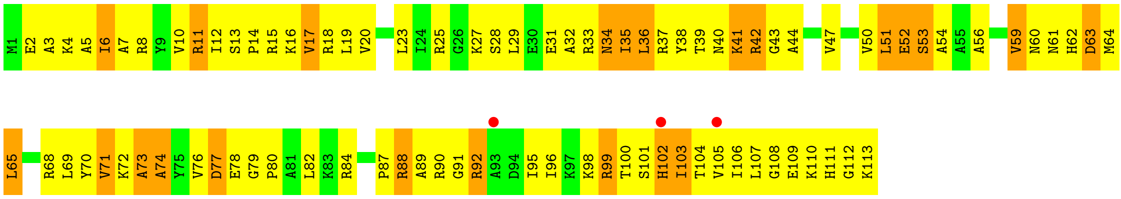




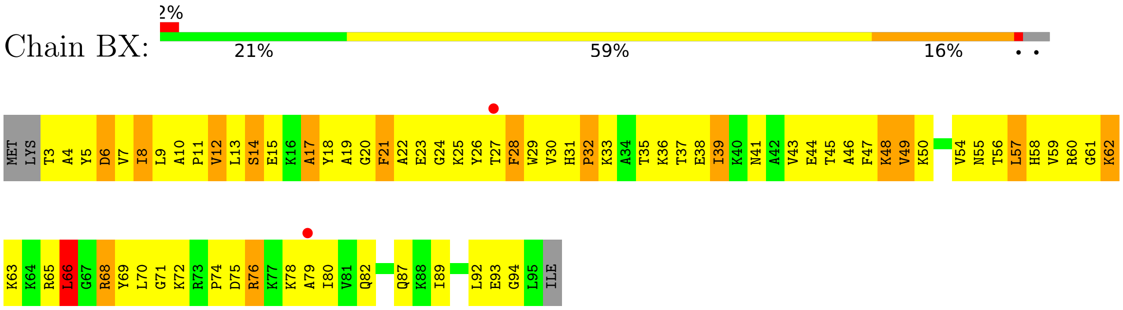
- Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain DW:

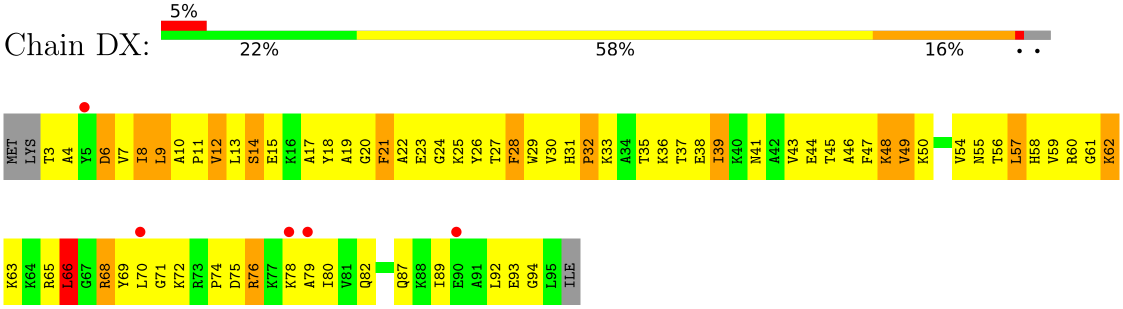




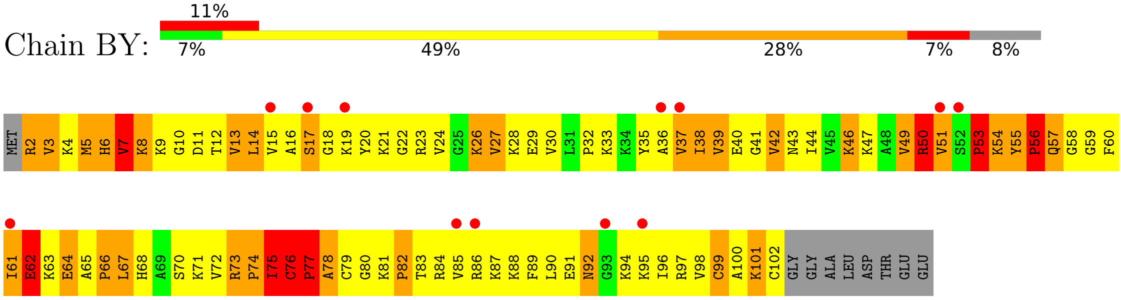
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



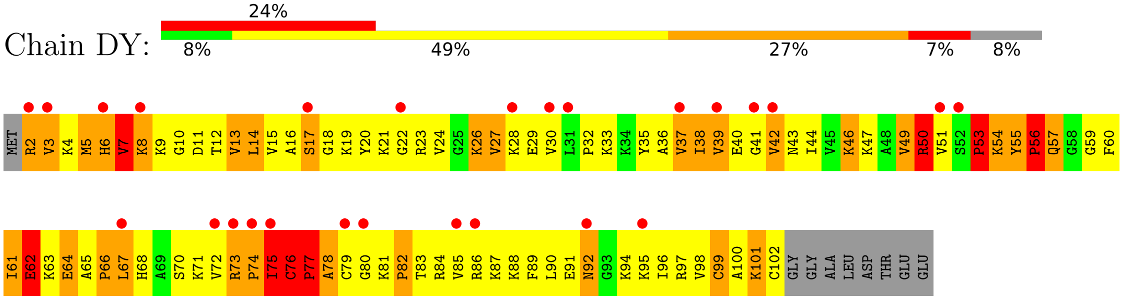
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



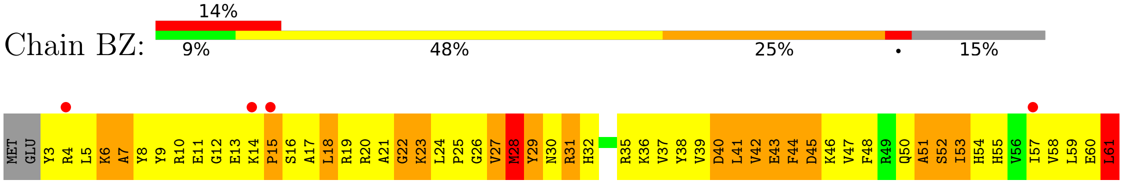
- Molecule 57: 50S RIBOSOMAL PROTEIN L24

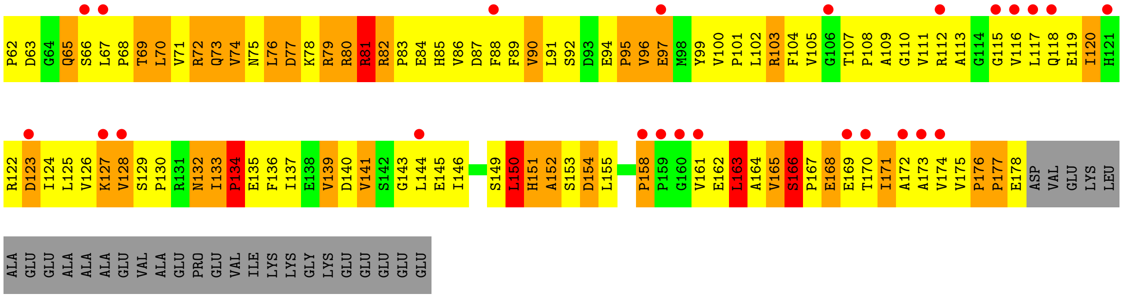


- Molecule 57: 50S RIBOSOMAL PROTEIN L24



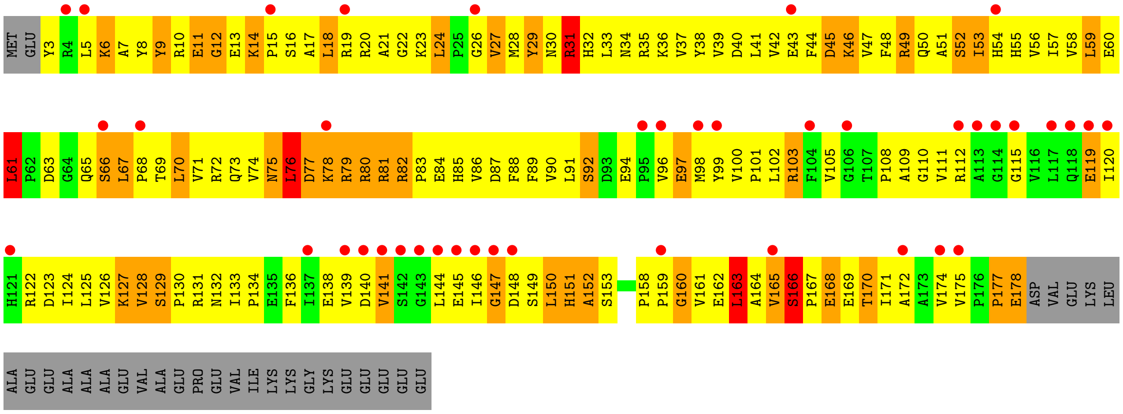
- Molecule 58: 50S RIBOSOMAL PROTEIN L25





- Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain DZ:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	289.57Å 268.36Å 403.88Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 49.91 – 3.48	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-3.60) 87.3 (49.91-3.48)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.281 , 0.315 0.277 , 0.311	Depositor DCC
R_{free} test set	35772 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	102.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 68.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.098 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	306876	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.21% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PSU, YG, GDP, 5MU, MG, KIR, H2U, 7MG, PAR

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	0.64	1/36190 (0.0%)	0.78	23/56486 (0.0%)
1	CA	0.64	0/36190	0.77	20/56486 (0.0%)
2	AB	0.44	0/1936	0.71	0/2611
2	CB	0.44	0/1936	0.72	0/2611
3	AC	0.46	0/1637	0.73	1/2207 (0.0%)
3	CC	0.47	0/1637	0.73	0/2207
4	AD	0.46	0/1733	0.75	1/2318 (0.0%)
4	CD	0.44	0/1733	0.73	2/2318 (0.1%)
5	AE	0.57	0/1163	0.79	1/1566 (0.1%)
5	CE	0.56	0/1163	0.78	0/1566
6	AF	0.42	0/856	0.67	0/1154
6	CF	0.42	0/856	0.67	0/1154
7	AG	0.41	0/1276	0.66	0/1709
7	CG	0.42	0/1276	0.66	0/1709
8	AH	0.51	0/1136	0.72	0/1527
8	CH	0.49	0/1136	0.74	0/1527
9	AI	0.39	0/1029	0.65	0/1379
9	CI	0.39	0/1029	0.65	0/1379
10	AJ	0.46	0/808	0.71	1/1087 (0.1%)
10	CJ	0.48	0/808	0.71	1/1087 (0.1%)
11	AK	0.48	0/900	0.73	0/1213
11	CK	0.48	0/900	0.73	0/1213
12	AL	0.52	0/987	0.81	0/1322
12	CL	0.54	0/987	0.81	0/1322
13	AM	0.43	0/999	0.75	0/1338
13	CM	0.43	0/999	0.74	0/1338
14	AN	0.52	0/501	0.73	0/664
14	CN	0.51	0/501	0.74	0/664
15	AO	0.45	0/745	0.73	0/992
15	CO	0.44	0/745	0.73	0/992
16	AP	0.48	0/717	0.72	0/965
16	CP	0.46	0/717	0.72	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
17	AQ	0.46	0/837	0.74	0/1119
17	CQ	0.48	0/837	0.74	0/1119
18	AR	0.50	0/579	0.75	1/768 (0.1%)
18	CR	0.49	0/579	0.75	1/768 (0.1%)
19	AS	0.47	0/643	0.67	0/867
19	CS	0.45	0/643	0.67	0/867
20	AT	0.38	0/765	0.70	0/1007
20	CT	0.36	0/765	0.70	0/1007
21	AU	0.55	0/213	0.63	0/279
21	CU	0.56	0/213	0.64	0/279
22	AV	0.53	0/1809	0.76	0/2819
22	AW	0.45	0/1809	0.73	0/2819
22	CV	0.49	0/1809	0.76	0/2819
22	CW	0.45	0/1809	0.72	0/2819
23	AX	0.71	0/304	0.83	0/471
23	CX	0.72	0/304	0.81	0/471
24	AY	0.50	1/1660 (0.1%)	0.72	1/2583 (0.0%)
24	CY	0.51	1/1660 (0.1%)	0.72	1/2583 (0.0%)
25	AZ	0.38	0/2957	0.65	0/4015
25	CZ	0.38	0/2957	0.65	0/4015
26	B0	0.40	0/671	0.67	0/892
26	D0	0.40	0/671	0.66	0/892
27	B1	0.57	0/739	0.91	0/983
27	D1	0.60	0/739	0.92	1/983 (0.1%)
28	B2	0.44	0/600	0.87	2/793 (0.3%)
28	D2	0.43	0/600	0.80	1/793 (0.1%)
29	B3	0.44	0/473	0.74	0/636
29	D3	0.42	0/473	0.75	0/636
30	B4	0.71	0/350	0.79	0/476
30	D4	0.73	1/350 (0.3%)	0.75	0/476
31	B5	0.44	0/473	0.72	0/639
31	D5	0.43	0/473	0.71	0/639
32	B6	0.53	0/440	0.91	0/586
32	D6	0.56	0/440	0.93	0/586
33	B7	0.50	0/427	0.75	0/563
33	D7	0.50	0/427	0.74	0/563
34	B8	0.51	0/516	0.78	0/681
34	D8	0.51	0/516	0.77	0/681
35	B9	0.42	0/310	0.66	0/407
35	D9	0.44	0/310	0.67	0/407
36	BA	0.61	2/69972 (0.0%)	0.76	36/109237 (0.0%)
36	DA	0.61	2/69972 (0.0%)	0.77	37/109237 (0.0%)
37	BB	0.46	0/2853	0.72	0/4451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	DB	0.45	0/2853	0.72	0/4451
38	BC	0.45	2/1774 (0.1%)	0.69	0/2391
38	DC	0.44	2/1774 (0.1%)	0.69	0/2391
39	BD	0.59	0/2195	0.86	1/2955 (0.0%)
39	DD	0.57	0/2195	0.86	0/2955
40	BE	0.48	0/1597	0.75	0/2155
40	DE	0.47	0/1597	0.75	0/2155
41	BF	0.45	0/1659	0.73	0/2246
41	DF	0.43	0/1659	0.72	0/2246
42	BG	0.46	0/1499	0.81	3/2016 (0.1%)
42	DG	0.50	1/1499 (0.1%)	0.77	0/2016
43	BH	0.37	0/1246	0.70	0/1684
43	DH	0.36	0/1246	0.70	0/1684
46	BN	0.42	0/1132	0.75	1/1527 (0.1%)
46	DN	0.43	0/1132	0.75	1/1527 (0.1%)
47	BO	0.49	0/943	0.79	0/1269
47	DO	0.52	0/943	0.78	0/1269
48	BP	0.49	0/1131	1.00	7/1504 (0.5%)
48	DP	0.48	0/1131	0.99	6/1504 (0.4%)
49	BQ	0.44	0/1143	0.71	0/1527
49	DQ	0.43	0/1143	0.72	0/1527
50	BR	0.41	0/974	0.74	0/1302
50	DR	0.39	0/974	0.74	0/1302
51	BS	0.41	0/779	0.72	0/1038
51	DS	0.41	0/779	0.72	0/1038
52	BT	0.47	0/1156	0.75	0/1544
52	DT	0.44	0/1156	0.75	0/1544
53	BU	0.43	0/975	0.74	0/1297
53	DU	0.45	0/975	0.75	0/1297
54	BV	0.39	0/790	0.73	0/1057
54	DV	0.40	0/790	0.73	0/1057
55	BW	0.44	0/907	0.71	0/1216
55	DW	0.42	0/907	0.72	0/1216
56	BX	0.47	0/740	0.71	0/995
56	DX	0.45	0/740	0.71	0/995
57	BY	0.44	0/789	0.81	1/1053 (0.1%)
57	DY	0.43	0/789	0.81	1/1053 (0.1%)
58	BZ	0.43	0/1435	0.77	0/1949
58	DZ	0.45	0/1435	0.78	0/1949
All	All	0.57	13/329754 (0.0%)	0.76	152/492708 (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	1	68
1	CA	0	63
22	AV	0	2
22	AW	0	3
22	CV	0	2
22	CW	0	3
23	AX	0	1
23	CX	0	1
30	B4	0	1
30	D4	0	1
36	BA	2	84
36	DA	1	84
46	BN	0	1
46	DN	0	1
All	All	4	315

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	1	G	OP3-P	-7.09	1.52	1.61
24	AY	1	G	OP3-P	-7.06	1.52	1.61
30	D4	47	GLN	C-N	-6.41	1.19	1.34
38	BC	218	MET	CG-SD	6.21	1.97	1.81
36	DA	2551	C	N1-C2	6.07	1.46	1.40

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1498	U	C2'-C3'-O3'	11.14	134.01	109.50
1	AA	1050	G	N9-C1'-C2'	-9.97	101.03	112.00
1	CA	1050	G	N9-C1'-C2'	-9.73	101.29	112.00
1	AA	961	U	N1-C1'-C2'	-9.15	101.93	112.00
1	CA	961	U	N1-C1'-C2'	-9.06	102.03	112.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1498	U	C3'
36	BA	1799	G	C3'
36	BA	1819	A	C3'

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Mol	Chain	Res	Type	Atom
36	DA	1819	A	C3'

5 of 315 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	109	A	Sidechain
1	AA	189(H)	G	Sidechain
1	AA	24	U	Sidechain
1	AA	37	U	Sidechain
1	AA	7	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	2215	0
1	CA	32329	0	16318	2218	0
2	AB	1901	0	1951	376	1
2	CB	1901	0	1951	383	1
3	AC	1613	0	1677	265	0
3	CC	1613	0	1677	260	0
4	AD	1703	0	1764	296	0
4	CD	1703	0	1765	305	0
5	AE	1147	0	1207	196	0
5	CE	1147	0	1207	198	0
6	AF	843	0	857	86	0
6	CF	843	0	857	101	0
7	AG	1257	0	1296	187	0
7	CG	1257	0	1296	187	0
8	AH	1116	0	1177	192	0
8	CH	1116	0	1177	204	0
9	AI	1010	0	1037	165	0
9	CI	1010	0	1037	168	0
10	AJ	795	0	840	197	0
10	CJ	795	0	840	209	0
11	AK	885	0	904	130	0
11	CK	885	0	904	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AL	971	0	1057	156	0
12	CL	971	0	1057	149	0
13	AM	988	0	1059	215	0
13	CM	988	0	1059	208	0
14	AN	492	0	529	130	0
14	CN	492	0	529	129	0
15	AO	734	0	771	94	0
15	CO	734	0	771	97	0
16	AP	701	0	720	116	0
16	CP	701	0	720	114	0
17	AQ	824	0	891	88	0
17	CQ	824	0	891	89	0
18	AR	574	0	644	97	0
18	CR	574	0	644	95	0
19	AS	630	0	652	129	0
19	CS	630	0	652	129	0
20	AT	763	0	861	148	0
20	CT	763	0	861	141	0
21	AU	209	0	221	30	0
21	CU	209	0	221	33	0
22	AV	1619	0	822	99	0
22	AW	1619	0	822	82	0
22	CV	1619	0	822	87	0
22	CW	1619	0	822	90	0
23	AX	272	0	142	23	0
23	CX	272	0	142	21	0
24	AY	1650	0	851	118	0
24	CY	1650	0	851	115	0
25	AZ	2900	0	2907	491	0
25	CZ	2900	0	2907	478	0
26	B0	662	0	688	112	0
26	D0	662	0	688	112	0
27	B1	732	0	808	156	0
27	D1	732	0	808	158	0
28	B2	598	0	653	166	0
28	D2	598	0	653	153	0
29	B3	468	0	523	74	0
29	D3	468	0	523	76	0
30	B4	341	0	337	72	0
30	D4	341	0	337	63	0
31	B5	459	0	480	98	0
31	D5	459	0	480	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	B6	433	0	461	157	0
32	D6	433	0	461	162	0
33	B7	419	0	467	71	0
33	D7	419	0	467	76	0
34	B8	508	0	576	141	0
34	D8	508	0	576	147	0
35	B9	307	0	335	74	0
35	D9	307	0	337	78	0
36	BA	62474	0	31497	4307	0
36	DA	62474	0	31497	4322	0
37	BB	2551	0	1295	152	0
37	DB	2551	0	1295	162	0
38	BC	1742	0	1800	269	1
38	DC	1742	0	1800	272	1
39	BD	2145	0	2234	441	0
39	DD	2145	0	2234	438	0
40	BE	1564	0	1629	331	0
40	DE	1564	0	1629	327	0
41	BF	1624	0	1677	362	0
41	DF	1624	0	1677	351	0
42	BG	1474	0	1535	396	0
42	DG	1474	0	1535	365	0
43	BH	1223	0	1282	214	0
43	DH	1223	0	1282	215	0
44	BJ	651	0	136	11	0
44	DJ	651	0	136	9	0
45	BK	701	0	157	35	0
45	DK	701	0	157	34	0
46	BN	1105	0	1180	233	0
46	DN	1105	0	1180	232	0
47	BO	933	0	996	121	0
47	DO	933	0	996	120	0
48	BP	1114	0	1187	309	0
48	DP	1114	0	1187	308	0
49	BQ	1122	0	1179	240	0
49	DQ	1122	0	1179	226	0
50	BR	960	0	1021	198	0
50	DR	960	0	1021	197	0
51	BS	771	0	832	195	0
51	DS	771	0	832	189	0
52	BT	1142	0	1202	274	0
52	DT	1142	0	1202	274	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	BU	958	0	1015	223	0
53	DU	958	0	1015	223	0
54	BV	779	0	852	167	0
54	DV	779	0	852	169	0
55	BW	896	0	953	153	0
55	DW	896	0	953	160	0
56	BX	726	0	778	118	0
56	DX	726	0	778	115	0
57	BY	776	0	870	208	0
57	DY	776	0	870	203	0
58	BZ	1403	0	1432	320	0
58	DZ	1403	0	1432	293	0
59	AA	42	0	45	4	0
59	CA	42	0	45	3	0
60	AD	1	0	0	1	0
60	AN	1	0	0	0	0
60	B4	1	0	0	0	0
60	B9	1	0	0	0	0
60	CD	1	0	0	0	0
60	CN	1	0	0	0	0
60	D4	1	0	0	0	0
60	D9	1	0	0	2	0
61	AY	1	0	0	0	0
61	CY	1	0	0	0	0
62	AZ	28	0	12	15	0
62	CZ	28	0	12	15	0
63	AZ	57	0	58	4	0
63	CZ	57	0	59	8	0
All	All	306876	0	208322	30310	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

The worst 5 of 30310 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)
25:AZ:356:PRO:O	25:AZ:359:VAL:CG2	1.74	1.32
27:B1:41:ARG:NH2	36:BA:1365:A:H5”	1.53	1.24
25:CZ:356:PRO:O	25:CZ:359:VAL:HG22	1.38	1.20
24:CY:41:G:H2’	24:CY:42:U:H5”	1.24	1.19
32:B6:45:LYS:H	32:B6:45:LYS:CD	1.48	1.19

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:65:GLY:O	38:BC:27:ARG:NH2[2_445]	1.63	0.57
2:CB:65:GLY:O	38:DC:27:ARG:NH2[2_646]	1.66	0.54

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	116 (50%)	72 (31%)	45 (19%)	0	2
2	CB	233/256 (91%)	115 (49%)	74 (32%)	44 (19%)	0	2
3	AC	205/239 (86%)	117 (57%)	52 (25%)	36 (18%)	0	2
3	CC	205/239 (86%)	113 (55%)	57 (28%)	35 (17%)	0	2
4	AD	206/209 (99%)	123 (60%)	49 (24%)	34 (16%)	0	3
4	CD	206/209 (99%)	122 (59%)	48 (23%)	36 (18%)	0	2
5	AE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	0	7
5	CE	149/162 (92%)	98 (66%)	37 (25%)	14 (9%)	0	8
6	AF	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	1	9
6	CF	99/101 (98%)	69 (70%)	21 (21%)	9 (9%)	1	9
7	AG	153/156 (98%)	86 (56%)	35 (23%)	32 (21%)	0	1
7	CG	153/156 (98%)	86 (56%)	37 (24%)	30 (20%)	0	2
8	AH	136/138 (99%)	88 (65%)	34 (25%)	14 (10%)	0	7
8	CH	136/138 (99%)	89 (65%)	35 (26%)	12 (9%)	1	9
9	AI	125/128 (98%)	80 (64%)	27 (22%)	18 (14%)	0	4
9	CI	125/128 (98%)	80 (64%)	27 (22%)	18 (14%)	0	4
10	AJ	97/105 (92%)	63 (65%)	20 (21%)	14 (14%)	0	4
10	CJ	97/105 (92%)	63 (65%)	20 (21%)	14 (14%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	117/129 (91%)	80 (68%)	29 (25%)	8 (7%)	1	15
11	CK	117/129 (91%)	77 (66%)	32 (27%)	8 (7%)	1	15
12	AL	123/135 (91%)	71 (58%)	32 (26%)	20 (16%)	0	3
12	CL	123/135 (91%)	73 (59%)	31 (25%)	19 (15%)	0	3
13	AM	123/126 (98%)	58 (47%)	39 (32%)	26 (21%)	0	1
13	CM	123/126 (98%)	58 (47%)	39 (32%)	26 (21%)	0	1
14	AN	58/61 (95%)	28 (48%)	17 (29%)	13 (22%)	0	1
14	CN	58/61 (95%)	29 (50%)	14 (24%)	15 (26%)	0	0
15	AO	86/89 (97%)	54 (63%)	16 (19%)	16 (19%)	0	2
15	CO	86/89 (97%)	55 (64%)	15 (17%)	16 (19%)	0	2
16	AP	82/88 (93%)	50 (61%)	18 (22%)	14 (17%)	0	2
16	CP	82/88 (93%)	50 (61%)	18 (22%)	14 (17%)	0	2
17	AQ	98/105 (93%)	70 (71%)	21 (21%)	7 (7%)	1	14
17	CQ	98/105 (93%)	69 (70%)	21 (21%)	8 (8%)	1	10
18	AR	68/88 (77%)	39 (57%)	17 (25%)	12 (18%)	0	2
18	CR	68/88 (77%)	39 (57%)	17 (25%)	12 (18%)	0	2
19	AS	77/93 (83%)	39 (51%)	27 (35%)	11 (14%)	0	4
19	CS	77/93 (83%)	39 (51%)	27 (35%)	11 (14%)	0	4
20	AT	97/106 (92%)	49 (50%)	30 (31%)	18 (19%)	0	2
20	CT	97/106 (92%)	50 (52%)	29 (30%)	18 (19%)	0	2
21	AU	23/27 (85%)	10 (44%)	7 (30%)	6 (26%)	0	0
21	CU	23/27 (85%)	10 (44%)	8 (35%)	5 (22%)	0	1
25	AZ	370/406 (91%)	254 (69%)	77 (21%)	39 (10%)	0	7
25	CZ	370/406 (91%)	252 (68%)	81 (22%)	37 (10%)	0	8
26	B0	82/85 (96%)	54 (66%)	20 (24%)	8 (10%)	0	8
26	D0	82/85 (96%)	54 (66%)	20 (24%)	8 (10%)	0	8
27	B1	92/98 (94%)	55 (60%)	22 (24%)	15 (16%)	0	3
27	D1	92/98 (94%)	54 (59%)	25 (27%)	13 (14%)	0	4
28	B2	69/72 (96%)	43 (62%)	10 (14%)	16 (23%)	0	0
28	D2	69/72 (96%)	44 (64%)	14 (20%)	11 (16%)	0	3
29	B3	58/60 (97%)	28 (48%)	15 (26%)	15 (26%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	D3	58/60 (97%)	28 (48%)	16 (28%)	14 (24%)	0	0
30	B4	43/71 (61%)	20 (46%)	15 (35%)	8 (19%)	0	2
30	D4	43/71 (61%)	20 (46%)	15 (35%)	8 (19%)	0	2
31	B5	57/60 (95%)	33 (58%)	13 (23%)	11 (19%)	0	2
31	D5	57/60 (95%)	32 (56%)	14 (25%)	11 (19%)	0	2
32	B6	48/54 (89%)	17 (35%)	14 (29%)	17 (35%)	0	0
32	D6	48/54 (89%)	18 (38%)	14 (29%)	16 (33%)	0	0
33	B7	47/49 (96%)	27 (57%)	12 (26%)	8 (17%)	0	2
33	D7	47/49 (96%)	27 (57%)	12 (26%)	8 (17%)	0	2
34	B8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	2
34	D8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	2
35	B9	35/37 (95%)	18 (51%)	9 (26%)	8 (23%)	0	1
35	D9	35/37 (95%)	18 (51%)	10 (29%)	7 (20%)	0	1
38	BC	226/229 (99%)	143 (63%)	53 (24%)	30 (13%)	0	4
38	DC	226/229 (99%)	141 (62%)	55 (24%)	30 (13%)	0	4
39	BD	273/276 (99%)	176 (64%)	63 (23%)	34 (12%)	0	5
39	DD	273/276 (99%)	172 (63%)	66 (24%)	35 (13%)	0	5
40	BE	203/206 (98%)	109 (54%)	45 (22%)	49 (24%)	0	0
40	DE	203/206 (98%)	108 (53%)	46 (23%)	49 (24%)	0	0
41	BF	206/210 (98%)	120 (58%)	47 (23%)	39 (19%)	0	2
41	DF	206/210 (98%)	121 (59%)	46 (22%)	39 (19%)	0	2
42	BG	179/182 (98%)	86 (48%)	52 (29%)	41 (23%)	0	1
42	DG	179/182 (98%)	96 (54%)	45 (25%)	38 (21%)	0	1
43	BH	158/180 (88%)	98 (62%)	36 (23%)	24 (15%)	0	3
43	DH	158/180 (88%)	99 (63%)	35 (22%)	24 (15%)	0	3
46	BN	137/140 (98%)	75 (55%)	39 (28%)	23 (17%)	0	2
46	DN	137/140 (98%)	74 (54%)	40 (29%)	23 (17%)	0	2
47	BO	120/122 (98%)	91 (76%)	17 (14%)	12 (10%)	0	8
47	DO	120/122 (98%)	93 (78%)	15 (12%)	12 (10%)	0	8
48	BP	144/150 (96%)	72 (50%)	35 (24%)	37 (26%)	0	0
48	DP	144/150 (96%)	71 (49%)	35 (24%)	38 (26%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	BQ	139/141 (99%)	77 (55%)	46 (33%)	16 (12%)	0	6
49	DQ	139/141 (99%)	81 (58%)	39 (28%)	19 (14%)	0	4
50	BR	115/118 (98%)	68 (59%)	25 (22%)	22 (19%)	0	2
50	DR	115/118 (98%)	70 (61%)	23 (20%)	22 (19%)	0	2
51	BS	97/112 (87%)	37 (38%)	35 (36%)	25 (26%)	0	0
51	DS	97/112 (87%)	36 (37%)	37 (38%)	24 (25%)	0	0
52	BT	136/146 (93%)	63 (46%)	40 (29%)	33 (24%)	0	0
52	DT	136/146 (93%)	63 (46%)	40 (29%)	33 (24%)	0	0
53	BU	115/118 (98%)	69 (60%)	34 (30%)	12 (10%)	0	7
53	DU	115/118 (98%)	66 (57%)	37 (32%)	12 (10%)	0	7
54	BV	99/101 (98%)	61 (62%)	19 (19%)	19 (19%)	0	2
54	DV	99/101 (98%)	61 (62%)	18 (18%)	20 (20%)	0	1
55	BW	111/113 (98%)	73 (66%)	24 (22%)	14 (13%)	0	5
55	DW	111/113 (98%)	74 (67%)	23 (21%)	14 (13%)	0	5
56	BX	91/96 (95%)	55 (60%)	20 (22%)	16 (18%)	0	2
56	DX	91/96 (95%)	54 (59%)	22 (24%)	15 (16%)	0	3
57	BY	99/110 (90%)	37 (37%)	29 (29%)	33 (33%)	0	0
57	DY	99/110 (90%)	38 (38%)	28 (28%)	33 (33%)	0	0
58	BZ	174/206 (84%)	87 (50%)	47 (27%)	40 (23%)	0	0
58	DZ	174/206 (84%)	96 (55%)	41 (24%)	37 (21%)	0	1
All	All	12280/13108 (94%)	7151 (58%)	3059 (25%)	2070 (17%)	0	2

5 of 2070 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	19	HIS
2	AB	76	GLN
2	AB	77	ALA
2	AB	93	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%)	178 (88%)	24 (12%)	5	27
2	CB	202/220 (92%)	179 (89%)	23 (11%)	5	29
3	AC	160/188 (85%)	148 (92%)	12 (8%)	13	45
3	CC	160/188 (85%)	148 (92%)	12 (8%)	13	45
4	AD	180/181 (99%)	147 (82%)	33 (18%)	1	10
4	CD	180/181 (99%)	146 (81%)	34 (19%)	1	9
5	AE	115/123 (94%)	103 (90%)	12 (10%)	7	33
5	CE	115/123 (94%)	103 (90%)	12 (10%)	7	33
6	AF	90/90 (100%)	79 (88%)	11 (12%)	5	26
6	CF	90/90 (100%)	78 (87%)	12 (13%)	4	23
7	AG	126/127 (99%)	113 (90%)	13 (10%)	7	34
7	CG	126/127 (99%)	113 (90%)	13 (10%)	7	34
8	AH	119/119 (100%)	100 (84%)	19 (16%)	2	16
8	CH	119/119 (100%)	101 (85%)	18 (15%)	3	19
9	AI	98/99 (99%)	86 (88%)	12 (12%)	5	26
9	CI	98/99 (99%)	86 (88%)	12 (12%)	5	26
10	AJ	88/92 (96%)	71 (81%)	17 (19%)	1	9
10	CJ	88/92 (96%)	71 (81%)	17 (19%)	1	9
11	AK	90/99 (91%)	81 (90%)	9 (10%)	7	35
11	CK	90/99 (91%)	82 (91%)	8 (9%)	9	40
12	AL	104/111 (94%)	82 (79%)	22 (21%)	1	7
12	CL	104/111 (94%)	82 (79%)	22 (21%)	1	7
13	AM	99/101 (98%)	88 (89%)	11 (11%)	6	31
13	CM	99/101 (98%)	88 (89%)	11 (11%)	6	31
14	AN	49/50 (98%)	40 (82%)	9 (18%)	1	10
14	CN	49/50 (98%)	40 (82%)	9 (18%)	1	10
15	AO	79/80 (99%)	69 (87%)	10 (13%)	4	24
15	CO	79/80 (99%)	68 (86%)	11 (14%)	3	22
16	AP	72/74 (97%)	65 (90%)	7 (10%)	8	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	36
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	17	52
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	13	46
18	AR	61/77 (79%)	56 (92%)	5 (8%)	11	42
18	CR	61/77 (79%)	56 (92%)	5 (8%)	11	42
19	AS	69/80 (86%)	59 (86%)	10 (14%)	3	20
19	CS	69/80 (86%)	59 (86%)	10 (14%)	3	20
20	AT	76/82 (93%)	63 (83%)	13 (17%)	2	13
20	CT	76/82 (93%)	63 (83%)	13 (17%)	2	13
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	33
21	CU	19/22 (86%)	17 (90%)	2 (10%)	7	33
25	AZ	314/339 (93%)	272 (87%)	42 (13%)	4	23
25	CZ	314/339 (93%)	273 (87%)	41 (13%)	4	23
26	B0	66/67 (98%)	52 (79%)	14 (21%)	1	7
26	D0	66/67 (98%)	51 (77%)	15 (23%)	1	5
27	B1	78/83 (94%)	59 (76%)	19 (24%)	0	4
27	D1	78/83 (94%)	59 (76%)	19 (24%)	0	4
28	B2	66/67 (98%)	49 (74%)	17 (26%)	0	4
28	D2	66/67 (98%)	56 (85%)	10 (15%)	3	19
29	B3	51/52 (98%)	44 (86%)	7 (14%)	3	22
29	D3	51/52 (98%)	44 (86%)	7 (14%)	3	22
30	B4	39/63 (62%)	26 (67%)	13 (33%)	0	2
30	D4	39/63 (62%)	26 (67%)	13 (33%)	0	2
31	B5	51/52 (98%)	47 (92%)	4 (8%)	12	44
31	D5	51/52 (98%)	47 (92%)	4 (8%)	12	44
32	B6	49/52 (94%)	41 (84%)	8 (16%)	2	15
32	D6	49/52 (94%)	40 (82%)	9 (18%)	1	10
33	B7	41/42 (98%)	32 (78%)	9 (22%)	1	6
33	D7	41/42 (98%)	33 (80%)	8 (20%)	1	9
34	B8	53/55 (96%)	45 (85%)	8 (15%)	3	19
34	D8	53/55 (96%)	45 (85%)	8 (15%)	3	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	B9	34/34 (100%)	30 (88%)	4 (12%)	5	28
35	D9	34/34 (100%)	30 (88%)	4 (12%)	5	28
38	BC	180/181 (99%)	157 (87%)	23 (13%)	4	24
38	DC	180/181 (99%)	157 (87%)	23 (13%)	4	24
39	BD	217/218 (100%)	180 (83%)	37 (17%)	2	13
39	DD	217/218 (100%)	178 (82%)	39 (18%)	1	11
40	BE	165/166 (99%)	142 (86%)	23 (14%)	3	22
40	DE	165/166 (99%)	143 (87%)	22 (13%)	4	23
41	BF	165/166 (99%)	152 (92%)	13 (8%)	12	44
41	DF	165/166 (99%)	152 (92%)	13 (8%)	12	44
42	BG	155/156 (99%)	130 (84%)	25 (16%)	2	16
42	DG	155/156 (99%)	129 (83%)	26 (17%)	2	14
43	BH	132/148 (89%)	118 (89%)	14 (11%)	6	32
43	DH	132/148 (89%)	119 (90%)	13 (10%)	8	36
46	BN	117/119 (98%)	103 (88%)	14 (12%)	5	27
46	DN	117/119 (98%)	102 (87%)	15 (13%)	4	24
47	BO	100/100 (100%)	90 (90%)	10 (10%)	7	35
47	DO	100/100 (100%)	90 (90%)	10 (10%)	7	35
48	BP	112/116 (97%)	88 (79%)	24 (21%)	1	7
48	DP	112/116 (97%)	89 (80%)	23 (20%)	1	7
49	BQ	111/111 (100%)	91 (82%)	20 (18%)	1	11
49	DQ	111/111 (100%)	91 (82%)	20 (18%)	1	11
50	BR	100/101 (99%)	86 (86%)	14 (14%)	3	21
50	DR	100/101 (99%)	82 (82%)	18 (18%)	1	11
51	BS	77/88 (88%)	66 (86%)	11 (14%)	3	21
51	DS	77/88 (88%)	66 (86%)	11 (14%)	3	21
52	BT	120/127 (94%)	99 (82%)	21 (18%)	2	12
52	DT	120/127 (94%)	100 (83%)	20 (17%)	2	14
53	BU	92/94 (98%)	84 (91%)	8 (9%)	10	41
53	DU	92/94 (98%)	84 (91%)	8 (9%)	10	41
54	BV	82/82 (100%)	66 (80%)	16 (20%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	DV	82/82 (100%)	66 (80%)	16 (20%)	1	9
55	BW	91/92 (99%)	79 (87%)	12 (13%)	4	23
55	DW	91/92 (99%)	79 (87%)	12 (13%)	4	23
56	BX	74/78 (95%)	67 (90%)	7 (10%)	8	37
56	DX	74/78 (95%)	67 (90%)	7 (10%)	8	37
57	BY	84/91 (92%)	68 (81%)	16 (19%)	1	9
57	DY	84/91 (92%)	68 (81%)	16 (19%)	1	9
58	BZ	155/179 (87%)	127 (82%)	28 (18%)	1	11
58	DZ	155/179 (87%)	131 (84%)	24 (16%)	2	18
All	All	10322/10862 (95%)	8852 (86%)	1470 (14%)	3	21

5 of 1470 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	CM	81	LEU
38	DC	72	VAL
16	CP	22	THR
13	CM	71	ARG
26	D0	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 331 such sidechains are listed below:

Mol	Chain	Res	Type
25	CZ	125	GLN
42	DG	40	ASN
26	D0	70	GLN
39	DD	96	HIS
49	DQ	12	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	288 (19%)	59 (3%)
1	CA	1503/1522 (98%)	284 (18%)	59 (3%)
22	AV	75/76 (98%)	20 (26%)	0
22	AW	75/76 (98%)	21 (28%)	2 (2%)
22	CV	75/76 (98%)	20 (26%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	CW	75/76 (98%)	21 (28%)	2 (2%)
23	AX	12/27 (44%)	4 (33%)	0
23	CX	12/27 (44%)	4 (33%)	0
24	AY	75/77 (97%)	29 (38%)	0
24	CY	75/77 (97%)	28 (37%)	0
36	BA	2900/2915 (99%)	647 (22%)	55 (1%)
36	DA	2900/2915 (99%)	653 (22%)	55 (1%)
37	BB	118/122 (96%)	29 (24%)	1 (0%)
37	DB	118/122 (96%)	29 (24%)	1 (0%)
All	All	9516/9630 (98%)	2077 (21%)	234 (2%)

5 of 2077 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	8	A
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 234 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2762	G
36	DA	2110	G
1	CA	575	G
36	DA	1992	G
36	DA	790	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

14 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	$\#\|Z\|>2$
24	YG	AY	37	24	31,42,43	1.39	4 (12%)	33,62,65	2.14	13 (39%)
24	H2U	AY	16	24	18,21,22	0.95	1 (5%)	21,30,33	1.79	4 (19%)
24	H2U	CY	20	24	18,21,22	0.82	0	21,30,33	1.77	4 (19%)
24	H2U	CY	17	24	18,21,22	0.85	0	21,30,33	1.90	4 (19%)
24	5MU	AY	54	24	19,22,23	0.24	0	28,32,35	0.39	0
24	H2U	AY	20	24	18,21,22	0.83	0	21,30,33	1.75	4 (19%)
24	7MG	AY	46	24	22,26,27	2.99	2 (9%)	29,39,42	1.55	2 (6%)
24	7MG	CY	46	24	22,26,27	3.05	2 (9%)	29,39,42	1.54	2 (6%)
24	5MU	CY	54	24	19,22,23	0.24	0	28,32,35	0.37	0
24	YG	CY	37	24	31,42,43	1.32	3 (9%)	33,62,65	2.13	11 (33%)
24	H2U	CY	16	24	18,21,22	0.88	1 (5%)	21,30,33	1.80	4 (19%)
24	PSU	AY	55	24	18,21,22	1.06	2 (11%)	22,30,33	1.94	5 (22%)
24	H2U	AY	17	24	18,21,22	0.84	0	21,30,33	1.89	4 (19%)
24	PSU	CY	55	24	18,21,22	1.06	2 (11%)	22,30,33	1.97	6 (27%)

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
24	YG	AY	37	24	-	2/20/42/43	0/3/4/4
24	H2U	AY	16	24	-	2/7/38/39	0/2/2/2
24	H2U	CY	20	24	-	3/7/38/39	0/2/2/2
24	H2U	CY	17	24	-	5/7/38/39	0/2/2/2
24	5MU	AY	54	24	-	0/7/25/26	0/2/2/2
24	H2U	AY	20	24	-	3/7/38/39	0/2/2/2
24	7MG	AY	46	24	-	0/7/37/38	0/3/3/3
24	7MG	CY	46	24	-	0/7/37/38	0/3/3/3
24	5MU	CY	54	24	-	0/7/25/26	0/2/2/2
24	YG	CY	37	24	-	2/20/42/43	0/3/4/4
24	H2U	CY	16	24	-	2/7/38/39	0/2/2/2
24	PSU	AY	55	24	-	1/7/25/26	0/2/2/2
24	H2U	AY	17	24	-	5/7/38/39	0/2/2/2
24	PSU	CY	55	24	-	1/7/25/26	0/2/2/2

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	46	7MG	C8-N9	-13.86	1.38	1.46
24	AY	46	7MG	C8-N9	-13.54	1.38	1.46
24	AY	37	YG	C12-N1	3.98	1.43	1.36
24	CY	37	YG	C12-N1	3.85	1.43	1.36
24	AY	37	YG	C8-N7	-3.51	1.29	1.35

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AY	46	7MG	N9-C8-N7	6.81	113.11	103.38
24	CY	46	7MG	N9-C8-N7	6.76	113.05	103.38
24	CY	17	H2U	C4-N3-C2	-5.43	121.29	125.79
24	CY	37	YG	C24-O23-C21	5.41	122.04	115.66
24	AY	16	H2U	C4-N3-C2	-5.34	121.36	125.79

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	17	H2U	O4'-C1'-N1-C2
24	AY	17	H2U	O4'-C1'-N1-C6
24	AY	20	H2U	O4'-C4'-C5'-O5'
24	AY	20	H2U	C3'-C4'-C5'-O5'
24	CY	17	H2U	O4'-C1'-N1-C2

There are no ring outliers.

12 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	37	YG	8	0
24	AY	16	H2U	3	0
24	CY	20	H2U	2	0
24	CY	17	H2U	1	0
24	AY	54	5MU	4	0
24	AY	20	H2U	2	0
24	CY	54	5MU	6	0
24	CY	37	YG	5	0
24	CY	16	H2U	3	0
24	AY	55	PSU	5	0
24	AY	17	H2U	1	0
24	CY	55	PSU	7	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
62	GDP	AZ	501	-	24,30,30	1.26	2 (8%)	30,47,47	1.69	6 (20%)
62	GDP	CZ	501	-	24,30,30	1.32	3 (12%)	30,47,47	1.70	6 (20%)
59	PAR	AA	1601	-	45,45,45	1.49	5 (11%)	64,67,67	1.42	8 (12%)
63	KIR	CZ	502	-	56,59,59	3.43	24 (42%)	62,84,84	1.66	14 (22%)
63	KIR	AZ	502	-	56,59,59	3.40	23 (41%)	62,84,84	1.65	10 (16%)
59	PAR	CA	1601	-	45,45,45	1.43	5 (11%)	64,67,67	1.36	9 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GDP	AZ	501	-	-	2/12/32/32	0/3/3/3
62	GDP	CZ	501	-	-	3/12/32/32	0/3/3/3
59	PAR	AA	1601	-	-	7/18/94/94	0/4/4/4
63	KIR	CZ	502	-	-	6/54/98/98	0/3/3/3
63	KIR	AZ	502	-	-	7/54/98/98	0/3/3/3
59	PAR	CA	1601	-	-	5/18/94/94	0/4/4/4

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	AZ	502	KIR	O18-C17	-14.60	1.22	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	CZ	502	KIR	O18-C17	-14.49	1.22	1.44
63	CZ	502	KIR	O30-C30	-12.32	1.18	1.42
63	AZ	502	KIR	O30-C30	-12.23	1.18	1.42
63	CZ	502	KIR	C22-C21	6.04	1.39	1.33

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	CZ	502	KIR	O29-C29-O34	-4.52	102.64	110.21
63	AZ	502	KIR	O29-C29-O34	-4.49	102.69	110.21
59	AA	1601	PAR	C14-O54-C54	4.47	122.47	113.69
63	CZ	502	KIR	C48-C32-C47	-4.43	101.40	107.72
59	AA	1601	PAR	O33-C14-C24	4.42	115.83	108.22

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AA	1601	PAR	C44-C54-C64-N64
59	AA	1601	PAR	O54-C54-C64-N64
62	AZ	501	GDP	PA-O3A-PB-O2B
62	AZ	501	GDP	PA-O3A-PB-O3B
62	CZ	501	GDP	PA-O3A-PB-O2B

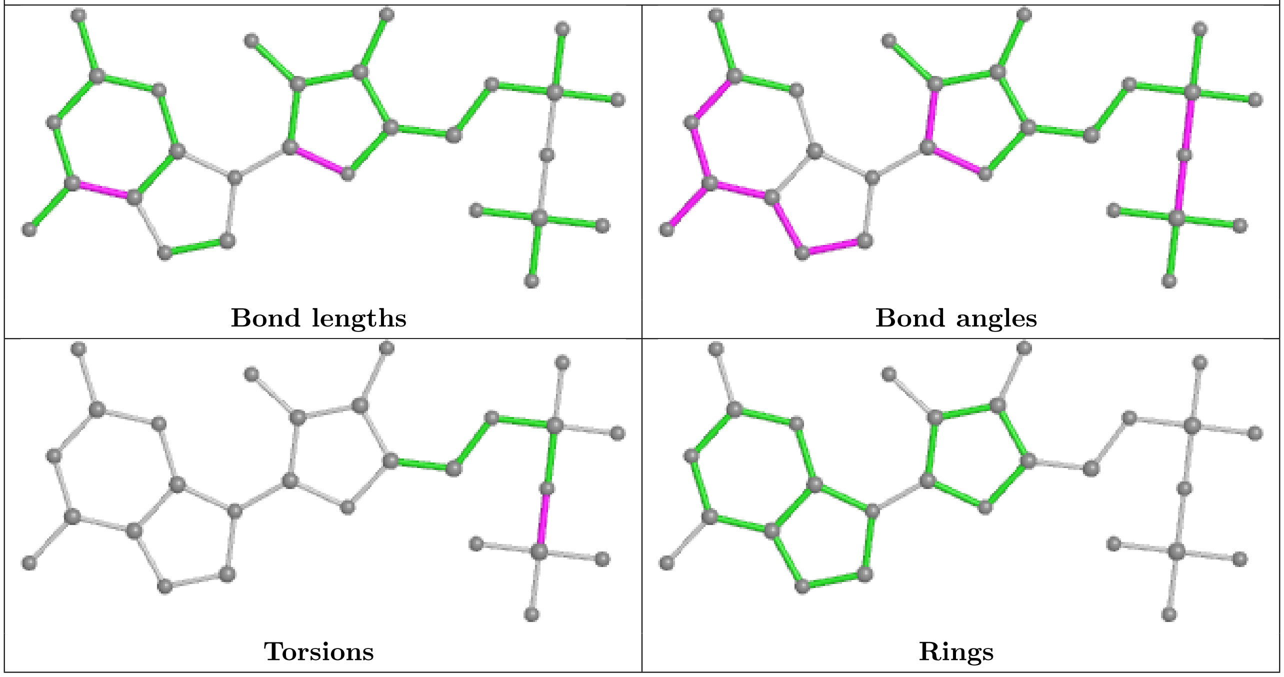
There are no ring outliers.

6 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	AZ	501	GDP	15	0
62	CZ	501	GDP	15	0
59	AA	1601	PAR	4	0
63	CZ	502	KIR	8	0
63	AZ	502	KIR	4	0
59	CA	1601	PAR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GDP AZ 501



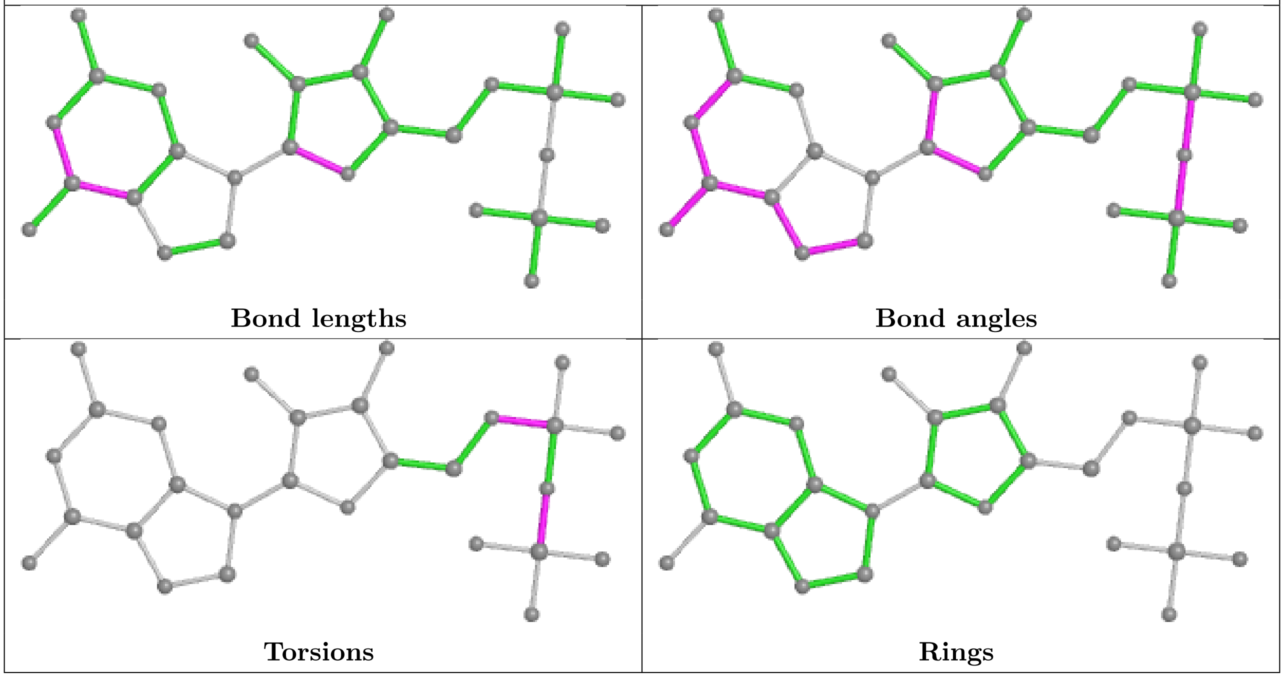
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP CZ 501



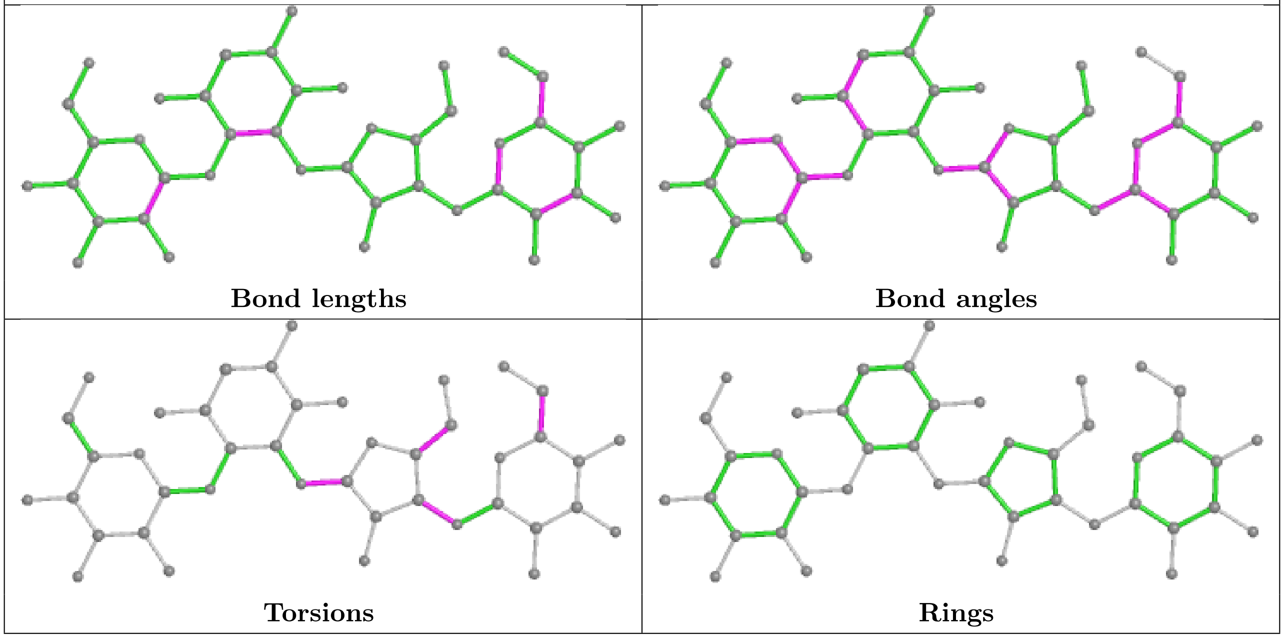
Bond lengths

Bond angles

Torsions

Rings

Ligand PAR AA 1601



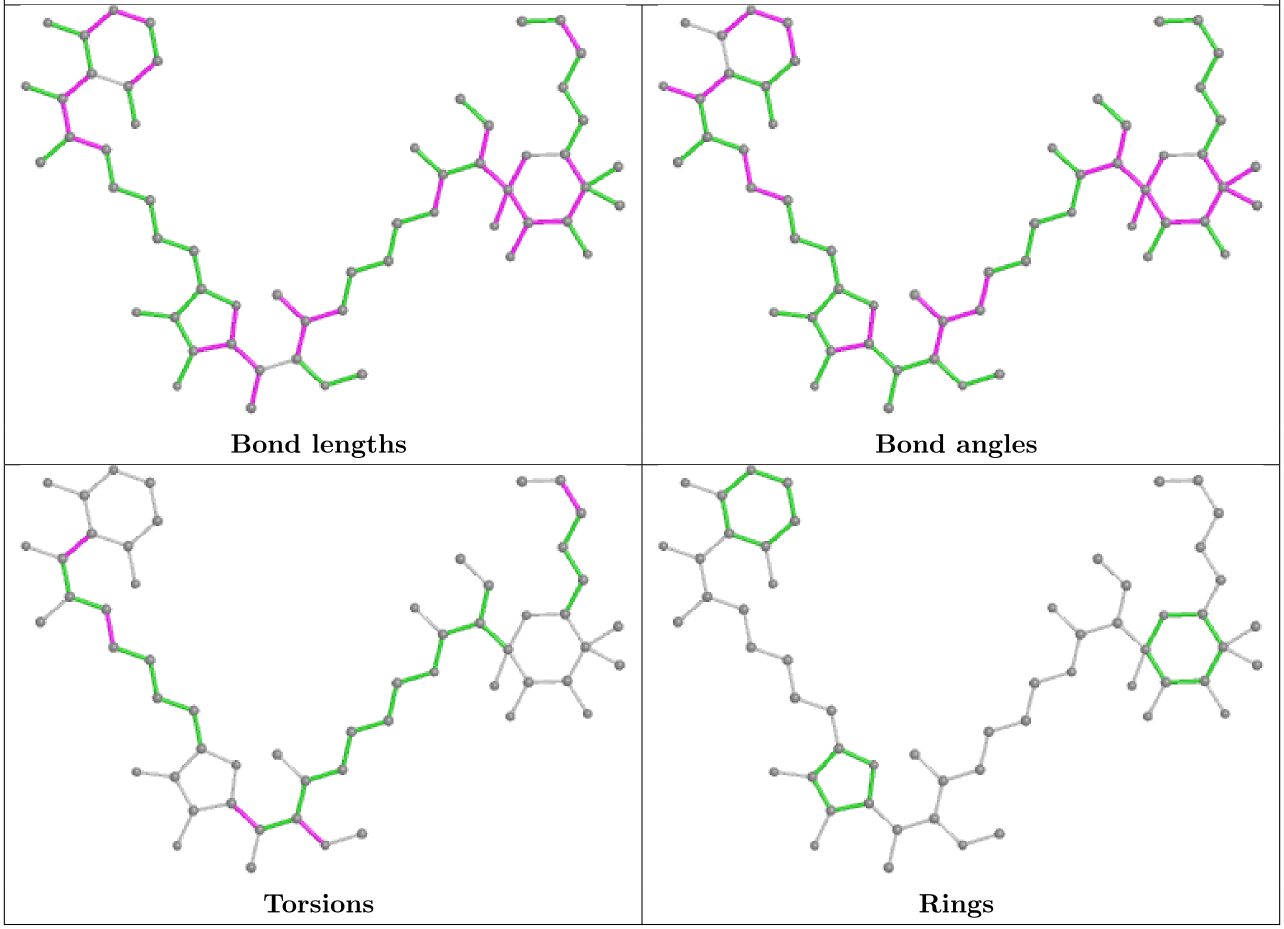
Bond lengths

Bond angles

Torsions

Rings

Ligand KIR CZ 502



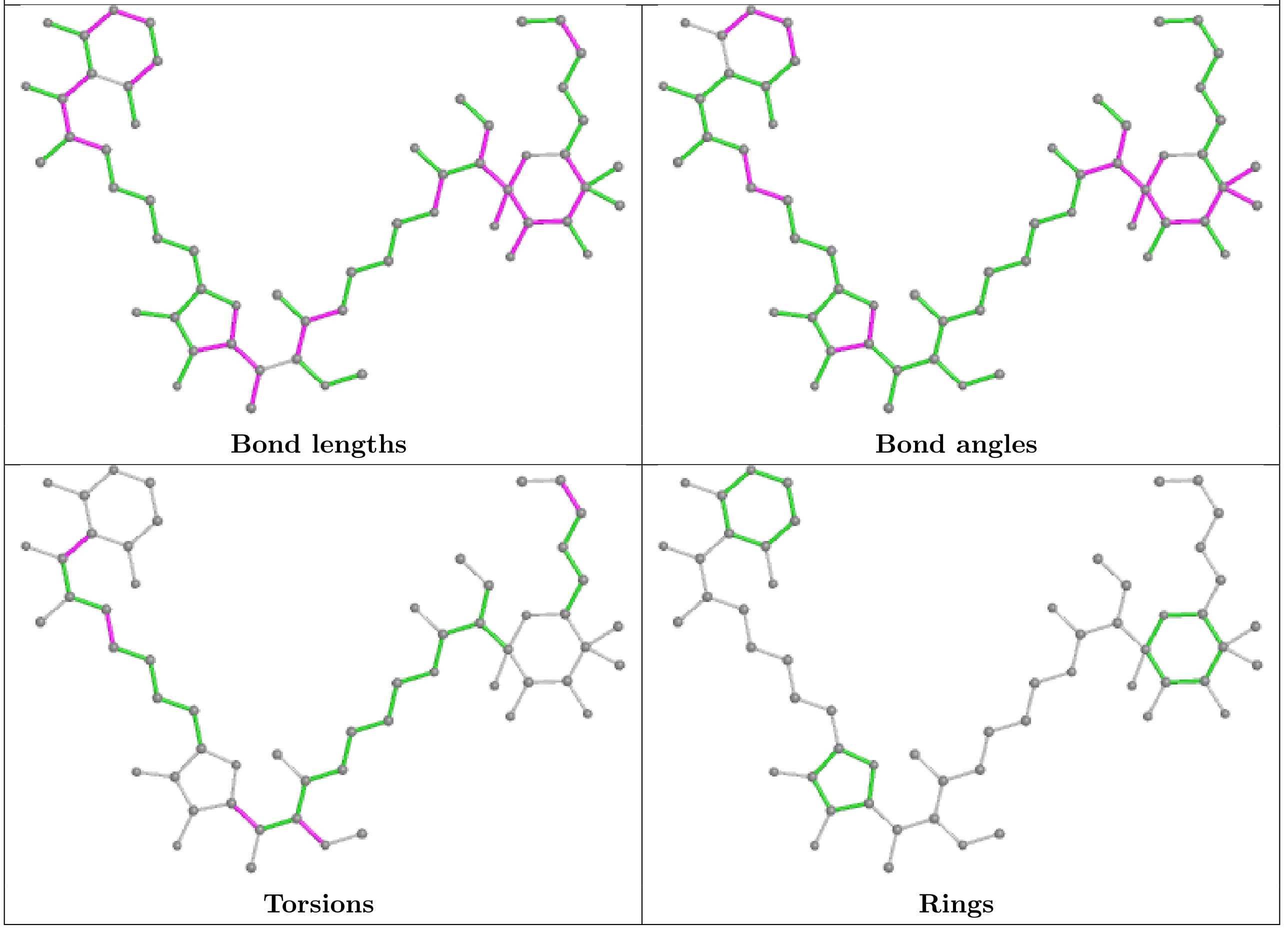
Bond lengths

Bond angles

Torsions

Rings

Ligand KIR AZ 502



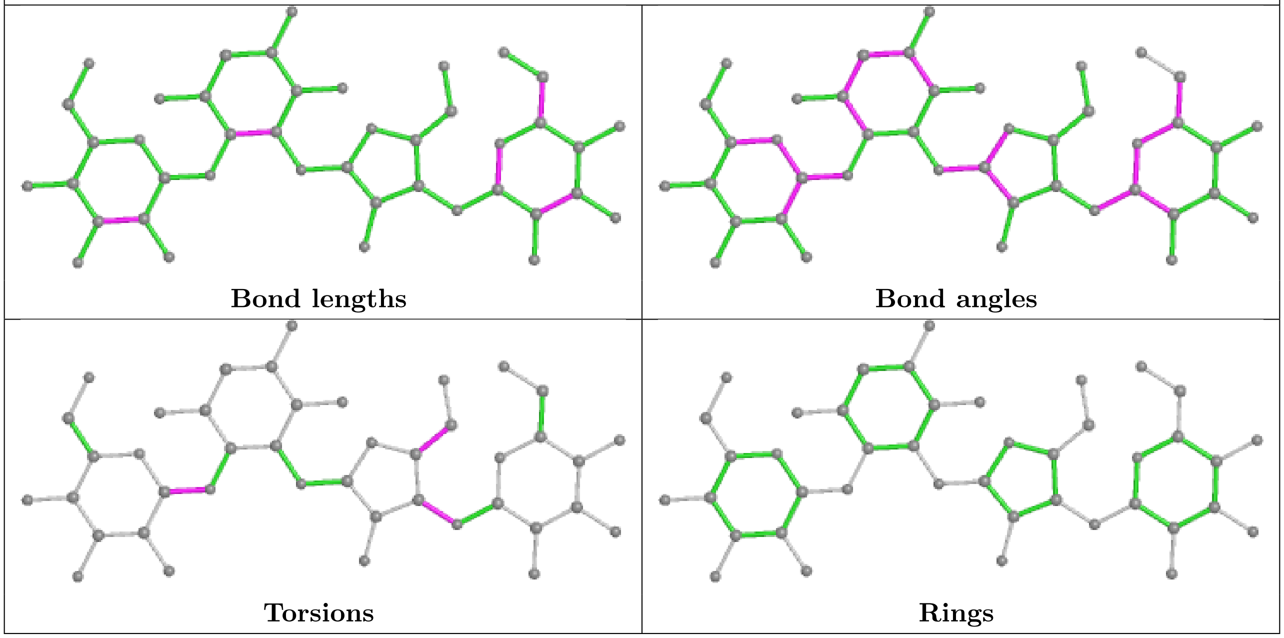
Bond lengths

Bond angles

Torsions

Rings

Ligand PAR CA 1601



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	D4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D4	47:GLN	C	48:ARG	N	1.19

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	1504/1522 (98%)	-0.07	10 (0%)	87	78	29, 82, 163, 200	0
1	CA	1504/1522 (98%)	-0.17	13 (0%)	84	73	28, 83, 163, 200	0
2	AB	235/256 (91%)	-0.06	3 (1%)	77	63	63, 102, 151, 161	0
2	CB	235/256 (91%)	-0.15	4 (1%)	70	55	63, 102, 151, 162	0
3	AC	207/239 (86%)	-0.19	1 (0%)	91	83	54, 91, 111, 117	0
3	CC	207/239 (86%)	-0.20	2 (0%)	82	70	59, 91, 111, 117	0
4	AD	208/209 (99%)	-0.23	1 (0%)	91	83	60, 91, 116, 122	0
4	CD	208/209 (99%)	-0.15	1 (0%)	91	83	61, 92, 117, 123	0
5	AE	151/162 (93%)	-0.30	0	100	100	44, 72, 90, 108	0
5	CE	151/162 (93%)	-0.25	1 (0%)	87	78	43, 73, 91, 109	0
6	AF	101/101 (100%)	-0.20	0	100	100	91, 102, 110, 118	0
6	CF	101/101 (100%)	-0.03	1 (0%)	82	70	92, 103, 111, 118	0
7	AG	155/156 (99%)	-0.10	3 (1%)	66	51	79, 104, 134, 141	0
7	CG	155/156 (99%)	-0.13	6 (3%)	39	25	81, 104, 134, 141	0
8	AH	138/138 (100%)	-0.04	1 (0%)	87	78	62, 80, 97, 116	0
8	CH	138/138 (100%)	-0.14	0	100	100	61, 82, 97, 115	0
9	AI	127/128 (99%)	0.08	5 (3%)	39	25	73, 126, 153, 158	0
9	CI	127/128 (99%)	0.11	3 (2%)	59	42	74, 126, 154, 159	0
10	AJ	99/105 (94%)	0.41	9 (9%)	9	5	79, 121, 149, 154	0
10	CJ	99/105 (94%)	0.42	10 (10%)	7	4	80, 121, 148, 153	0
11	AK	119/129 (92%)	-0.10	4 (3%)	45	30	63, 84, 125, 150	0
11	CK	119/129 (92%)	-0.01	4 (3%)	45	30	65, 85, 126, 151	0
12	AL	125/135 (92%)	-0.24	1 (0%)	86	75	47, 70, 100, 125	0
12	CL	125/135 (92%)	-0.09	1 (0%)	86	75	52, 71, 101, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	125/126 (99%)	0.12	6 (4%) 30 19	79, 119, 143, 159	0
13	CM	125/126 (99%)	0.12	5 (4%) 38 25	80, 118, 143, 159	0
14	AN	60/61 (98%)	-0.22	1 (1%) 70 55	60, 77, 96, 101	0
14	CN	60/61 (98%)	-0.12	1 (1%) 70 55	61, 77, 95, 103	0
15	AO	88/89 (98%)	-0.05	1 (1%) 80 68	69, 92, 109, 112	0
15	CO	88/89 (98%)	0.00	2 (2%) 60 44	72, 91, 109, 112	0
16	AP	84/88 (95%)	-0.05	1 (1%) 79 66	76, 89, 119, 137	0
16	CP	84/88 (95%)	0.01	2 (2%) 59 42	74, 89, 118, 137	0
17	AQ	100/105 (95%)	-0.05	0 100 100	65, 92, 115, 121	0
17	CQ	100/105 (95%)	0.03	2 (2%) 65 49	67, 92, 115, 121	0
18	AR	70/88 (79%)	-0.20	1 (1%) 75 61	55, 86, 114, 121	0
18	CR	70/88 (79%)	-0.22	1 (1%) 75 61	57, 87, 115, 121	0
19	AS	79/93 (84%)	0.42	10 (12%) 3 2	82, 120, 143, 146	0
19	CS	79/93 (84%)	0.27	7 (8%) 9 5	83, 120, 144, 146	0
20	AT	99/106 (93%)	-0.14	4 (4%) 38 25	94, 109, 129, 132	0
20	CT	99/106 (93%)	-0.15	1 (1%) 82 70	93, 109, 129, 132	0
21	AU	25/27 (92%)	0.64	3 (12%) 4 3	104, 116, 137, 139	0
21	CU	25/27 (92%)	0.38	1 (4%) 38 25	104, 116, 136, 138	0
22	AV	76/76 (100%)	-0.15	0 100 100	54, 120, 170, 179	0
22	AW	76/76 (100%)	-0.06	1 (1%) 77 63	82, 147, 186, 199	0
22	CV	76/76 (100%)	-0.21	0 100 100	54, 121, 170, 179	0
22	CW	76/76 (100%)	0.06	3 (3%) 39 25	84, 148, 185, 199	0
23	AX	13/27 (48%)	0.32	1 (7%) 13 8	45, 63, 136, 154	0
23	CX	13/27 (48%)	0.16	0 100 100	47, 62, 136, 154	0
24	AY	70/77 (90%)	0.23	2 (2%) 51 35	74, 155, 194, 200	0
24	CY	70/77 (90%)	0.47	6 (8%) 10 6	76, 156, 194, 200	0
25	AZ	374/406 (92%)	0.49	36 (9%) 8 4	97, 139, 158, 177	0
25	CZ	374/406 (92%)	0.78	67 (17%) 1 0	98, 139, 158, 176	0
26	B0	84/85 (98%)	0.16	0 100 100	104, 116, 128, 137	0
26	D0	84/85 (98%)	0.27	2 (2%) 59 42	104, 116, 129, 137	0
27	B1	94/98 (95%)	-0.21	3 (3%) 47 32	41, 71, 107, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
27	D1	94/98 (95%)	-0.19	1 (1%) 80 68	63, 85, 115, 122	0
28	B2	71/72 (98%)	-0.24	0 100 100	84, 115, 128, 130	0
28	D2	71/72 (98%)	0.14	3 (4%) 36 23	104, 125, 144, 163	0
29	B3	60/60 (100%)	0.85	9 (15%) 2 1	106, 122, 132, 148	0
29	D3	60/60 (100%)	0.48	5 (8%) 11 7	107, 122, 132, 148	0
30	B4	45/71 (63%)	0.75	8 (17%) 1 1	107, 169, 196, 198	0
30	D4	45/71 (63%)	0.61	6 (13%) 3 2	107, 170, 195, 197	0
31	B5	59/60 (98%)	0.63	5 (8%) 10 6	89, 116, 175, 187	0
31	D5	59/60 (98%)	0.42	6 (10%) 6 4	90, 115, 175, 186	0
32	B6	50/54 (92%)	0.47	7 (14%) 2 2	78, 119, 146, 152	0
32	D6	50/54 (92%)	0.48	6 (12%) 4 3	79, 119, 147, 152	0
33	B7	49/49 (100%)	-0.18	0 100 100	59, 77, 144, 152	0
33	D7	49/49 (100%)	-0.41	0 100 100	60, 78, 145, 152	0
34	B8	64/65 (98%)	0.12	3 (4%) 31 19	80, 104, 124, 138	0
34	D8	64/65 (98%)	0.24	3 (4%) 31 19	83, 104, 125, 138	0
35	B9	37/37 (100%)	0.21	2 (5%) 25 16	104, 117, 124, 128	0
35	D9	37/37 (100%)	0.71	4 (10%) 5 3	103, 118, 125, 126	0
36	BA	2901/2915 (99%)	-0.04	49 (1%) 70 55	31, 100, 192, 200	0
36	DA	2901/2915 (99%)	-0.05	59 (2%) 65 49	31, 101, 192, 200	0
37	BB	119/122 (97%)	0.04	3 (2%) 57 41	103, 142, 169, 175	0
37	DB	119/122 (97%)	-0.15	0 100 100	102, 142, 168, 174	0
38	BC	228/229 (99%)	0.37	16 (7%) 16 9	92, 122, 168, 178	0
38	DC	228/229 (99%)	0.54	27 (11%) 4 3	92, 122, 167, 179	0
39	BD	275/276 (99%)	-0.13	2 (0%) 87 78	30, 67, 96, 110	0
39	DD	275/276 (99%)	-0.17	2 (0%) 87 78	38, 68, 96, 109	0
40	BE	205/206 (99%)	0.18	9 (4%) 34 21	67, 106, 143, 154	0
40	DE	205/206 (99%)	0.12	5 (2%) 59 42	67, 106, 143, 153	0
41	BF	208/210 (99%)	0.14	10 (4%) 30 19	61, 123, 160, 167	0
41	DF	208/210 (99%)	0.28	11 (5%) 26 16	62, 123, 160, 166	0
42	BG	181/182 (99%)	0.08	10 (5%) 25 15	103, 128, 146, 163	0
42	DG	181/182 (99%)	0.34	14 (7%) 13 8	111, 133, 151, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	BH	160/180 (88%)	0.67	27 (16%) 1 1	131, 155, 174, 176	0
43	DH	160/180 (88%)	0.92	27 (16%) 1 1	131, 155, 174, 176	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	139/140 (99%)	0.20	6 (4%) 35 22	103, 123, 148, 155	0
46	DN	139/140 (99%)	0.22	9 (6%) 18 11	103, 123, 148, 155	0
47	BO	122/122 (100%)	-0.14	0 100 100	60, 80, 96, 104	0
47	DO	122/122 (100%)	-0.05	0 100 100	61, 80, 96, 106	0
48	BP	146/150 (97%)	0.02	6 (4%) 37 24	71, 113, 133, 140	0
48	DP	146/150 (97%)	0.35	14 (9%) 8 4	70, 114, 133, 139	0
49	BQ	141/141 (100%)	0.10	5 (3%) 44 29	73, 106, 130, 159	0
49	DQ	141/141 (100%)	0.14	3 (2%) 63 48	73, 105, 129, 159	0
50	BR	117/118 (99%)	0.11	5 (4%) 35 22	81, 105, 123, 143	0
50	DR	117/118 (99%)	0.18	4 (3%) 45 30	82, 105, 124, 143	0
51	BS	99/112 (88%)	0.22	3 (3%) 50 34	96, 133, 155, 162	0
51	DS	99/112 (88%)	0.35	5 (5%) 28 17	97, 133, 156, 162	0
52	BT	138/146 (94%)	0.09	6 (4%) 35 22	72, 112, 166, 181	0
52	DT	138/146 (94%)	0.21	10 (7%) 15 9	73, 111, 166, 181	0
53	BU	117/118 (99%)	0.17	4 (3%) 45 30	87, 120, 141, 147	0
53	DU	117/118 (99%)	-0.07	3 (2%) 56 40	88, 119, 141, 148	0
54	BV	101/101 (100%)	0.77	18 (17%) 1 1	105, 144, 159, 164	0
54	DV	101/101 (100%)	0.73	18 (17%) 1 1	106, 145, 159, 165	0
55	BW	113/113 (100%)	0.14	9 (7%) 12 7	81, 109, 132, 136	0
55	DW	113/113 (100%)	0.17	3 (2%) 54 38	81, 109, 131, 136	0
56	BX	93/96 (96%)	0.04	2 (2%) 62 45	96, 108, 124, 128	0
56	DX	93/96 (96%)	0.14	5 (5%) 25 16	97, 109, 125, 130	0
57	BY	101/110 (91%)	0.66	12 (11%) 4 3	124, 145, 165, 170	0
57	DY	101/110 (91%)	1.18	26 (25%) 0 0	123, 145, 163, 170	0
58	BZ	176/206 (85%)	0.71	28 (15%) 1 1	107, 133, 161, 164	0
58	DZ	176/206 (85%)	1.00	41 (23%) 0 0	109, 139, 168, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	22002/23378 (94%)	0.06	838 (3%)	40	26	28, 105, 164, 200	0

The worst 5 of 838 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	DQ	140	ALA	16.1
31	B5	60	VAL	14.7
57	DY	52	SER	12.2
1	AA	89	C	11.2
36	DA	654(I)	C	11.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	H2U	CY	16	20/21	0.53	0.47	199,199,200,200	0
24	H2U	AY	17	20/21	0.58	0.40	195,199,199,200	0
24	H2U	AY	16	20/21	0.62	0.66	198,199,200,200	0
24	PSU	CY	55	20/21	0.66	0.31	172,180,180,180	0
24	H2U	CY	17	20/21	0.67	0.48	196,199,200,200	0
24	H2U	CY	20	20/21	0.72	0.18	195,198,200,200	0
24	PSU	AY	55	20/21	0.76	0.19	171,180,181,182	0
24	7MG	CY	46	24/25	0.78	0.24	186,189,190,190	0
24	7MG	AY	46	24/25	0.78	0.22	186,189,190,190	0
24	H2U	AY	20	20/21	0.83	0.21	196,198,200,200	0
24	5MU	AY	54	21/22	0.85	0.23	164,166,168,171	0
24	5MU	CY	54	21/22	0.87	0.35	165,167,168,171	0
24	YG	CY	37	39/40	0.90	0.26	77,108,122,122	0
24	YG	AY	37	39/40	0.90	0.30	77,108,121,122	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
61	MG	CY	101	1/1	-0.22	2.02	181,181,181,181	0
61	MG	AY	101	1/1	0.32	0.24	109,109,109,109	0
62	GDP	CZ	501	28/28	0.84	0.19	117,126,128,128	0
63	KIR	AZ	502	57/57	0.85	0.46	98,106,116,117	0
62	GDP	AZ	501	28/28	0.89	0.20	117,124,126,126	0
63	KIR	CZ	502	57/57	0.89	0.44	99,106,116,117	0
59	PAR	AA	1601	42/42	0.94	0.20	40,44,48,49	0
59	PAR	CA	1601	42/42	0.94	0.21	41,46,64,65	0
60	ZN	D4	101	1/1	0.94	0.12	133,133,133,133	0
60	ZN	D9	101	1/1	0.96	0.09	126,126,126,126	0
60	ZN	B4	101	1/1	0.97	0.15	97,97,97,97	0
60	ZN	CN	101	1/1	0.98	0.19	100,100,100,100	0
60	ZN	AD	301	1/1	0.99	0.28	52,52,52,52	0
60	ZN	B9	101	1/1	0.99	0.18	113,113,113,113	0
60	ZN	CD	301	1/1	0.99	0.29	56,56,56,56	0
60	ZN	AN	101	1/1	1.00	0.16	45,45,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.