wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 3, 2024 – 02:11 am GMT

PDB ID : 4V5Q
Title : The crystal structure of EF-Tu and G24A-tRNA-Trp bound to a near- cognate codon on the 70S ribosome
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.
Deposited on : 2010-12-07
Resolution : 3.10 Å(reported)

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

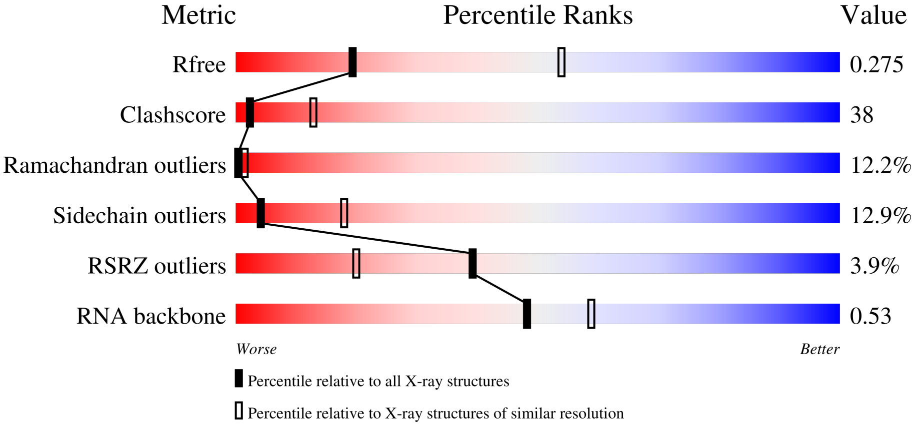
MolProbity	4.02b-467
Mogul	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	1.13
EDS	2.36
buster-report	1.1.7 (2018)
Percentile statistics	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	5.8.0158
CCP4	7.0.044 (Gargrove)
Ideal geometry (proteins)	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

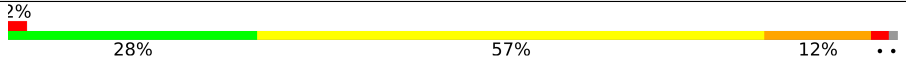
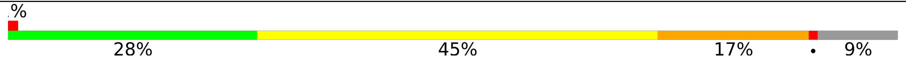
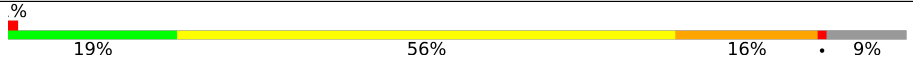
The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	37% 38% 11% 14%
3	CC	239	26% 48% 12% 14%
4	AD	209	4% 25% 55% 19% •
4	CD	209	4% 15% 61% 21% •
5	AE	162	50% 37% 5% • 7%
5	CE	162	32% 56% 5% 7%
6	AF	101	% 39% 50% 12%
6	CF	101	% 26% 58% 15% •
7	AG	156	3% 39% 51% 10% •
7	CG	156	3% 46% 42% 12% •
8	AH	138	57% 37% 7%
8	CH	138	35% 57% 7% •
9	AI	128	% 36% 48% 14% ••
9	CI	128	8% 31% 55% 12% • •
10	AJ	105	28% 48% 17% • 7%
10	CJ	105	9% 20% 54% 17% • 7%
11	AK	129	2% 43% 41% 8% 8%
11	CK	129	2% 35% 47% 9% • 8%
12	AL	132	% 33% 48% 11% • 6%
12	CL	132	2% 43% 39% 11% • 6%
13	AM	126	4% 28% 52% 16% • •
13	CM	126	6% 19% 65% 12% • •
14	AN	61	2% 36% 41% 16% 5% •
14	CN	61	3% 28% 49% 16% 5% •
15	AO	89	42% 49% 7% ••

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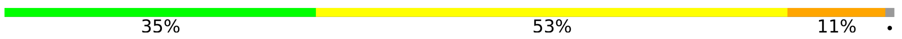
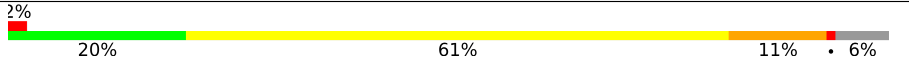
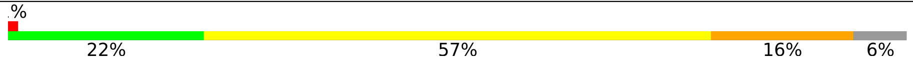
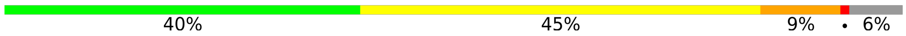
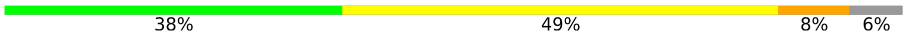
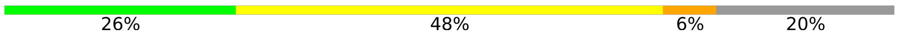
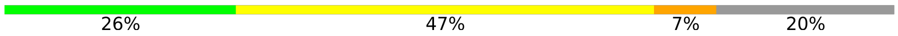
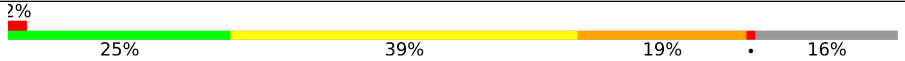
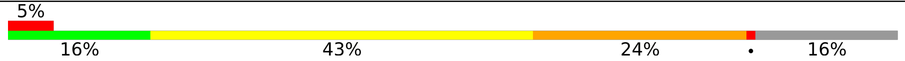
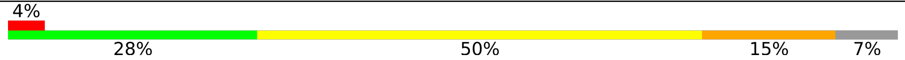
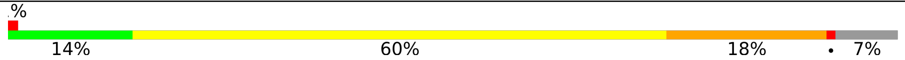
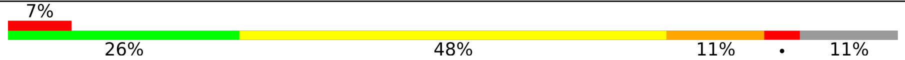
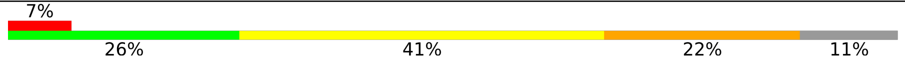
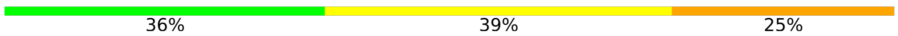
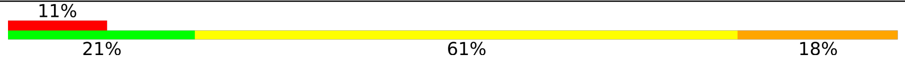
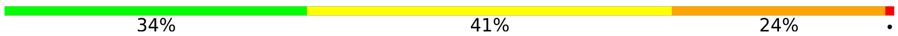
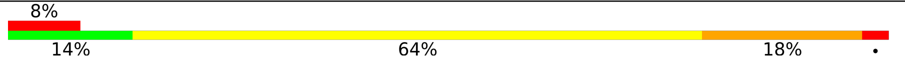
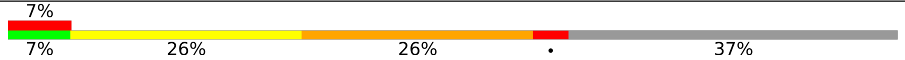
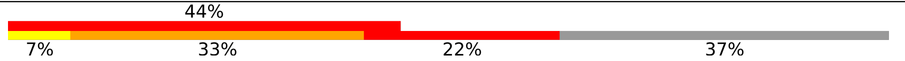
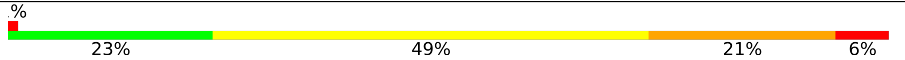
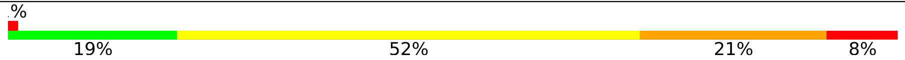
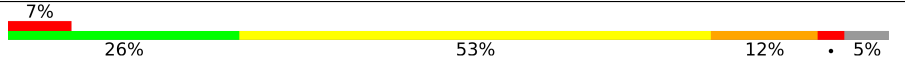
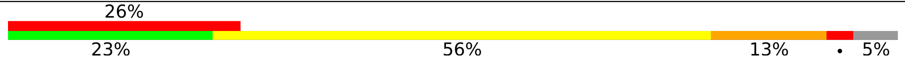
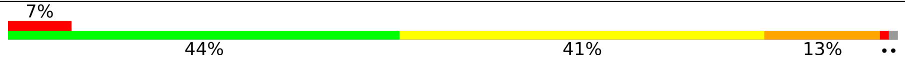
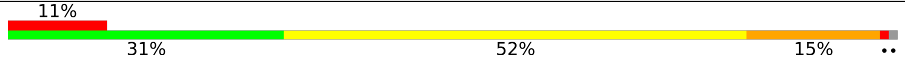
Mol	Chain	Length	Quality of chain
15	CO	89	 35% 53% 11% •
16	AP	88	 2% 20% 61% 11% • 6%
16	CP	88	 % 22% 57% 16% 6%
17	AQ	105	 40% 45% 9% • 6%
17	CQ	105	 38% 49% 8% 6%
18	AR	88	 26% 48% 6% 20%
18	CR	88	 26% 47% 7% 20%
19	AS	93	 2% 25% 39% 19% • 16%
19	CS	93	 5% 16% 43% 24% • 16%
20	AT	106	 4% 28% 50% 15% 7%
20	CT	106	 % 14% 60% 18% • 7%
21	AU	27	 7% 26% 48% 11% • 11%
21	CU	27	 7% 26% 41% 22% 11%
22	AV	76	 36% 39% 25%
22	AW	76	 11% 21% 61% 18%
22	CV	76	 34% 41% 24% •
22	CW	76	 8% 14% 64% 18% •
23	AX	27	 7% 7% 26% 26% • 37%
23	CX	27	 44% 7% 33% 22% 37%
24	AY	77	 % 23% 49% 21% 6%
24	CY	77	 % 19% 52% 21% 8%
25	AZ	405	 7% 26% 53% 12% • 5%
25	CZ	405	 26% 23% 56% 13% • 5%
26	B0	85	 7% 44% 41% 13% ••
26	D0	85	 11% 31% 52% 15% ••

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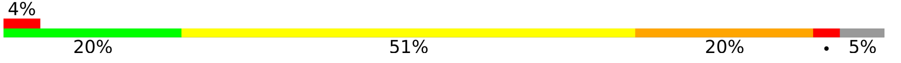
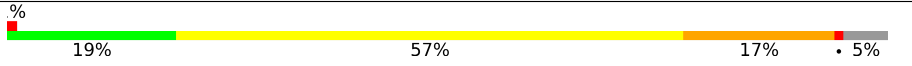
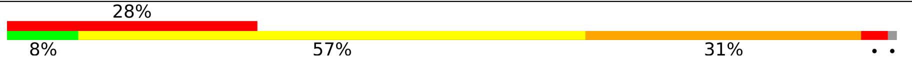
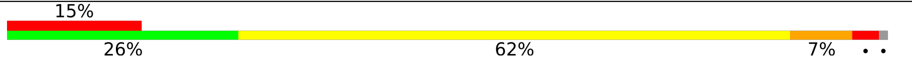
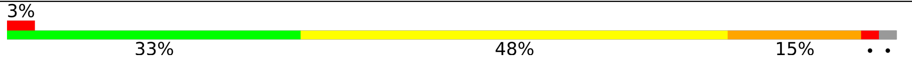
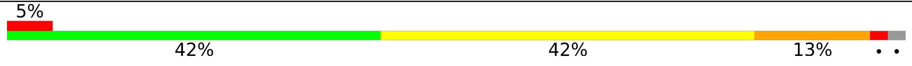
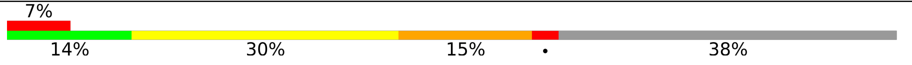
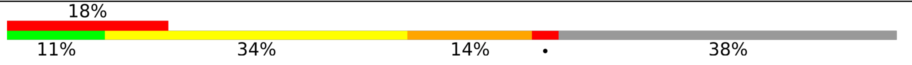
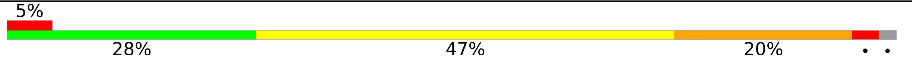
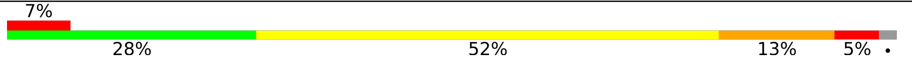
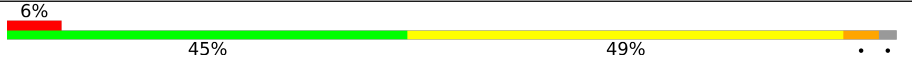
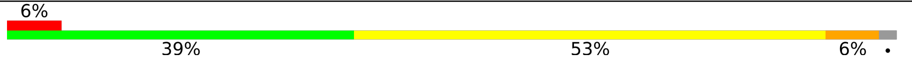
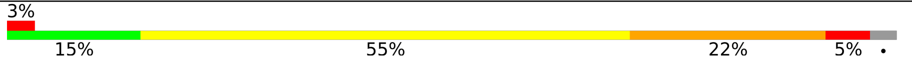
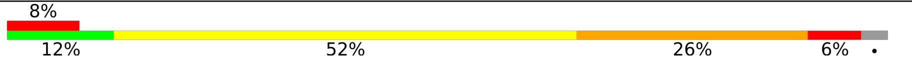
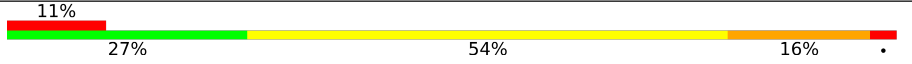
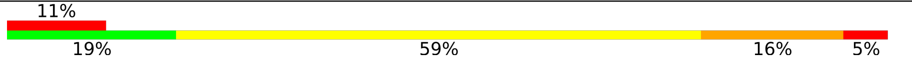
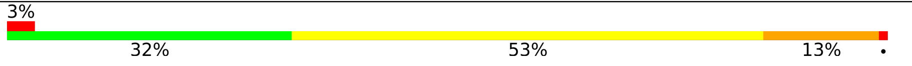
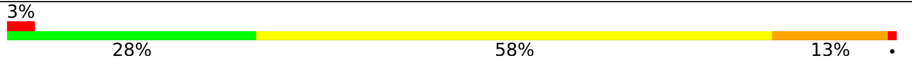
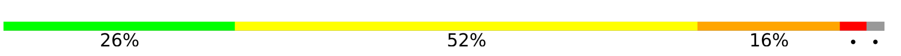
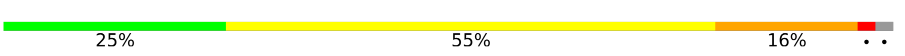
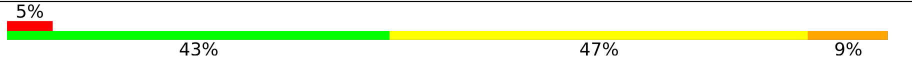
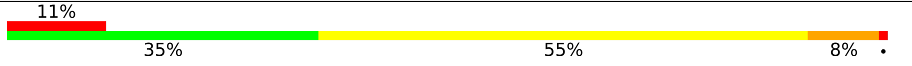
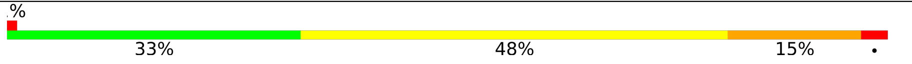
Mol	Chain	Length	Quality of chain
27	B1	98	
27	D1	98	
28	B2	72	
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229	
39	BD	276	

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Mol	Chain	Length	Quality of chain
39	DD	276	% 30% 51% 17% •
40	BE	206	2% 23% 53% 20% • •
40	DE	206	3% 17% 58% 22% • •
41	BF	210	7% 30% 54% 12% • •
41	DF	210	8% 26% 61% 11% •
42	BG	182	5% 21% 50% 27% • •
42	DG	182	4% 16% 57% 25% • •
43	BH	180	12% 28% 41% 18% • 12%
43	DH	180	6% 25% 45% 18% • 12%
44	BJ	173	58% 17% 25%
44	DJ	173	54% 21% 25%
45	BK	147	80% 16% 5%
45	DK	147	83% 12% 5%
46	BN	140	23% 56% 19% • •
46	DN	140	24% 54% 18% • •
47	BO	122	42% 47% 10% •
47	DO	122	40% 48% 10% •
48	BP	150	9% 17% 51% 25% • •
48	DP	150	14% 18% 49% 28% • •
49	BQ	141	2% 35% 52% 11% •
49	DQ	141	% 34% 52% 13% •
50	BR	118	2% 24% 53% 20% • •
50	DR	118	% 24% 56% 17% • •
51	BS	112	3% 12% 50% 23% • 12%
51	DS	112	7% 14% 41% 28% • 12%

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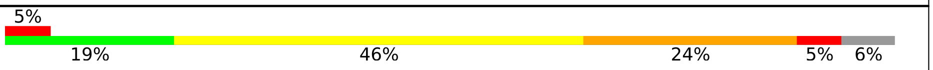
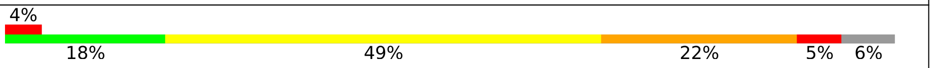
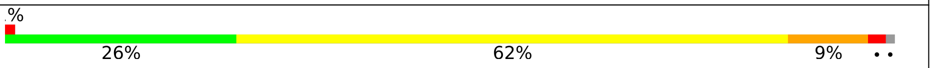
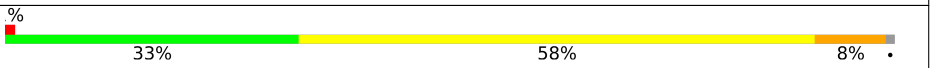
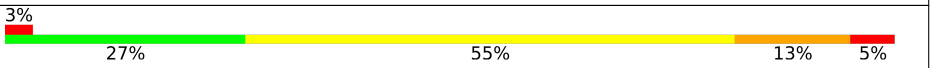
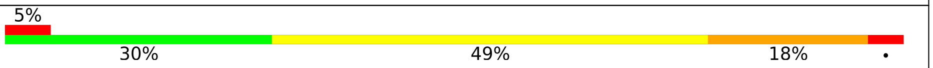
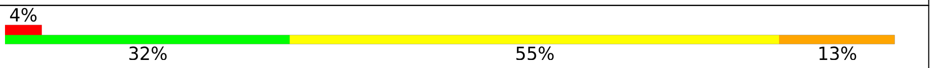
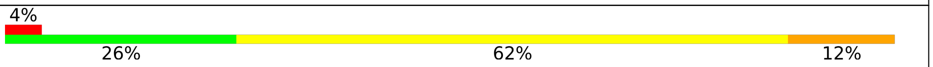
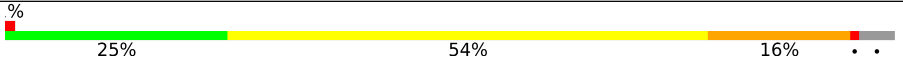
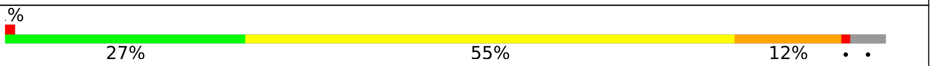
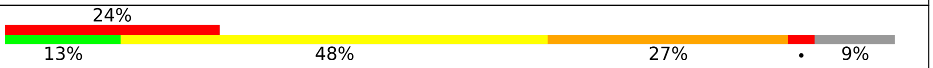
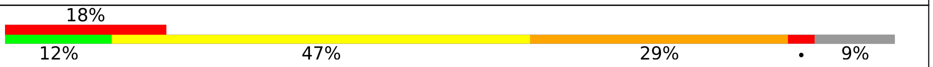
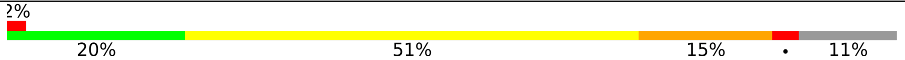
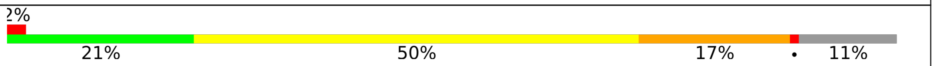
Mol	Chain	Length	Quality of chain
52	BT	146	
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	

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
59	ZN	AN	101	-	-	X	-
60	GDP	AZ	501	-	-	X	-
60	GDP	CZ	501	-	-	X	-
61	KIR	CZ	502	-	-	-	X

2 Entry composition ⓘ

There are 61 unique types of molecules in this entry. The entry contains 307194 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total 1900	C 1213	N 341	O 341	S 5	0	0	0
2	CB	234	Total 1900	C 1213	N 341	O 341	S 5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total 1612	C 1016	N 314	O 281	S 1	0	0	0
3	CC	206	Total 1612	C 1016	N 314	O 281	S 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AE	150	1146	724	217	201	4	0	0	0
5	CE	150	1146	724	217	201	4	0	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	AJ	98	794	499	156	138	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total 794	C 499	N 156	O 138	S 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total 970	C 611	N 195	O 163	S 1	0	0	0
12	CL	124	Total 970	C 611	N 195	O 163	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	124	Total 987	C 611	N 205	O 169	S 2	0	0	0
13	CM	124	Total 987	C 611	N 205	O 169	S 2	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	AP	83	Total C N O S 700 443 139 117 1	0	0	0
16	CP	83	Total C N O S 700 443 139 117 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	AQ	99	Total C N O S 823 528 151 142 2	0	0	0
17	CQ	99	Total C N O S 823 528 151 142 2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	AS	78	Total C N O S 629 403 114 110 2	0	0	0
19	CS	78	Total C N O S 629 403 114 110 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	AT	99	Total C N O S 763 470 162 129 2	0	0	0
20	CT	99	Total C N O S 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
21	AU	24	Total	C	N	O	0	0	0
			208	128	50	30			
21	CU	24	Total	C	N	O	0	0	0
			208	128	50	30			

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

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

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	17	Total	C	N	O	P	0	0	0
			361	164	68	113	16			
23	CX	17	Total	C	N	O	P	0	0	0
			361	164	68	113	16			

- Molecule 24 is a RNA chain called A-SITE TRNA G24A TRP-TRNA TRP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AY	77	Total	C	N	O	P	S	0	0	0
			1644	742	289	535	76	2			
24	CY	77	Total	C	N	O	P	S	0	0	0
			1644	742	289	535	76	2			

- Molecule 25 is a protein called ELONGATION FACTOR TU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AZ	385	Total	C	N	O	S	0	0	0
			2984	1885	524	563	12			
25	CZ	385	Total	C	N	O	S	0	0	0
			2984	1885	524	563	12			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B1	93	Total 731	C 460	N 145	O 125	S 1	0	0	0
27	D1	93	Total 731	C 460	N 145	O 125	S 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B3	59	Total 467	C 298	N 90	O 78	S 1	0	0	0
29	D3	59	Total 467	C 298	N 90	O 78	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	44	Total 340	C 218	N 57	O 61	S 4	0	0	0
30	D4	44	Total 340	C 218	N 57	O 61	S 4	0	0	0

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

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

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

- 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 433 270 88 71 4	0	0	0
32	D6	50	Total C N O S 433 270 88 71 4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
33	B7	48	Total C N O S 418 257 104 55 2	0	0	0
33	D7	48	Total C N O S 418 257 104 55 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
34	B8	63	Total C N O S 507 326 101 78 2	0	0	0
34	D8	63	Total C N O S 507 326 101 78 2	0	0	0

- 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 307 188 68 47 4	0	0	0
35	D9	37	Total C N O S 307 188 68 47 4	0	0	0

- 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 62477 27807 11683 20087 2900	0	0	0
36	DA	2901	Total C N O P 62477 27807 11683 20087 2900	0	0	0

- 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	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
40	DE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			
41	DF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			
43	DH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O	0	0	0
			651	391	130	130			
44	DJ	130	Total	C	N	O	0	0	0
			651	391	130	130			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BK	140	Total	C	N	O	0	0	0
			700	420	140	140			
45	DK	140	Total	C	N	O	0	0	0
			700	420	140	140			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
46	DN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
51	BS	98	770	486	154	130	0	0	0
51	DS	98	770	486	154	130	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	BT	137	1141	710	234	196	1	0	0	0
52	DT	137	1141	710	234	196	1	0	0	0

- 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 958 604 202 151 1	0	0	0
53	DU	117	Total C N O S 958 604 202 151 1	0	0	0

- 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 779 501 142 135 1	0	0	0
54	DV	101	Total C N O S 779 501 142 135 1	0	0	0

- 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 896 563 176 155 2	0	0	0
55	DW	113	Total C N O S 896 563 176 155 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
56	BX	92	Total C N O 725 471 131 123	0	0	0
56	DX	92	Total C N O 725 471 131 123	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
57	BY	100	Total C N O S 775 500 148 123 4	0	0	0
57	DY	100	Total C N O S 775 500 148 123 4	0	0	0

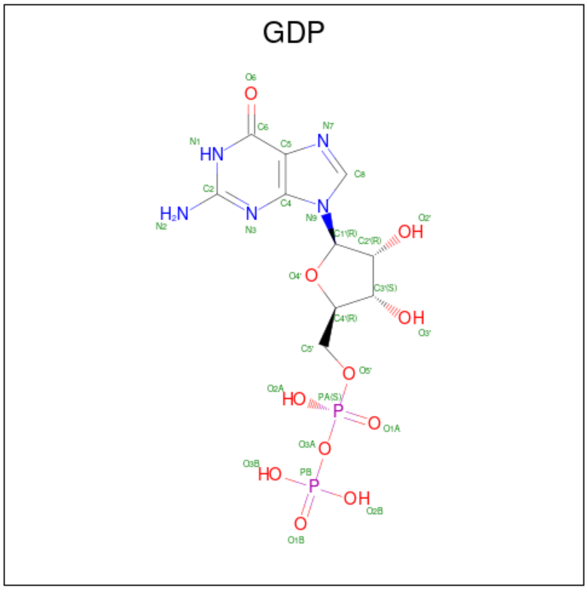
- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	183	Total 1459	C 932	N 260	O 265	S 2	0	0	0
58	DZ	183	Total 1459	C 932	N 260	O 265	S 2	0	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

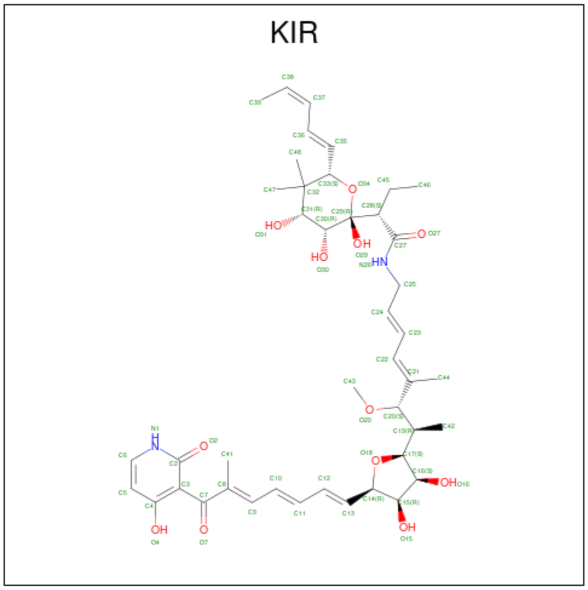
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	1	Total 1	Zn 1	0	0
59	AN	1	Total 1	Zn 1	0	0
59	B4	1	Total 1	Zn 1	0	0
59	B9	1	Total 1	Zn 1	0	0
59	CD	1	Total 1	Zn 1	0	0
59	CN	1	Total 1	Zn 1	0	0
59	D4	1	Total 1	Zn 1	0	0
59	D9	1	Total 1	Zn 1	0	0

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 61 is KIRROMYCIN (three-letter code: KIR) (formula: $C_{43}H_{60}N_2O_{12}$).



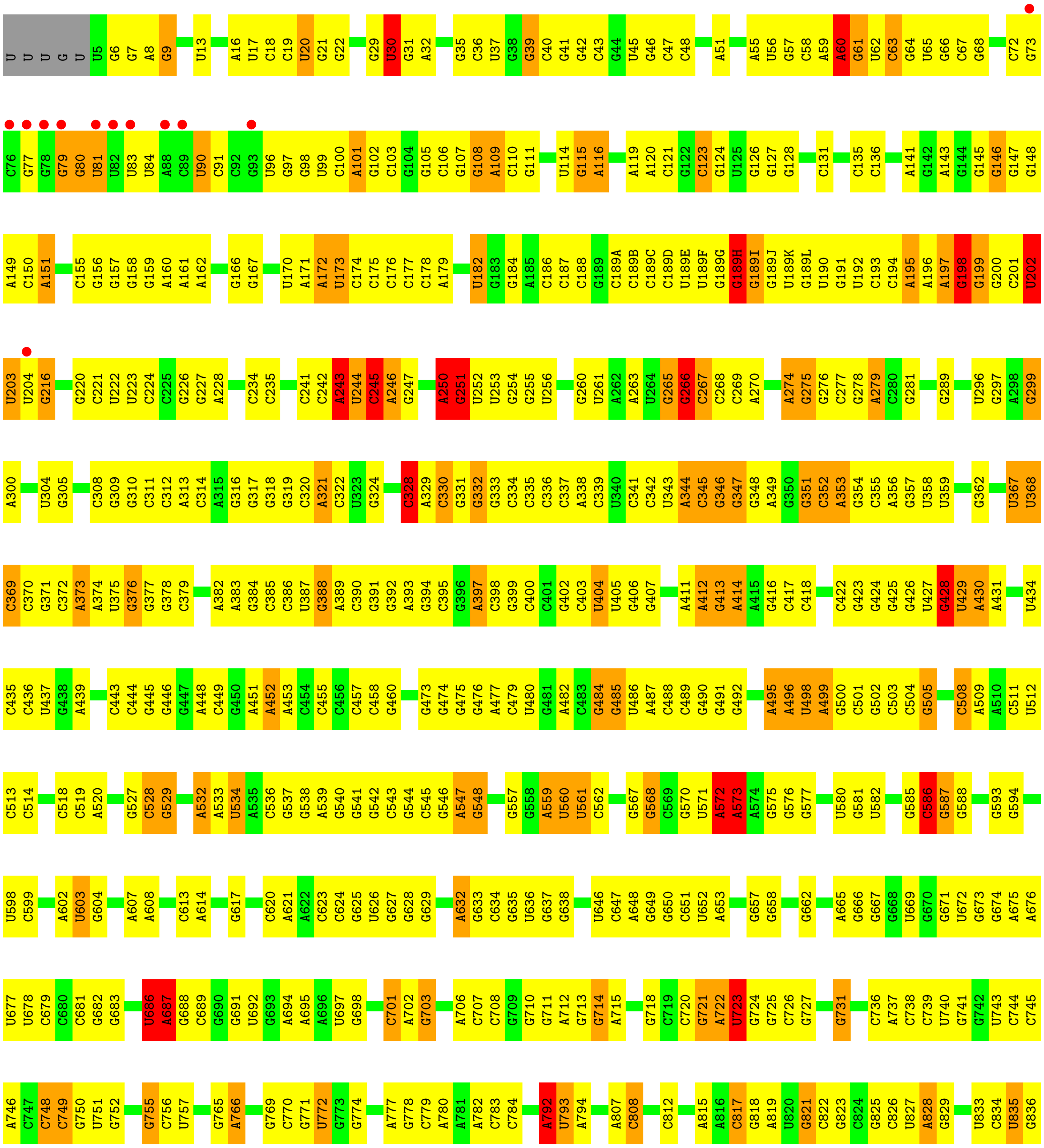
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
61	AZ	1	Total	C	N	O	0	0
			57	43	2	12		
61	CZ	1	Total	C	N	O	0	0
			57	43	2	12		

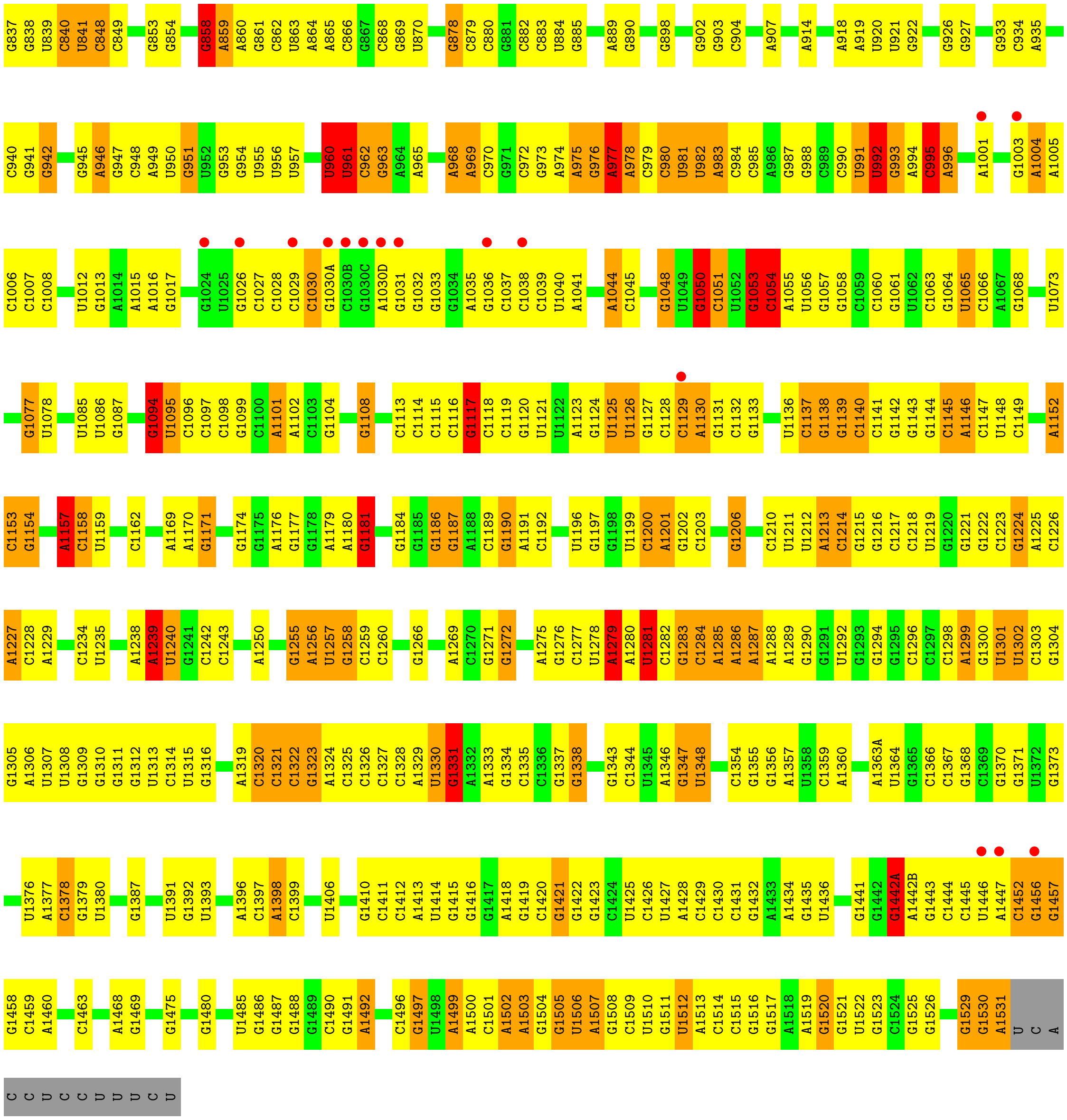
3 Residue-property plots ⓘ

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

- Molecule 1: 16S RRNA

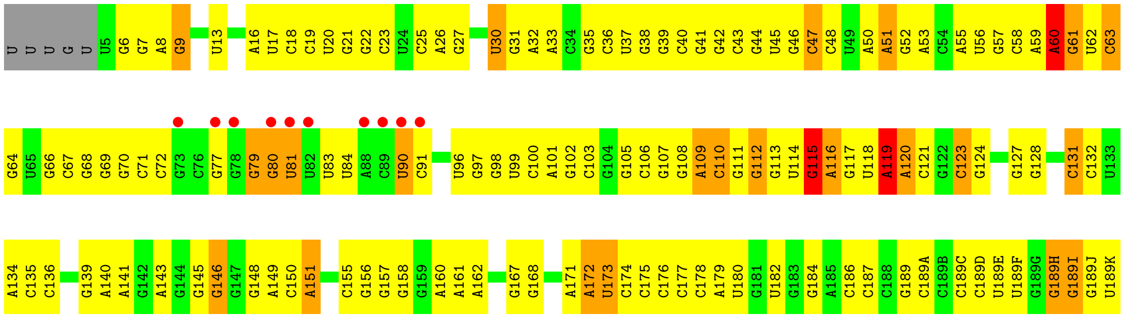
Chain AA:

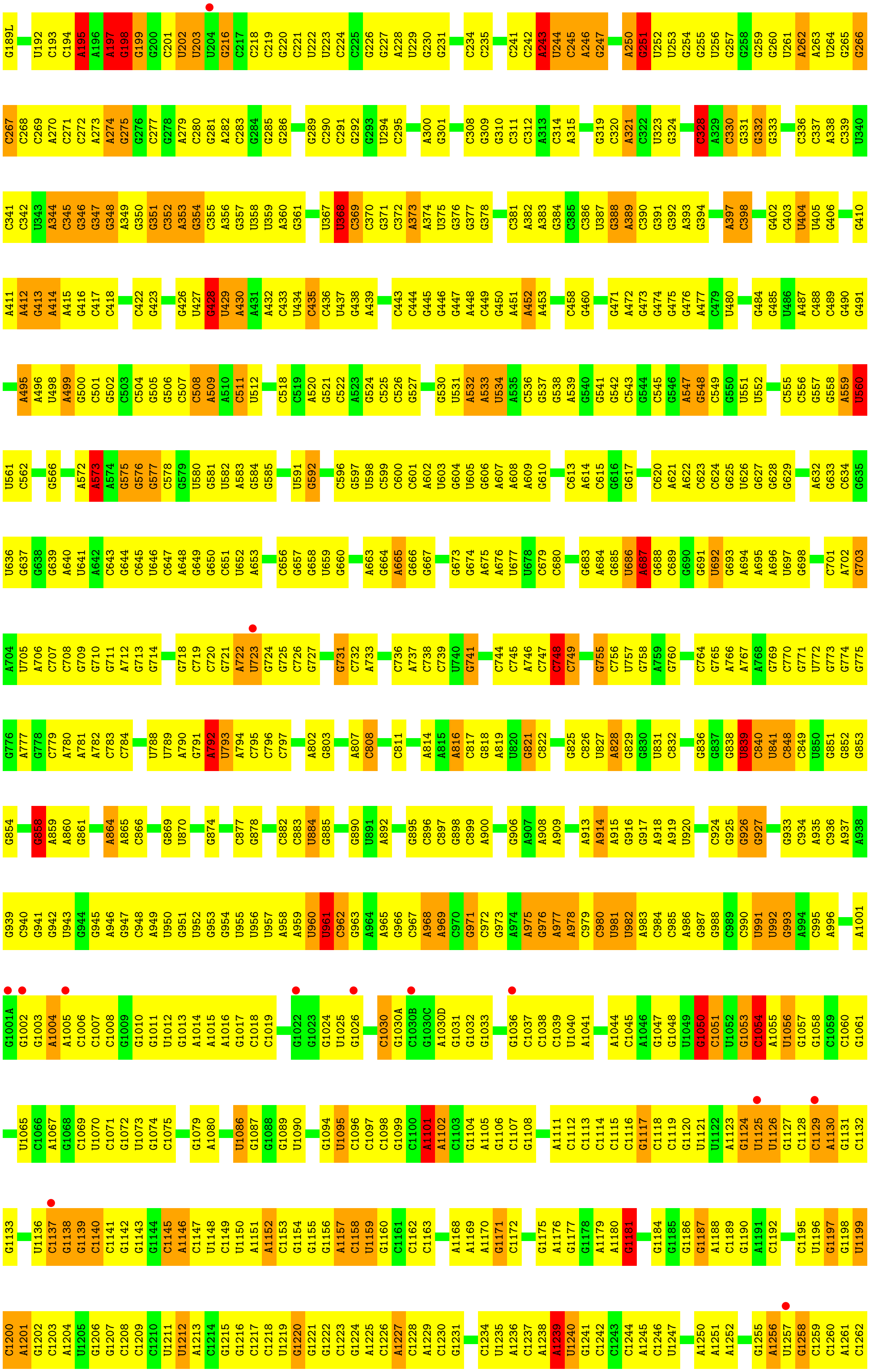




• Molecule 1: 16S RRNA

Chain CA:

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C267 C268 C269 A270 C271 C272 A273 A274 G275 G276 C277 G278 A279 C280 G281 A282 C283 G284 G285 G286 G289 C290 C291 G292 G293 U294 C295 A300 G301 C308 G309 C310 C311 C312 A313 C314 A315 G319 C320 A321 C322 U323 G324 C328 A329 C330 C331 G332 G333 C336 C337 A338 C339 U340
C341 C342 U343 A344 C345 G346 G347 G348 A349 G350 G351 C352 A353 G354 C355 A356 G357 U358 U359 A360 G361 U367 U368 C369 C370 G371 C372 A373 A374 U375 G376 G377 G378 C381 A382 A383 G384 C385 C386 U387 G388 A389 C390 G391 G392 A393 G394 A397 C398 G402 C403 U404 U405 G406 G410
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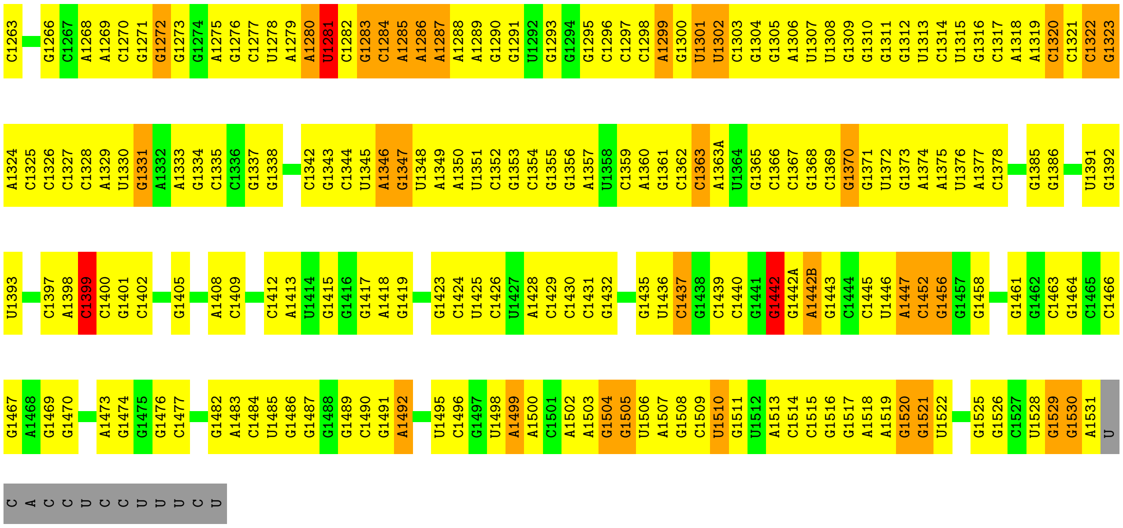
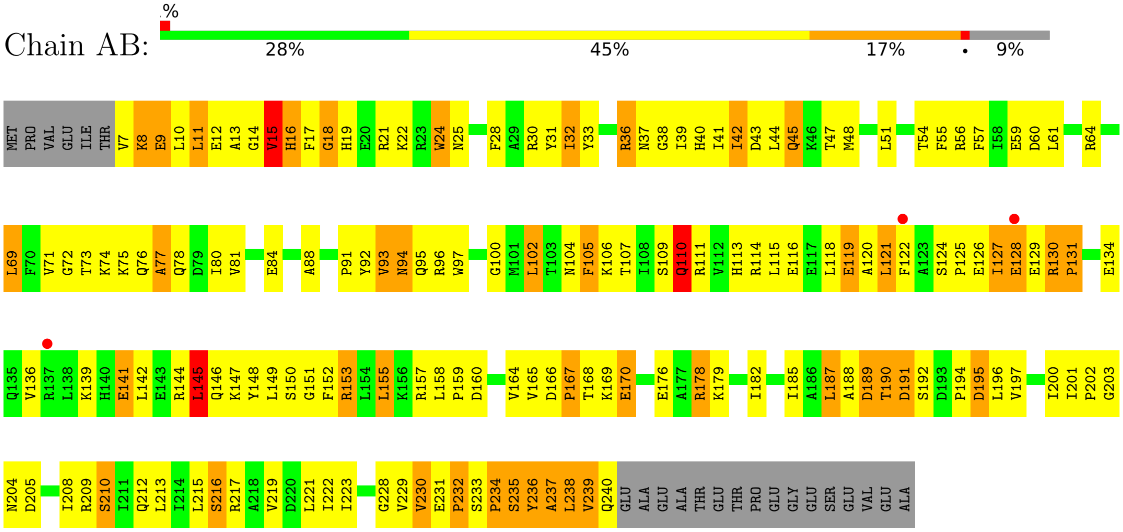
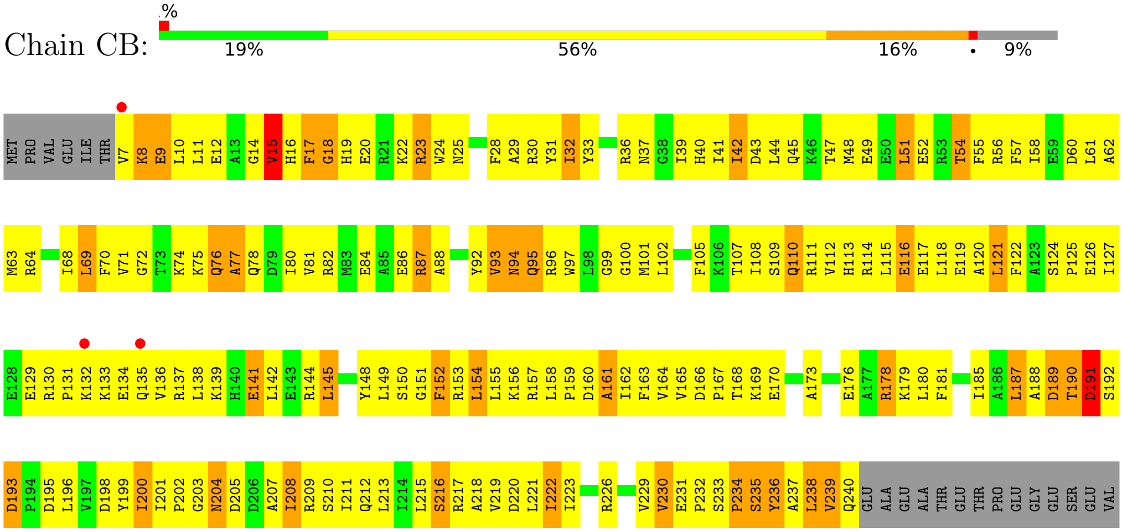
A495 A496 U498 A499 G500 C501 G502 C503 C504 G505 G506 C507 C508 A509 A510 C511 U512 C518 C519 A520 G521 C522 A523 G524 C525 C526 G527 G530 U531 A532 A533 U534 A535 C536 G537 G538 A539 G540 G541 G542 C543 G544 C545 G546 A547 G548 C549 G550 U551 U552 C555 C556 G557 G558 A559 U560
U561 C562 G566 A572 A573 A574 G575 G576 G577 C578 G579 U580 G581 U582 A583 G584 G585 U591 G592 C596 G597 U598 C599 C600 C601 A602 U603 G604 U605 G606 A607 A608 A609 G610 C613 A614 C615 G616 G617 C620 A621 A622 C623 G624 G625 U626 G627 G628 G629 A632 G633 C634 G635
U636 G637 G638 G639 A640 U641 A642 C643 G644 C645 U646 C647 A648 G649 G650 C651 U652 A653 C656 G657 G658 U659 G660 A663 G664 A665 G666 G667 G673 G674 A675 A676 U677 U678 C679 C680 G683 A684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 U697 G698 C701 A702 G703
A704 U705 A706 C707 G708 G709 G710 G711 A712 G713 G714 G718 C719 C720 G721 A722 U723 G724 G725 C726 G727 G731 C732 A733 C736 A737 C738 C739 U740 G741 C744 C745 A746 C747 C748 C749 G755 C756 U757 G758 A759 G760 C764 G765 A766 A767 A768 G769 C770 G771 U772 G773 G774 G775
G776 A777 G778 C779 A780 A781 A782 C783 C784 U788 U789 A790 G791 A792 U793 A794 C795 C796 C797 A802 G803 A807 C808 C811 A814 A815 A816 C817 G818 A819 U820 G821 C822 G825 C826 U827 A828 G829 G830 U831 C832 G836 G837 G838 U839 C840 U841 C848 C849 U850 G851 G852 G853
G854 G858 A859 A860 G861 A864 A865 C866 G869 U870 G874 C877 G878 C882 C883 U884 G885 G890 U891 A892 G895 C896 C897 G898 C899 A900 G906 A907 A908 A909 A913 A914 A915 G916 G917 A918 A919 U920 C924 G925 G926 G927 G933 C934 A935 C936 A937 A938
G939 C940 G941 G942 U943 G944 G945 A946 G947 C948 A949 U950 G951 U952 G953 G954 U955 U956 G957 A958 A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 G987 G988 C989 C990 U991 U992 G993 A994 C995 A996 A1001
G1001A G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 G1010 G1011 U1012 G1013 A1014 A1015 G1016 G1017 C1018 C1019 G1022 G1023 C1024 U1025 G1026 C1030 G1030A G1030B G1030C A1030D G1031 G1032 G1033 G1036 C1037 C1038 C1039 U1040 A1041 A1044 C1045 A1046 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061
U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1074 C1075 G1079 A1080 U1086 G1087 G1088 G1089 U1090 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 A1111 C1112 C1113 C1114 C1115 C1116 G1117 C1118 C1119 G1120 U1121 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132
G1133 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 C1163 A1168 A1169 A1170 G1171 C1172 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1184 G1185 G1186 G1187 A1188 C1189 G1190 A1191 C1192 C1195 U1196 G1197 G1198 U1199
C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 C1234 U1235 A1236 C1237 A1238 A1239 U1240 G1241 C1242 C1243 C1244 G1245 C1246 U1247 A1250 A1251 A1252 G1255 A1256 U1257 G1258 C1259 C1260 A1261 C1262



• Molecule 2: 30S RIBOSOMAL PROTEIN S2

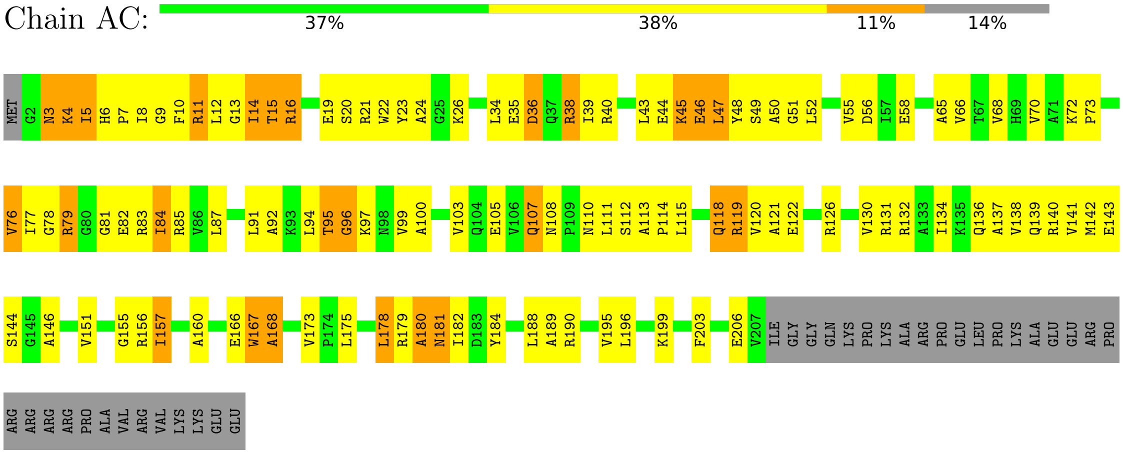


• Molecule 2: 30S RIBOSOMAL PROTEIN S2



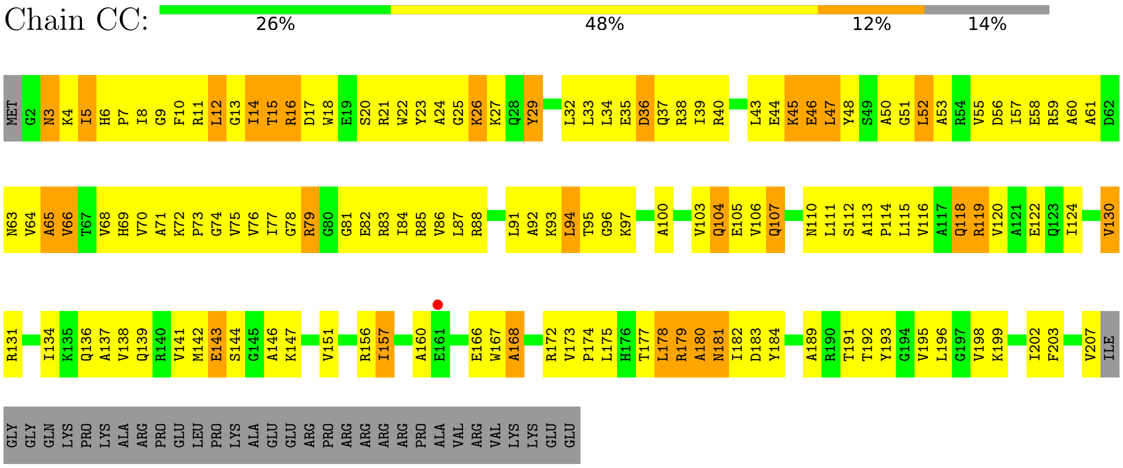
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:



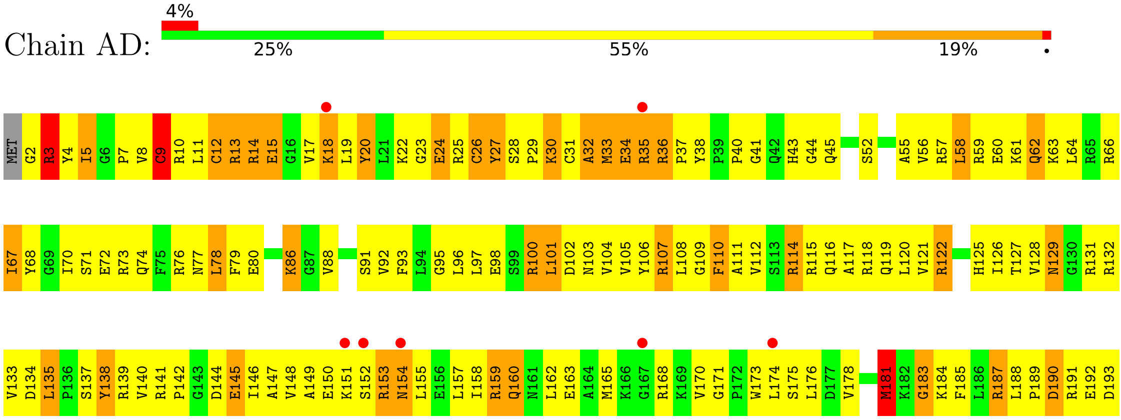
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

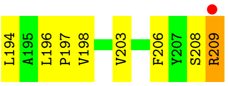
Chain CC:



- Molecule 4: 30S RIBOSOMAL PROTEIN S4

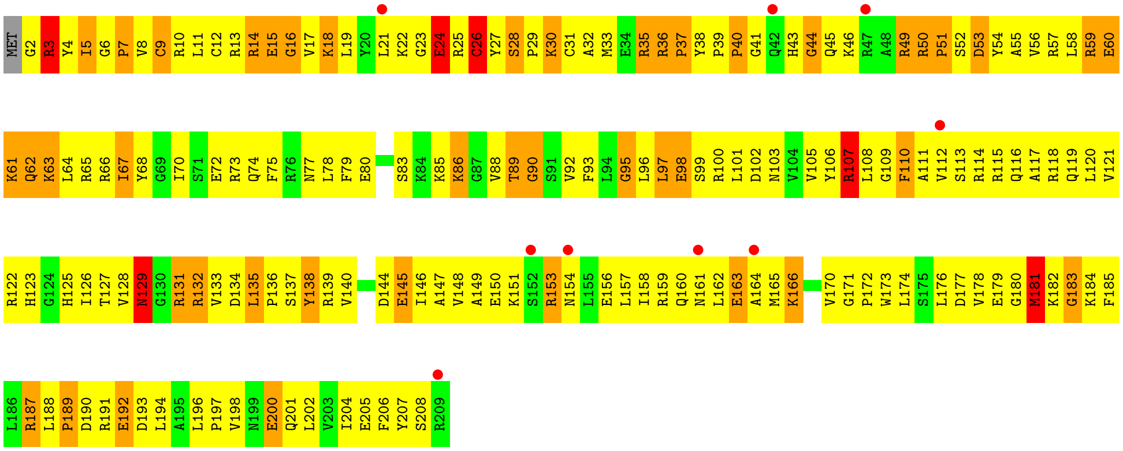
Chain AD:





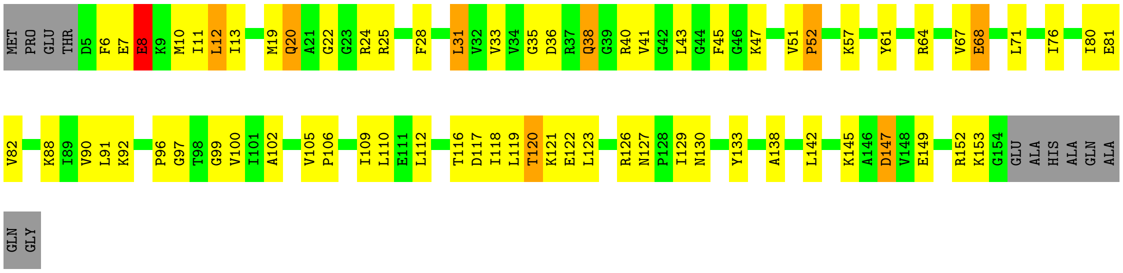
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD:



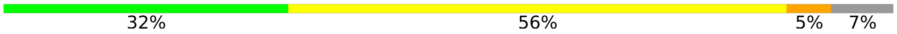
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

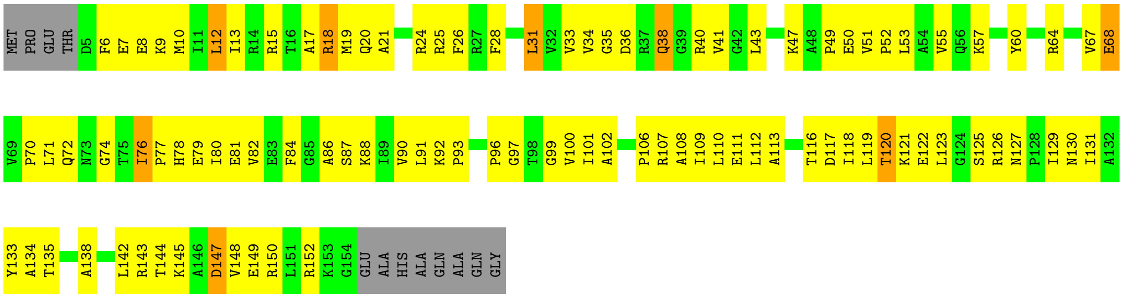
Chain AE:



- Molecule 5: 30S RIBOSOMAL PROTEIN S5

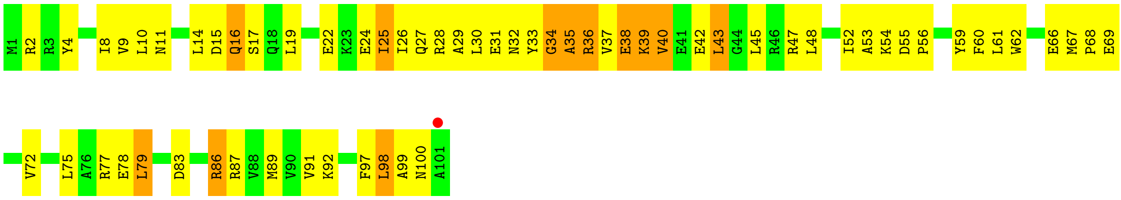
Chain CE:





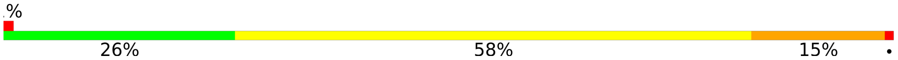
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

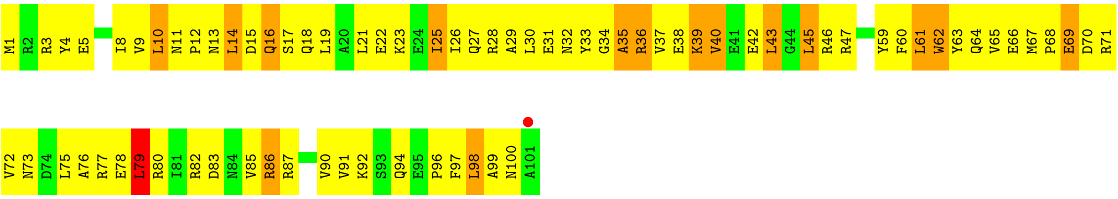
Chain AF:



- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF:



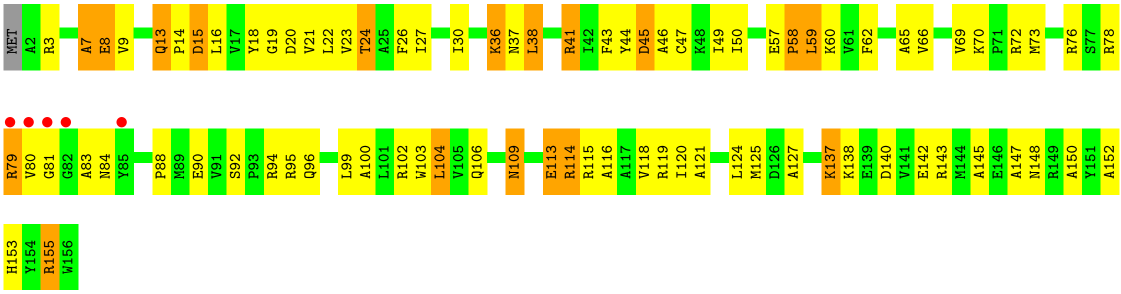


- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:

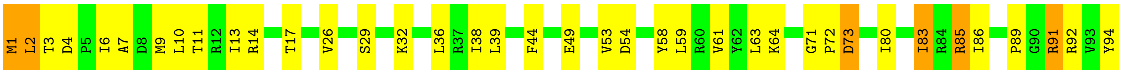
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG:



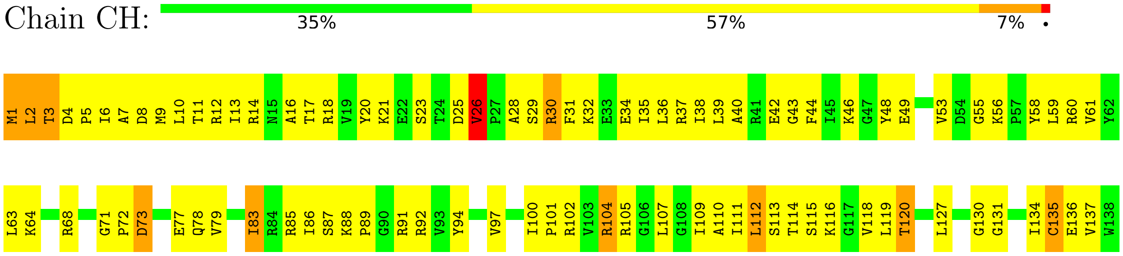
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



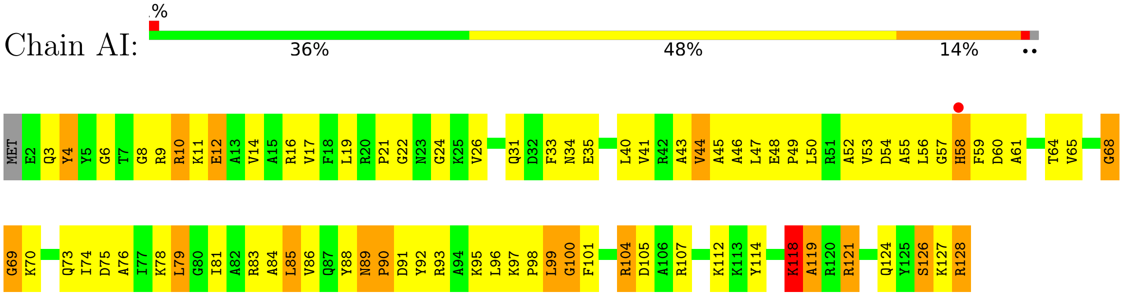
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:



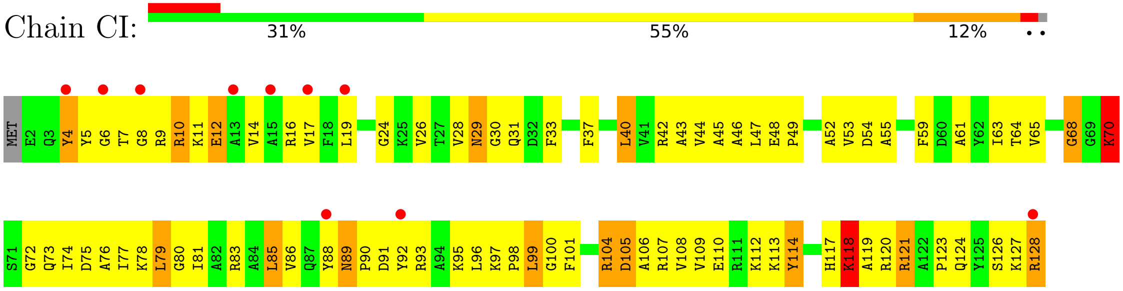
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



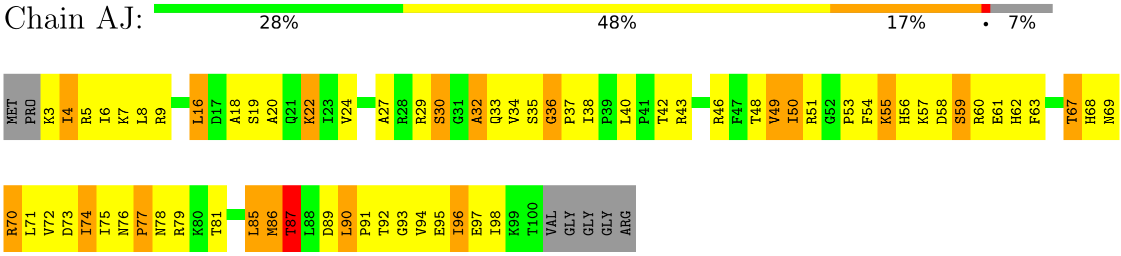
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



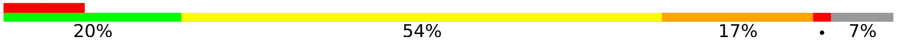
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

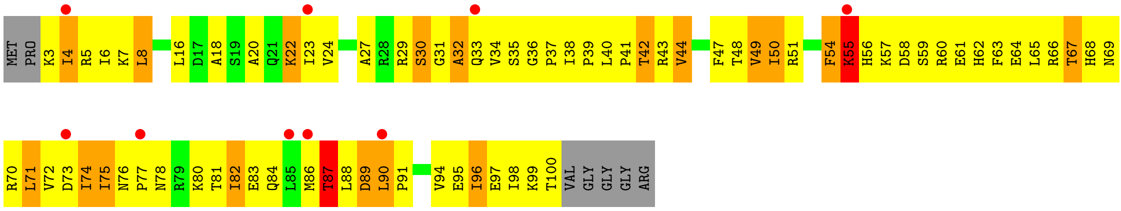
Chain AJ:



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

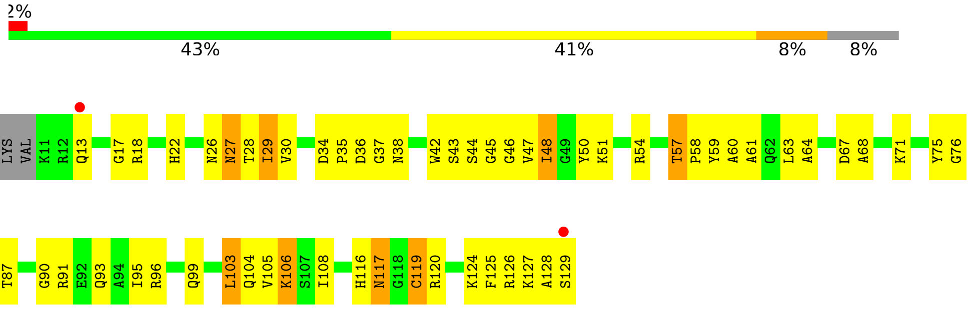
Chain CJ:





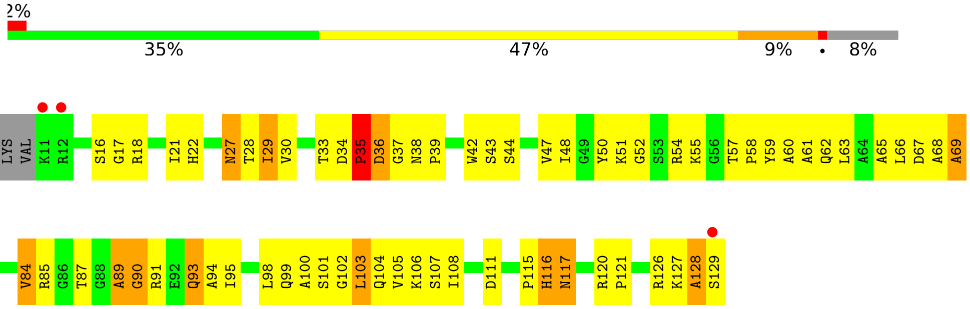
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



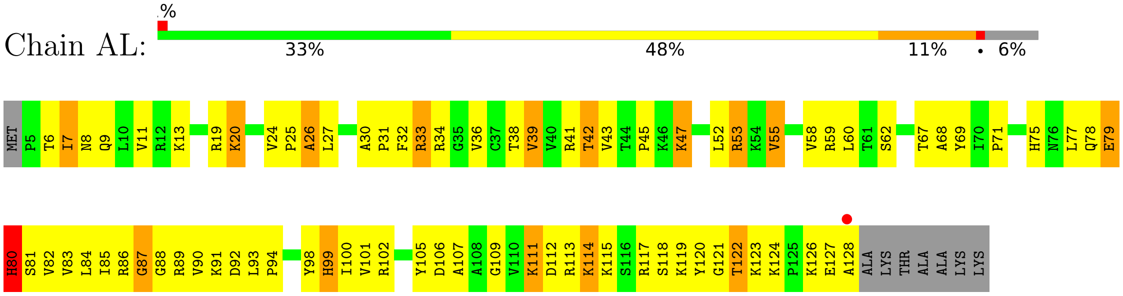
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



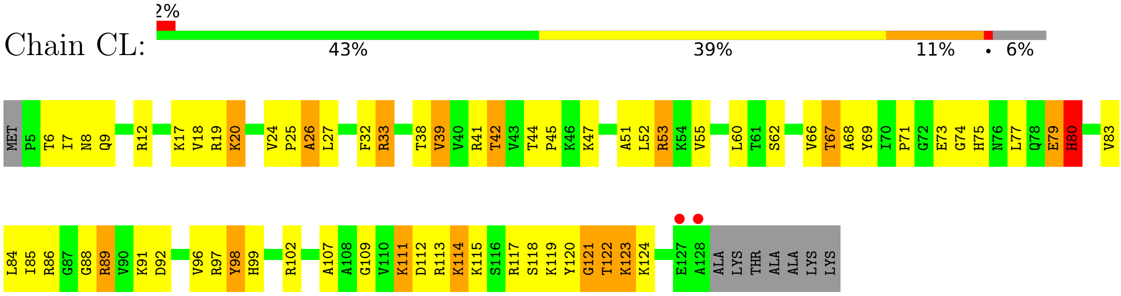
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



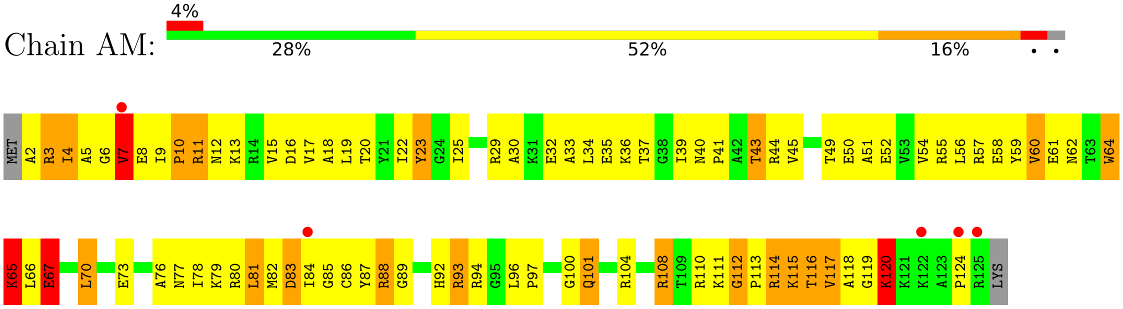
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL:



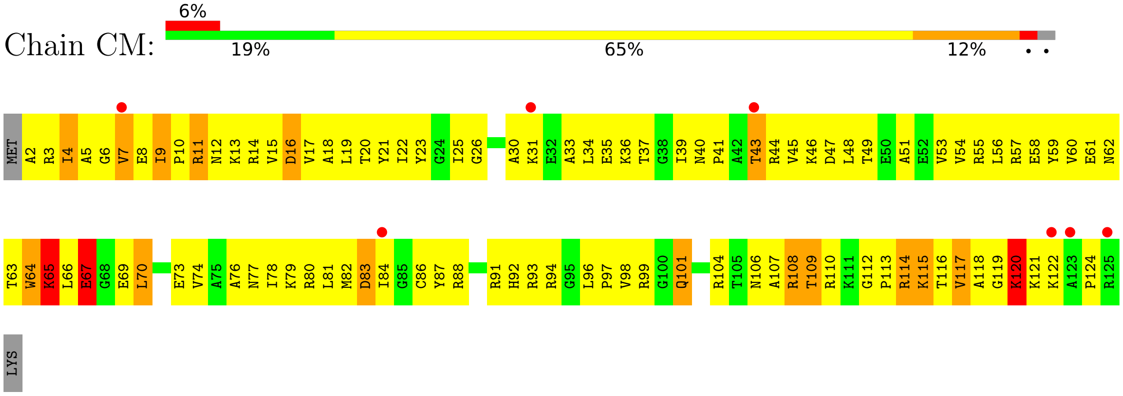
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



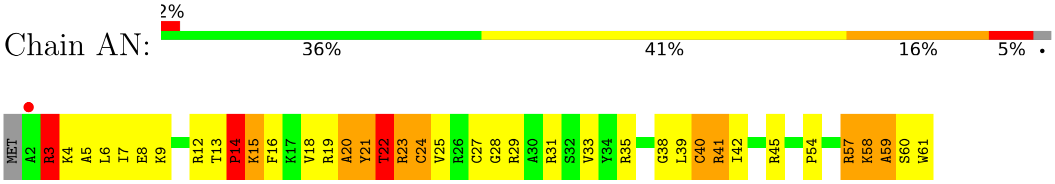
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



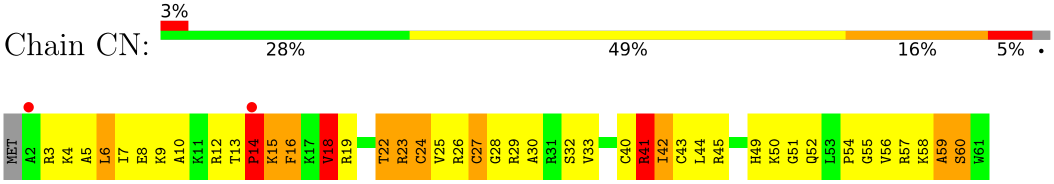
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AN:



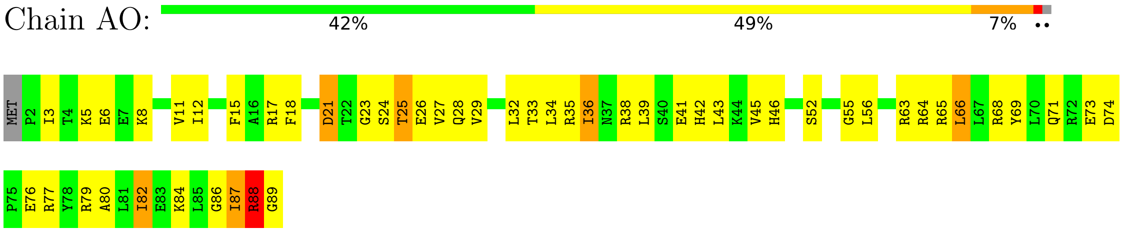
- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain CN:



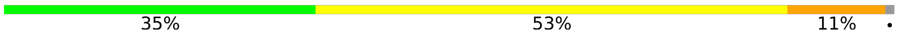
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

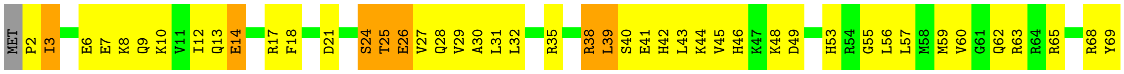
Chain AO:



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

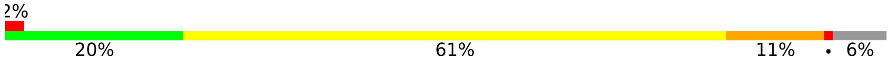
Chain CO:

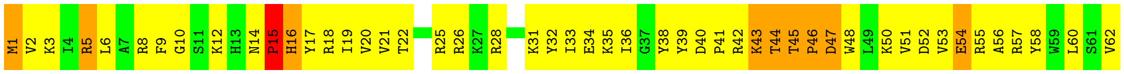




- Molecule 16: 30S RIBOSOMAL PROTEIN S16

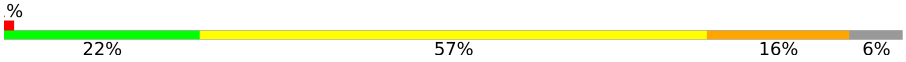
Chain AP:

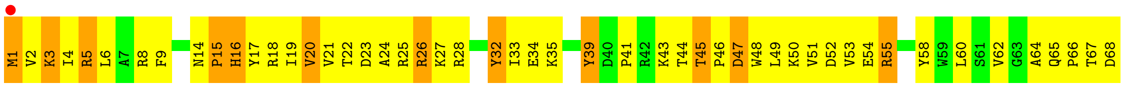


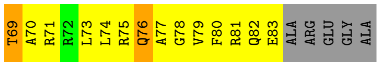


- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:





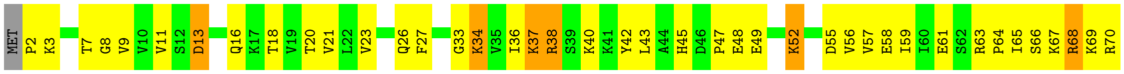


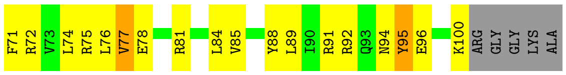
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:

- Molecule 17: 30S RIBOSOMAL PROTEIN S17

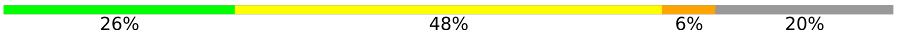
Chain CQ:

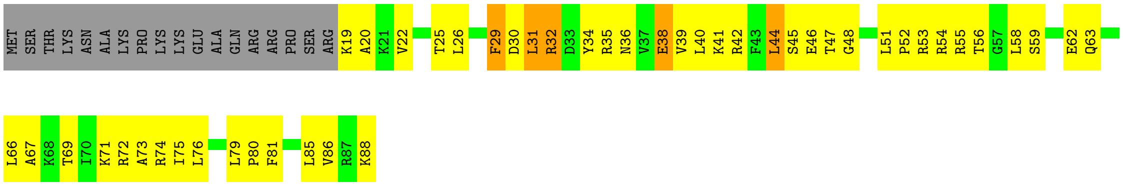




- Molecule 18: 30S RIBOSOMAL PROTEIN S18

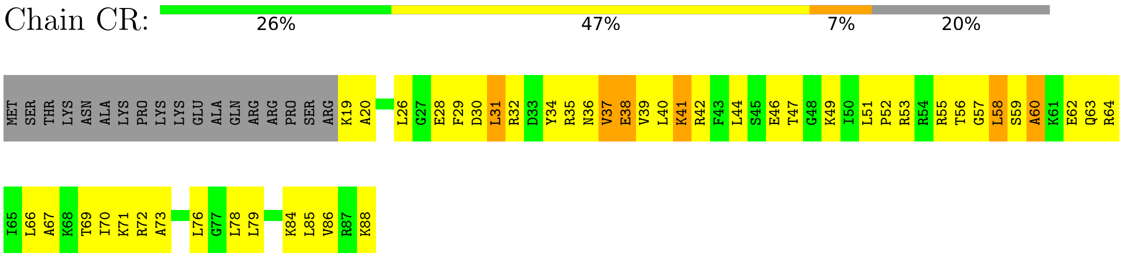
Chain AR:





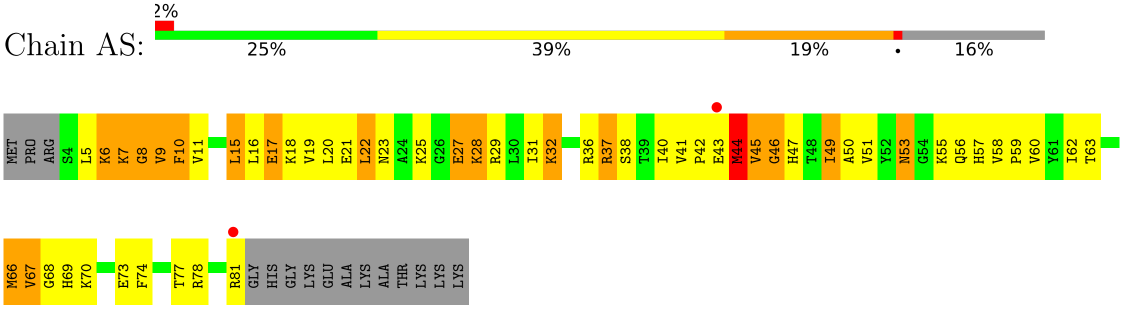
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:



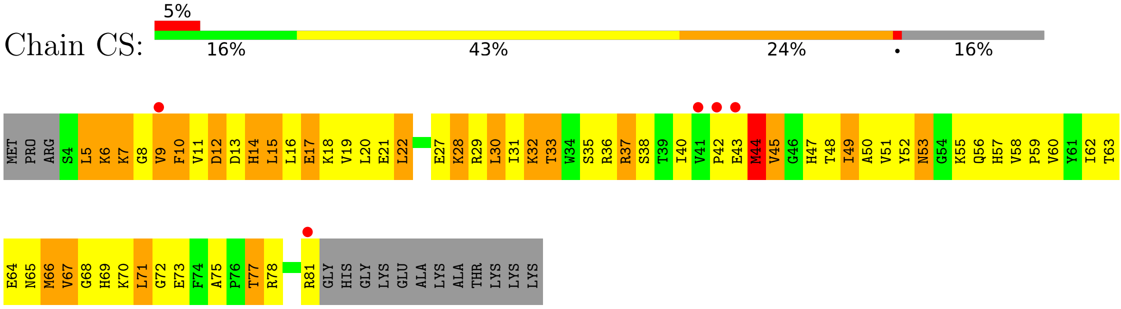
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



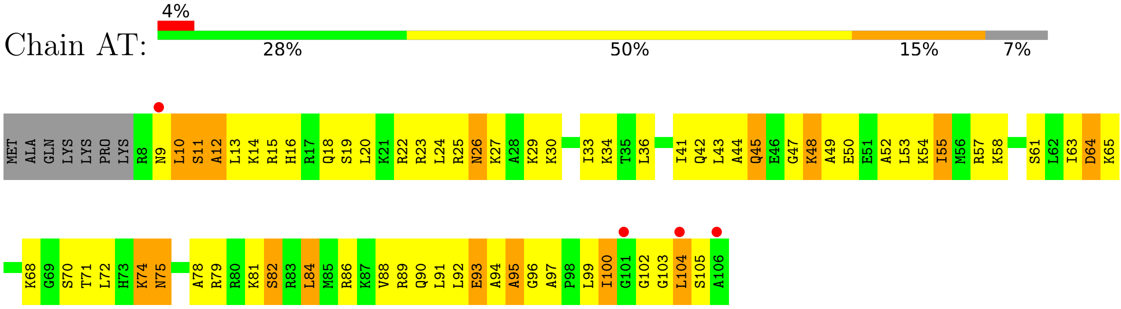
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:



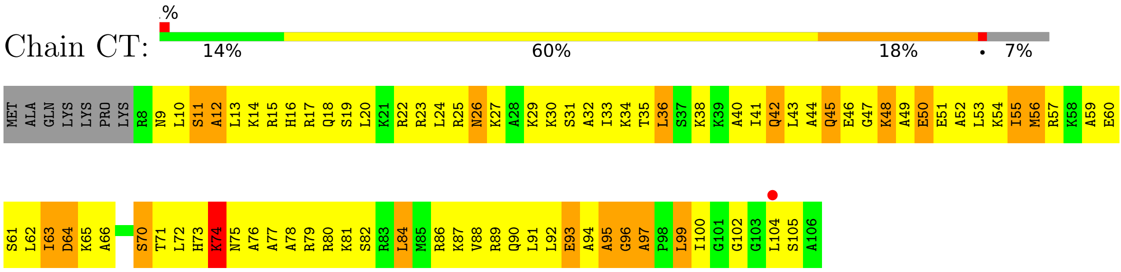
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



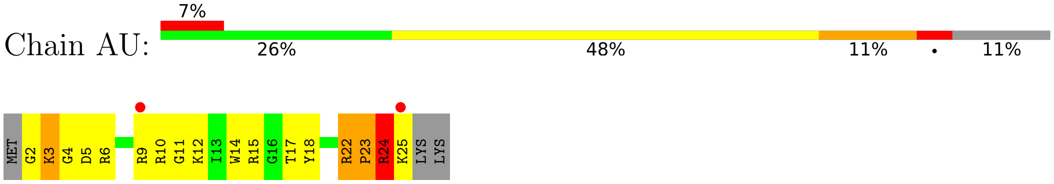
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CT:



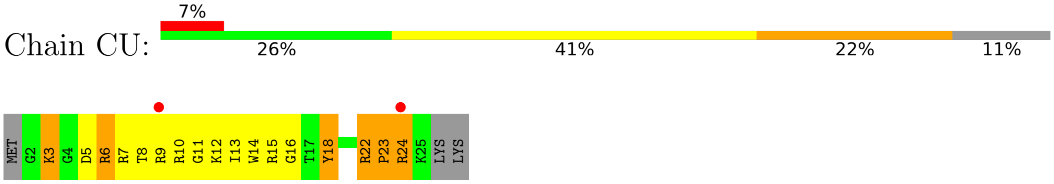
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



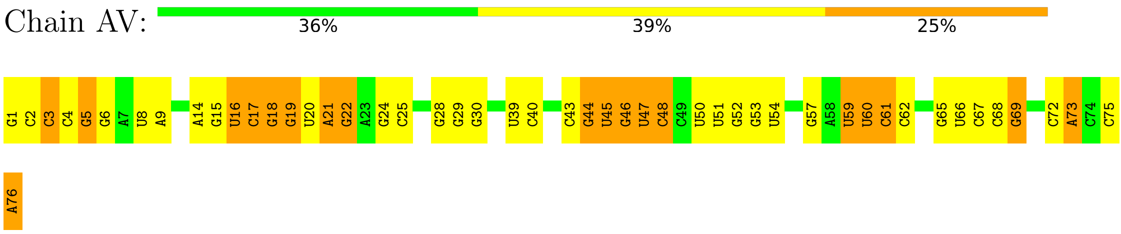
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



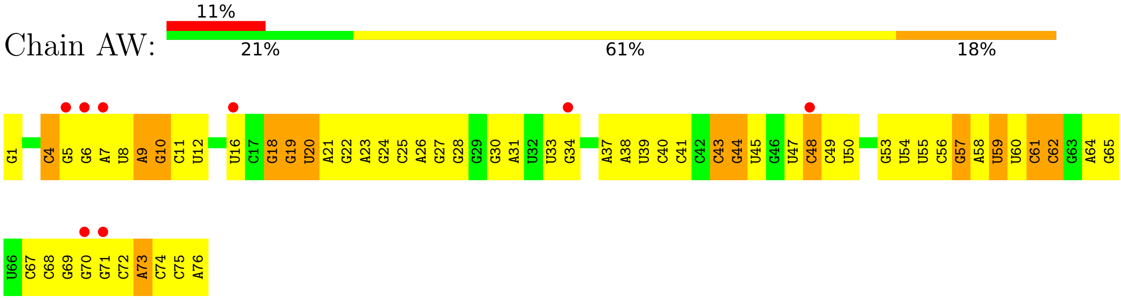
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AV:



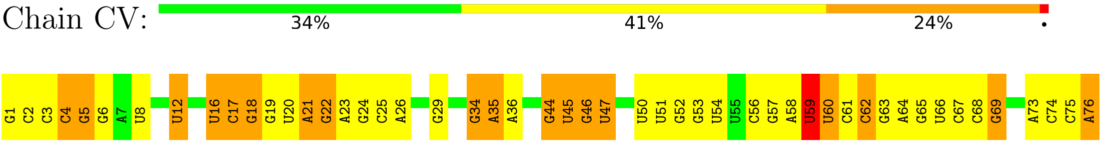
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AW:

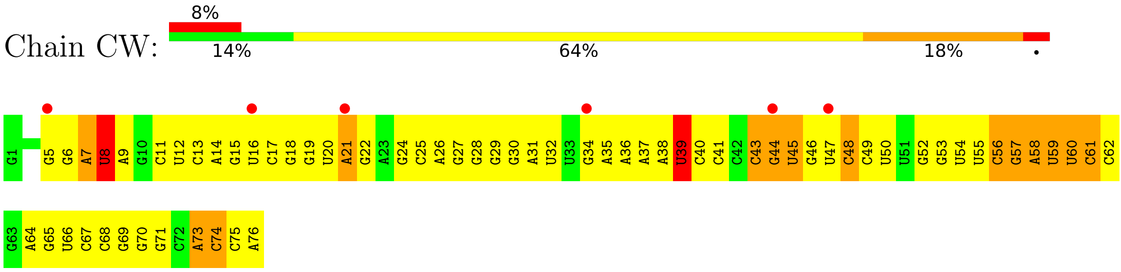


- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

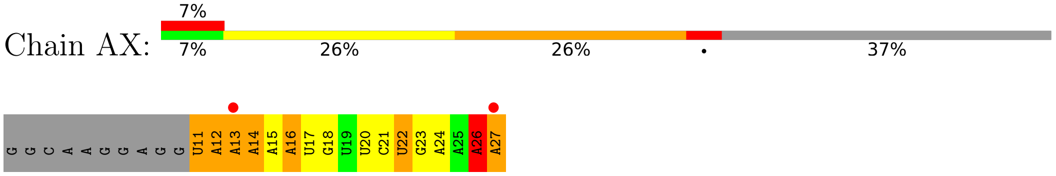
Chain CV:



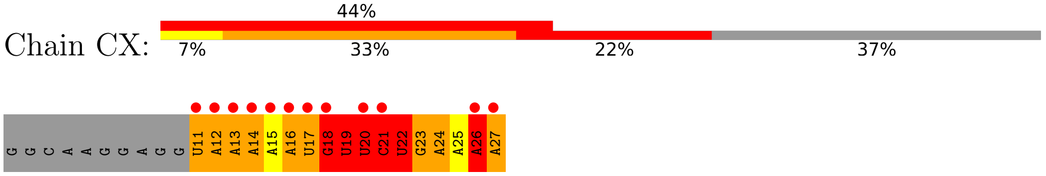
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



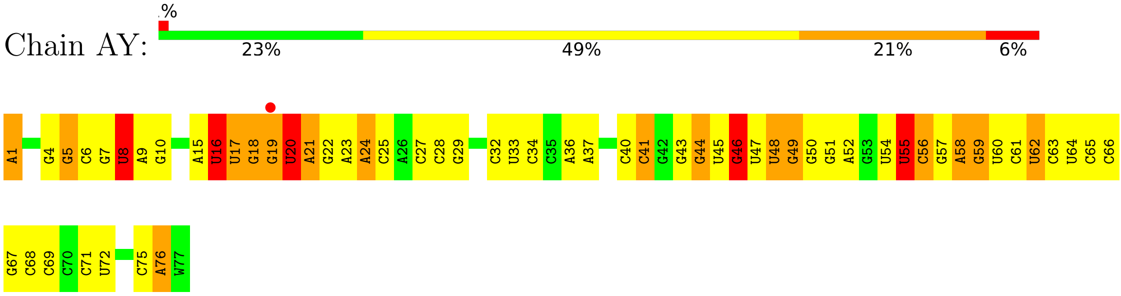
- Molecule 23: MRNA



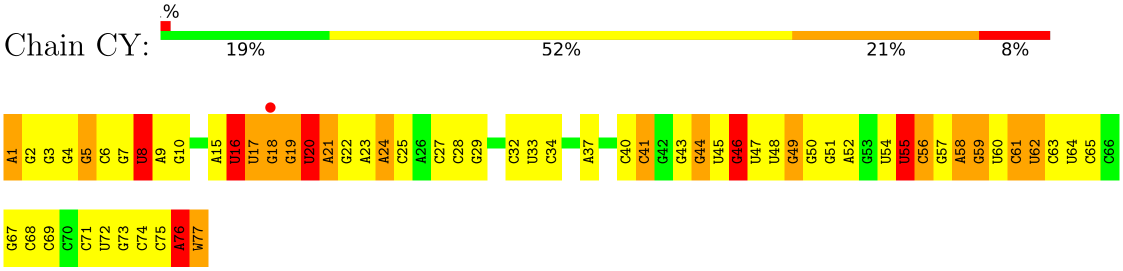
- Molecule 23: MRNA



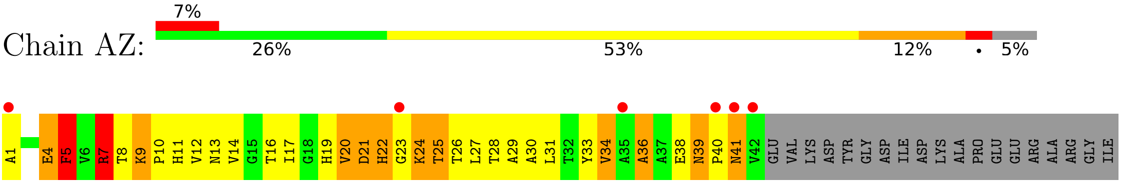
- Molecule 24: A-SITE TRNA G24A TRP-TRNA TRP

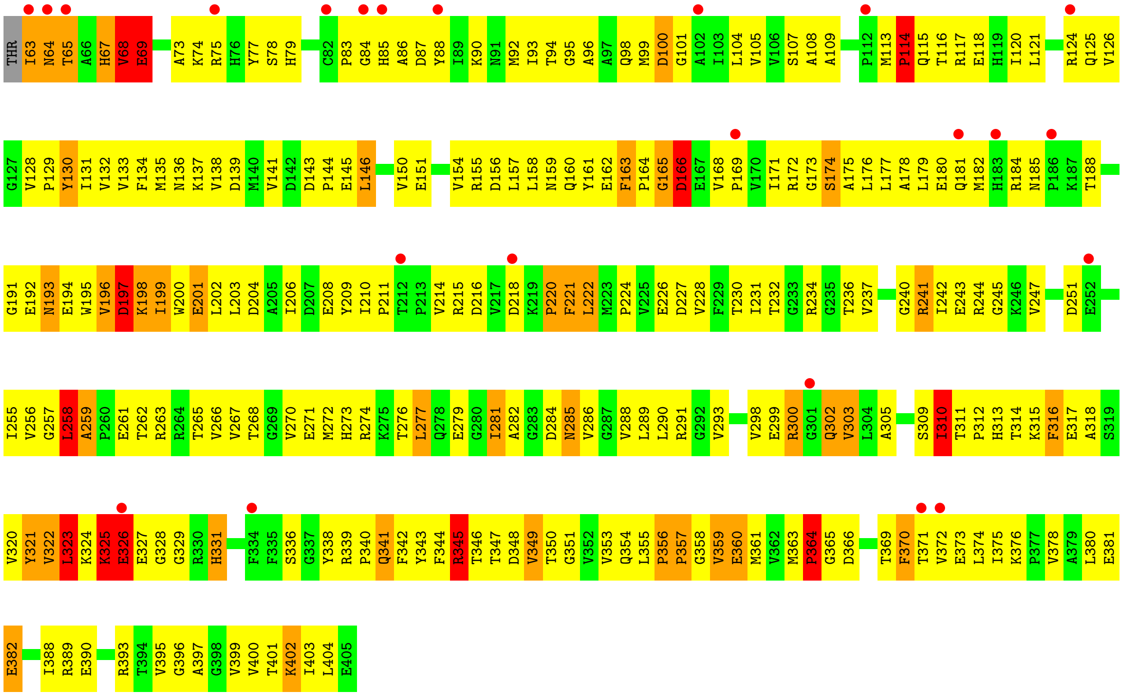


- Molecule 24: A-SITE TRNA G24A TRP-TRNA TRP



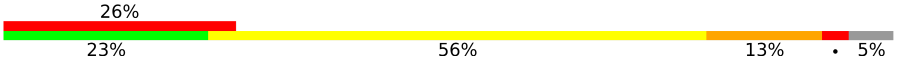
- Molecule 25: ELONGATION FACTOR TU

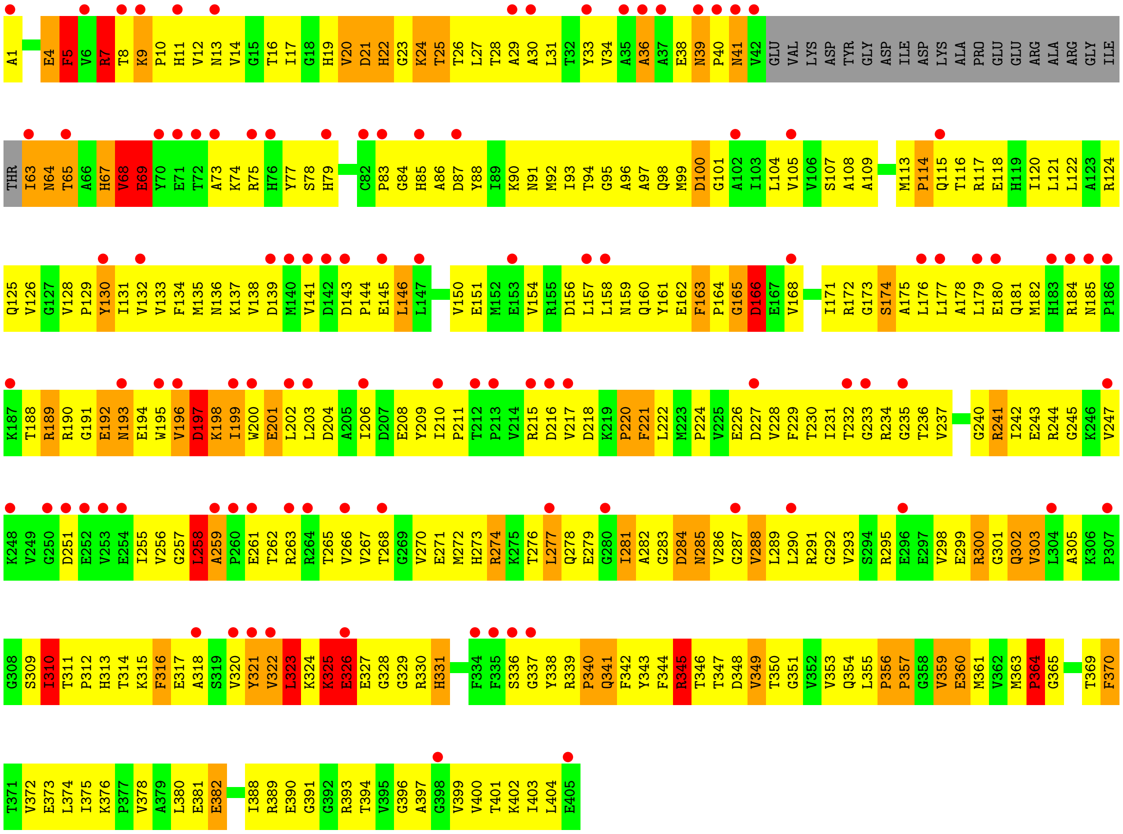




- Molecule 25: ELONGATION FACTOR TU

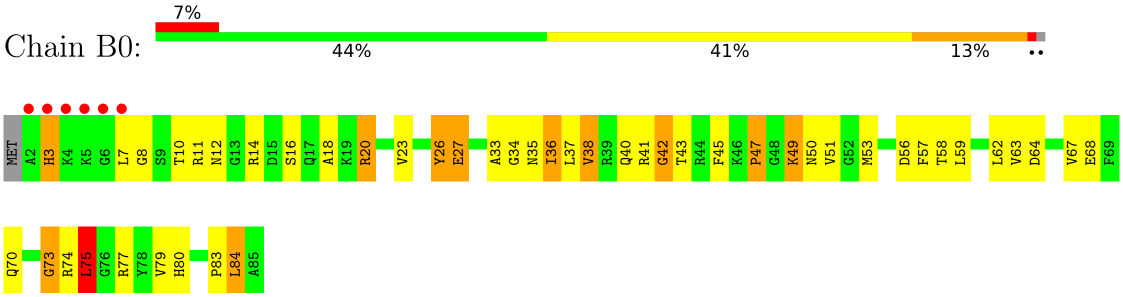
Chain CZ:





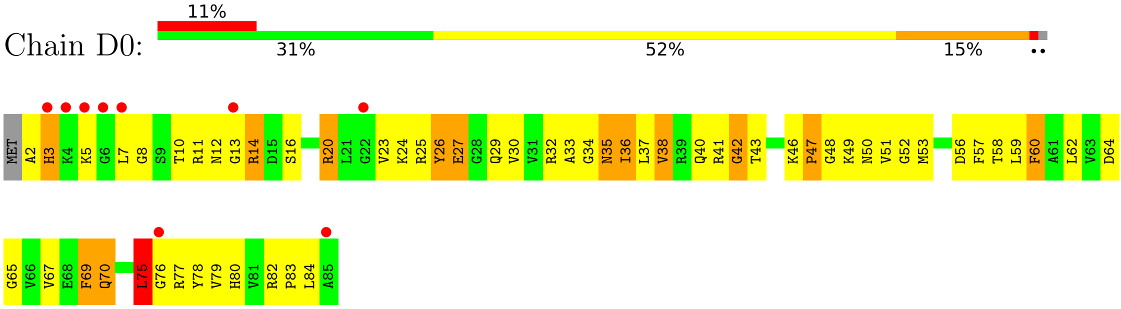
- Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain B0:



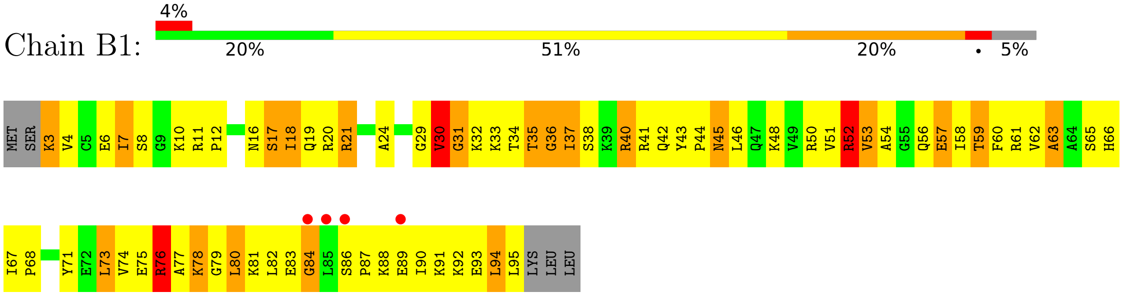
- Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain D0:



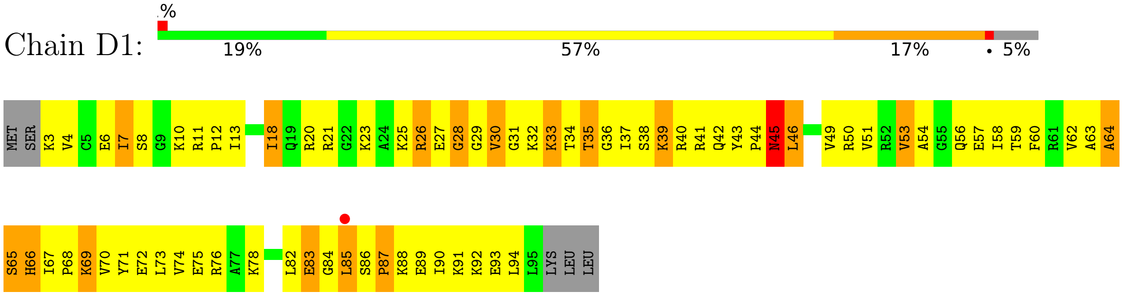
- Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain B1:



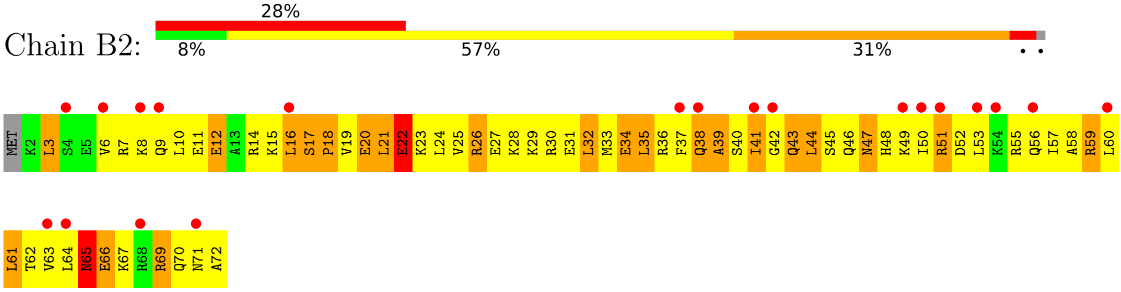
- Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain D1:



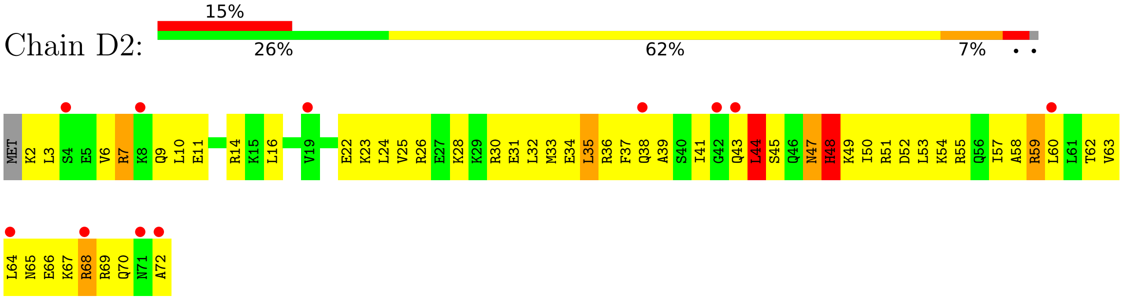
- Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain B2:



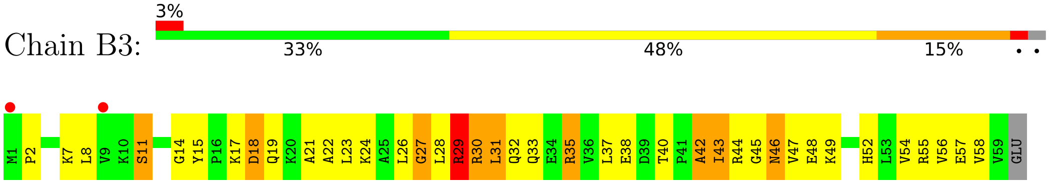
- Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain D2:



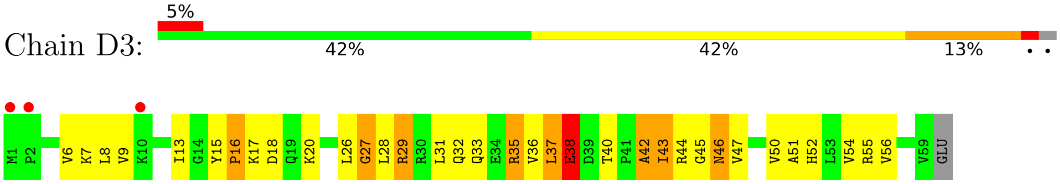
- Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain B3:



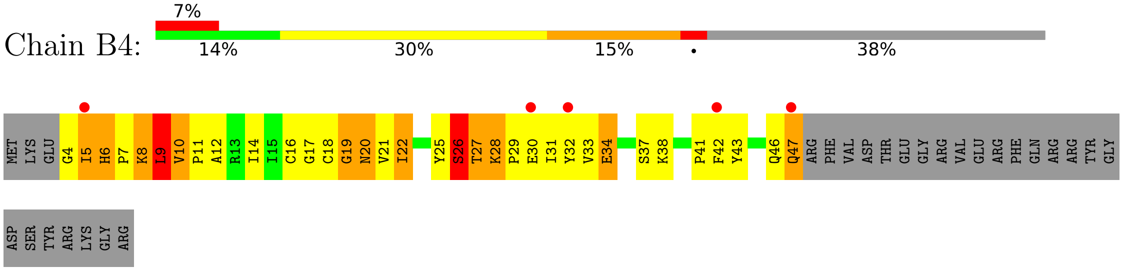
- Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain D3:



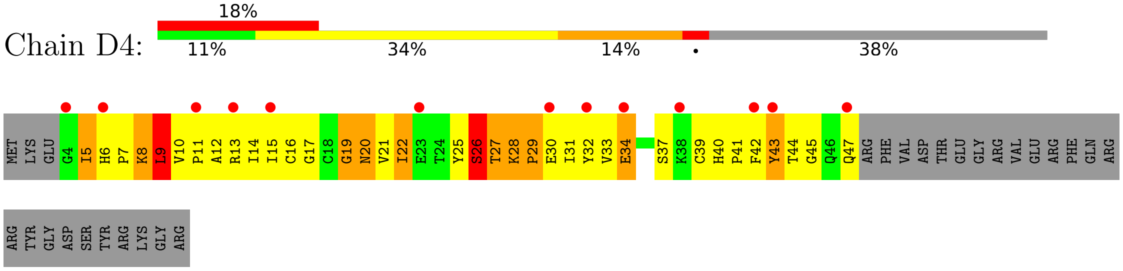
- Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain B4:



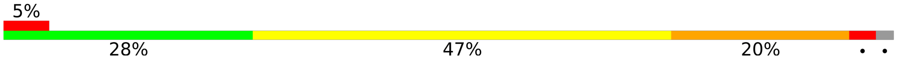
- Molecule 30: 50S RIBOSOMAL PROTEIN L31

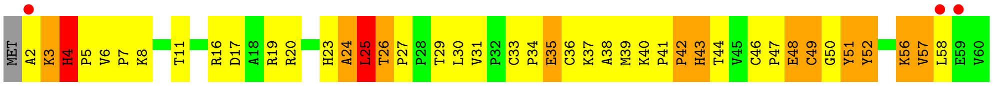
Chain D4:



- Molecule 31: 50S RIBOSOMAL PROTEIN L32

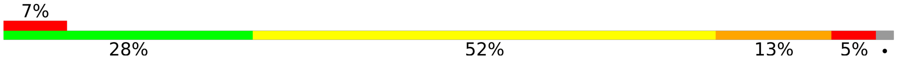
Chain B5:





- Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain D5:

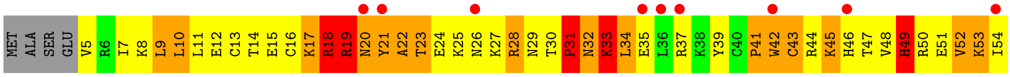


- Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain B6:

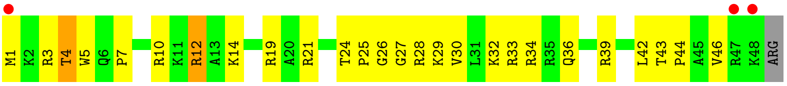
- Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain D6:



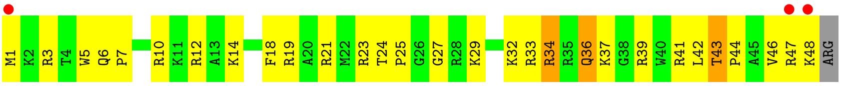
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain B7:



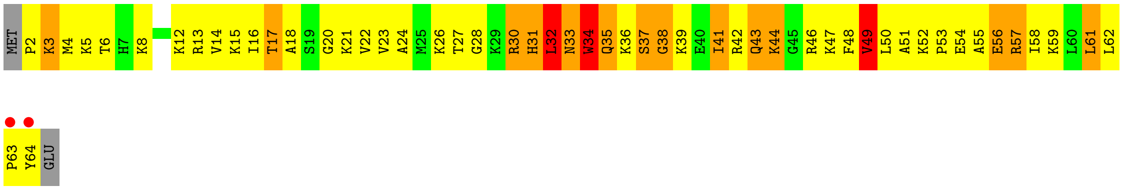
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain D7:

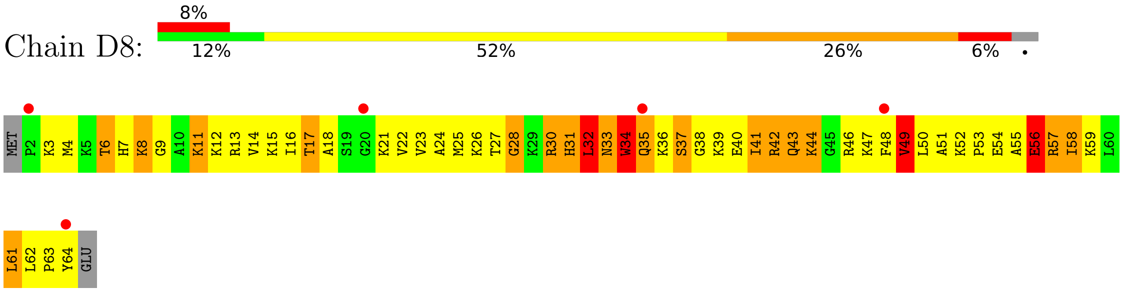


- Molecule 34: 50S RIBOSOMAL PROTEIN L35

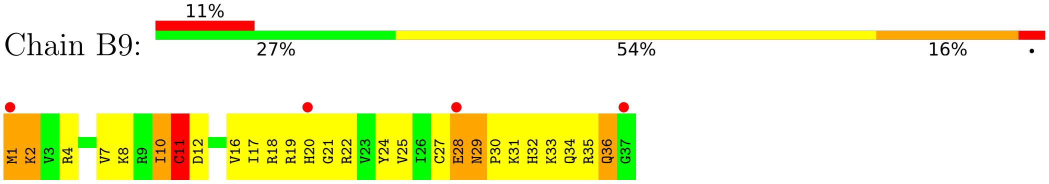
Chain B8:



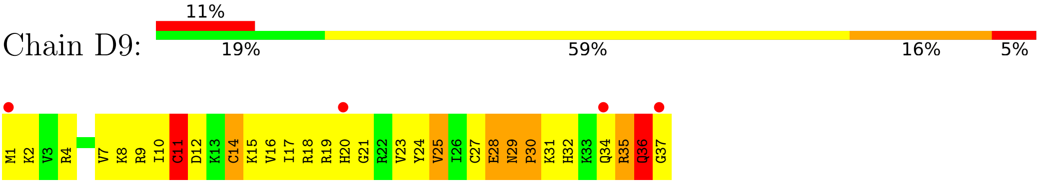
- Molecule 34: 50S RIBOSOMAL PROTEIN L35



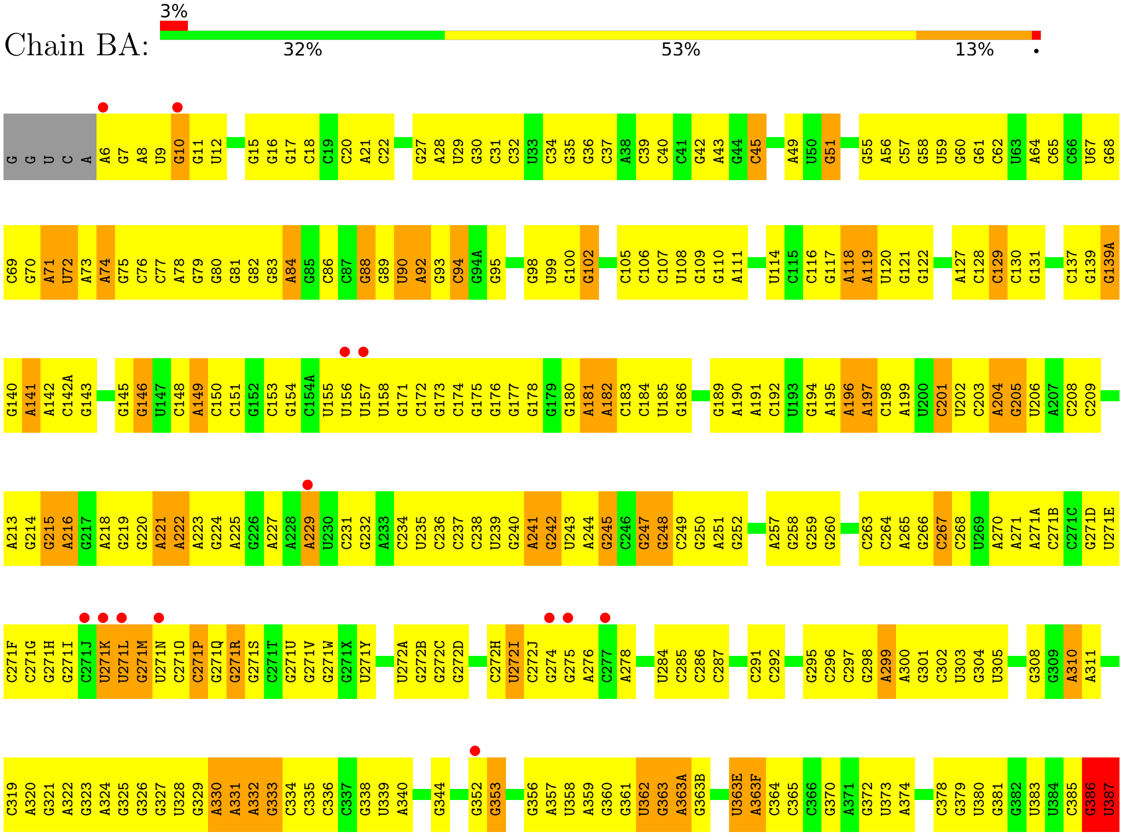
- Molecule 35: 50S RIBOSOMAL PROTEIN L36

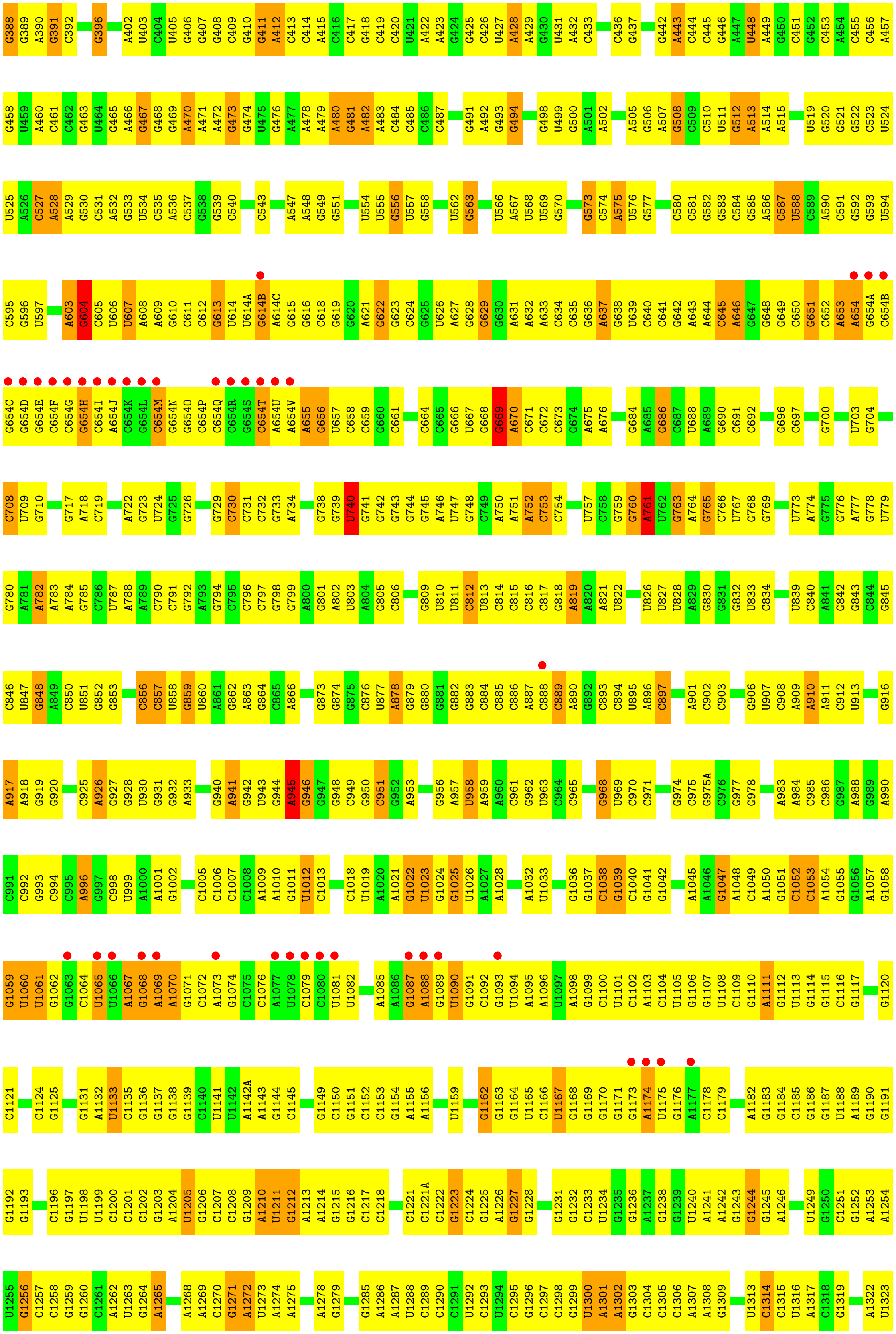


- Molecule 35: 50S RIBOSOMAL PROTEIN L36



- Molecule 36: 23S RIBOSOMAL RNA

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C708 U709 G710 G717 A718 C719 A722 G723 U724 G725 G726 C729 C730 C731 C732 G733 A734 G738 C739 U740 G741 G742 G743 G744 G745 A746 U747 G748 C749 A750 A751 A752 C753 C754 U757 C758 G759 G760 A761 U762 G763 A764 G765 C766 U767 G768 G769 U773 A774 G775 G776 A777 G778 U779
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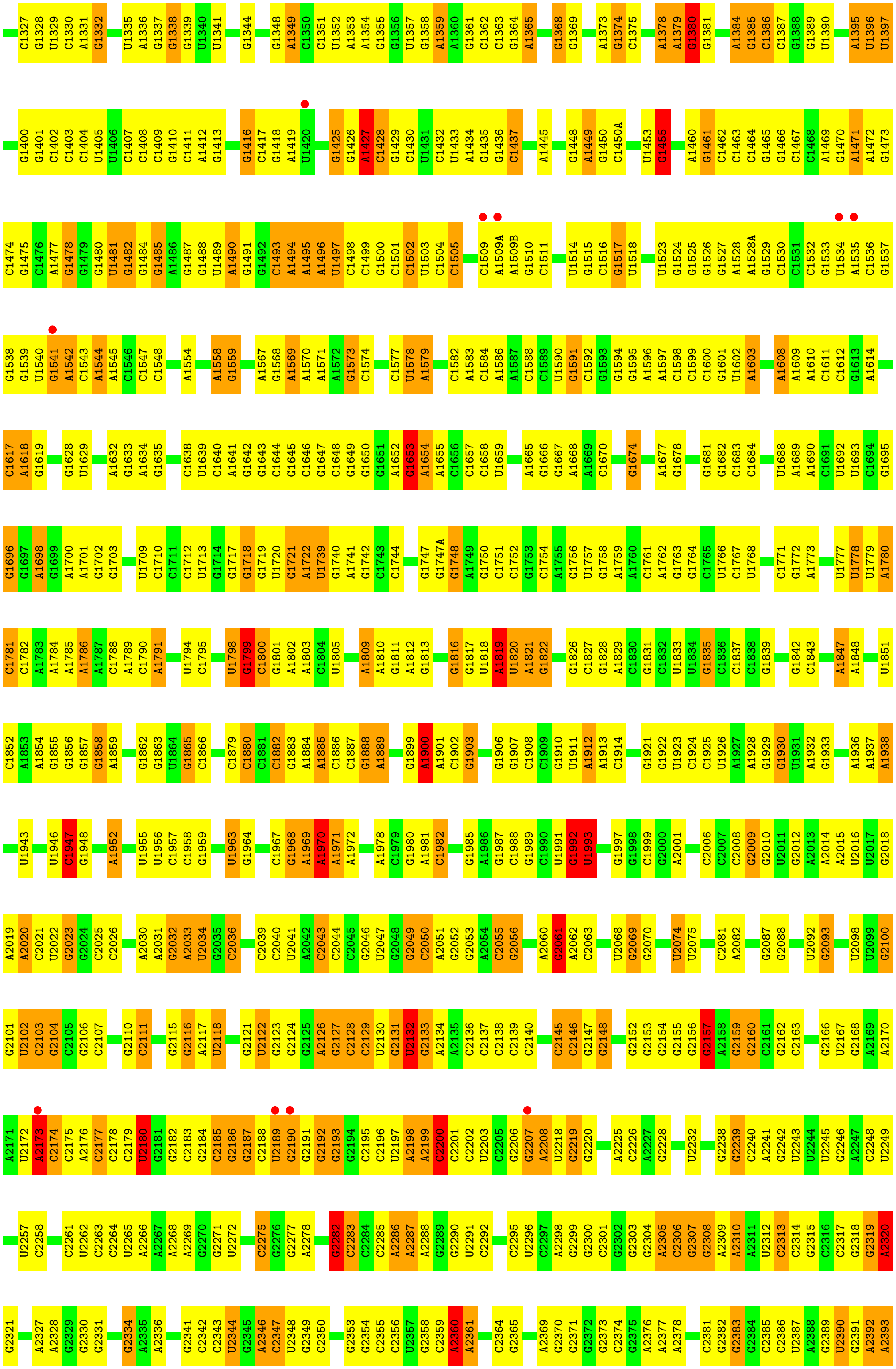
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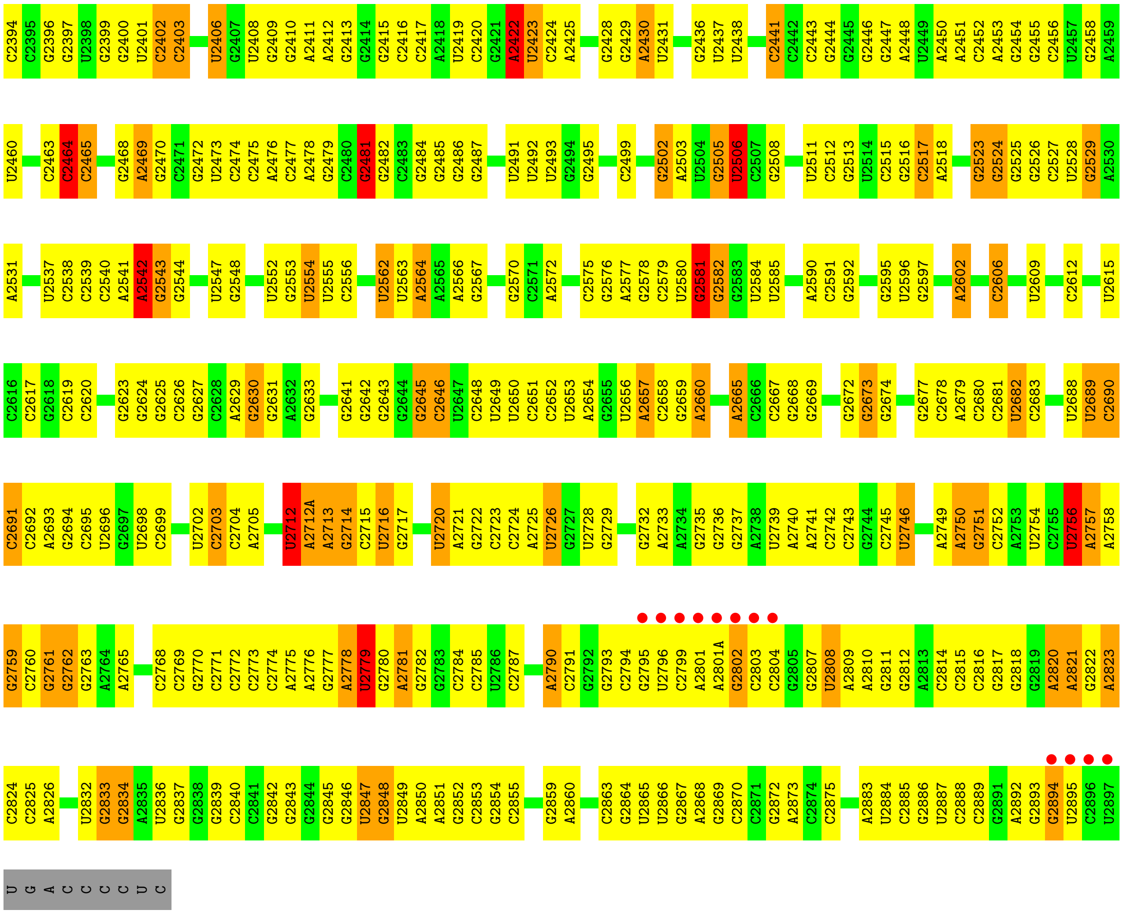
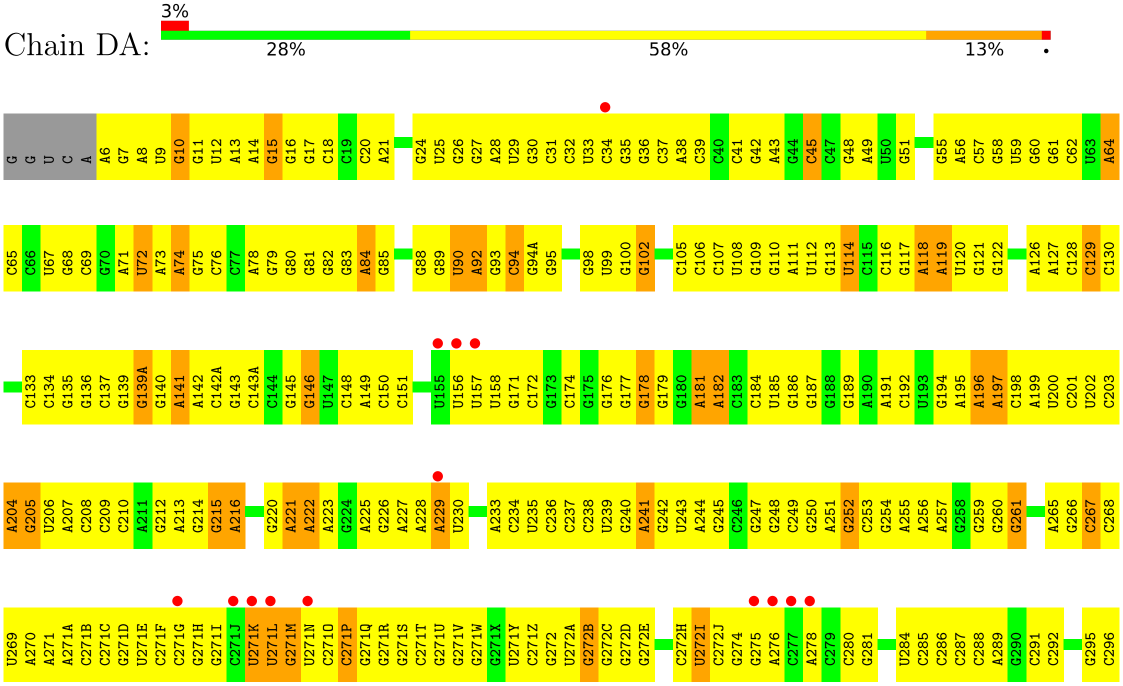
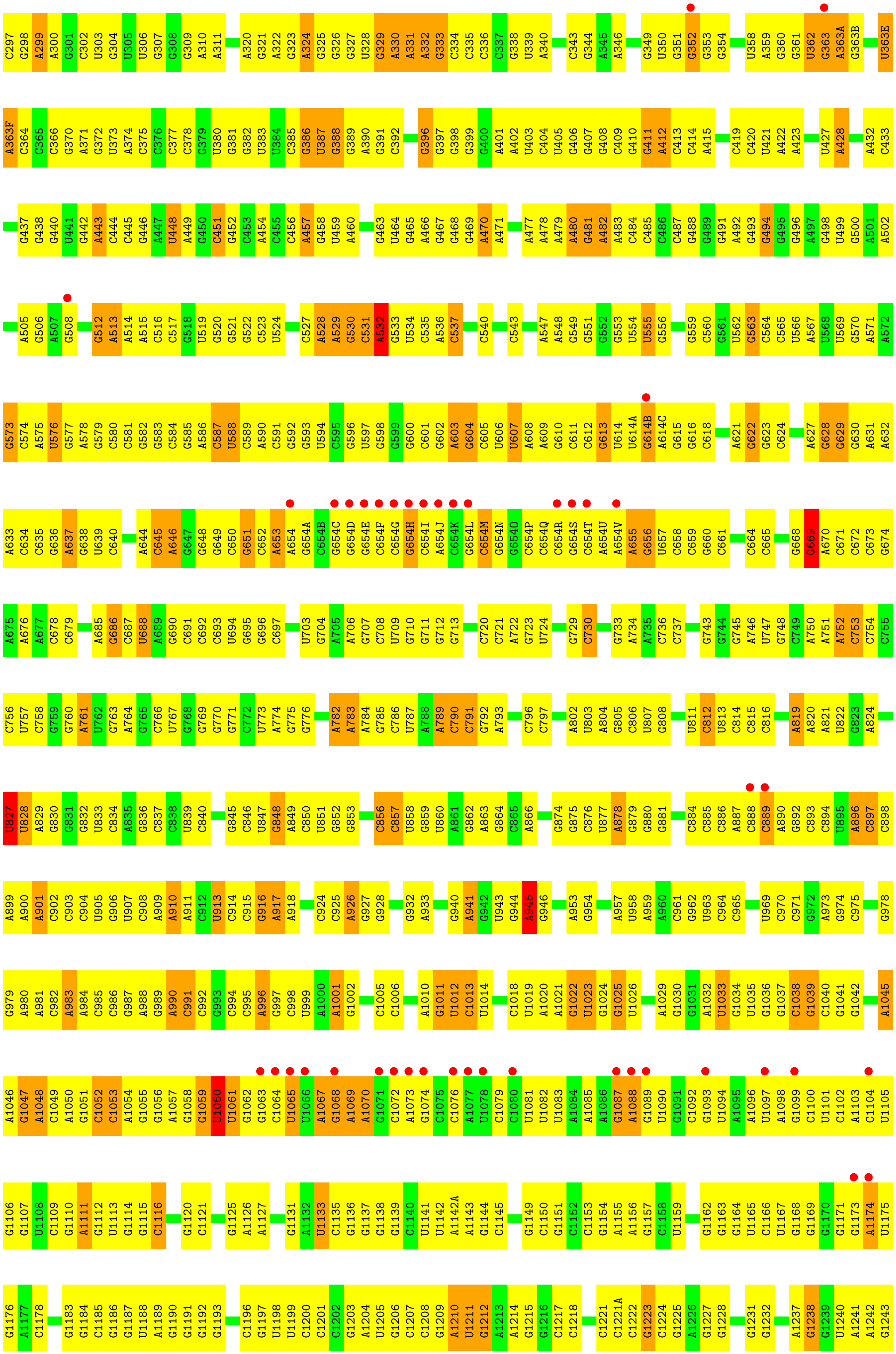


- Molecule 36: 23S RIBOSOMAL RNA

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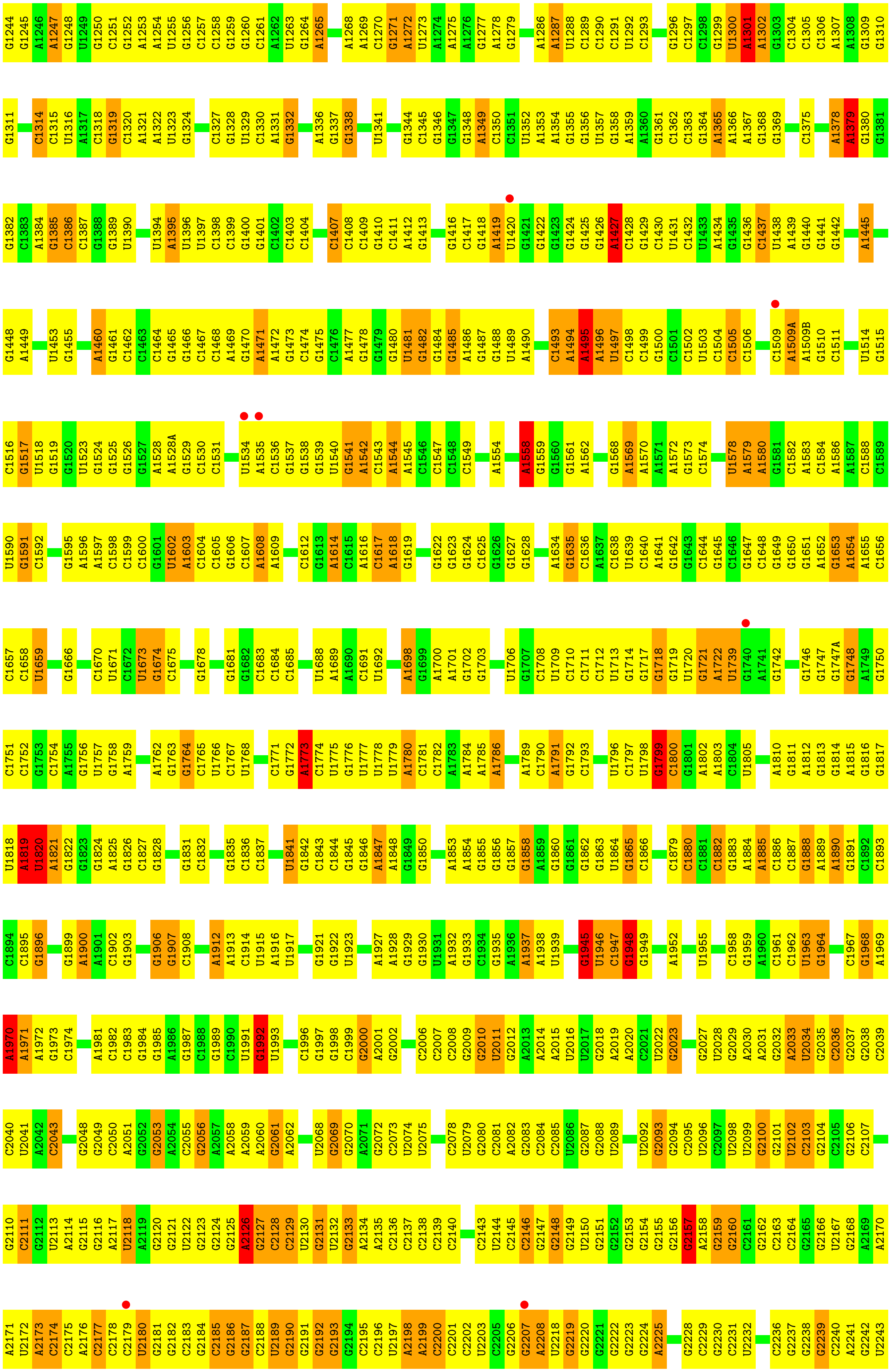
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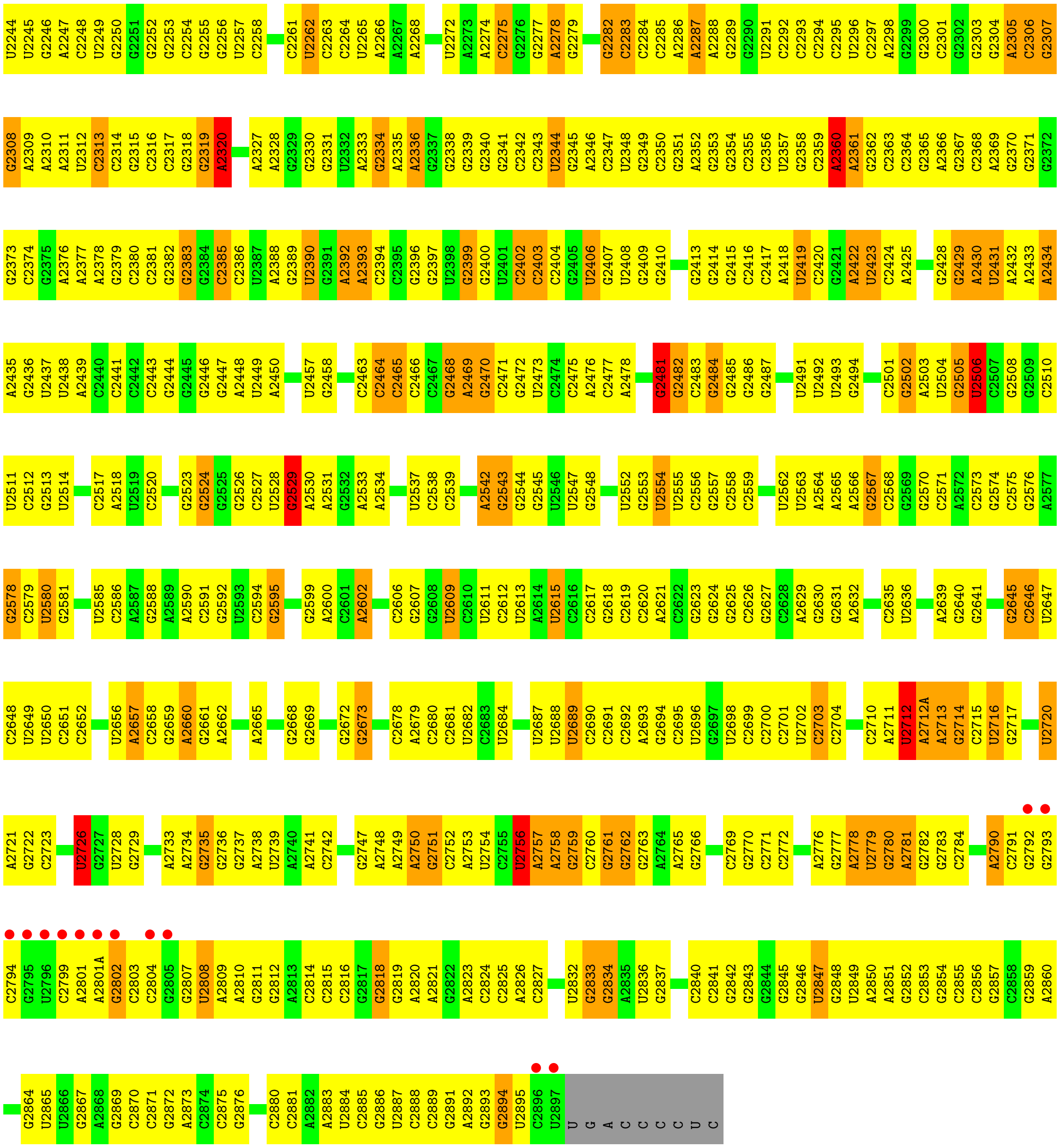

- Molecule 37: 5S RIBOSOMAL RNA

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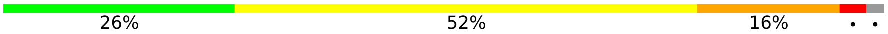

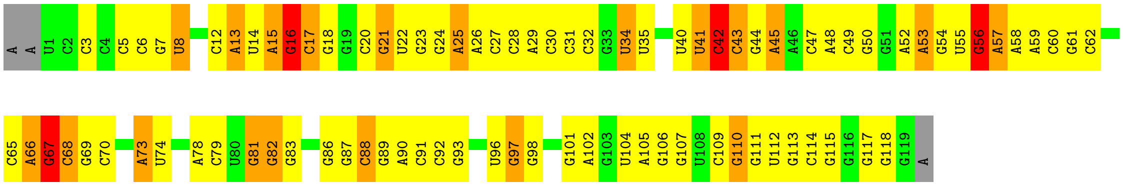

- Molecule 37: 5S RIBOSOMAL RNA

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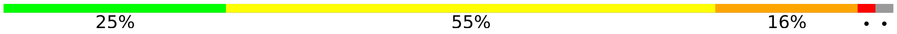

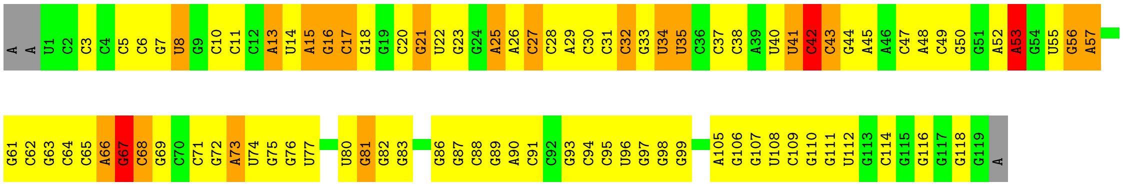

• Molecule 38: 50S RIBOSOMAL PROTEIN L1

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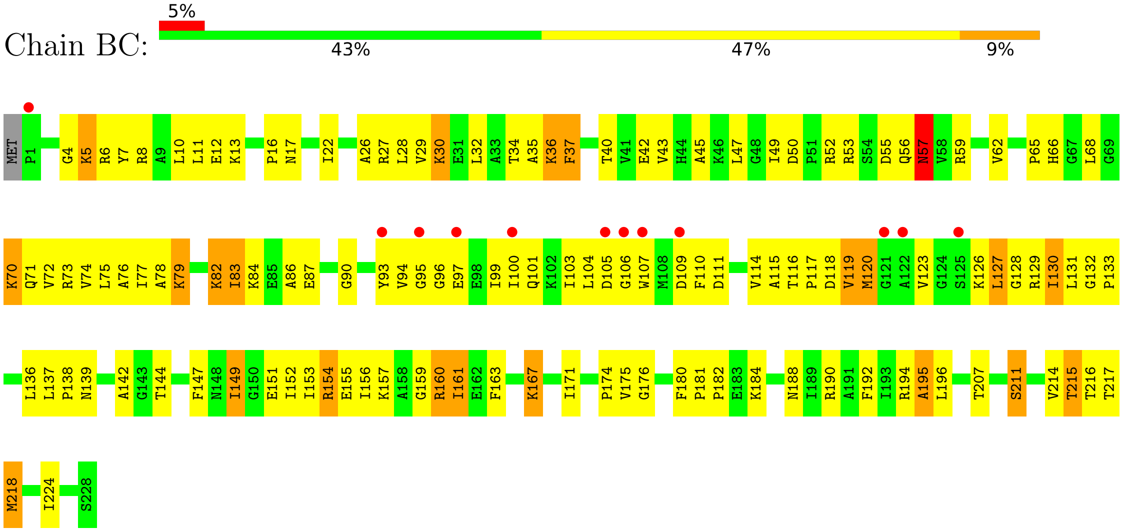

• Molecule 38: 50S RIBOSOMAL PROTEIN L1

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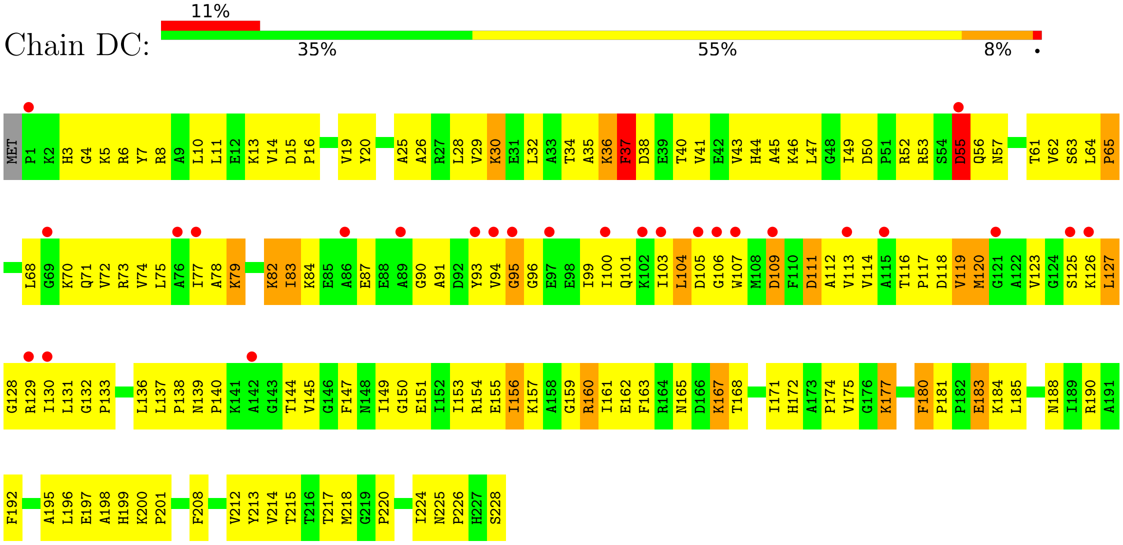

• Molecule 39: 50S RIBOSOMAL PROTEIN L2

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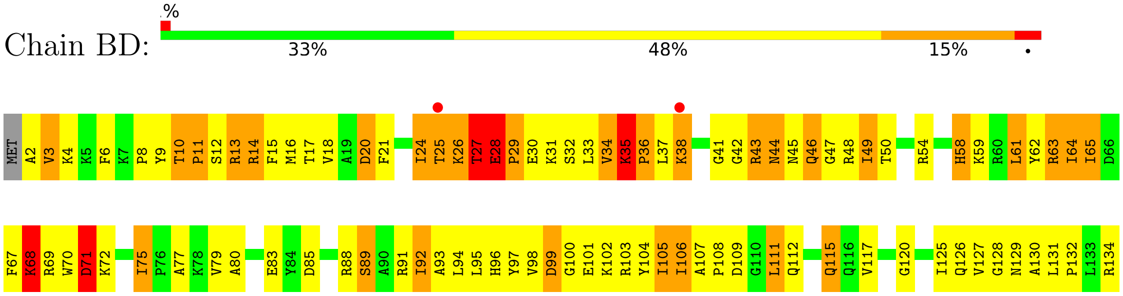
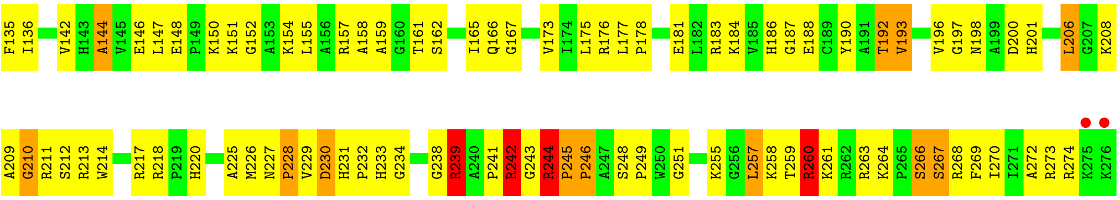
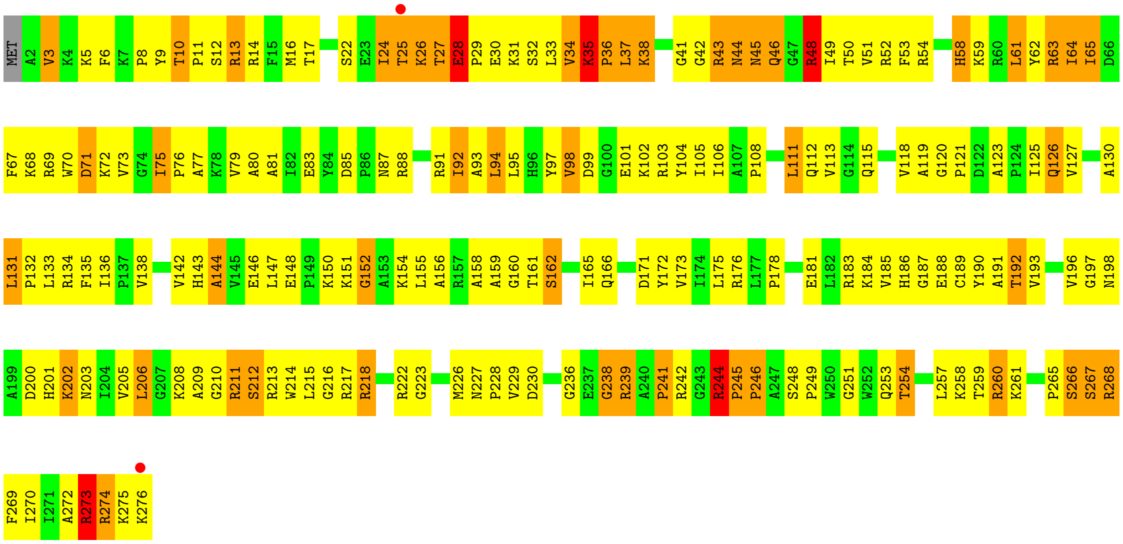




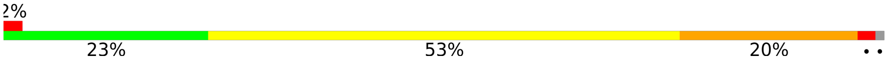
- Molecule 39: 50S RIBOSOMAL PROTEIN L2

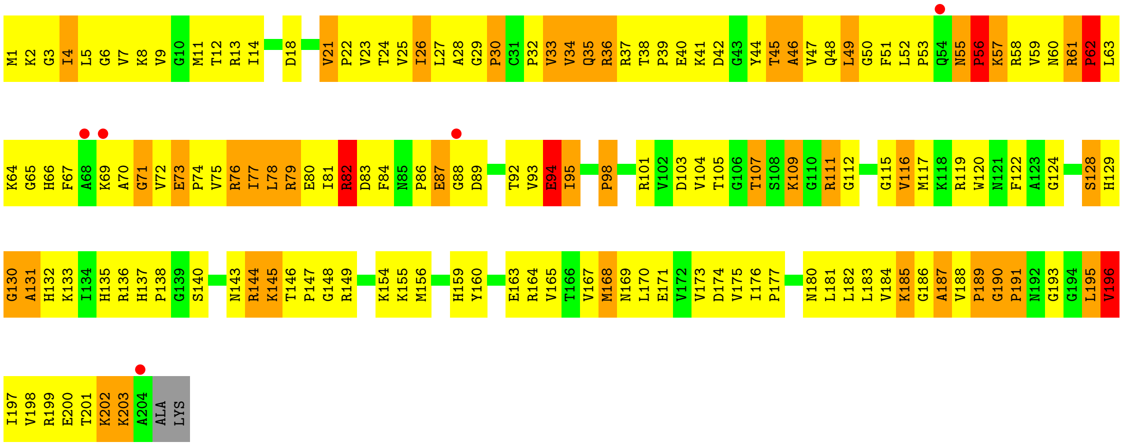
Chain DD:



- Molecule 40: 50S RIBOSOMAL PROTEIN L3

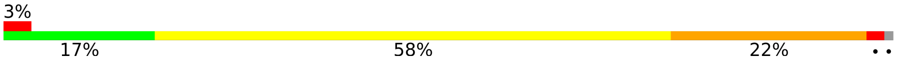
Chain BE:

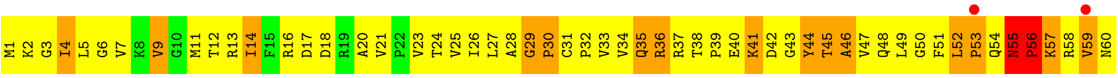


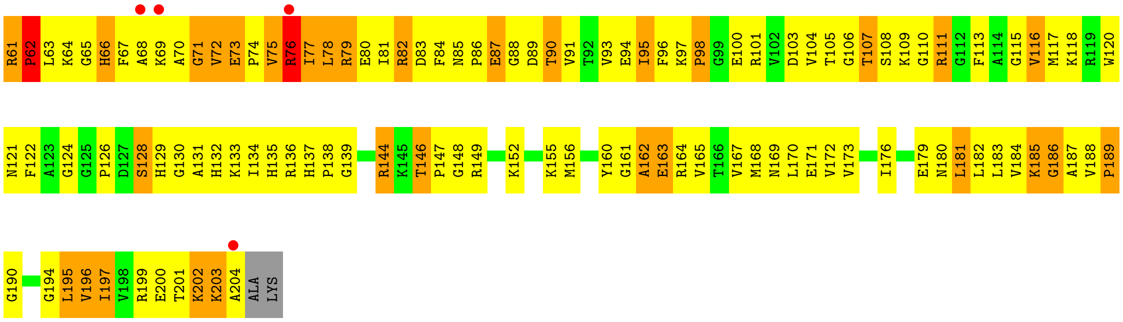


- Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain DE:

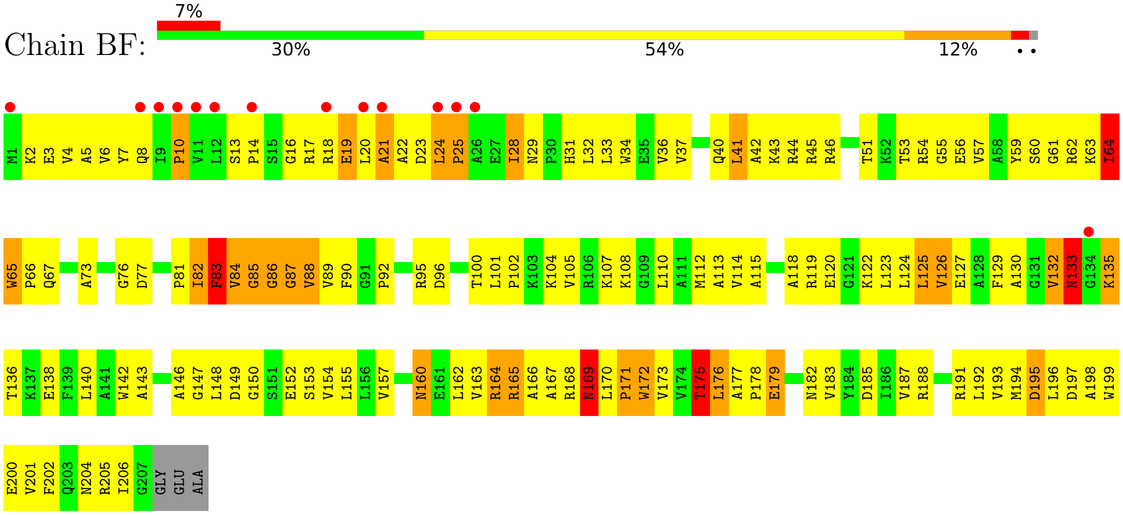






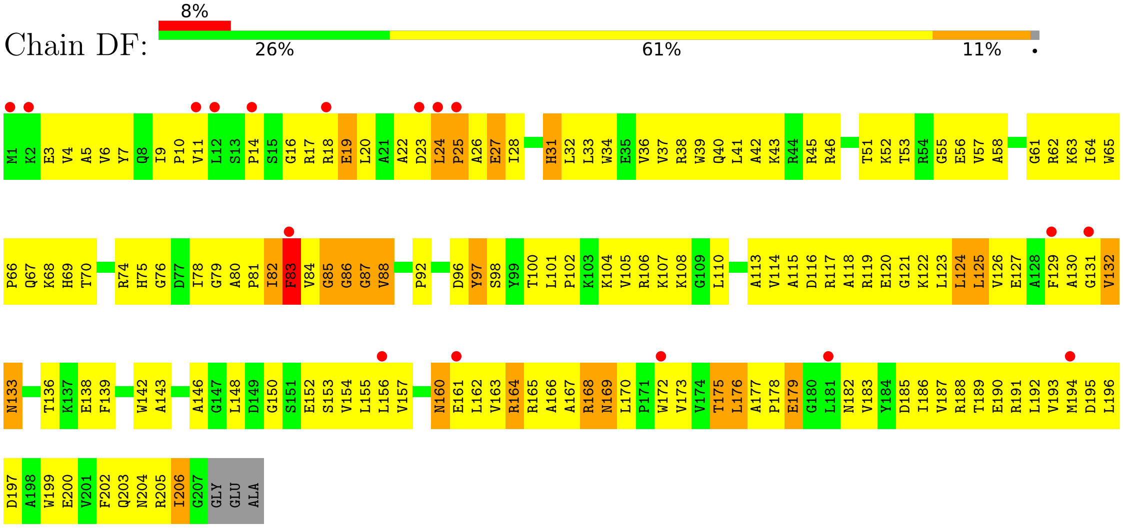
- Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain BF:



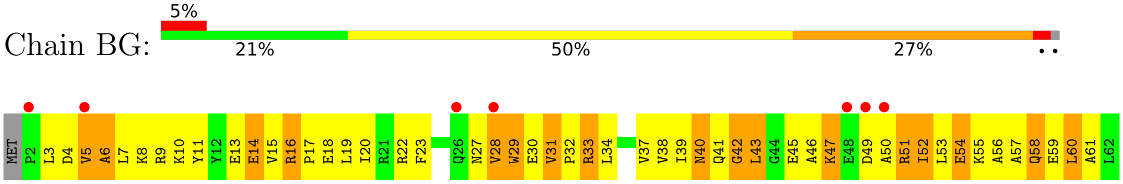
- Molecule 41: 50S RIBOSOMAL PROTEIN L4

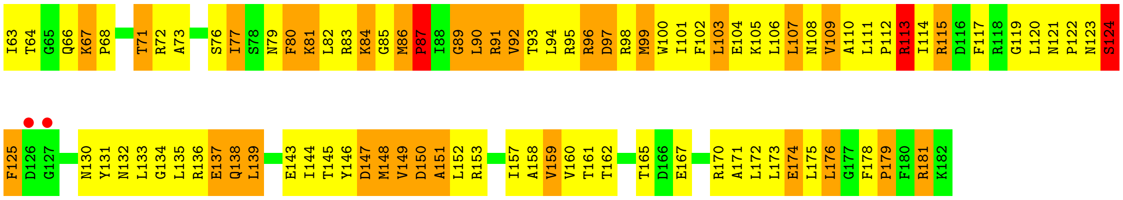
Chain DF:



- Molecule 42: 50S RIBOSOMAL PROTEIN L5

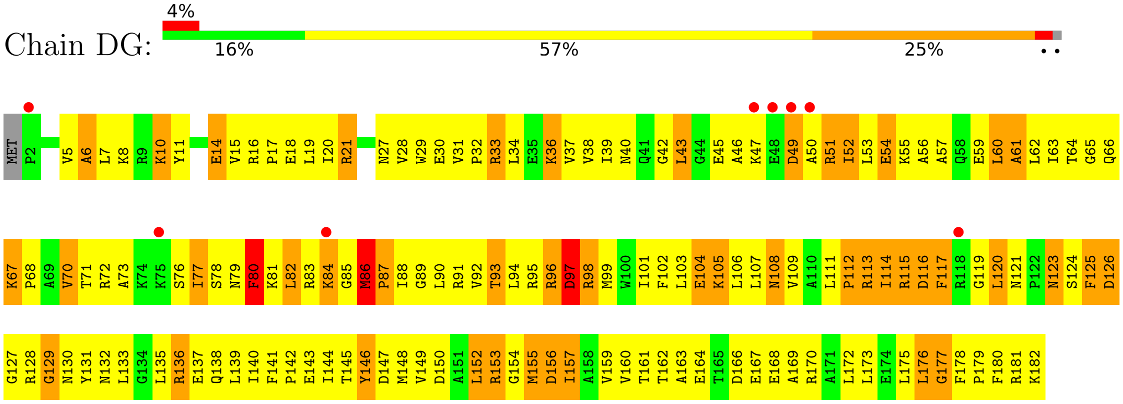
Chain BG:





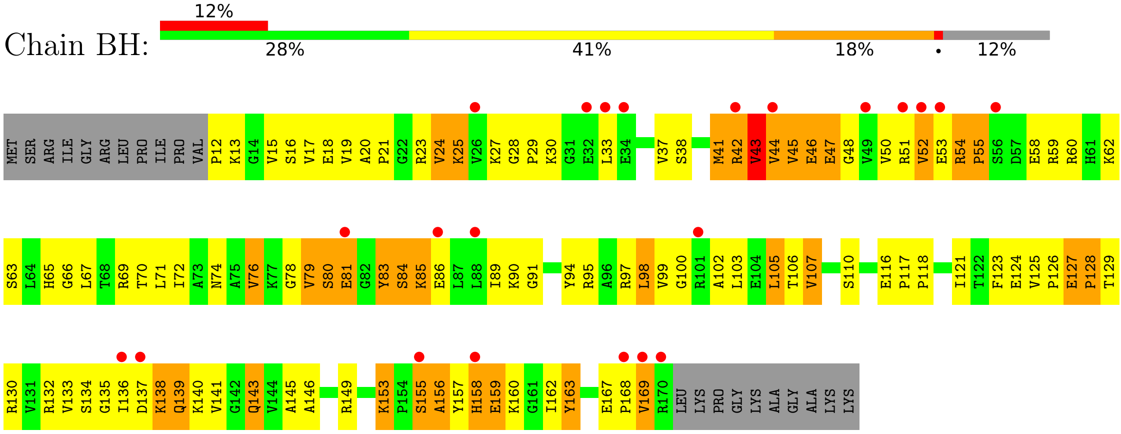
- Molecule 42: 50S RIBOSOMAL PROTEIN L5

Chain DG:



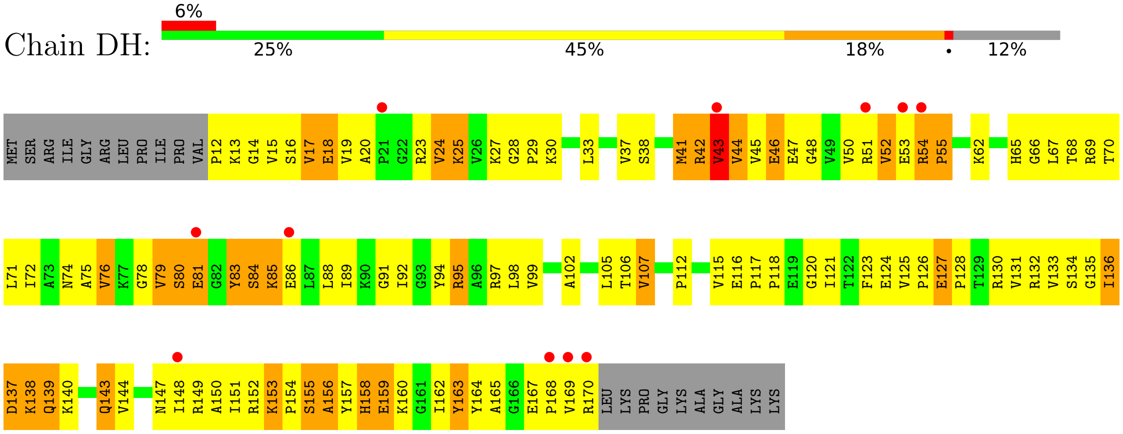
- Molecule 43: 50S RIBOSOMAL PROTEIN L6

Chain BH:

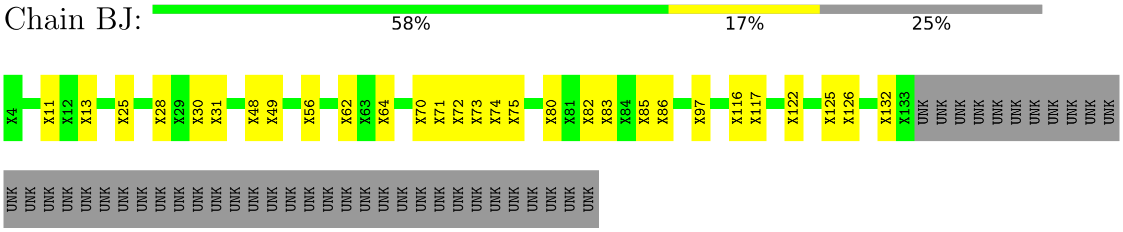


- Molecule 43: 50S RIBOSOMAL PROTEIN L6

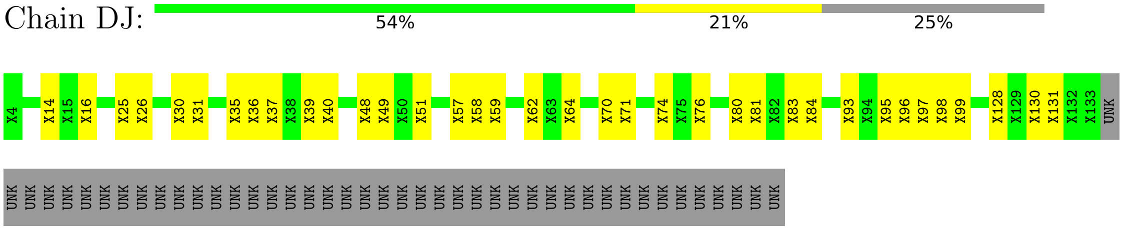
Chain DH:



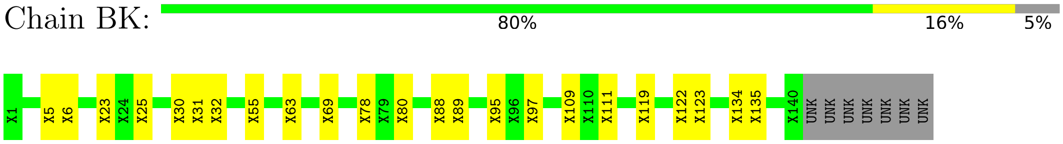
- Molecule 44: 50S RIBOSOMAL PROTEIN L10



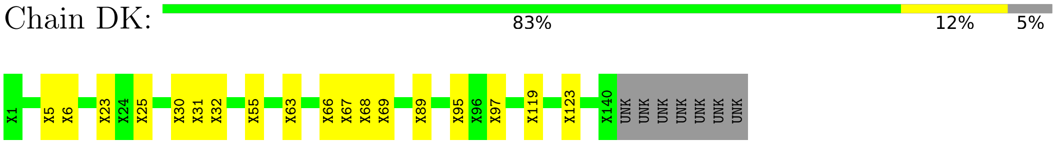
- Molecule 44: 50S RIBOSOMAL PROTEIN L10



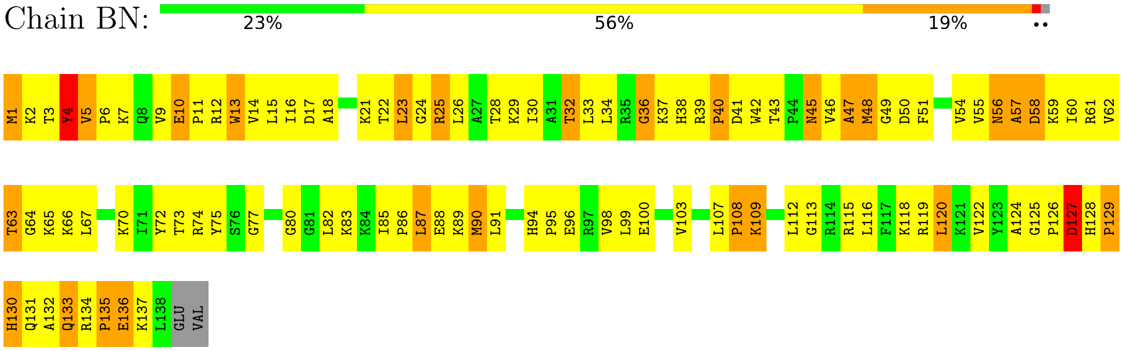
- Molecule 45: 50S RIBOSOMAL PROTEIN L11



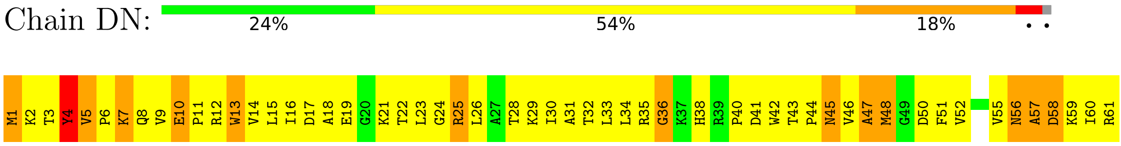
- Molecule 45: 50S RIBOSOMAL PROTEIN L11

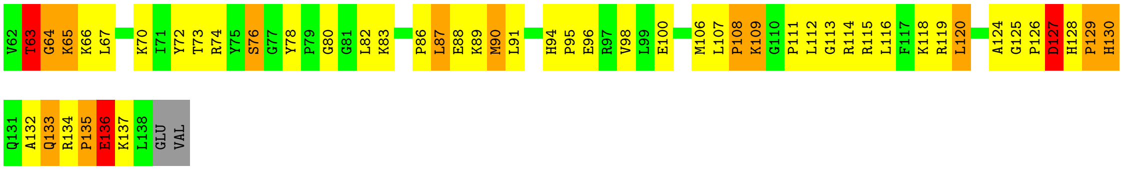


- Molecule 46: 50S RIBOSOMAL PROTEIN L13

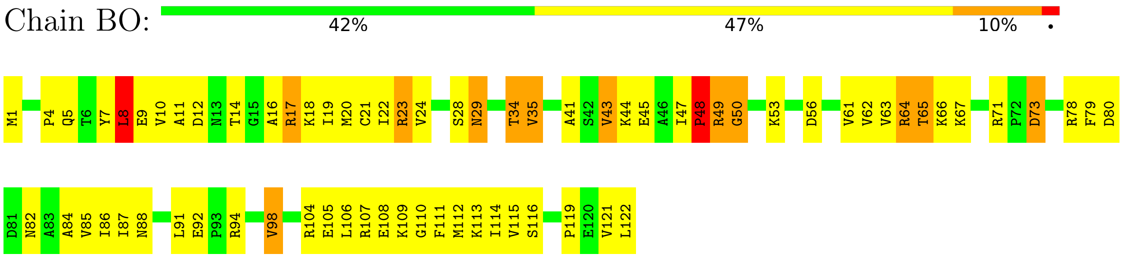


- Molecule 46: 50S RIBOSOMAL PROTEIN L13

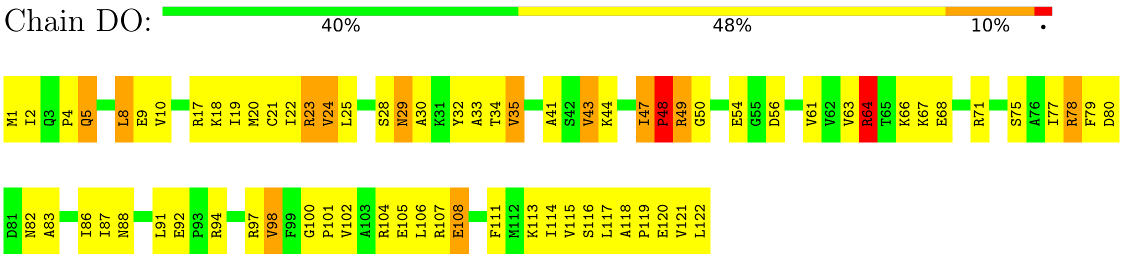




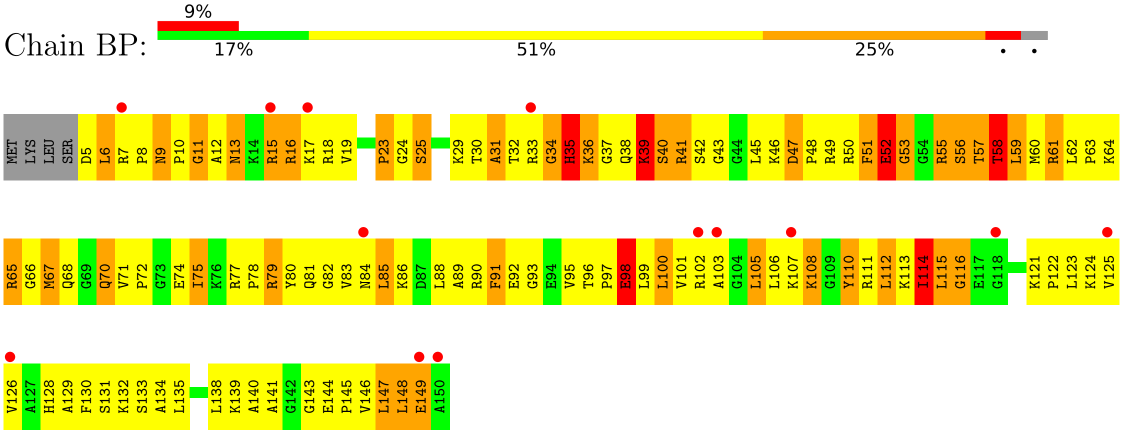
- Molecule 47: 50S RIBOSOMAL PROTEIN L14



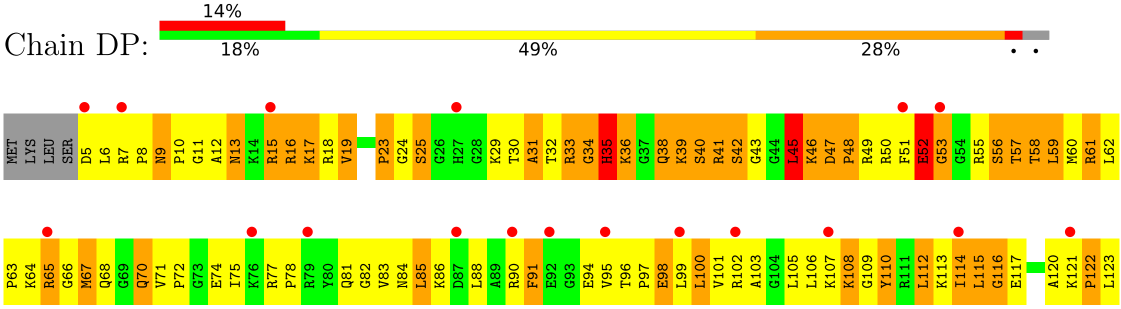
- Molecule 47: 50S RIBOSOMAL PROTEIN L14



- Molecule 48: 50S RIBOSOMAL PROTEIN L15

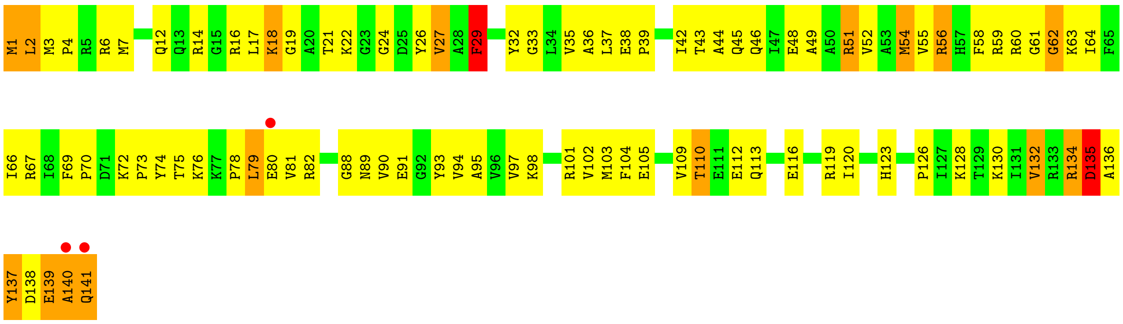


- Molecule 48: 50S RIBOSOMAL PROTEIN L15



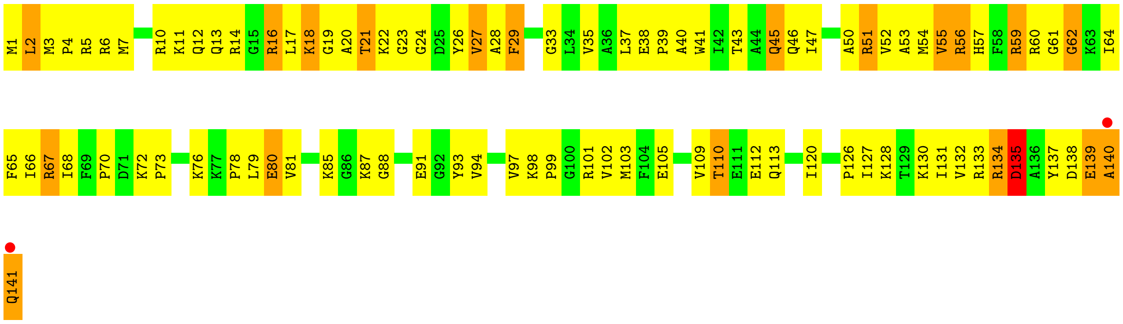
- Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



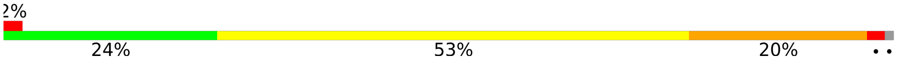
- Molecule 49: 50S RIBOSOMAL PROTEIN L16

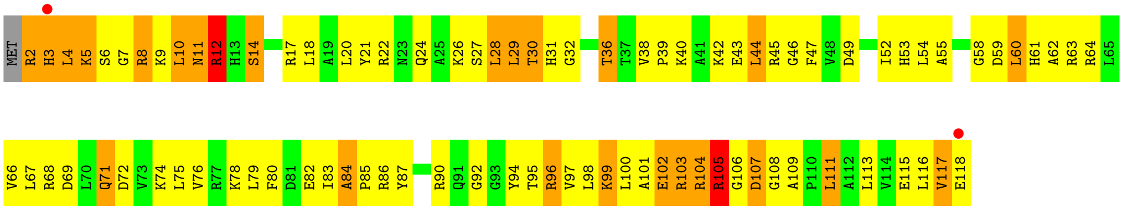
Chain DQ:



- Molecule 50: 50S RIBOSOMAL PROTEIN L17

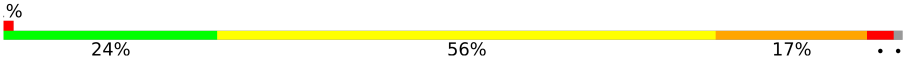
Chain BR:

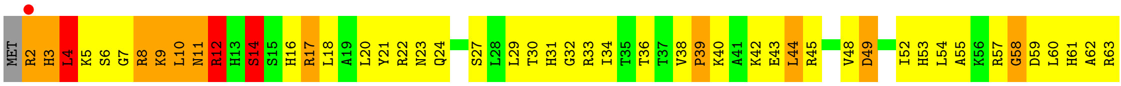


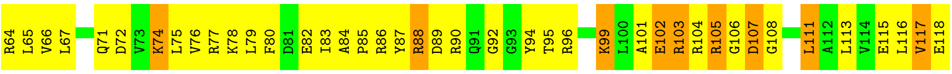


- Molecule 50: 50S RIBOSOMAL PROTEIN L17

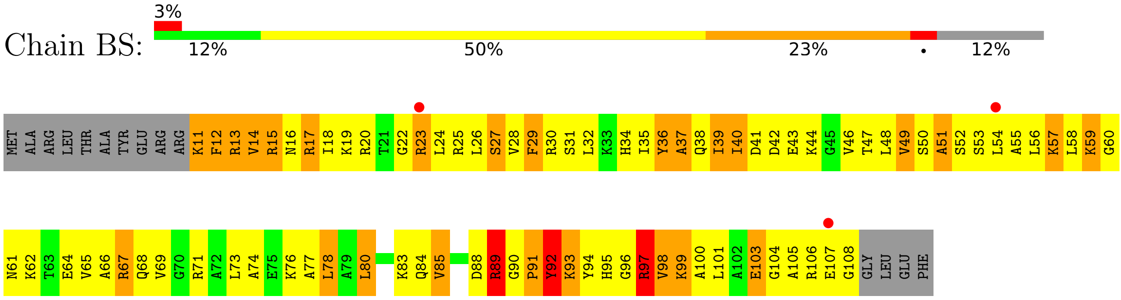
Chain DR:



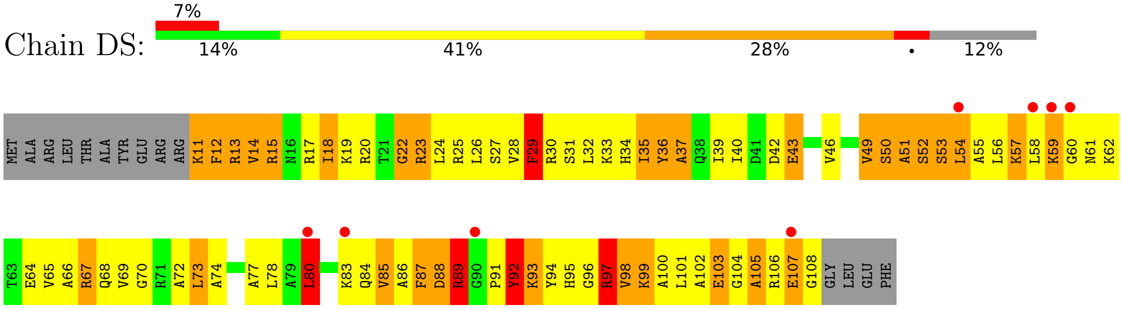




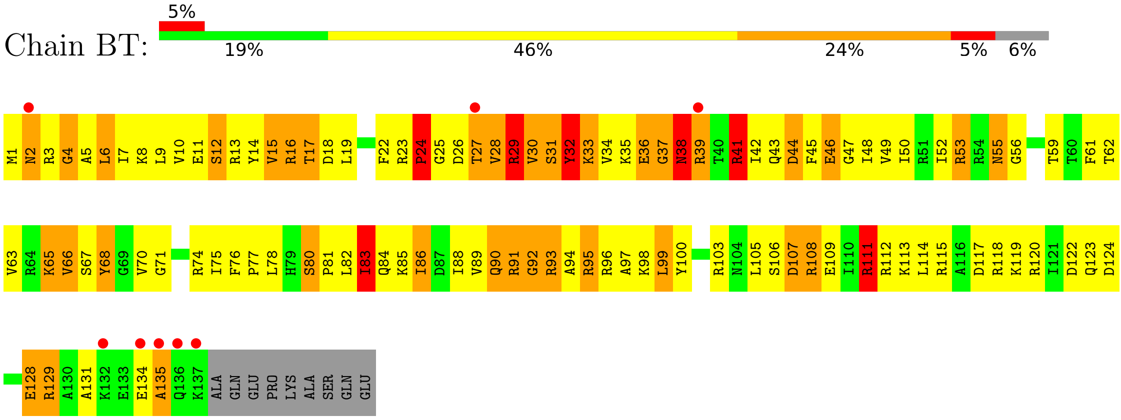
- Molecule 51: 50S RIBOSOMAL PROTEIN L18



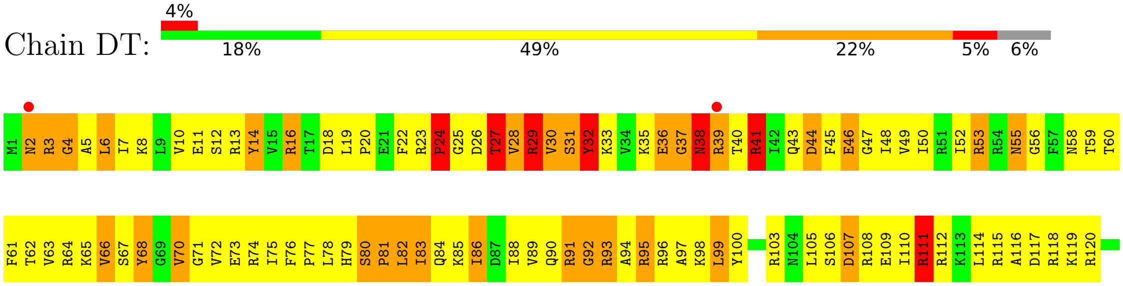
- Molecule 51: 50S RIBOSOMAL PROTEIN L18

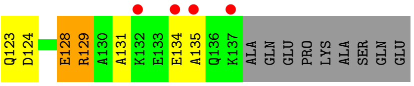


- Molecule 52: 50S RIBOSOMAL PROTEIN L19



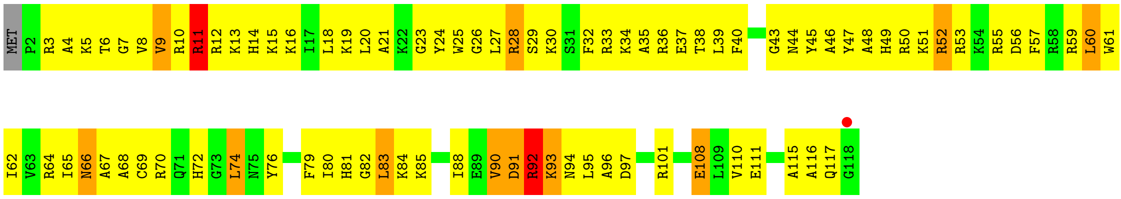
- Molecule 52: 50S RIBOSOMAL PROTEIN L19





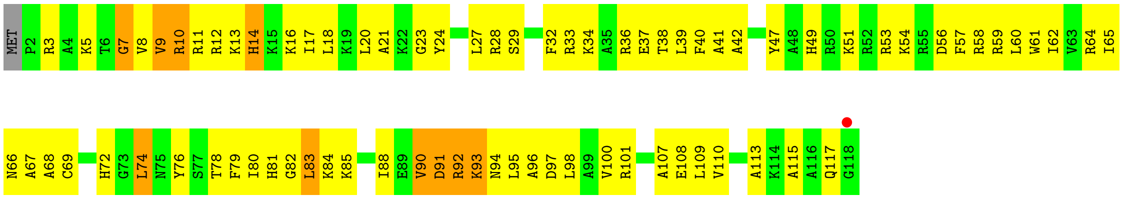
- Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:



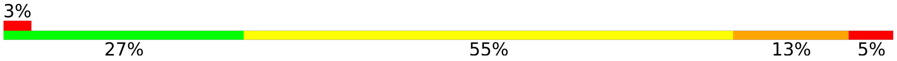
- Molecule 53: 50S RIBOSOMAL PROTEIN L20

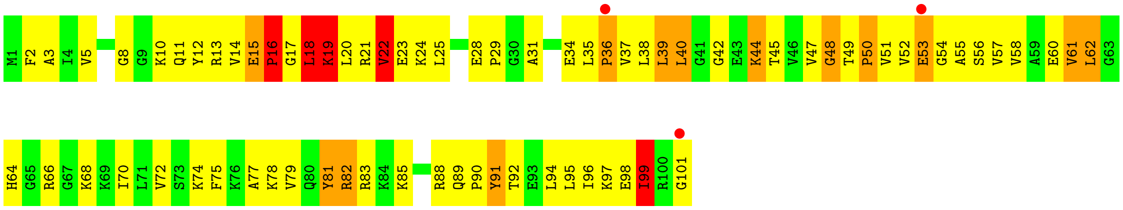
Chain DU:



- Molecule 54: 50S RIBOSOMAL PROTEIN L21

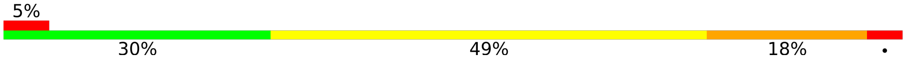
Chain BV:

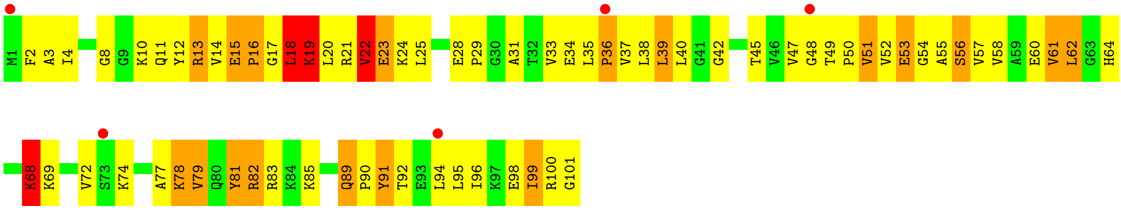




- Molecule 54: 50S RIBOSOMAL PROTEIN L21

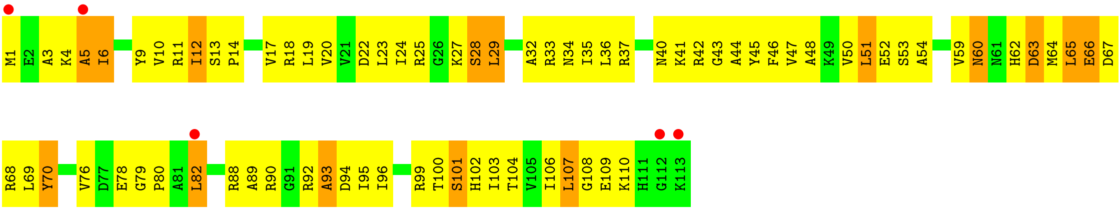
Chain DV:



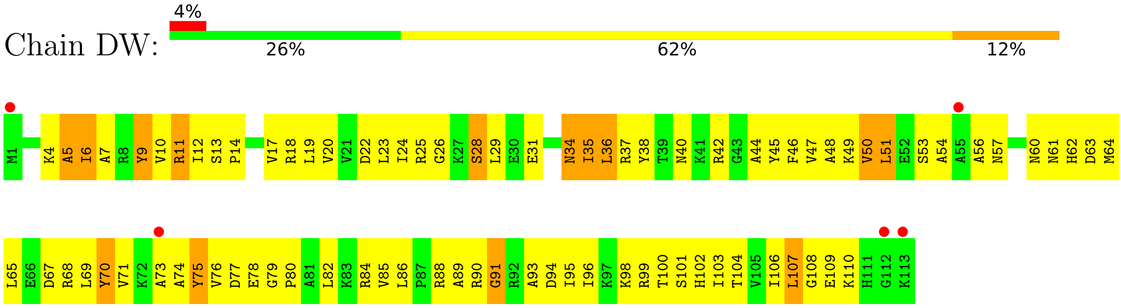


- Molecule 55: 50S RIBOSOMAL PROTEIN L22

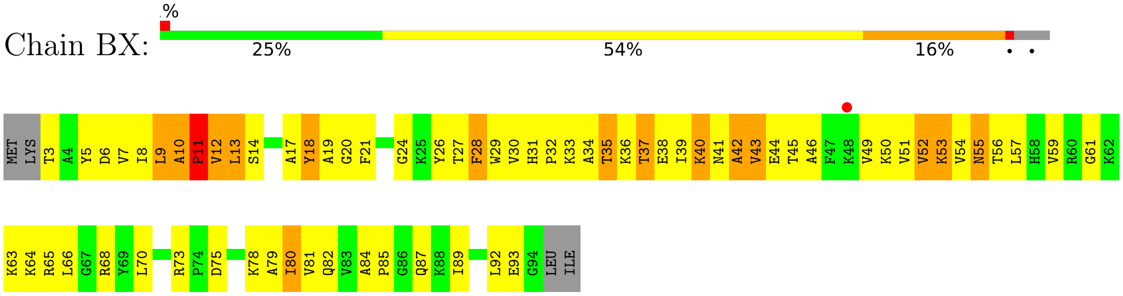
Chain BW:



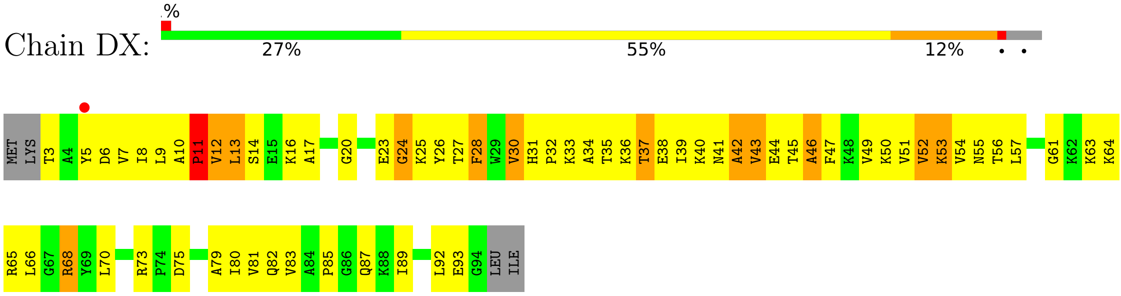
- Molecule 55: 50S RIBOSOMAL PROTEIN L22



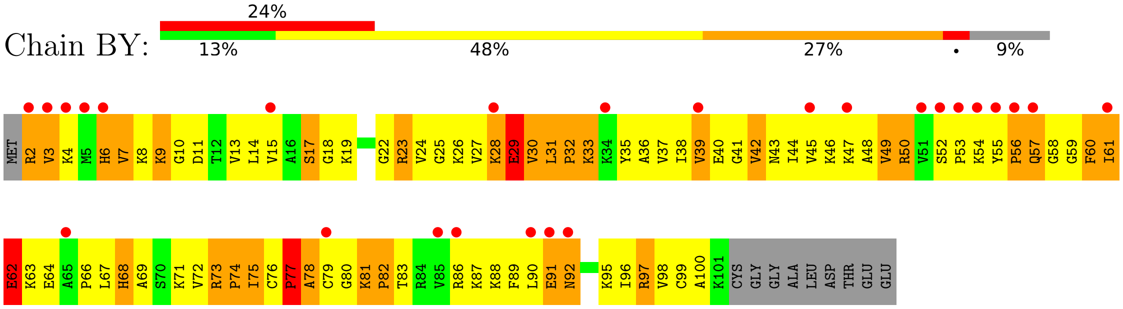
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



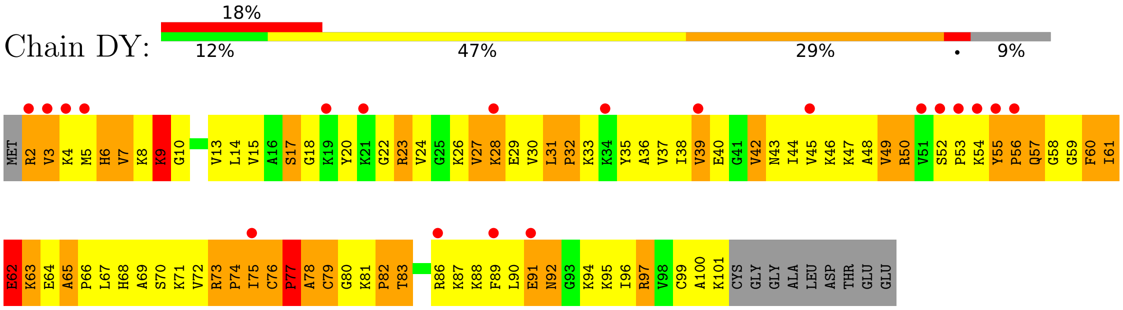
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



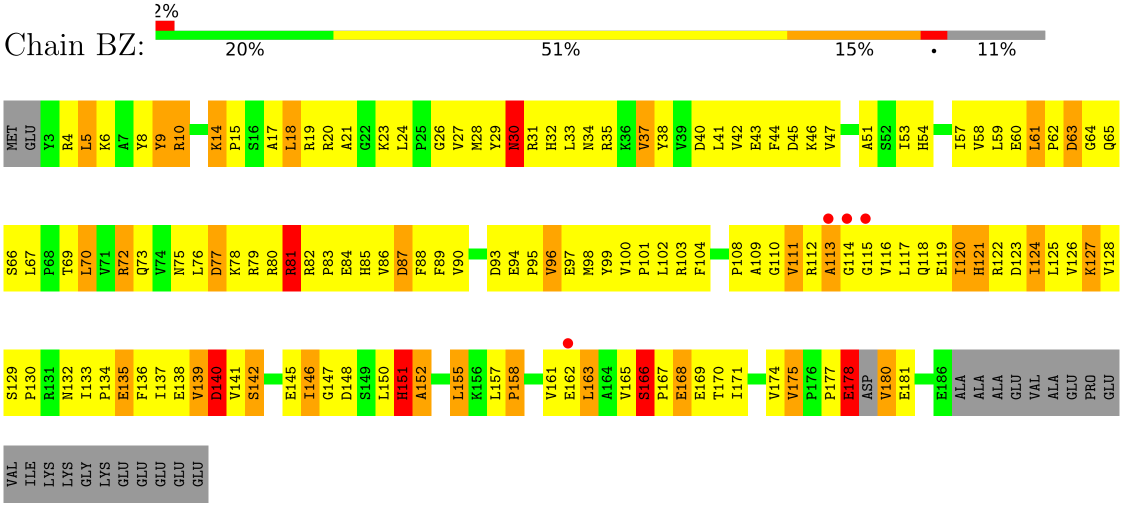
- Molecule 57: 50S RIBOSOMAL PROTEIN L24



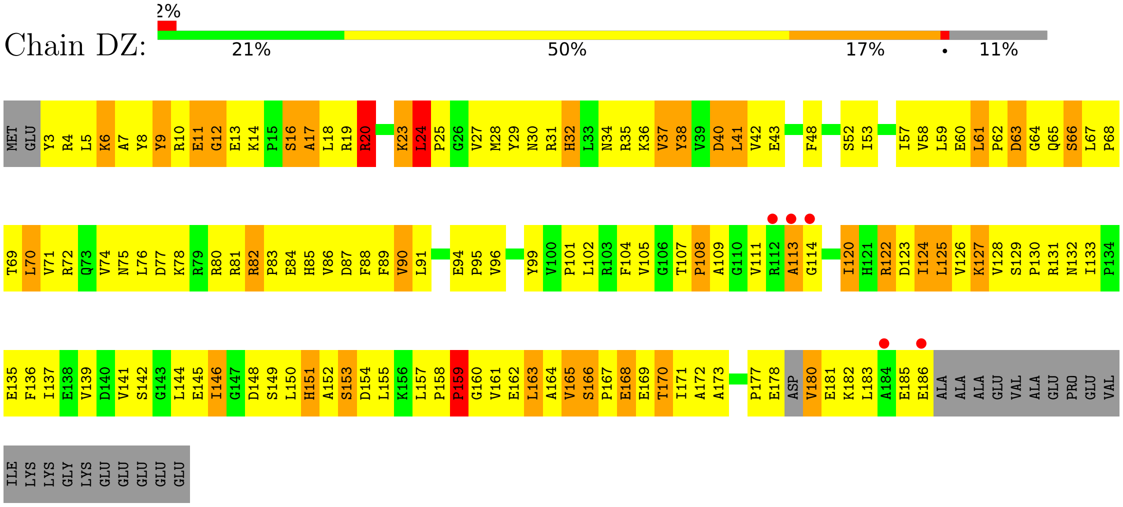
- Molecule 57: 50S RIBOSOMAL PROTEIN L24



• Molecule 58: 50S RIBOSOMAL PROTEIN L25



• Molecule 58: 50S RIBOSOMAL PROTEIN L25



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	289.90Å 269.40Å 404.50Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-3.10) 91.8 (49.22-2.80)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.238 , 0.275 0.238 , 0.275	Depositor DCC
R_{free} test set	69565 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	65.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 74.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	307194	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: KIR, GDP, 4SU, MIA, 7MG, ZN, PSU, 5MU, H2U, OMC

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	0.67	10/36190 (0.0%)	0.79	44/56486 (0.1%)
1	CA	0.54	3/36190 (0.0%)	0.74	25/56486 (0.0%)
2	AB	0.55	0/1935	0.76	0/2609
2	CB	0.43	0/1935	0.70	0/2609
3	AC	0.65	1/1636 (0.1%)	0.83	0/2205
3	CC	0.43	0/1636	0.70	0/2205
4	AD	0.48	1/1733 (0.1%)	0.75	1/2318 (0.0%)
4	CD	0.44	1/1733 (0.1%)	0.71	0/2318
5	AE	0.65	1/1162 (0.1%)	0.81	0/1564
5	CE	0.52	0/1162	0.77	0/1564
6	AF	0.50	0/856	0.70	1/1154 (0.1%)
6	CF	0.38	0/856	0.67	0/1154
7	AG	0.52	0/1276	0.73	1/1709 (0.1%)
7	CG	0.39	0/1276	0.63	0/1709
8	AH	0.57	0/1136	0.80	0/1527
8	CH	0.49	0/1136	0.79	0/1527
9	AI	0.55	0/1029	0.82	0/1379
9	CI	0.41	0/1029	0.68	0/1379
10	AJ	0.55	0/807	0.85	0/1085
10	CJ	0.40	0/807	0.75	1/1085 (0.1%)
11	AK	0.60	1/900 (0.1%)	0.80	0/1213
11	CK	0.46	0/900	0.76	1/1213 (0.1%)
12	AL	0.52	0/986	0.82	1/1320 (0.1%)
12	CL	0.44	0/986	0.77	0/1320
13	AM	0.51	0/998	0.80	0/1336
13	CM	0.39	0/998	0.74	0/1336
14	AN	0.70	1/501 (0.2%)	0.98	1/664 (0.2%)
14	CN	0.53	1/501 (0.2%)	0.86	1/664 (0.2%)
15	AO	0.52	0/745	0.77	0/992
15	CO	0.44	0/745	0.66	0/992
16	AP	0.46	0/716	0.74	0/963
16	CP	0.40	0/716	0.70	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.54	0/836	0.76	0/1117
17	CQ	0.45	0/836	0.76	0/1117
18	AR	0.56	0/579	0.73	0/768
18	CR	0.46	0/579	0.72	0/768
19	AS	0.55	0/642	0.76	0/865
19	CS	0.40	0/642	0.76	0/865
20	AT	0.42	0/765	0.69	0/1007
20	CT	0.36	0/765	0.71	0/1007
21	AU	0.55	0/212	0.87	0/277
21	CU	0.48	0/212	0.80	0/277
22	AV	0.68	0/1809	0.79	0/2819
22	AW	0.47	0/1809	0.74	0/2819
22	CV	0.92	5/1809 (0.3%)	0.90	7/2819 (0.2%)
22	CW	0.41	0/1809	0.73	0/2819
23	AX	0.79	0/405	0.91	2/629 (0.3%)
23	CX	1.78	13/405 (3.2%)	1.64	16/629 (2.5%)
24	AY	0.49	1/1618 (0.1%)	0.71	0/2514
24	CY	0.64	2/1618 (0.1%)	0.76	0/2514
25	AZ	0.84	12/3042 (0.4%)	0.99	15/4129 (0.4%)
25	CZ	0.90	14/3042 (0.5%)	1.02	17/4129 (0.4%)
26	B0	0.47	0/671	0.78	0/892
26	D0	0.42	0/671	0.74	0/892
27	B1	0.51	0/738	0.81	1/981 (0.1%)
27	D1	0.42	0/738	0.76	0/981
28	B2	0.38	0/600	0.73	0/793
28	D2	0.35	0/600	0.60	0/793
29	B3	0.40	0/472	0.67	0/634
29	D3	0.38	0/472	0.68	0/634
30	B4	0.46	0/349	0.66	0/474
30	D4	0.51	0/349	0.62	0/474
31	B5	0.44	0/473	0.73	0/639
31	D5	0.43	0/473	0.74	0/639
32	B6	0.70	0/440	0.94	0/586
32	D6	0.58	0/440	0.85	0/586
33	B7	0.49	0/426	0.73	0/561
33	D7	0.44	0/426	0.74	1/561 (0.2%)
34	B8	0.58	0/515	0.89	1/679 (0.1%)
34	D8	0.52	0/515	0.87	1/679 (0.1%)
35	B9	0.56	0/310	0.73	0/407
35	D9	0.69	1/310 (0.3%)	0.81	0/407
36	BA	0.56	7/69976 (0.0%)	0.74	36/109244 (0.0%)
36	DA	0.51	3/69976 (0.0%)	0.73	25/109244 (0.0%)
37	BB	0.51	0/2853	0.77	3/4451 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	DB	0.48	0/2853	0.76	0/4451
38	BC	0.46	2/1774 (0.1%)	0.65	0/2391
38	DC	0.41	2/1774 (0.1%)	0.61	0/2391
39	BD	0.62	0/2195	0.93	3/2955 (0.1%)
39	DD	0.51	0/2195	0.86	1/2955 (0.0%)
40	BE	0.46	0/1596	0.77	1/2153 (0.0%)
40	DE	0.45	0/1596	0.75	1/2153 (0.0%)
41	BF	0.40	0/1658	0.65	0/2244
41	DF	0.40	0/1658	0.64	0/2244
42	BG	0.48	0/1499	0.78	0/2016
42	DG	0.40	0/1499	0.70	0/2016
43	BH	0.37	0/1245	0.66	0/1682
43	DH	0.35	0/1245	0.66	0/1682
46	BN	0.39	0/1131	0.72	0/1525
46	DN	0.39	0/1131	0.70	0/1525
47	BO	0.53	0/943	0.74	1/1269 (0.1%)
47	DO	0.51	1/943 (0.1%)	0.74	0/1269
48	BP	0.46	0/1131	0.96	4/1504 (0.3%)
48	DP	0.42	0/1131	0.93	4/1504 (0.3%)
49	BQ	0.52	0/1143	0.73	0/1527
49	DQ	0.51	0/1143	0.69	0/1527
50	BR	0.41	0/974	0.81	2/1302 (0.2%)
50	DR	0.38	0/974	0.77	2/1302 (0.2%)
51	BS	0.45	0/778	0.79	0/1036
51	DS	0.41	0/778	0.76	1/1036 (0.1%)
52	BT	0.48	0/1155	0.78	1/1542 (0.1%)
52	DT	0.44	0/1155	0.77	1/1542 (0.1%)
53	BU	0.42	0/975	0.69	0/1297
53	DU	0.44	0/975	0.69	0/1297
54	BV	0.38	0/790	0.68	0/1057
54	DV	0.37	0/790	0.67	0/1057
55	BW	0.39	0/907	0.76	0/1216
55	DW	0.39	0/907	0.68	0/1216
56	BX	0.45	0/739	0.70	0/993
56	DX	0.41	0/739	0.67	0/993
57	BY	0.36	0/788	0.69	0/1051
57	DY	0.38	0/788	0.70	0/1051
58	BZ	0.50	0/1491	0.75	0/2024
58	DZ	0.46	0/1491	0.72	0/2024
All	All	0.55	83/330116 (0.0%)	0.75	224/493186 (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	90
1	CA	2	54
5	AE	0	1
22	AV	0	1
22	CV	0	2
22	CW	0	2
23	AX	0	2
23	CX	0	6
24	CY	0	1
25	AZ	0	2
25	CZ	0	2
36	BA	2	87
36	DA	0	79
37	BB	0	4
37	DB	0	3
39	BD	0	1
46	BN	0	1
All	All	5	338

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CV	34	G	C5-C6	-23.91	1.18	1.42
25	CZ	69	GLU	CB-CG	17.54	1.85	1.52
25	AZ	69	GLU	CB-CG	16.36	1.83	1.52
25	AZ	68	VAL	CA-C	12.52	1.85	1.52
25	CZ	68	VAL	CA-C	11.51	1.82	1.52

The worst 5 of 224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AZ	356	PRO	C-N-CD	-26.29	62.77	120.60
25	CZ	356	PRO	C-N-CD	-25.87	63.68	120.60
25	AZ	197	ASP	CB-CG-OD2	-14.50	105.25	118.30
25	AZ	69	GLU	N-CA-CB	-13.90	85.58	110.60
25	CZ	69	GLU	N-CA-CB	-13.63	86.07	110.60

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	508	C	C3’
36	BA	1300	U	C3’
36	BA	1820	U	C3’
1	CA	508	C	C3’
1	CA	1399	C	C3’

5 of 338 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	108	G	Sidechain
1	AA	123	C	Sidechain
1	AA	13	U	Sidechain
1	AA	189(G)	G	Sidechain
1	AA	20	U	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	1034	0
1	CA	32329	0	16318	1280	0
2	AB	1900	0	1951	204	0
2	CB	1900	0	1951	237	0
3	AC	1612	0	1677	145	0
3	CC	1612	0	1677	183	0
4	AD	1703	0	1763	229	0
4	CD	1703	0	1763	265	0
5	AE	1146	0	1207	75	0
5	CE	1146	0	1207	108	0
6	AF	843	0	857	71	0
6	CF	843	0	857	94	0
7	AG	1257	0	1296	88	0
7	CG	1257	0	1296	87	0
8	AH	1116	0	1177	64	0
8	CH	1116	0	1177	92	0
9	AI	1010	0	1037	111	0
9	CI	1010	0	1037	117	0
10	AJ	794	0	840	126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	CJ	794	0	840	169	0
11	AK	885	0	904	67	0
11	CK	885	0	904	77	0
12	AL	970	0	1057	112	0
12	CL	970	0	1057	87	0
13	AM	987	0	1059	122	0
13	CM	987	0	1059	139	0
14	AN	492	0	531	62	0
14	CN	492	0	530	77	0
15	AO	734	0	771	47	0
15	CO	734	0	771	56	0
16	AP	700	0	720	92	0
16	CP	700	0	720	102	0
17	AQ	823	0	891	70	0
17	CQ	823	0	891	76	0
18	AR	574	0	644	51	0
18	CR	574	0	644	54	0
19	AS	629	0	652	81	0
19	CS	629	0	652	104	0
20	AT	763	0	861	105	0
20	CT	763	0	861	110	0
21	AU	208	0	221	32	0
21	CU	208	0	221	29	0
22	AV	1619	0	822	74	0
22	AW	1619	0	822	75	0
22	CV	1619	0	822	78	0
22	CW	1619	0	822	90	0
23	AX	361	0	184	27	0
23	CX	361	0	184	30	0
24	AY	1644	0	853	71	0
24	CY	1644	0	853	130	0
25	AZ	2984	0	2997	433	0
25	CZ	2984	0	2997	513	0
26	B0	662	0	688	75	0
26	D0	662	0	688	96	0
27	B1	731	0	808	88	0
27	D1	731	0	808	116	0
28	B2	598	0	653	179	0
28	D2	598	0	653	81	0
29	B3	467	0	523	57	0
29	D3	467	0	523	40	0
30	B4	340	0	336	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	D4	340	0	335	55	0
31	B5	459	0	480	82	0
31	D5	459	0	480	86	0
32	B6	433	0	461	143	0
32	D6	433	0	461	147	0
33	B7	418	0	467	35	0
33	D7	418	0	467	40	0
34	B8	507	0	576	118	0
34	D8	507	0	576	134	0
35	B9	307	0	335	35	0
35	D9	307	0	336	49	0
36	BA	62477	0	31497	2270	0
36	DA	62477	0	31497	2492	0
37	BB	2551	0	1295	108	0
37	DB	2551	0	1295	108	0
38	BC	1742	0	1800	152	0
38	DC	1742	0	1800	181	0
39	BD	2145	0	2234	297	0
39	DD	2145	0	2234	321	0
40	BE	1563	0	1629	227	0
40	DE	1563	0	1629	256	0
41	BF	1623	0	1677	197	0
41	DF	1623	0	1677	209	0
42	BG	1474	0	1535	241	0
42	DG	1474	0	1535	275	0
43	BH	1222	0	1282	171	0
43	DH	1222	0	1282	159	0
44	BJ	651	0	170	19	0
44	DJ	651	0	162	25	0
45	BK	700	0	175	15	0
45	DK	700	0	171	13	0
46	BN	1104	0	1180	160	0
46	DN	1104	0	1180	159	0
47	BO	933	0	996	92	0
47	DO	933	0	996	100	0
48	BP	1114	0	1187	291	0
48	DP	1114	0	1187	301	0
49	BQ	1122	0	1179	141	0
49	DQ	1122	0	1179	138	0
50	BR	960	0	1021	131	0
50	DR	960	0	1021	136	0
51	BS	770	0	832	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	DS	770	0	832	159	0
52	BT	1141	0	1202	234	0
52	DT	1141	0	1202	211	0
53	BU	958	0	1015	141	0
53	DU	958	0	1015	152	0
54	BV	779	0	852	135	0
54	DV	779	0	852	124	0
55	BW	896	0	953	100	0
55	DW	896	0	953	97	0
56	BX	725	0	778	98	0
56	DX	725	0	778	107	0
57	BY	775	0	870	176	0
57	DY	775	0	870	164	0
58	BZ	1459	0	1488	216	0
58	DZ	1459	0	1488	206	0
59	AD	1	0	0	0	0
59	AN	1	0	0	2	0
59	B4	1	0	0	0	0
59	B9	1	0	0	0	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D9	1	0	0	1	0
60	AZ	28	0	12	12	0
60	CZ	28	0	12	13	0
61	AZ	57	0	59	11	0
61	CZ	57	0	59	14	0
All	All	307194	0	208701	19681	0

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 38.

The worst 5 of 19681 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:CZ:69:GLU:CB	25:CZ:69:GLU:CG	1.85	1.54
25:AZ:69:GLU:CG	25:AZ:69:GLU:CB	1.83	1.52
25:CZ:68:VAL:C	25:CZ:68:VAL:CA	1.82	1.46
25:AZ:68:VAL:C	25:AZ:68:VAL:CA	1.85	1.45
25:CZ:198:LYS:HE3	25:CZ:201:GLU:OE1	1.33	1.29

There are no symmetry-related clashes.

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	232/256 (91%)	168 (72%)	35 (15%)	29 (12%)	0	1
2	CB	232/256 (91%)	154 (66%)	50 (22%)	28 (12%)	0	1
3	AC	204/239 (85%)	161 (79%)	29 (14%)	14 (7%)	1	7
3	CC	204/239 (85%)	147 (72%)	40 (20%)	17 (8%)	1	5
4	AD	206/209 (99%)	139 (68%)	44 (21%)	23 (11%)	0	2
4	CD	206/209 (99%)	128 (62%)	44 (21%)	34 (16%)	0	0
5	AE	148/162 (91%)	138 (93%)	8 (5%)	2 (1%)	11	40
5	CE	148/162 (91%)	122 (82%)	25 (17%)	1 (1%)	22	57
6	AF	99/101 (98%)	78 (79%)	15 (15%)	6 (6%)	1	9
6	CF	99/101 (98%)	75 (76%)	13 (13%)	11 (11%)	0	2
7	AG	153/156 (98%)	121 (79%)	20 (13%)	12 (8%)	1	5
7	CG	153/156 (98%)	121 (79%)	24 (16%)	8 (5%)	2	12
8	AH	136/138 (99%)	124 (91%)	8 (6%)	4 (3%)	4	24
8	CH	136/138 (99%)	117 (86%)	12 (9%)	7 (5%)	2	13
9	AI	125/128 (98%)	85 (68%)	26 (21%)	14 (11%)	0	2
9	CI	125/128 (98%)	79 (63%)	31 (25%)	15 (12%)	0	1
10	AJ	96/105 (91%)	72 (75%)	15 (16%)	9 (9%)	0	3
10	CJ	96/105 (91%)	71 (74%)	16 (17%)	9 (9%)	0	3
11	AK	117/129 (91%)	103 (88%)	13 (11%)	1 (1%)	17	52
11	CK	117/129 (91%)	88 (75%)	23 (20%)	6 (5%)	2	13
12	AL	122/132 (92%)	97 (80%)	15 (12%)	10 (8%)	1	5
12	CL	122/132 (92%)	92 (75%)	22 (18%)	8 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	AM	122/126 (97%)	75 (62%)	31 (25%)	16 (13%)	0	1
13	CM	122/126 (97%)	72 (59%)	35 (29%)	15 (12%)	0	1
14	AN	58/61 (95%)	40 (69%)	10 (17%)	8 (14%)	0	1
14	CN	58/61 (95%)	34 (59%)	15 (26%)	9 (16%)	0	0
15	AO	86/89 (97%)	68 (79%)	13 (15%)	5 (6%)	1	10
15	CO	86/89 (97%)	68 (79%)	15 (17%)	3 (4%)	3	20
16	AP	81/88 (92%)	50 (62%)	21 (26%)	10 (12%)	0	1
16	CP	81/88 (92%)	49 (60%)	22 (27%)	10 (12%)	0	1
17	AQ	97/105 (92%)	84 (87%)	9 (9%)	4 (4%)	3	16
17	CQ	97/105 (92%)	80 (82%)	11 (11%)	6 (6%)	1	9
18	AR	68/88 (77%)	52 (76%)	12 (18%)	4 (6%)	1	10
18	CR	68/88 (77%)	51 (75%)	12 (18%)	5 (7%)	1	6
19	AS	76/93 (82%)	50 (66%)	16 (21%)	10 (13%)	0	1
19	CS	76/93 (82%)	45 (59%)	20 (26%)	11 (14%)	0	1
20	AT	97/106 (92%)	62 (64%)	24 (25%)	11 (11%)	0	2
20	CT	97/106 (92%)	64 (66%)	19 (20%)	14 (14%)	0	1
21	AU	22/27 (82%)	16 (73%)	3 (14%)	3 (14%)	0	1
21	CU	22/27 (82%)	14 (64%)	5 (23%)	3 (14%)	0	1
25	AZ	381/405 (94%)	272 (71%)	66 (17%)	43 (11%)	0	2
25	CZ	381/405 (94%)	270 (71%)	68 (18%)	43 (11%)	0	2
26	B0	82/85 (96%)	65 (79%)	10 (12%)	7 (8%)	1	5
26	D0	82/85 (96%)	62 (76%)	12 (15%)	8 (10%)	0	3
27	B1	91/98 (93%)	58 (64%)	18 (20%)	15 (16%)	0	0
27	D1	91/98 (93%)	64 (70%)	12 (13%)	15 (16%)	0	0
28	B2	69/72 (96%)	34 (49%)	20 (29%)	15 (22%)	0	0
28	D2	69/72 (96%)	44 (64%)	19 (28%)	6 (9%)	1	4
29	B3	57/60 (95%)	42 (74%)	9 (16%)	6 (10%)	0	3
29	D3	57/60 (95%)	39 (68%)	10 (18%)	8 (14%)	0	1
30	B4	42/71 (59%)	25 (60%)	10 (24%)	7 (17%)	0	0
30	D4	42/71 (59%)	17 (40%)	17 (40%)	8 (19%)	0	0
31	B5	57/60 (95%)	40 (70%)	7 (12%)	10 (18%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	D5	57/60 (95%)	40 (70%)	8 (14%)	9 (16%)	0	0
32	B6	48/54 (89%)	20 (42%)	10 (21%)	18 (38%)	0	0
32	D6	48/54 (89%)	20 (42%)	14 (29%)	14 (29%)	0	0
33	B7	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
33	D7	46/49 (94%)	40 (87%)	6 (13%)	0	100	100
34	B8	61/65 (94%)	31 (51%)	18 (30%)	12 (20%)	0	0
34	D8	61/65 (94%)	27 (44%)	19 (31%)	15 (25%)	0	0
35	B9	35/37 (95%)	19 (54%)	11 (31%)	5 (14%)	0	1
35	D9	35/37 (95%)	17 (49%)	13 (37%)	5 (14%)	0	1
38	BC	226/229 (99%)	176 (78%)	33 (15%)	17 (8%)	1	6
38	DC	226/229 (99%)	170 (75%)	37 (16%)	19 (8%)	1	5
39	BD	273/276 (99%)	199 (73%)	46 (17%)	28 (10%)	0	3
39	DD	273/276 (99%)	197 (72%)	43 (16%)	33 (12%)	0	1
40	BE	202/206 (98%)	125 (62%)	45 (22%)	32 (16%)	0	0
40	DE	202/206 (98%)	129 (64%)	38 (19%)	35 (17%)	0	0
41	BF	205/210 (98%)	145 (71%)	34 (17%)	26 (13%)	0	1
41	DF	205/210 (98%)	129 (63%)	54 (26%)	22 (11%)	0	2
42	BG	179/182 (98%)	110 (62%)	33 (18%)	36 (20%)	0	0
42	DG	179/182 (98%)	99 (55%)	53 (30%)	27 (15%)	0	0
43	BH	157/180 (87%)	97 (62%)	31 (20%)	29 (18%)	0	0
43	DH	157/180 (87%)	99 (63%)	27 (17%)	31 (20%)	0	0
46	BN	136/140 (97%)	91 (67%)	27 (20%)	18 (13%)	0	1
46	DN	136/140 (97%)	89 (65%)	27 (20%)	20 (15%)	0	0
47	BO	120/122 (98%)	97 (81%)	15 (12%)	8 (7%)	1	7
47	DO	120/122 (98%)	97 (81%)	15 (12%)	8 (7%)	1	7
48	BP	144/150 (96%)	77 (54%)	36 (25%)	31 (22%)	0	0
48	DP	144/150 (96%)	78 (54%)	34 (24%)	32 (22%)	0	0
49	BQ	139/141 (99%)	112 (81%)	20 (14%)	7 (5%)	2	13
49	DQ	139/141 (99%)	112 (81%)	17 (12%)	10 (7%)	1	6
50	BR	115/118 (98%)	81 (70%)	15 (13%)	19 (16%)	0	0
50	DR	115/118 (98%)	73 (64%)	27 (24%)	15 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BS	96/112 (86%)	44 (46%)	29 (30%)	23 (24%)	0	0
51	DS	96/112 (86%)	44 (46%)	22 (23%)	30 (31%)	0	0
52	BT	135/146 (92%)	76 (56%)	28 (21%)	31 (23%)	0	0
52	DT	135/146 (92%)	71 (53%)	35 (26%)	29 (22%)	0	0
53	BU	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	5
53	DU	115/118 (98%)	74 (64%)	34 (30%)	7 (6%)	1	9
54	BV	99/101 (98%)	65 (66%)	21 (21%)	13 (13%)	0	1
54	DV	99/101 (98%)	67 (68%)	19 (19%)	13 (13%)	0	1
55	BW	111/113 (98%)	78 (70%)	17 (15%)	16 (14%)	0	1
55	DW	111/113 (98%)	72 (65%)	23 (21%)	16 (14%)	0	1
56	BX	90/96 (94%)	63 (70%)	15 (17%)	12 (13%)	0	1
56	DX	90/96 (94%)	58 (64%)	22 (24%)	10 (11%)	0	2
57	BY	98/110 (89%)	43 (44%)	28 (29%)	27 (28%)	0	0
57	DY	98/110 (89%)	43 (44%)	26 (26%)	29 (30%)	0	0
58	BZ	181/206 (88%)	117 (65%)	38 (21%)	26 (14%)	0	1
58	DZ	181/206 (88%)	114 (63%)	42 (23%)	25 (14%)	0	1
All	All	12270/13100 (94%)	8441 (69%)	2326 (19%)	1503 (12%)	0	1

5 of 1503 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	8	LYS
2	AB	9	GLU
2	AB	15	VAL
2	AB	127	ILE
2	AB	131	PRO

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	20
2	CB	202/220 (92%)	177 (88%)	25 (12%)	4	19
3	AC	160/188 (85%)	142 (89%)	18 (11%)	6	23
3	CC	160/188 (85%)	144 (90%)	16 (10%)	7	28
4	AD	180/181 (99%)	151 (84%)	29 (16%)	2	10
4	CD	180/181 (99%)	153 (85%)	27 (15%)	3	12
5	AE	115/123 (94%)	106 (92%)	9 (8%)	12	40
5	CE	115/123 (94%)	105 (91%)	10 (9%)	10	36
6	AF	90/90 (100%)	79 (88%)	11 (12%)	5	19
6	CF	90/90 (100%)	77 (86%)	13 (14%)	3	14
7	AG	126/127 (99%)	113 (90%)	13 (10%)	7	27
7	CG	126/127 (99%)	116 (92%)	10 (8%)	12	40
8	AH	119/119 (100%)	108 (91%)	11 (9%)	9	33
8	CH	119/119 (100%)	112 (94%)	7 (6%)	19	50
9	AI	98/99 (99%)	89 (91%)	9 (9%)	9	33
9	CI	98/99 (99%)	88 (90%)	10 (10%)	7	27
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	4	18
10	CJ	88/92 (96%)	74 (84%)	14 (16%)	2	11
11	AK	90/99 (91%)	77 (86%)	13 (14%)	3	14
11	CK	90/99 (91%)	77 (86%)	13 (14%)	3	14
12	AL	104/109 (95%)	91 (88%)	13 (12%)	4	18
12	CL	104/109 (95%)	93 (89%)	11 (11%)	6	26
13	AM	99/101 (98%)	85 (86%)	14 (14%)	3	15
13	CM	99/101 (98%)	85 (86%)	14 (14%)	3	15
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3	14
14	CN	49/50 (98%)	43 (88%)	6 (12%)	5	19
15	AO	79/80 (99%)	69 (87%)	10 (13%)	4	18
15	CO	79/80 (99%)	69 (87%)	10 (13%)	4	18
16	AP	72/74 (97%)	68 (94%)	4 (6%)	21	52
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	30
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13	42
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	53	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	61/77 (79%)	54 (88%)	7 (12%)	5	22
18	CR	61/77 (79%)	54 (88%)	7 (12%)	5	22
19	AS	69/80 (86%)	58 (84%)	11 (16%)	2	11
19	CS	69/80 (86%)	54 (78%)	15 (22%)	1	4
20	AT	76/82 (93%)	66 (87%)	10 (13%)	4	17
20	CT	76/82 (93%)	67 (88%)	9 (12%)	5	21
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	26
21	CU	19/22 (86%)	16 (84%)	3 (16%)	2	11
25	AZ	322/338 (95%)	282 (88%)	40 (12%)	4	19
25	CZ	322/338 (95%)	281 (87%)	41 (13%)	4	18
26	B0	66/67 (98%)	53 (80%)	13 (20%)	1	6
26	D0	66/67 (98%)	55 (83%)	11 (17%)	2	9
27	B1	78/83 (94%)	68 (87%)	10 (13%)	4	18
27	D1	78/83 (94%)	70 (90%)	8 (10%)	7	27
28	B2	66/67 (98%)	55 (83%)	11 (17%)	2	9
28	D2	66/67 (98%)	60 (91%)	6 (9%)	9	33
29	B3	51/52 (98%)	44 (86%)	7 (14%)	3	16
29	D3	51/52 (98%)	45 (88%)	6 (12%)	5	21
30	B4	39/63 (62%)	28 (72%)	11 (28%)	0	1
30	D4	39/63 (62%)	29 (74%)	10 (26%)	0	1
31	B5	51/52 (98%)	44 (86%)	7 (14%)	3	16
31	D5	51/52 (98%)	45 (88%)	6 (12%)	5	21
32	B6	49/52 (94%)	32 (65%)	17 (35%)	0	0
32	D6	49/52 (94%)	36 (74%)	13 (26%)	0	1
33	B7	41/42 (98%)	37 (90%)	4 (10%)	8	29
33	D7	41/42 (98%)	35 (85%)	6 (15%)	3	13
34	B8	53/55 (96%)	43 (81%)	10 (19%)	1	6
34	D8	53/55 (96%)	43 (81%)	10 (19%)	1	6
35	B9	34/34 (100%)	28 (82%)	6 (18%)	2	8
35	D9	34/34 (100%)	29 (85%)	5 (15%)	3	13
38	BC	180/181 (99%)	168 (93%)	12 (7%)	16	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DC	180/181 (99%)	165 (92%)	15 (8%)	11	38
39	BD	217/218 (100%)	176 (81%)	41 (19%)	1	6
39	DD	217/218 (100%)	185 (85%)	32 (15%)	3	13
40	BE	165/166 (99%)	137 (83%)	28 (17%)	2	9
40	DE	165/166 (99%)	137 (83%)	28 (17%)	2	9
41	BF	165/166 (99%)	147 (89%)	18 (11%)	6	25
41	DF	165/166 (99%)	152 (92%)	13 (8%)	12	40
42	BG	155/156 (99%)	130 (84%)	25 (16%)	2	10
42	DG	155/156 (99%)	127 (82%)	28 (18%)	1	7
43	BH	132/148 (89%)	122 (92%)	10 (8%)	13	41
43	DH	132/148 (89%)	123 (93%)	9 (7%)	16	45
46	BN	117/119 (98%)	102 (87%)	15 (13%)	4	18
46	DN	117/119 (98%)	99 (85%)	18 (15%)	2	11
47	BO	100/100 (100%)	92 (92%)	8 (8%)	12	40
47	DO	100/100 (100%)	90 (90%)	10 (10%)	7	28
48	BP	112/116 (97%)	89 (80%)	23 (20%)	1	5
48	DP	112/116 (97%)	92 (82%)	20 (18%)	2	8
49	BQ	111/111 (100%)	94 (85%)	17 (15%)	2	12
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	4	18
50	BR	100/101 (99%)	88 (88%)	12 (12%)	5	20
50	DR	100/101 (99%)	89 (89%)	11 (11%)	6	25
51	BS	77/88 (88%)	65 (84%)	12 (16%)	2	11
51	DS	77/88 (88%)	61 (79%)	16 (21%)	1	5
52	BT	120/127 (94%)	101 (84%)	19 (16%)	2	11
52	DT	120/127 (94%)	102 (85%)	18 (15%)	3	12
53	BU	92/94 (98%)	84 (91%)	8 (9%)	10	36
53	DU	92/94 (98%)	85 (92%)	7 (8%)	13	41
54	BV	82/82 (100%)	69 (84%)	13 (16%)	2	11
54	DV	82/82 (100%)	66 (80%)	16 (20%)	1	6
55	BW	91/92 (99%)	85 (93%)	6 (7%)	16	47
55	DW	91/92 (99%)	85 (93%)	6 (7%)	16	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	BX	74/78 (95%)	65 (88%)	9 (12%)	5	19
56	DX	74/78 (95%)	68 (92%)	6 (8%)	11	39
57	BY	84/91 (92%)	72 (86%)	12 (14%)	3	14
57	DY	84/91 (92%)	73 (87%)	11 (13%)	4	17
58	BZ	161/179 (90%)	134 (83%)	27 (17%)	2	9
58	DZ	161/179 (90%)	138 (86%)	23 (14%)	3	14
All	All	10350/10856 (95%)	9014 (87%)	1336 (13%)	4	18

5 of 1336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	CZ	166	ASP
42	DG	150	ASP
25	CZ	370	PHE
25	CZ	163	PHE
38	DC	70	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 314 such sidechains are listed below:

Mol	Chain	Res	Type
28	D2	48	HIS
48	DP	84	ASN
29	D3	52	HIS
40	DE	54	GLN
53	DU	14	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	227 (15%)	50 (3%)
1	CA	1503/1522 (98%)	229 (15%)	41 (2%)
22	AV	75/76 (98%)	20 (26%)	0
22	AW	75/76 (98%)	20 (26%)	0
22	CV	75/76 (98%)	19 (25%)	2 (2%)
22	CW	75/76 (98%)	22 (29%)	2 (2%)
23	AX	17/27 (62%)	8 (47%)	1 (5%)
23	CX	17/27 (62%)	9 (52%)	1 (5%)
24	AY	74/77 (96%)	24 (32%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	CY	74/77 (96%)	25 (33%)	1 (1%)
36	BA	2900/2915 (99%)	511 (17%)	48 (1%)
36	DA	2900/2915 (99%)	513 (17%)	43 (1%)
37	BB	118/122 (96%)	26 (22%)	4 (3%)
37	DB	118/122 (96%)	26 (22%)	4 (3%)
All	All	9524/9630 (98%)	1679 (17%)	198 (2%)

5 of 1679 RNA backbone outliers are listed below:

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

5 of 198 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	274	A
1	CA	1285	A
1	CA	428	G
1	CA	792	A
24	CY	20	H2U

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

18 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	H2U	CY	17	24	18,21,22	0.87	0	21,30,33	1.85	5 (23%)
24	4SU	AY	8	24	18,21,22	1.98	3 (16%)	26,30,33	1.78	5 (19%)
24	H2U	CY	16	24	18,21,22	0.89	0	21,30,33	1.77	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	4SU	CY	8	24	18,21,22	2.09	3 (16%)	26,30,33	1.80	4 (15%)
24	H2U	AY	17	24	18,21,22	0.78	0	21,30,33	1.78	5 (23%)
24	MIA	CY	37	24	24,31,32	1.47	3 (12%)	26,44,47	1.50	4 (15%)
24	OMC	AY	32	24	19,22,23	0.62	0	26,31,34	0.43	0
24	H2U	AY	20	24	18,21,22	0.86	1 (5%)	21,30,33	1.92	5 (23%)
24	5MU	AY	54	24	19,22,23	0.28	0	28,32,35	0.40	0
24	OMC	CY	32	24	19,22,23	0.68	0	26,31,34	0.45	0
24	MIA	AY	37	24	24,31,32	1.31	2 (8%)	26,44,47	1.83	4 (15%)
24	5MU	CY	54	24	19,22,23	0.30	0	28,32,35	0.41	0
24	PSU	CY	55	24	18,21,22	1.10	2 (11%)	22,30,33	1.75	4 (18%)
24	H2U	CY	20	24	18,21,22	0.84	0	21,30,33	1.98	6 (28%)
24	PSU	AY	55	24	18,21,22	1.00	2 (11%)	22,30,33	1.81	4 (18%)
24	7MG	CY	46	24	22,26,27	2.99	2 (9%)	29,39,42	1.58	2 (6%)
24	H2U	AY	16	24	18,21,22	0.80	0	21,30,33	1.75	4 (19%)
24	7MG	AY	46	24	22,26,27	3.06	2 (9%)	29,39,42	1.56	2 (6%)

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	H2U	CY	17	24	-	5/7/38/39	0/2/2/2
24	4SU	AY	8	24	-	1/7/25/26	0/2/2/2
24	H2U	CY	16	24	-	2/7/38/39	0/2/2/2
24	4SU	CY	8	24	-	1/7/25/26	0/2/2/2
24	H2U	AY	17	24	-	5/7/38/39	0/2/2/2
24	MIA	CY	37	24	-	1/11/33/34	0/3/3/3
24	OMC	AY	32	24	-	0/9/27/28	0/2/2/2
24	H2U	AY	20	24	-	5/7/38/39	0/2/2/2
24	5MU	AY	54	24	-	1/7/25/26	0/2/2/2
24	OMC	CY	32	24	-	0/9/27/28	0/2/2/2
24	MIA	AY	37	24	-	1/11/33/34	0/3/3/3
24	5MU	CY	54	24	-	1/7/25/26	0/2/2/2
24	PSU	CY	55	24	-	2/7/25/26	0/2/2/2
24	H2U	CY	20	24	-	5/7/38/39	0/2/2/2
24	PSU	AY	55	24	-	2/7/25/26	0/2/2/2
24	7MG	CY	46	24	-	4/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	H2U	AY	16	24	-	2/7/38/39	0/2/2/2
24	7MG	AY	46	24	-	4/7/37/38	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	46	7MG	C8-N9	-13.78	1.38	1.46
24	CY	46	7MG	C8-N9	-13.46	1.38	1.46
24	CY	8	4SU	C4-N3	5.70	1.43	1.37
24	CY	37	MIA	C2-S10	5.33	1.80	1.75
24	AY	8	4SU	C4-N3	5.21	1.43	1.37

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	CY	46	7MG	N9-C8-N7	6.92	113.28	103.38
24	AY	46	7MG	N9-C8-N7	6.83	113.14	103.38
24	AY	37	MIA	C11-S10-C2	6.40	107.05	102.27
24	CY	20	H2U	C4-N3-C2	-4.97	121.67	125.79
24	CY	17	H2U	C4-N3-C2	-4.84	121.78	125.79

There are no chirality outliers.

5 of 42 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'-C1'-N1-C6
24	AY	37	MIA	N6-C12-C13-C14
24	AY	55	PSU	C4'-C5'-O5'-P

There are no ring outliers.

14 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	8	4SU	3	0
24	CY	16	H2U	1	0
24	CY	8	4SU	3	0
24	AY	32	OMC	1	0
24	AY	20	H2U	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	54	5MU	3	0
24	CY	32	OMC	1	0
24	CY	54	5MU	3	0
24	CY	55	PSU	2	0
24	CY	20	H2U	3	0
24	AY	55	PSU	2	0
24	CY	46	7MG	1	0
24	AY	16	H2U	1	0
24	AY	46	7MG	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
60	GDP	AZ	501	-	24,30,30	1.11	3 (12%)	30,47,47	1.77	9 (30%)
61	KIR	AZ	502	-	56,59,59	3.56	22 (39%)	62,84,84	1.67	13 (20%)
61	KIR	CZ	502	-	56,59,59	3.66	24 (42%)	62,84,84	1.66	12 (19%)
60	GDP	CZ	501	-	24,30,30	1.11	2 (8%)	30,47,47	1.75	8 (26%)

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
60	GDP	AZ	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	KIR	AZ	502	-	-	8/54/98/98	0/3/3/3
61	KIR	CZ	502	-	-	8/54/98/98	0/3/3/3
60	GDP	CZ	501	-	-	1/12/32/32	0/3/3/3

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AZ	502	KIR	O18-C17	-14.95	1.22	1.44
61	CZ	502	KIR	O18-C17	-14.23	1.23	1.44
61	CZ	502	KIR	O30-C30	-12.29	1.18	1.42
61	AZ	502	KIR	O30-C30	-12.09	1.18	1.42
61	CZ	502	KIR	C32-C31	6.53	1.63	1.54

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	AZ	501	GDP	PA-O3A-PB	-4.73	116.58	132.83
61	AZ	502	KIR	O29-C29-O34	-4.61	102.49	110.21
60	CZ	501	GDP	PA-O3A-PB	-4.57	117.13	132.83
61	AZ	502	KIR	C48-C32-C47	-4.42	101.41	107.72
61	CZ	502	KIR	C48-C32-C47	-4.40	101.44	107.72

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	AZ	501	GDP	C5'-O5'-PA-O1A
60	CZ	501	GDP	C5'-O5'-PA-O1A
61	AZ	502	KIR	O18-C17-C19-C42
61	CZ	502	KIR	O18-C17-C19-C42
61	AZ	502	KIR	C11-C10-C9-C8

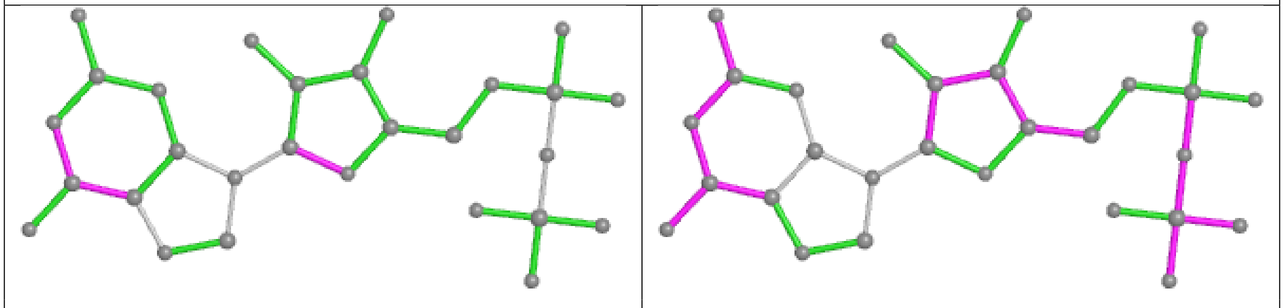
There are no ring outliers.

4 monomers are involved in 50 short contacts:

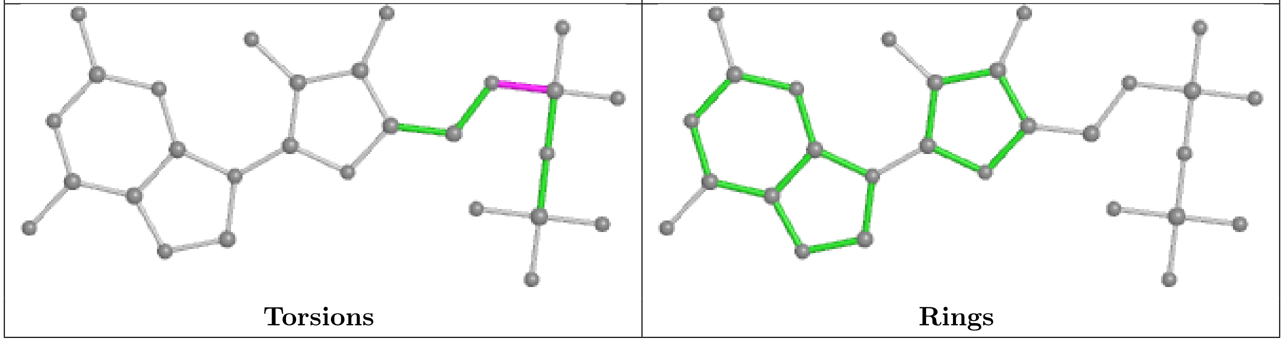
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	AZ	501	GDP	12	0
61	AZ	502	KIR	11	0
61	CZ	502	KIR	14	0
60	CZ	501	GDP	13	0

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

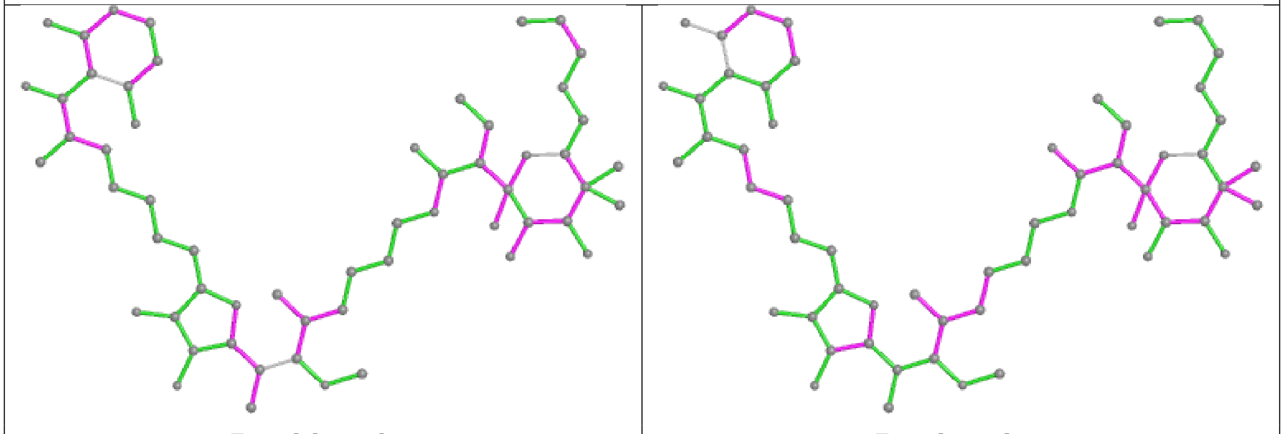


Bond lengths **Bond angles**



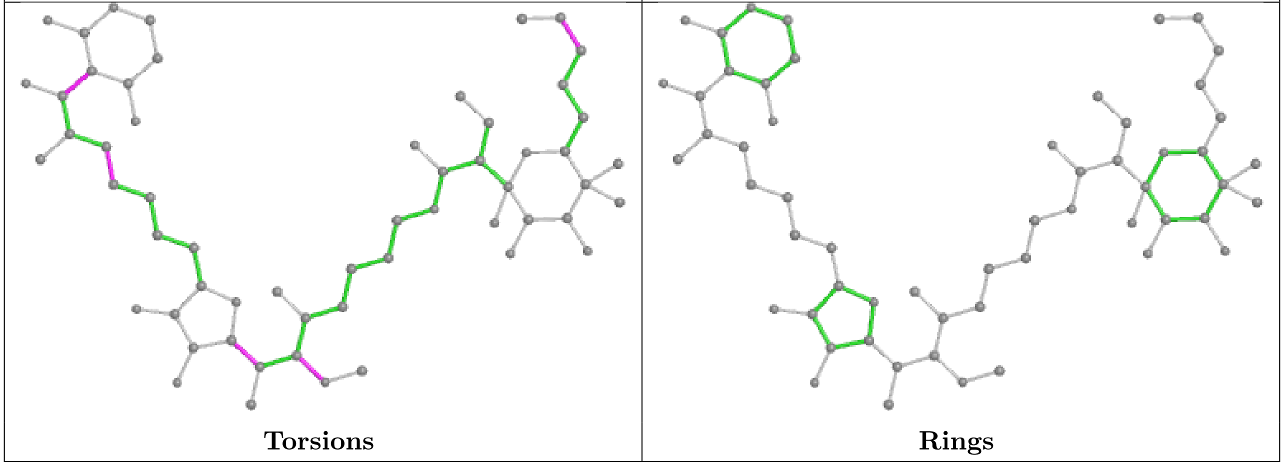
Torsions **Rings**

Ligand KIR AZ 502



Bond lengths

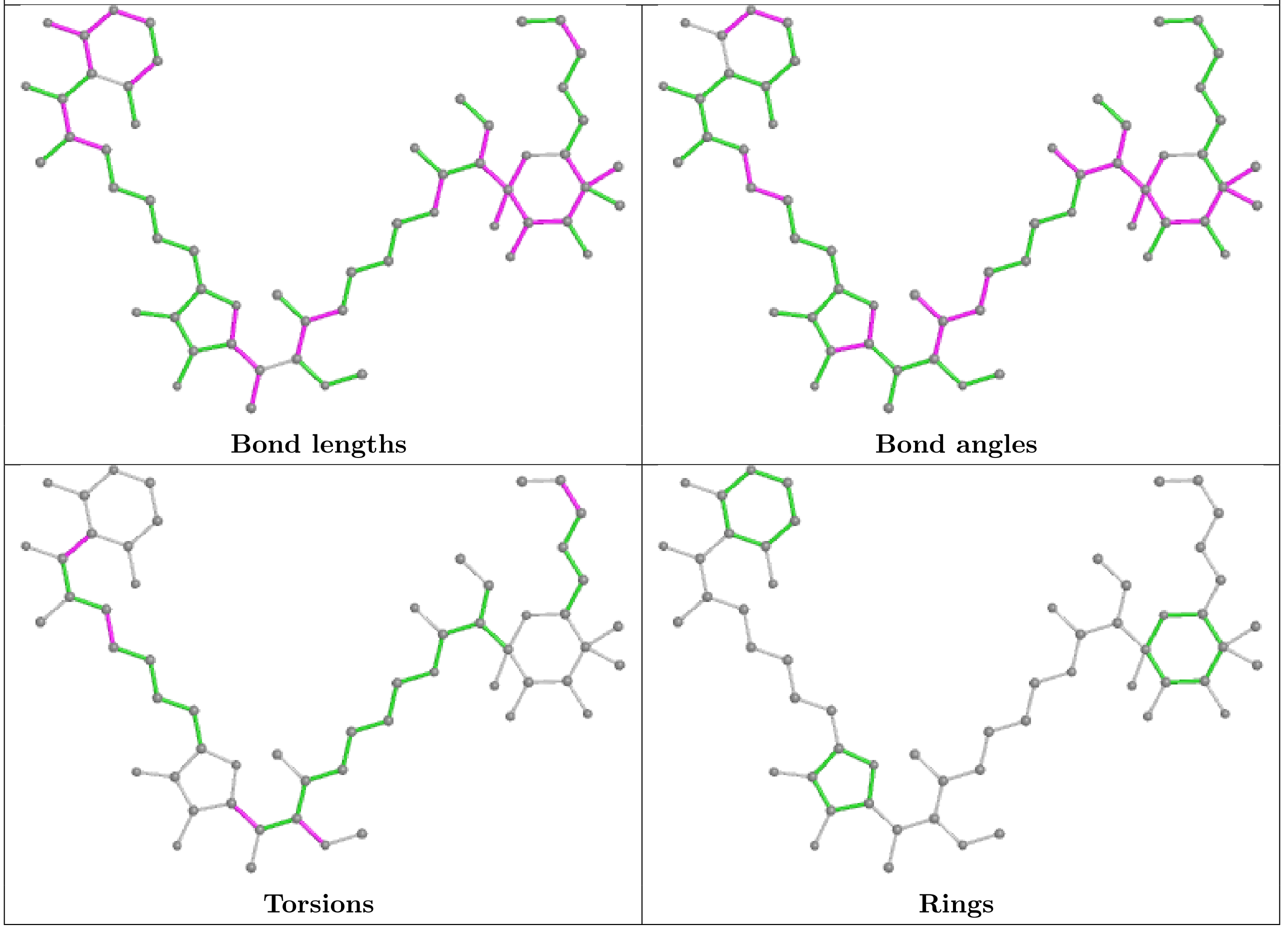
Bond angles



Torsions

Rings

Ligand KIR CZ 502



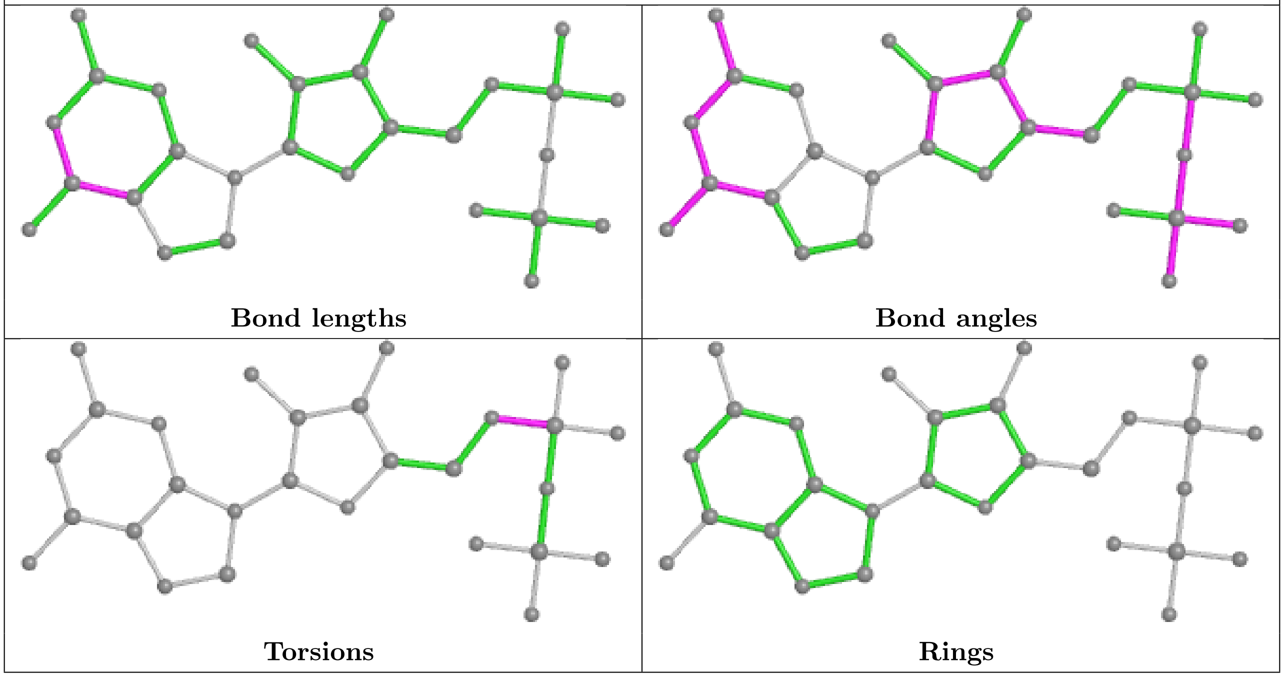
Bond lengths

Bond angles

Torsions

Rings

Ligand GDP CZ 501



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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%)	-0.27	28 (1%)	66	46	22, 58, 151, 200	0
1	CA	1504/1522 (98%)	-0.24	23 (1%)	73	54	39, 79, 157, 200	0
2	AB	234/256 (91%)	-0.32	3 (1%)	77	59	33, 66, 135, 154	0
2	CB	234/256 (91%)	-0.27	3 (1%)	77	59	50, 89, 142, 150	0
3	AC	206/239 (86%)	-0.59	0	100	100	25, 49, 78, 88	0
3	CC	206/239 (86%)	-0.44	1 (0%)	91	81	53, 80, 106, 113	0
4	AD	208/209 (99%)	0.07	8 (3%)	40	20	59, 88, 122, 126	0
4	CD	208/209 (99%)	0.15	9 (4%)	35	17	79, 105, 125, 135	0
5	AE	150/162 (92%)	-0.62	0	100	100	30, 45, 71, 97	0
5	CE	150/162 (92%)	-0.47	0	100	100	48, 63, 85, 102	0
6	AF	101/101 (100%)	-0.50	1 (0%)	82	67	48, 74, 94, 105	0
6	CF	101/101 (100%)	-0.14	1 (0%)	82	67	79, 98, 111, 119	0
7	AG	155/156 (99%)	-0.37	5 (3%)	47	25	39, 65, 96, 117	0
7	CG	155/156 (99%)	-0.08	5 (3%)	47	25	71, 95, 115, 127	0
8	AH	138/138 (100%)	-0.55	0	100	100	32, 49, 69, 74	0
8	CH	138/138 (100%)	-0.44	0	100	100	46, 64, 80, 87	0
9	AI	127/128 (99%)	-0.20	1 (0%)	86	72	32, 68, 111, 124	0
9	CI	127/128 (99%)	0.41	10 (7%)	12	5	66, 106, 132, 139	0
10	AJ	98/105 (93%)	-0.10	0	100	100	33, 70, 112, 125	0
10	CJ	98/105 (93%)	0.43	9 (9%)	9	3	66, 109, 144, 148	0
11	AK	119/129 (92%)	-0.43	2 (1%)	70	49	32, 50, 92, 118	0
11	CK	119/129 (92%)	-0.23	3 (2%)	57	34	52, 76, 100, 120	0
12	AL	124/132 (93%)	-0.28	1 (0%)	86	72	33, 61, 85, 124	0
12	CL	124/132 (93%)	-0.17	2 (1%)	72	51	47, 72, 99, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	124/126 (98%)	-0.09	5 (4%) 38 19	43, 72, 103, 131	0
13	CM	124/126 (98%)	0.04	7 (5%) 24 11	76, 99, 122, 142	0
14	AN	60/61 (98%)	-0.29	1 (1%) 70 49	30, 53, 78, 84	0
14	CN	60/61 (98%)	0.05	2 (3%) 46 24	65, 83, 102, 105	0
15	AO	88/89 (98%)	-0.51	0 100 100	36, 54, 82, 88	0
15	CO	88/89 (98%)	-0.31	0 100 100	44, 68, 90, 98	0
16	AP	83/88 (94%)	-0.02	2 (2%) 59 37	61, 74, 98, 133	0
16	CP	83/88 (94%)	0.16	1 (1%) 79 61	74, 90, 110, 132	0
17	AQ	99/105 (94%)	-0.37	0 100 100	40, 60, 79, 89	0
17	CQ	99/105 (94%)	-0.22	0 100 100	53, 71, 91, 102	0
18	AR	70/88 (79%)	-0.43	0 100 100	39, 60, 90, 99	0
18	CR	70/88 (79%)	-0.26	0 100 100	56, 81, 108, 118	0
19	AS	78/93 (83%)	-0.05	2 (2%) 56 33	52, 73, 117, 127	0
19	CS	78/93 (83%)	0.14	5 (6%) 19 8	81, 97, 126, 132	0
20	AT	99/106 (93%)	0.13	4 (4%) 38 19	55, 80, 126, 130	0
20	CT	99/106 (93%)	0.09	1 (1%) 82 67	74, 90, 120, 122	0
21	AU	24/27 (88%)	-0.02	2 (8%) 11 4	41, 55, 79, 99	0
21	CU	24/27 (88%)	0.60	2 (8%) 11 4	74, 92, 105, 113	0
22	AV	76/76 (100%)	-0.46	0 100 100	35, 72, 107, 124	0
22	AW	76/76 (100%)	0.37	8 (10%) 6 2	64, 140, 185, 199	0
22	CV	76/76 (100%)	-0.29	0 100 100	51, 86, 120, 137	0
22	CW	76/76 (100%)	0.42	6 (7%) 12 5	94, 170, 191, 200	0
23	AX	17/27 (62%)	0.45	2 (11%) 4 2	31, 91, 142, 143	0
23	CX	17/27 (62%)	2.24	12 (70%) 0 0	69, 122, 155, 157	0
24	AY	68/77 (88%)	0.24	1 (1%) 73 54	57, 140, 177, 197	0
24	CY	68/77 (88%)	0.36	1 (1%) 73 54	73, 142, 175, 198	0
25	AZ	385/405 (95%)	0.63	29 (7%) 14 5	87, 124, 151, 169	0
25	CZ	385/405 (95%)	1.37	104 (27%) 0 0	111, 133, 156, 170	0
26	B0	84/85 (98%)	0.15	6 (7%) 16 6	58, 73, 107, 122	0
26	D0	84/85 (98%)	0.48	9 (10%) 6 2	69, 86, 113, 123	0
27	B1	93/98 (94%)	0.02	4 (4%) 35 17	45, 69, 129, 134	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB($Å^2$)	Q<0.9
27	D1	93/98 (94%)	0.15	1 (1%) 80 64	59, 86, 133, 139	0
28	B2	71/72 (98%)	1.37	20 (28%) 0 0	130, 143, 155, 158	0
28	D2	71/72 (98%)	0.49	11 (15%) 2 1	100, 122, 136, 143	0
29	B3	59/60 (98%)	0.20	2 (3%) 45 24	65, 81, 106, 122	0
29	D3	59/60 (98%)	0.30	3 (5%) 28 13	60, 93, 106, 126	0
30	B4	44/71 (61%)	0.67	5 (11%) 5 2	111, 140, 167, 173	0
30	D4	44/71 (61%)	1.16	13 (29%) 0 0	136, 163, 184, 186	0
31	B5	59/60 (98%)	0.15	3 (5%) 28 13	62, 87, 148, 163	0
31	D5	59/60 (98%)	0.24	4 (6%) 17 7	63, 92, 145, 154	0
32	B6	50/54 (92%)	0.50	4 (8%) 12 5	57, 84, 103, 110	0
32	D6	50/54 (92%)	0.93	9 (18%) 1 0	73, 97, 116, 122	0
33	B7	48/49 (97%)	0.14	3 (6%) 20 8	51, 64, 101, 121	0
33	D7	48/49 (97%)	0.08	3 (6%) 20 8	64, 73, 104, 125	0
34	B8	63/65 (96%)	0.23	2 (3%) 47 25	56, 73, 91, 115	0
34	D8	63/65 (96%)	0.39	5 (7%) 12 5	72, 85, 101, 120	0
35	B9	37/37 (100%)	0.57	4 (10%) 5 2	73, 85, 103, 104	0
35	D9	37/37 (100%)	1.12	4 (10%) 5 2	67, 96, 107, 120	0
36	BA	2901/2915 (99%)	-0.15	76 (2%) 56 33	26, 77, 181, 200	0
36	DA	2901/2915 (99%)	-0.10	77 (2%) 54 31	37, 87, 180, 200	0
37	BB	119/122 (97%)	-0.48	0 100 100	59, 85, 112, 132	0
37	DB	119/122 (97%)	-0.44	0 100 100	69, 101, 126, 132	0
38	BC	228/229 (99%)	0.01	12 (5%) 26 12	50, 79, 160, 173	0
38	DC	228/229 (99%)	0.47	26 (11%) 5 2	68, 102, 170, 180	0
39	BD	275/276 (99%)	-0.41	4 (1%) 73 54	30, 49, 83, 105	0
39	DD	275/276 (99%)	-0.32	2 (0%) 87 75	42, 61, 91, 111	0
40	BE	204/206 (99%)	-0.02	5 (2%) 57 34	50, 79, 128, 140	0
40	DE	204/206 (99%)	0.00	6 (2%) 51 28	47, 84, 133, 138	0
41	BF	207/210 (98%)	0.32	14 (6%) 17 7	53, 112, 162, 170	0
41	DF	207/210 (98%)	0.43	17 (8%) 11 4	62, 118, 161, 170	0
42	BG	181/182 (99%)	-0.04	9 (4%) 28 13	63, 86, 117, 130	0
42	DG	181/182 (99%)	0.05	8 (4%) 34 17	89, 108, 136, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
43	BH	159/180 (88%)	0.74	22 (13%)	2	1	92, 134, 152, 156	0
43	DH	159/180 (88%)	0.53	11 (6%)	16	7	87, 129, 146, 154	0
44	BJ	0/173	-	-			-	-
44	DJ	0/173	-	-			-	-
45	BK	0/147	-	-			-	-
45	DK	0/147	-	-			-	-
46	BN	138/140 (98%)	-0.08	0	100	100	63, 89, 125, 134	0
46	DN	138/140 (98%)	-0.18	0	100	100	69, 90, 125, 133	0
47	BO	122/122 (100%)	-0.44	0	100	100	46, 63, 77, 85	0
47	DO	122/122 (100%)	-0.38	0	100	100	47, 67, 83, 89	0
48	BP	146/150 (97%)	0.52	13 (8%)	9	3	55, 103, 133, 150	0
48	DP	146/150 (97%)	0.72	21 (14%)	2	1	64, 115, 137, 153	0
49	BQ	141/141 (100%)	-0.22	3 (2%)	63	43	46, 64, 86, 128	0
49	DQ	141/141 (100%)	-0.22	2 (1%)	75	56	51, 66, 90, 126	0
50	BR	117/118 (99%)	0.06	2 (1%)	70	49	60, 85, 107, 126	0
50	DR	117/118 (99%)	0.06	1 (0%)	84	69	57, 90, 105, 123	0
51	BS	98/112 (87%)	0.13	3 (3%)	49	26	63, 90, 116, 126	0
51	DS	98/112 (87%)	0.44	8 (8%)	11	4	77, 102, 126, 128	0
52	BT	137/146 (93%)	-0.02	8 (5%)	23	10	58, 84, 142, 167	0
52	DT	137/146 (93%)	-0.03	6 (4%)	34	17	63, 90, 147, 169	0
53	BU	117/118 (99%)	-0.05	1 (0%)	84	69	64, 79, 111, 128	0
53	DU	117/118 (99%)	-0.03	1 (0%)	84	69	63, 86, 110, 124	0
54	BV	101/101 (100%)	0.28	3 (2%)	50	27	62, 116, 129, 136	0
54	DV	101/101 (100%)	0.38	5 (4%)	28	13	71, 115, 134, 136	0
55	BW	113/113 (100%)	0.10	5 (4%)	34	17	65, 90, 116, 141	0
55	DW	113/113 (100%)	0.31	5 (4%)	34	17	73, 93, 123, 145	0
56	BX	92/96 (95%)	0.22	1 (1%)	80	64	75, 95, 110, 118	0
56	DX	92/96 (95%)	0.20	1 (1%)	80	64	82, 100, 116, 120	0
57	BY	100/110 (90%)	1.25	26 (26%)	0	0	108, 134, 162, 168	0
57	DY	100/110 (90%)	1.13	20 (20%)	1	0	107, 136, 160, 169	0
58	BZ	183/206 (88%)	-0.13	4 (2%)	62	41	56, 83, 120, 132	0
58	DZ	183/206 (88%)	-0.05	5 (2%)	54	31	62, 88, 120, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	21996/23370 (94%)	-0.02	860 (3%)	39	20	22, 84, 151, 200	0

The worst 5 of 860 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	CZ	183	HIS	12.4
41	BF	24	LEU	11.5
25	AZ	85	HIS	10.9
49	BQ	141	GLN	10.5
36	BA	1077	A	9.4

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	0.60	0.45	194,198,199,199	0
24	H2U	AY	16	20/21	0.61	0.47	196,198,199,200	0
24	H2U	CY	17	20/21	0.62	0.57	199,199,200,200	0
24	H2U	AY	17	20/21	0.68	0.36	199,199,200,200	0
24	PSU	CY	55	20/21	0.69	0.29	158,161,162,162	0
24	PSU	AY	55	20/21	0.77	0.25	156,161,162,162	0
24	4SU	AY	8	20/21	0.77	0.21	142,144,146,146	0
24	H2U	CY	20	20/21	0.79	0.38	188,191,192,192	0
24	5MU	AY	54	21/22	0.81	0.20	139,150,152,154	0
24	4SU	CY	8	20/21	0.81	0.27	143,145,147,148	0
24	H2U	AY	20	20/21	0.83	0.43	186,189,193,193	0
24	5MU	CY	54	21/22	0.84	0.26	139,149,151,155	0
24	7MG	AY	46	24/25	0.84	0.27	145,150,151,151	0
24	7MG	CY	46	24/25	0.85	0.30	148,153,154,154	0
24	OMC	CY	32	21/22	0.87	0.29	108,114,121,121	0
24	OMC	AY	32	21/22	0.89	0.20	101,105,115,115	0
24	MIA	AY	37	29/30	0.91	0.25	64,78,89,98	0
24	MIA	CY	37	29/30	0.92	0.23	80,87,95,99	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

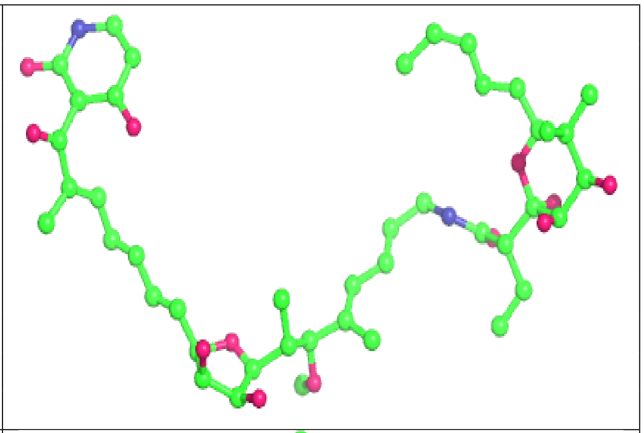
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

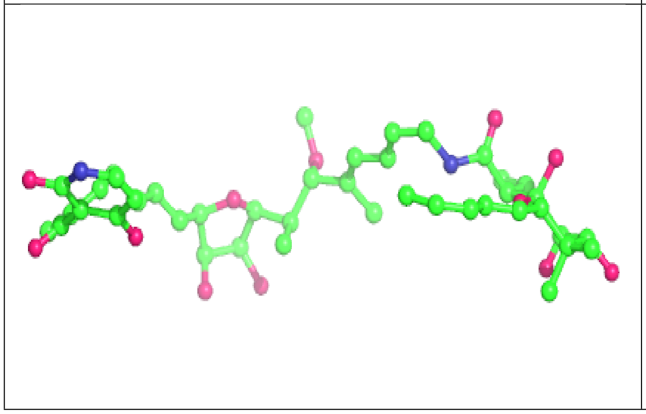
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
61	KIR	CZ	502	57/57	0.67	0.62	122,131,140,141	0
60	GDP	AZ	501	28/28	0.69	0.31	129,133,138,138	0
60	GDP	CZ	501	28/28	0.70	0.26	137,140,141,141	0
61	KIR	AZ	502	57/57	0.81	0.36	115,122,129,130	0
59	ZN	D4	101	1/1	0.85	0.12	196,196,196,196	0
59	ZN	D9	101	1/1	0.90	0.17	141,141,141,141	0
59	ZN	B9	101	1/1	0.92	0.12	113,113,113,113	0
59	ZN	B4	101	1/1	0.95	0.13	112,112,112,112	0
59	ZN	AN	101	1/1	0.98	0.18	48,48,48,48	0
59	ZN	AD	301	1/1	0.99	0.27	74,74,74,74	0
59	ZN	CD	301	1/1	0.99	0.28	79,79,79,79	0
59	ZN	CN	101	1/1	0.99	0.17	77,77,77,77	0

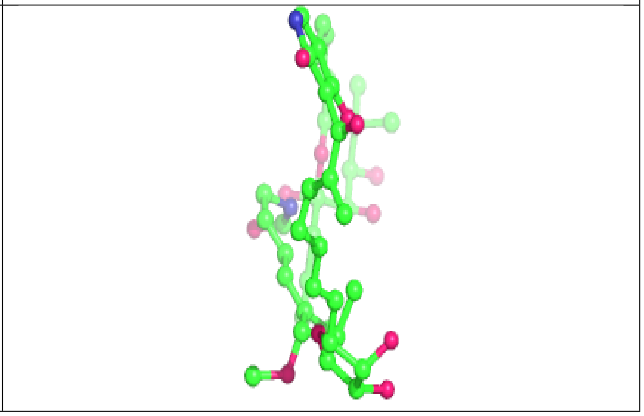
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around KIR CZ 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

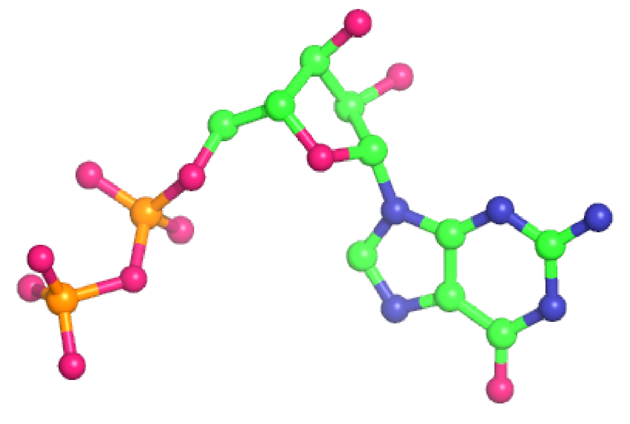


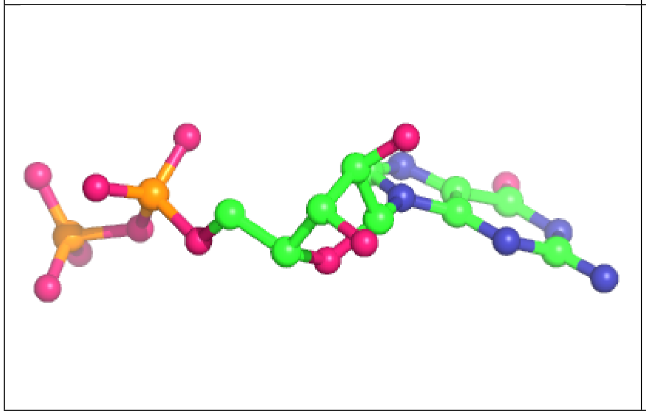


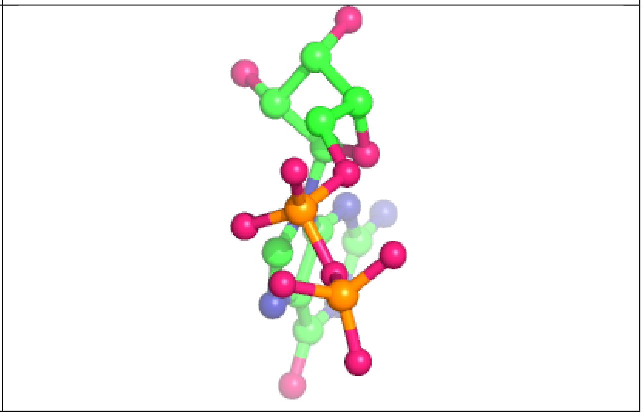


Electron density around GDP AZ 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

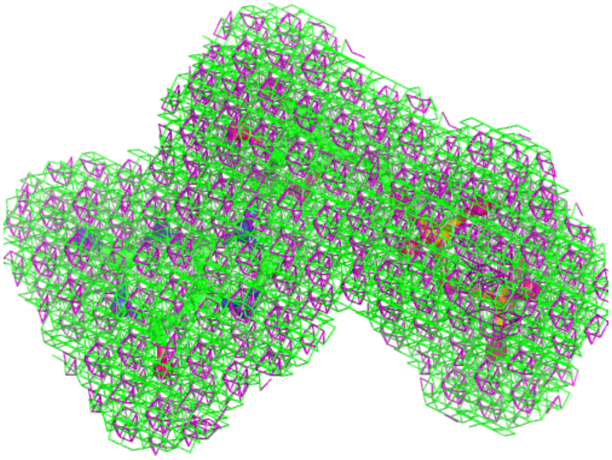


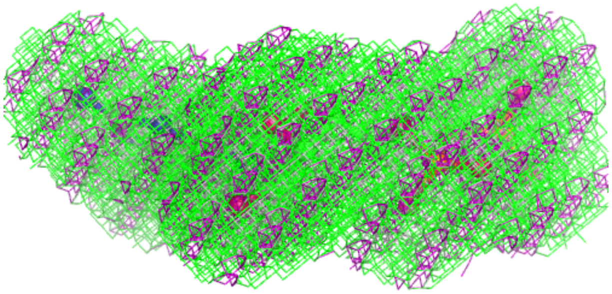


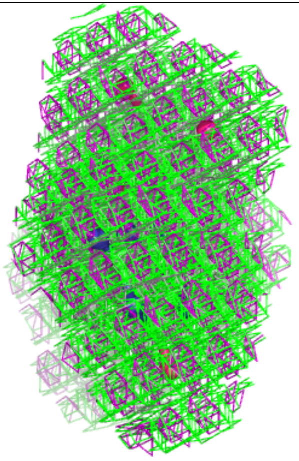


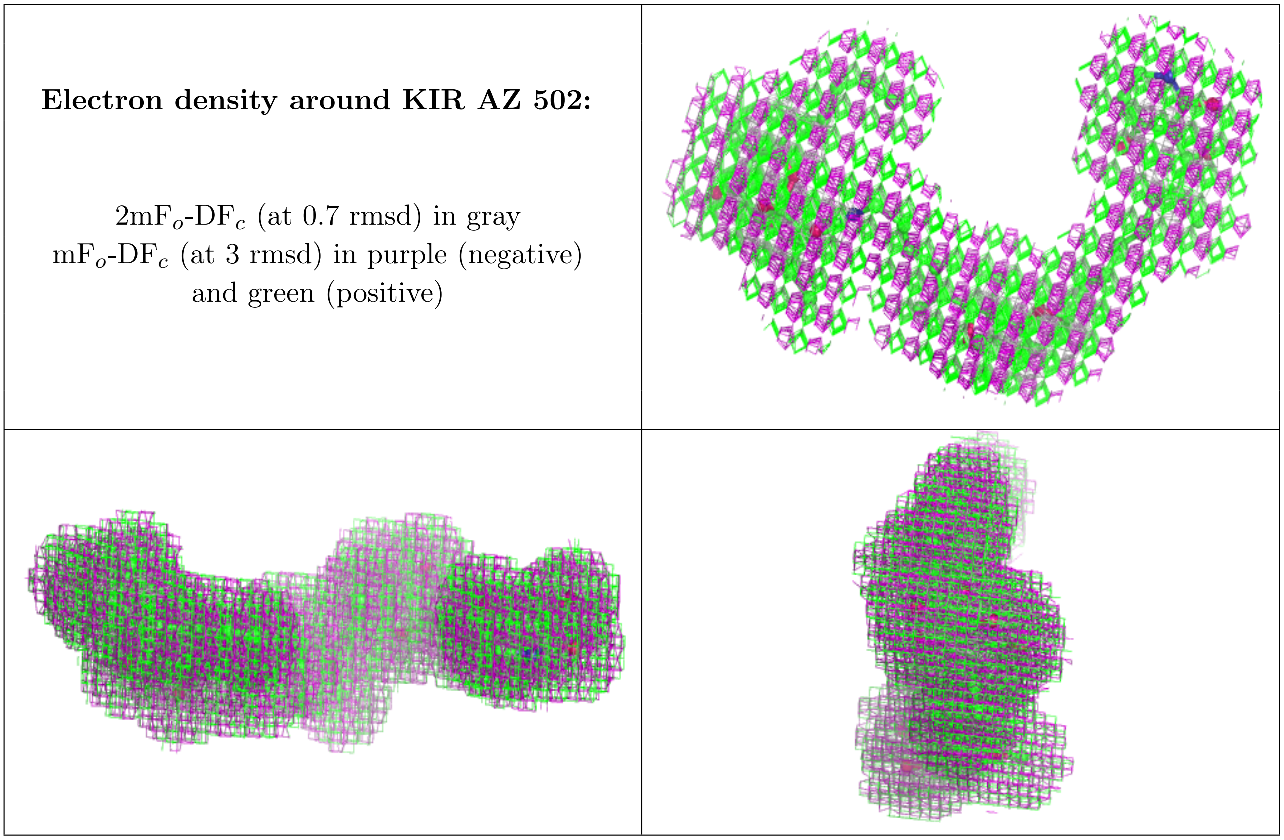
Electron density around GDP CZ 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)









Electron density around KIR AZ 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.